



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 01:48 PM UTC

PDB ID : 6HIZ / pdb_00006hiz
EMDB ID : EMD-0233
Title : Cryo-EM structure of the Trypanosoma brucei mitochondrial ribosome - This entry contains the head of the small mitoribosomal subunit
Authors : Ramrath, D.J.F.; Niemann, M.; Leibundgut, M.; Bieri, P.; Prange, C.; Horn, E.K.; Leitner, A.; Boehringer, A.; Schneider, A.; Ban, N.
Deposited on : 2018-08-31
Resolution : 3.08 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

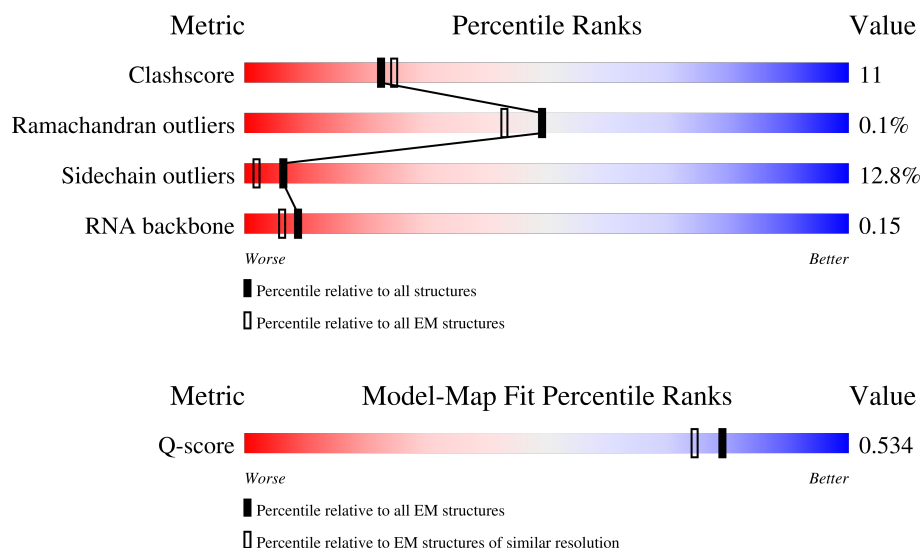
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



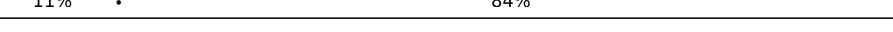
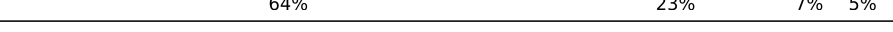
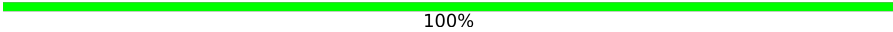
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14000 (2.58 - 3.58)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	DA	1788	
2	DL	307	
3	DB	1181	

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Mol	Chain	Length	Quality of chain
4	DC	1165	
5	DE	747	
6	DF	666	
7	DG	631	
8	DH	581	
9	DJ	396	
10	DK	324	
11	DT	247	
12	DV	183	
13	DW	179	
14	DX	169	
15	DY	163	
16	CC	74	
17	CI	443	
18	CJ	817	
19	CK	326	
20	CN	166	
21	CR	320	
22	CS	244	
23	Cg	498	
24	Ci	181	
25	Ck	874	
26	CA	611	
27	UO	5	
28	UP	7	

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 76845 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called mS48.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	DA	131	Total	C	N	O	S	0	0
			993	629	174	186	4		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	894	HIS	ASN	conflict	UNP Q57UJ2
DA	1181	THR	ILE	conflict	UNP Q57UJ2
DA	1333	ALA	VAL	conflict	UNP Q57UJ2
DA	1700	ARG	HIS	conflict	UNP Q57UJ2
DA	1761	LYS	ARG	conflict	UNP Q57UJ2

- Molecule 2 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	DL	143	Total	C	N	O	S	0	0
			1153	733	215	202	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DL	274	THR	ALA	conflict	UNP Q38BS2

- Molecule 3 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	DB	1111	Total	C	N	O	S	0	0
			9148	5691	1717	1711	29		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DB	23	VAL	ALA	conflict	UNP Q586P5

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Chain	Residue	Modelled	Actual	Comment	Reference
DB	359	ILE	THR	conflict	UNP Q586P5
DB	384	GLN	HIS	conflict	UNP Q586P5
DB	402	THR	ILE	conflict	UNP Q586P5
DB	423	THR	ALA	conflict	UNP Q586P5
DB	586	ARG	HIS	conflict	UNP Q586P5
DB	593	ARG	LYS	conflict	UNP Q586P5
DB	647	SER	GLY	conflict	UNP Q586P5

- Molecule 4 is a protein called mS50.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	DC	1095	Total	C	N	O	S	0	0
			8748	5519	1544	1654	31		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	53	ALA	THR	conflict	UNP Q57YB5
DC	365	LYS	GLU	conflict	UNP Q57YB5
DC	385	THR	ALA	conflict	UNP Q57YB5
DC	405	ILE	VAL	conflict	UNP Q57YB5
DC	641	SER	PRO	conflict	UNP Q57YB5
DC	651	LYS	GLU	conflict	UNP Q57YB5
DC	731	GLU	ASP	conflict	UNP Q57YB5
DC	814	GLN	HIS	conflict	UNP Q57YB5
DC	1097	ALA	VAL	conflict	UNP Q57YB5
DC	1113	THR	ILE	conflict	UNP Q57YB5

- Molecule 5 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	DE	590	Total	C	N	O	S	0	0
			4831	3075	874	863	19		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DE	514	THR	SER	conflict	UNP Q386Q7

- Molecule 6 is a protein called mS53.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	DF	590	Total	C	N	O	S	0	0
			4747	2979	896	847	25		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DF	18	THR	ALA	conflict	UNP Q38ET1
DF	258	ASP	ASN	conflict	UNP Q38ET1
DF	372	ASN	ASP	conflict	UNP Q38ET1
DF	406	ASN	SER	conflict	UNP Q38ET1
DF	510	ASP	GLY	conflict	UNP Q38ET1
DF	577	ALA	VAL	conflict	UNP Q38ET1
DF	636	UNK	GLY	conflict	UNP Q38ET1
DF	638	LYS	ARG	conflict	UNP Q38ET1

- Molecule 7 is a protein called mS54.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	DG	566	Total	C	N	O	S	0	0
			4575	2875	835	834	31		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DG	428	ASN	SER	conflict	UNP Q57ZP8
DG	429	GLY	SER	conflict	UNP Q57ZP8

- Molecule 8 is a protein called mS55.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	DH	564	Total	C	N	O	S	0	0
			4578	2872	850	834	22		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DH	191	HIS	GLN	conflict	UNP Q580V1
DH	194	PRO	ARG	conflict	UNP Q580V1
DH	488	GLY	SER	conflict	UNP Q580V1

- Molecule 9 is a protein called mS57.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	DJ	315	Total	C	N	O	S	0	0
			2572	1646	452	460	14		

- Molecule 10 is a protein called mS58.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	DK	255	Total	C	N	O	S	0	0
			2007	1260	365	377	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DK	61	SER	PRO	conflict	UNP Q38BP1
DK	257	GLY	SER	conflict	UNP Q38BP1

- Molecule 11 is a protein called mS67.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	DT	239	Total	C	N	O	S	0	0
			2058	1321	364	362	11		

- Molecule 12 is a protein called mS69.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	DV	160	Total	C	N	O	S	0	0
			1346	855	252	235	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DV	163	ALA	THR	conflict	UNP Q57UZ6

- Molecule 13 is a protein called mS70.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	DW	161	Total	C	N	O	S	0	0
			1359	866	260	228	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DW	74	THR	MET	conflict	UNP Q383N9

- Molecule 14 is a protein called mS71.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	DX	141	Total	C	N	O	S	0	0
			1196	762	226	201	7		

- Molecule 15 is a protein called mS72.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	DY	154	Total	C	N	O	S	0	0
			1293	827	245	216	5		

- Molecule 16 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CC	74	Total	C	N	O	S	0	0
			646	451	96	98	1		

- Molecule 17 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CI	222	Total	C	N	O	S	0	0
			1754	1101	330	313	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	279	UNK	ARG	conflict	UNP Q57W62
CI	370	ALA	VAL	conflict	UNP Q57W62

- Molecule 18 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CJ	800	Total	C	N	O	S	0	0
			6516	4119	1151	1216	30		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CJ	311	LEU	TYR	conflict	UNP Q57Z45
CJ	484	HIS	ARG	conflict	UNP Q57Z45
CJ	488	SER	ASN	conflict	UNP Q57Z45
CJ	594	GLU	VAL	conflict	UNP Q57Z45

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Chain	Residue	Modelled	Actual	Comment	Reference
CJ	629	ARG	LYS	conflict	UNP Q57Z45

- Molecule 19 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CK	52	Total	C	N	O	S	0	0
			438	272	90	74	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CK	3	ARG	GLN	conflict	UNP Q389T7
CK	138	UNK	ILE	conflict	UNP Q389T7

- Molecule 20 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CN	157	Total	C	N	O	S	0	0
			1322	843	251	220	8		

- Molecule 21 is a protein called uS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CR	44	Total	C	N	O	S	0	0
			353	217	64	71	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CR	8	ILE	VAL	conflict	UNP Q38AS2

- Molecule 22 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CS	142	Total	C	N	O	S	0	0
			1175	761	210	198	6		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CS	-71	MET	-	initiating methionine	UNP Q584T8

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Chain	Residue	Modelled	Actual	Comment	Reference
CS	-70	ALA	-	expression tag	UNP Q584T8
CS	-69	PHE	-	expression tag	UNP Q584T8
CS	-68	ARG	-	expression tag	UNP Q584T8
CS	-67	ASN	-	expression tag	UNP Q584T8
CS	-66	THR	-	expression tag	UNP Q584T8
CS	-65	PHE	-	expression tag	UNP Q584T8
CS	-64	THR	-	expression tag	UNP Q584T8
CS	-63	THR	-	expression tag	UNP Q584T8
CS	-62	PRO	-	expression tag	UNP Q584T8
CS	-61	GLY	-	expression tag	UNP Q584T8
CS	-60	LYS	-	expression tag	UNP Q584T8
CS	-59	PHE	-	expression tag	UNP Q584T8
CS	-58	SER	-	expression tag	UNP Q584T8
CS	-57	THR	-	expression tag	UNP Q584T8
CS	-56	VAL	-	expression tag	UNP Q584T8
CS	-55	SER	-	expression tag	UNP Q584T8
CS	-54	LYS	-	expression tag	UNP Q584T8
CS	-53	ASN	-	expression tag	UNP Q584T8
CS	-52	ILE	-	expression tag	UNP Q584T8
CS	-51	VAL	-	expression tag	UNP Q584T8
CS	-50	LEU	-	expression tag	UNP Q584T8
CS	-49	LEU	-	expression tag	UNP Q584T8
CS	-48	LEU	-	expression tag	UNP Q584T8
CS	-47	ILE	-	expression tag	UNP Q584T8
CS	-46	TRP	-	expression tag	UNP Q584T8
CS	-45	ARG	-	expression tag	UNP Q584T8
CS	-44	VAL	-	expression tag	UNP Q584T8
CS	-43	LYS	-	expression tag	UNP Q584T8
CS	-42	VAL	-	expression tag	UNP Q584T8
CS	-41	PHE	-	expression tag	UNP Q584T8
CS	-40	LEU	-	expression tag	UNP Q584T8
CS	-39	ARG	-	expression tag	UNP Q584T8
CS	-38	ALA	-	expression tag	UNP Q584T8
CS	-37	GLU	-	expression tag	UNP Q584T8
CS	-36	GLY	-	expression tag	UNP Q584T8
CS	-35	PHE	-	expression tag	UNP Q584T8
CS	-34	ALA	-	expression tag	UNP Q584T8
CS	-33	HIS	-	expression tag	UNP Q584T8
CS	-32	SER	-	expression tag	UNP Q584T8
CS	-31	LEU	-	expression tag	UNP Q584T8
CS	-30	VAL	-	expression tag	UNP Q584T8
CS	-29	MET	-	expression tag	UNP Q584T8

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Chain	Residue	Modelled	Actual	Comment	Reference
CS	-28	LEU	-	expression tag	UNP Q584T8
CS	-27	PRO	-	expression tag	UNP Q584T8
CS	-26	VAL	-	expression tag	UNP Q584T8
CS	-25	SER	-	expression tag	UNP Q584T8
CS	-24	LEU	-	expression tag	UNP Q584T8
CS	-23	TYR	-	expression tag	UNP Q584T8
CS	-22	SER	-	expression tag	UNP Q584T8
CS	-21	LYS	-	expression tag	UNP Q584T8
CS	-20	ILE	-	expression tag	UNP Q584T8
CS	-19	LEU	-	expression tag	UNP Q584T8
CS	-18	LEU	-	expression tag	UNP Q584T8
CS	-17	CYS	-	expression tag	UNP Q584T8
CS	-16	ASP	-	expression tag	UNP Q584T8
CS	-15	VAL	-	expression tag	UNP Q584T8
CS	-14	LYS	-	expression tag	UNP Q584T8
CS	-13	LYS	-	expression tag	UNP Q584T8
CS	-12	LYS	-	expression tag	UNP Q584T8
CS	-11	ILE	-	expression tag	UNP Q584T8
CS	-10	VAL	-	expression tag	UNP Q584T8
CS	-9	TYR	-	expression tag	UNP Q584T8
CS	-8	PHE	-	expression tag	UNP Q584T8
CS	-7	HIS	-	expression tag	UNP Q584T8
CS	-6	CYS	-	expression tag	UNP Q584T8
CS	-5	CYS	-	expression tag	UNP Q584T8
CS	-4	THR	-	expression tag	UNP Q584T8
CS	-3	ARG	-	expression tag	UNP Q584T8
CS	-2	LYS	-	expression tag	UNP Q584T8
CS	-1	LYS	-	expression tag	UNP Q584T8
CS	0	SER	-	expression tag	UNP Q584T8

- Molecule 23 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Cg	482	Total	C	N	O	S	0	0
			3904	2499	684	701	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cg	181	VAL	ALA	conflict	UNP Q585C2
Cg	498	ARG	MET	conflict	UNP Q585C2

- Molecule 24 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ci	165	Total	C	N	O	S	0	0
			1348	848	247	244	9		

- Molecule 25 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ck	703	Total	C	N	O	S	0	0
			5596	3503	1017	1050	26		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ck	107	SER	LEU	conflict	UNP Q387C7
Ck	144	PHE	LEU	conflict	UNP Q387C7
Ck	253	TYR	PHE	conflict	UNP Q387C7
Ck	339	GLU	VAL	conflict	UNP Q387C7
Ck	871	GLY	GLU	conflict	UNP Q387C7

- Molecule 26 is a RNA chain called RNA (143-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CA	143	Total	C	N	O	P	0	0
			3030	1364	522	1001	143		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	473	U	G	conflict	GB 343546

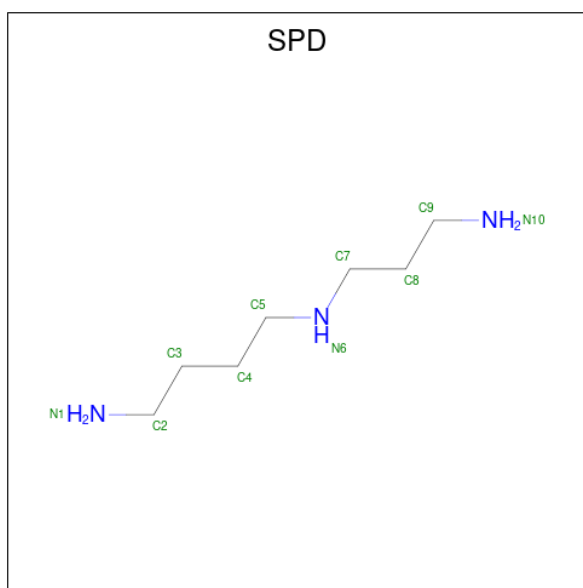
- Molecule 27 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	UO	5	Total	C	N	O	0	0
			30	20	5	5		

- Molecule 28 is a protein called Unknown protein.

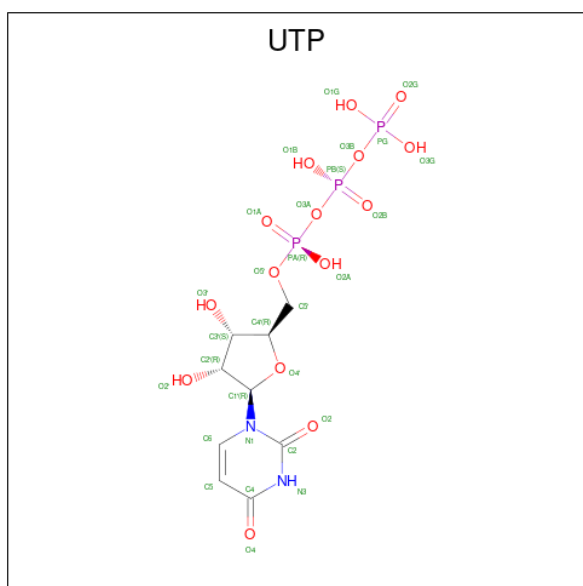
Mol	Chain	Residues	Atoms				AltConf	Trace
28	UP	7	Total	C	N	O	0	0
			42	28	7	7		

- Molecule 29 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



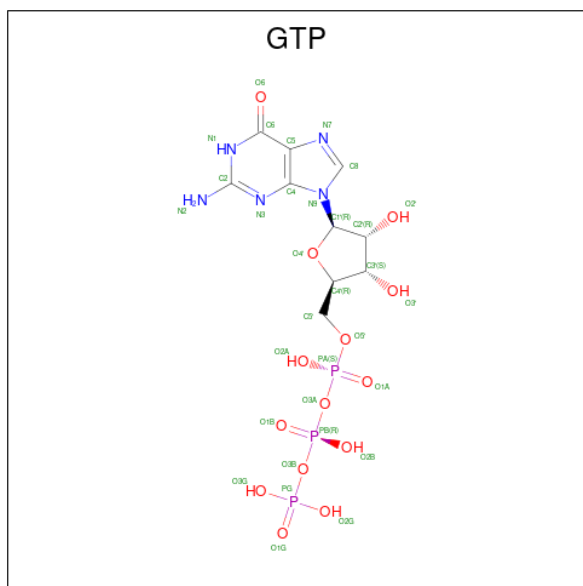
Mol	Chain	Residues	Atoms			AltConf
29	DL	1	Total	C	N	0
			10	7	3	
29	CA	1	Total	C	N	0
			10	7	3	

- Molecule 30 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).



Mol	Chain	Residues	Atoms					AltConf
30	DJ	1	Total	C	N	O	P	0
			29	9	2	15	3	

- Molecule 31 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
31	Cg	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	Cg	1	Total	Mg	0
			1	1	
32	CA	2	Total	Mg	0
			2	2	

- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	Cg	3	Total	O	0
			3	3	

PRO	LEU	PHE	GLN	ARG	PHE	GLU	ARG	GLY	LEU	LEU	LEU	GLU	PRO	ARG	ALA	ASN	LEU	LYS	PHE	PHE	THR	SER	ARG	ALA	SER	GLN	GLN	SER	THR	LEU	GLU	ARG	ARG	G266	H267	M268	M269	T270	P271	H272	T273	T274	L275	H276	G277	R278	W282	T286	W287	L294	G295	P296	P302	G303	M304	T305	PRO	GLY	ASP
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• Molecule 3: mS49

Chain DB:  66% 23% 5% 6%

MET	ILE	ARG	ARG	ASN	VAL	CYS	GLY	ASP	GLY	ALA	ARG	LEU	GLU	W72	ALA	PRO	ASN	ILE	ALA	ALA	THR	PHE	SER	ALA	SER	GLN	GLN	SER	THR	GLN	LEU	GLY	ARG	SER	ASP	P121	H122	LYS	PRO	SER	ASN	PHE	SER	SER	VAL	ARG	ARG	SER	GLU	ASN	ALA	ASN	GLY	ASP	ALA	THR	SER	PRO	GLY	ALA
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THR	ALA	GLY	GLU	ASN	PRO	ALA	SER	SER	GLY	D71	W72	R78	A91	H92	K93	D94	D98	V99	Q220	H221	R110	M114	G115	G116	A117	V118	A119	Y120	H122	I123	E128	Y129	E130	E131	V137	W138	L139	D140	H141	R145	M146	H153	R154	L157	R173	V183
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S186	V189	H190	P191	I192	Q193	Q194	S204	A205	L206	Q209	R214	R215	I217	A218	E219	Q220	H221	T228	D231	R232	G116	D233	D236	S249	L255	V276	Q281	M285	T295	Q301	L302	P303	P308	S309	L318	S321	T326	P327	A333
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R339	T341	V342	V343	Q355	I357	N358	I359	T365	E368	G382	R383	A386	L387	V388	Q389	D394	Q395	T397	K400	H401	T402	N403	F413	O414	Q415	N416	T423	D424	H427	N428	P429	R433	S434	T435	E436	V439	O440	N445	D448	T449	M450
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R451	R452	E453	D454	R455	L456	Q461	D462	L463	T464	E465	Y471	G472	V473	P474	L478	V479	V483	H486	R487	N488	R489	A490	R493	P494	L495	L507	N510	R511	Y512	Y513	R514	E517	G518	F519	S520	M522	P526	E527	F528	L529	E532	Q539	R544	R545	R546
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L547	A548	L549	L550	H551	G552	L553	E554	A557	N558	E559	T560	A561	Q562	R564	H569	D572	E573	L574	F580	E584	M585	R586	V587	N588	D589	D590	E591	M592	E597	L608	P609	V614	A622	S623	L626	M635	G636	T637	R641	S646	G647	R648	L656
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R662	V663	G664	R665	V671	V672	Q684	P685	Q686	L689	S693	E716	M719	K720	R722	Y731	V735	V743	V744	L755	T756	V757	S758	E765	A768	V769	N774	T776	V783	Y784	N785	L786	L787	P788	N789	S790	R793	Y794	V795	P796	Q800	L801
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D802	E805	T810	D815	R816	E820	E829	P830	P823	L826	L830	N831	Y832	G833	T834	Y837	R841	D849	S850	T851	M852	G859	Q860	R861	T867	H868	L876	P877	V878	R881	P885	Q891	R892	L893	Q898	Y901	I902	Y903	Q904	Y905	Q908	P909	F910
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L917	V918	V920	A921	F922	Q923	M929	E930	E939	M937	Q940	R941	H944	G945	P946	R948	T949	V950	S954	R955	N958	P959	M962	R963	R964	V968	T969	K975	H981	L983	D984	R990	D993	T994	V995	T1001	T1002	Q1004	I1005	D1009	T1012	R1013
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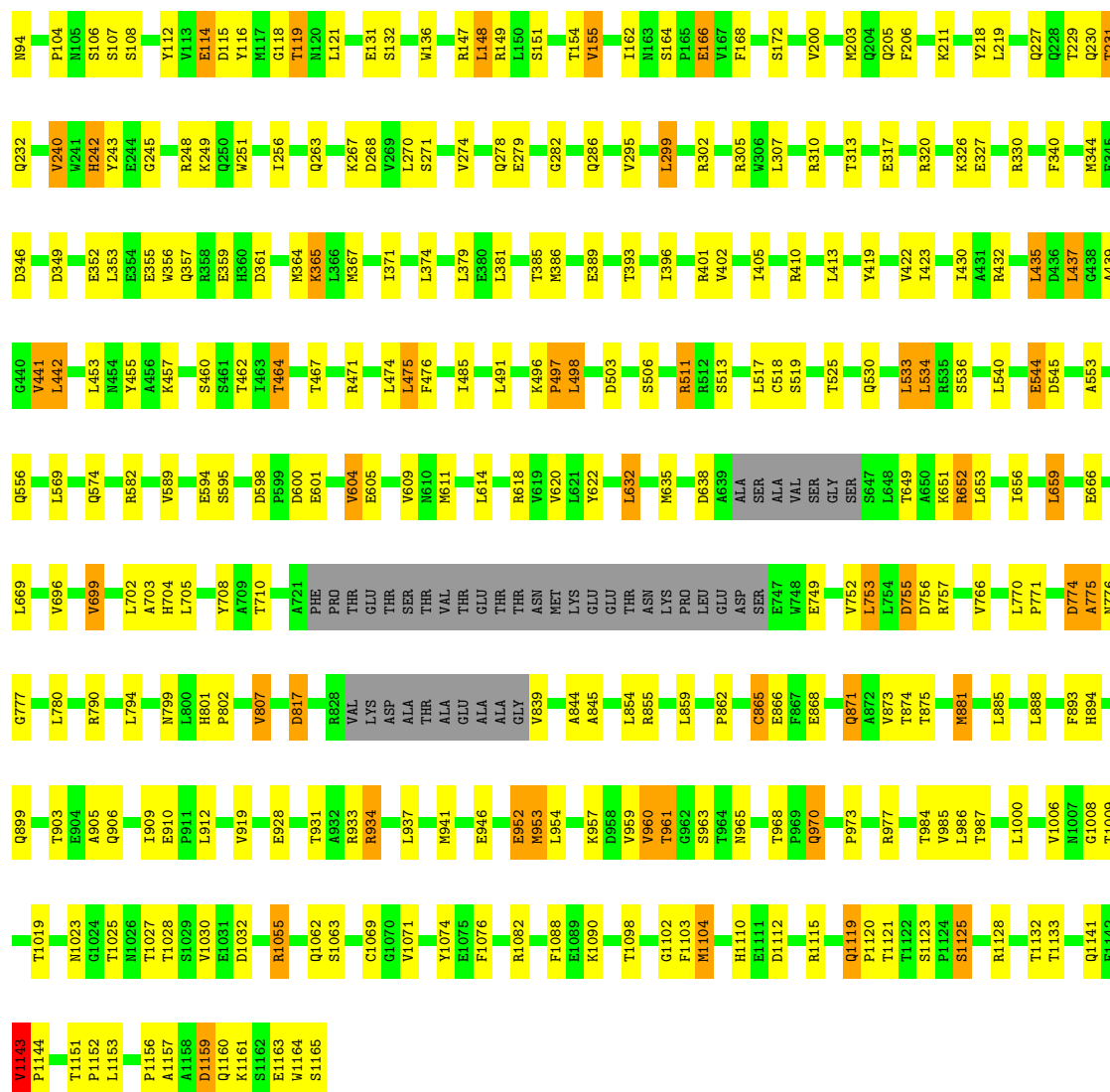
D1020	R1023	S1026	T1027	S1028	R1029	R1030	R1031	D1032	Y1033	I1034	Q1035	I1039	Y1042	T1043	P1044	V1047	Q1051	A1052	A1053	Q1054	Q1055	P1056	D1065	M1066	T1067	G1068	T1069	V1079	R1080	Y1081	K1082	L1100	Q1101	Y1102	V1103	D1104	G1105	V1106	T1107	P1108	W1109	K1110	T1117	H1125	P1126	M1127
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R1132	P1133	E1134	V1135	A1136	M1137	V1142	G1143	L1144	L1145	P1146	D1153	T1156	G1157	K1158	V1159	K1160	D1164	S1165	V1166	R1167	D1168	K1172	T1173	L1181
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• Molecule 4: mS50

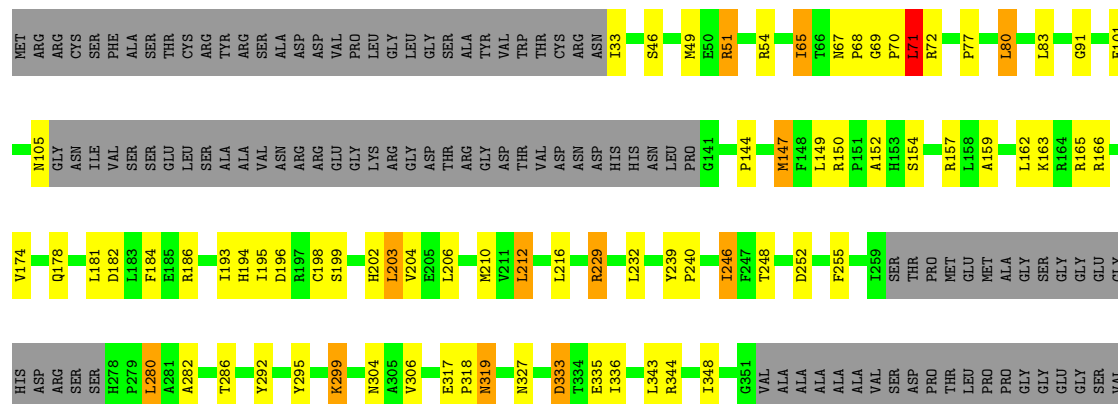
Chain DC:  67% 23% 5% 6%

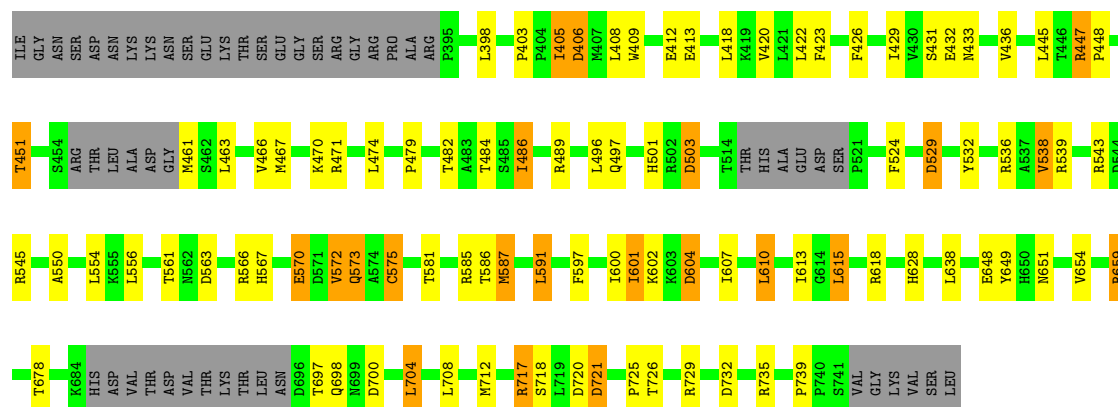
MET	PHE	ARG	VAL	ARG	ARG	LEU	ALA	GLY	PHE	ILE	GLN	CYS	SER	PRO	CYS	GLY	LYS	MET	GLY	PRO	LEU	LYS	GLN	THR	ARG	ARG	Y29	T30	D36	R46	E50	A56	E57	V58	I61	W71	D77	P78	H81	T82	P85	T86	M87	L88	G89	G90	K91	F92	R93
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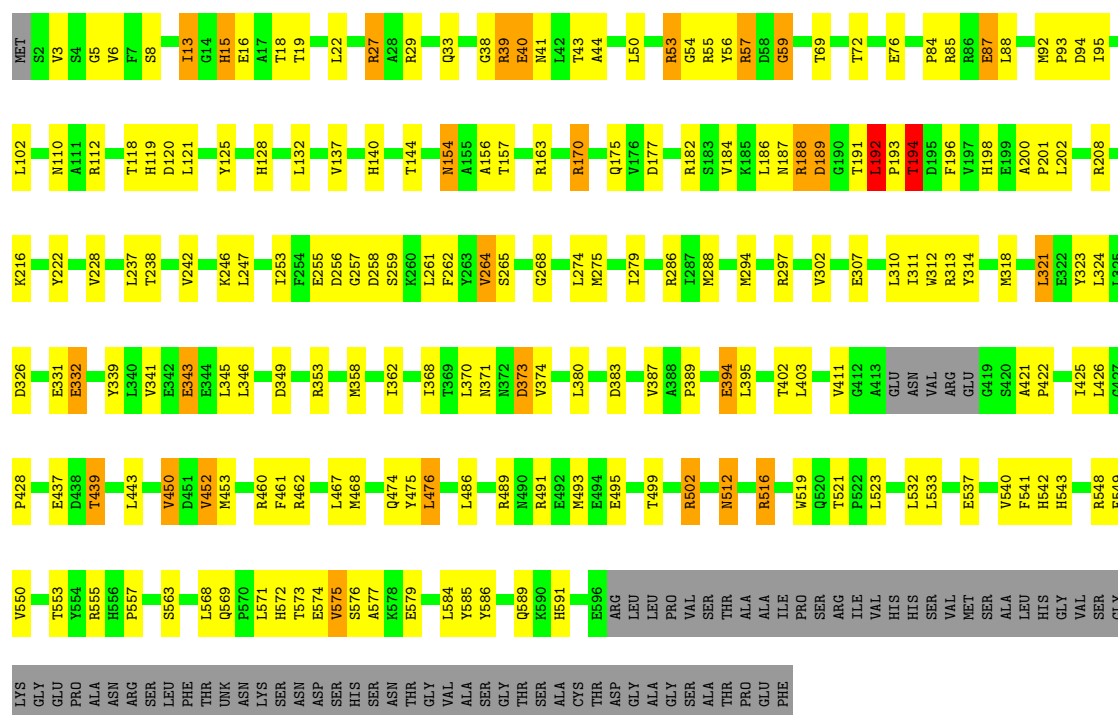
• Molecule 5: mS52

Chain DE: 56% 18% 5% 21%

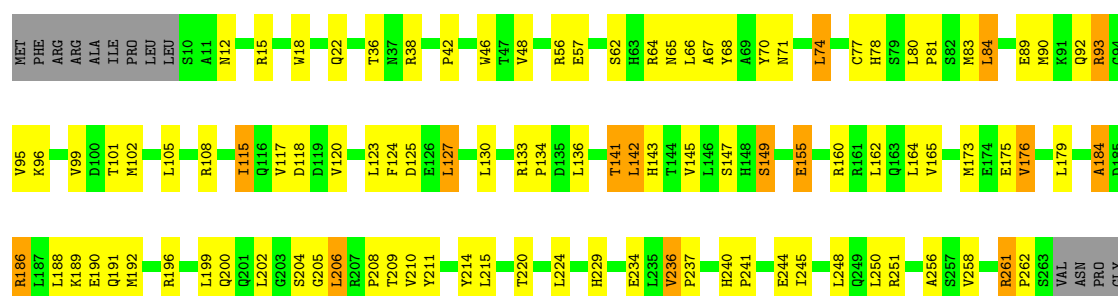




• Molecule 6: mS53

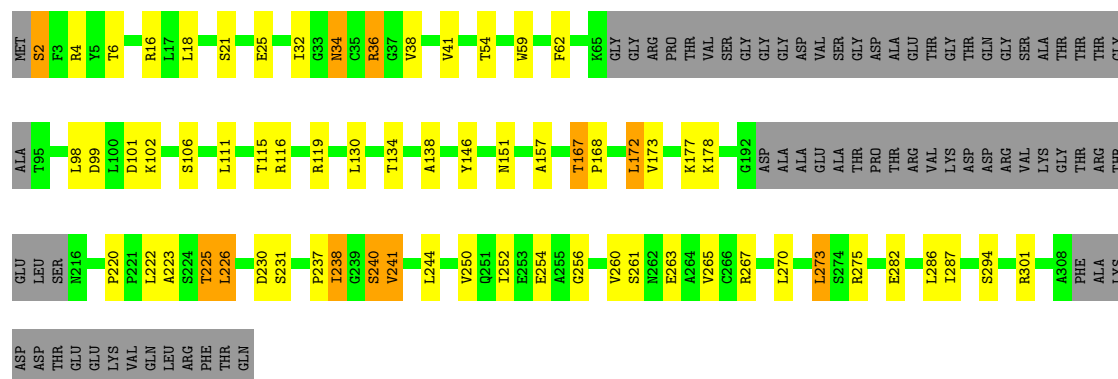


• Molecule 7: mS54



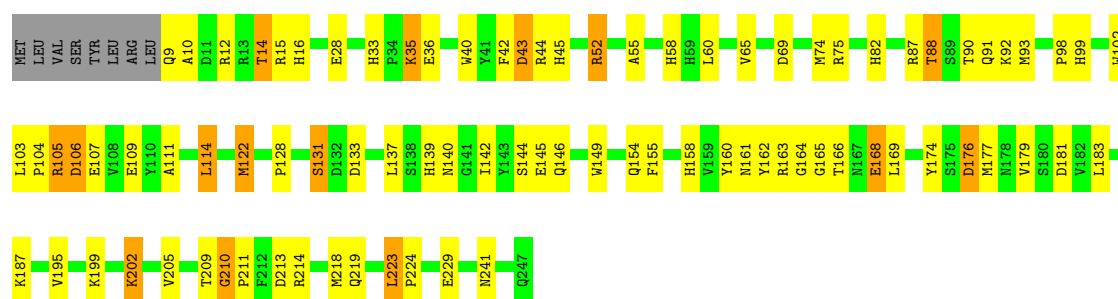
- Molecule 10: mS58

Chain DK:  59% 17% 21%



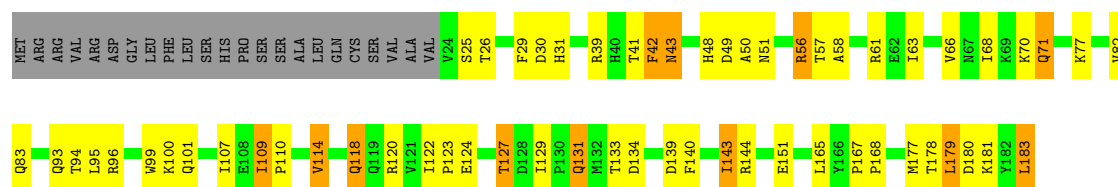
- Molecule 11: mS67

Chain DT:  62% 29% 6% 1%



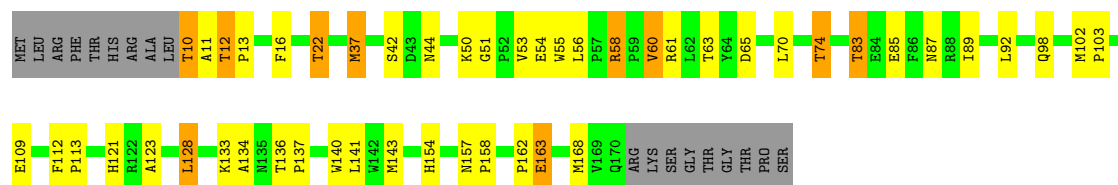
- Molecule 12: mS69

Chain DV:  55% 26% 7% 13%



- Molecule 13: mS70

Chain DW:  63% 22% 6% 10%



- Molecule 14: mS71

777	778	779	780	781	782	783	784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850	851	852	853	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000
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T93	R96	Q99	E102	Q106	F109	T110	R111	H112	V113	T124	T125	Q128	D133	Y138	V141	R148	R161	R162	K163																											
MET	LEU	ARG	SER	THR	LEU	THR	SER	LEU	R10	T11	T14	S15	P20	S23	W32	A33	D34	P35	E36	R37	M38	V39	R40	L43	T47	L48	G49	V50	D51	Q52	L53	P54	T58	Q62	R63	D64	L65	C71	V77	G78	D79	S80	T81	K84	R87	T92

M4
 I7
 V10
 T14
 I15
 L16
 Q17
 K18
 Y19
 T20
 F21
 K22
 L36
 L44
 L45
 W46
 L47
 I50
 H51
 I52
 I55
 F62
 L65
 N66
 N67
 F68
 E69
 Y70
 L71
 I72
 I73
 L74
 I75
 S76
 T77

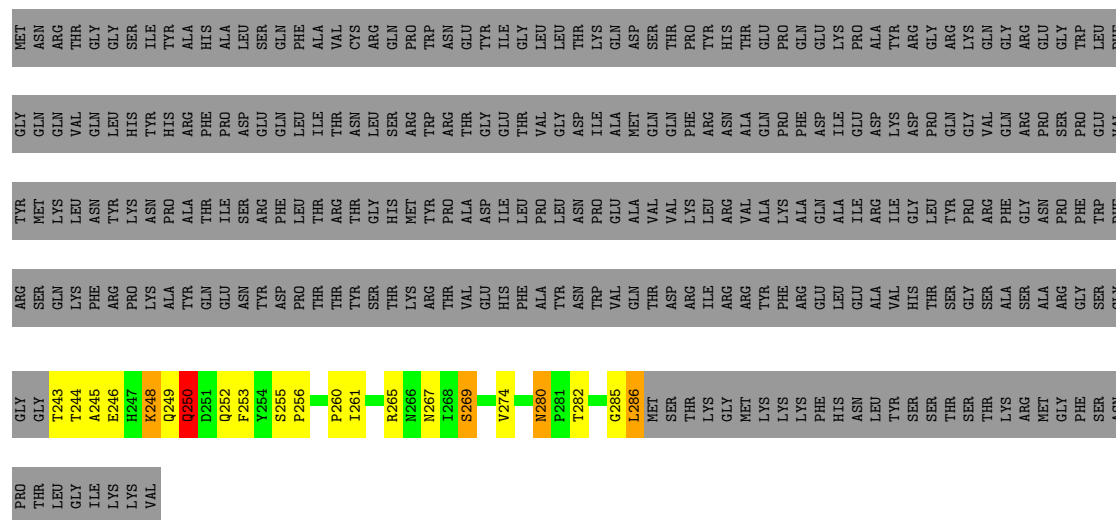
M356	M366	PHE	THR	ASN	THR	ALA	GLU	M1
A361	THR	ASN	PHE	GLN	GLU	GLN	THR	Q2
	VAL	LEU	LEU	ILE	GLY	ILE	PRO	K3
I372	LEU	GLY	GLU	GLY	GLU	GLY	MET	L4
E375	LYS	TRP	TRP	GLU	GLU	VAL	TRP	T9
	ASP	MET	MET	VAL	VAL	GLY	GLY	A10
R392	ALA	ARG	GLY	ALA	LEU	ALA	GLU	R14
V400	LYS	THR	THR	LEU	LEU	ALA	VAL	L15
	VAL	GLU	GLU	PHE	PHE	ALA	PRO	F16
T406	ALA	THR	THR	PRO	PRO	ALA	ALA	R17
R407	GLY	ARG	ARG	GLU	GLU	HIS	HIS	L18
L410	ASP	ALA	ALA	LEU	LEU	ASN	ASN	K32
K411	SER	LYS	PHE	CYS	CYS	LEU	LEU	S33
K412	ARG	THR	THR	TYR	TYR	THR	THR	D34
L415	HIS	GLU	GLU	GLU	GLU	GLU	SER	G35
	T289	HIS	HIS	ALA	ALA	GLN	SER	E36
T290	LYS	ALA	LEU	ALA	ALA	ARG	ARG	L38
	R293	LEU	PHE	LEU	LEU	ASP	ASP	V39
T294	GLU	GLU	GLU	LEU	VAL	LEU	GLU	R40
D295	PHE	PHE	PHE	VAL	GLN	ARG	LEU	V41
	SER	SER	SER	THR	THR	ASP	LEU	R42
	ARG	ARG	ARG	THR	THR	GLU	LEU	S43
	HIS	LYS	LYS	GLY	GLY	LEU	LEU	S54
	T303	ARG	ARG	LEU	LEU	THR	THR	S57
G304	ARG	ARG	LYS	GLY	GLY	ALA	ALA	E58
I305	PHE	ASN	PHE	CYS	CYS	ILE	GLN	R59
A306	ASN	THR	THR	ILE	ILE	SER	SER	
G308	ARG	ARG	ARG	ARG	ARG	ARG	LEU	
R309	ASP	ASP	ASP	ARG	ARG	PRO	LYS	E62
G310	ASP	VAL	VAL	VAL	VAL	VAL	GLU	
C311	VAL	ARG	ARG	SER	SER	SER	ALA	R65
R312	ARG	VAL	VAL	ALA	ALA	ALA	TRP	P66
D313	VAL	MET	MET	ALA	ALA	MET	MET	L67
G314	MET	PHE	PHE	SER	SER	ARG	GLU	
E315	GLY	GLU	GLU	GLN	GLN	VAL	VAL	
	ASN	ASN	ASN	GLN	GLN	SER	GLY	
T320	THR	THR	THR	LEU	LEU	GLY	GLU	
A321	ARG	ARG	ARG	SER	SER	ASN	ASN	
L322	LEU	LEU	LEU	ARG	ARG	VAL	VAL	
I323	MET	MET	MET	THR	THR	PHE	PHE	
R324	SER	SER	SER	ILE	ILE	ALA	ALA	
E325	LYS	LYS	LYS	THR	THR	GLN	GLN	
N326	ALA	ALA	ALA	ALA	ALA	SER	SER	
	THR	THR	THR	GLY	GLY	VAL	VAL	
	LEU	LEU	LEU	VAL	VAL	GLN	GLN	
	ALA	ALA	ALA	GLY	GLY	THR	THR	
	ASP	ASP	ASP	LEU	LEU	ALA	ALA	
	SER	SER	SER	ASP	ASP	SER	SER	
	ALA	ALA	ALA	ASN	ASN	VAL	VAL	
	ASP	ASP	ASP	ALA	ALA	GLY	GLY	
	THR	THR	THR	PRO	PRO	TYR	TYR	
	SER	SER	SER	GLY	GLY	ASP	ASP	
	HIS	HIS	HIS	THR	THR	LEU	LEU	
	SER	SER	SER	THR	THR	ASP	ASP	
	THR	THR	THR	ALA	ALA	GLY	GLY	
	ASN	ASN	ASN	THR	THR	ASN	ASN	
	GLY	GLY	GLY	VAL	VAL	GLN	GLN	
	ALA	ALA	ALA	GLY	GLY	THR	THR	
	ASN	ASN	ASN	ALA	ALA	ASN	ASN	
	GLY	GLY	GLY	THR	THR	GLY	GLY	
	THR	THR	THR	ALA	ALA	THR	THR	
	ASN	ASN	ASN	THR	THR	ASN	ASN	
	GLY	GLY	GLY	VAL	VAL	GLN	GLN	
	ALA	ALA	ALA	GLY	GLY	THR	THR	
	ASN	ASN	ASN	ALA	ALA	ASN	ASN	
	GLY	GLY	GLY	THR	THR	GLY	GLY	
	THR	THR	THR	ALA	ALA	THR	THR	
	ASN	ASN	ASN	THR	THR	ASN	ASN	
	GLY	GLY	GLY	VAL	VAL	GLN	GLN	

Chain CJ: 64% 29% 5%



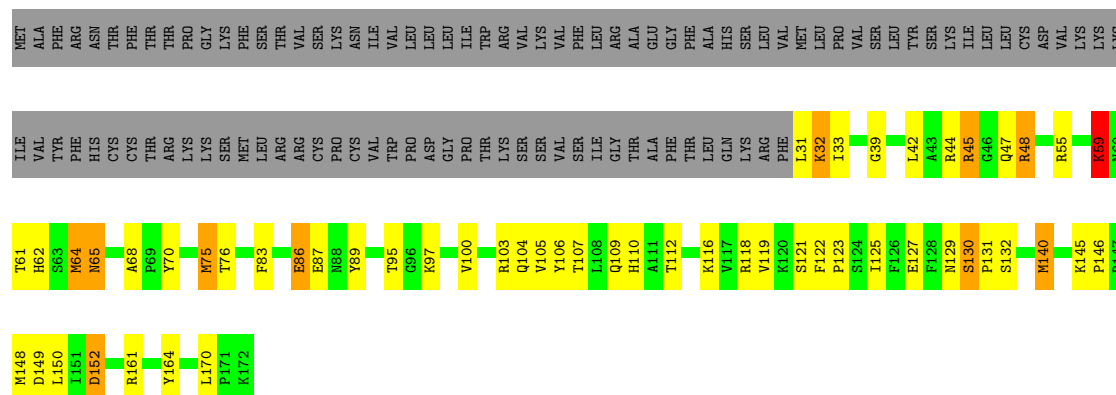
• Molecule 21: uS18m

Chain CR: 7% 5% • 86%



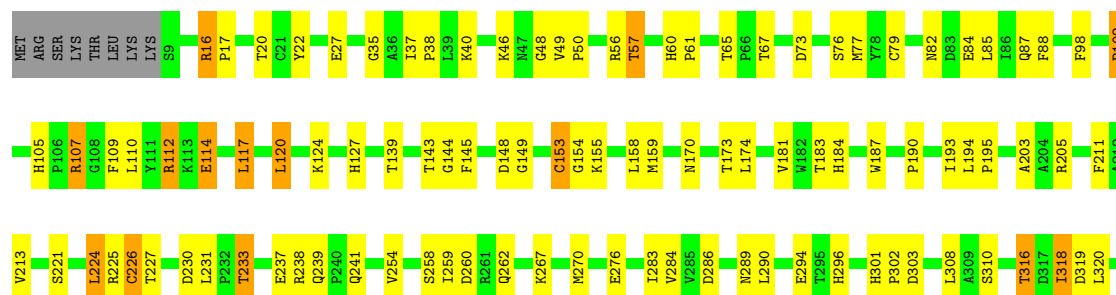
• Molecule 22: uS19m

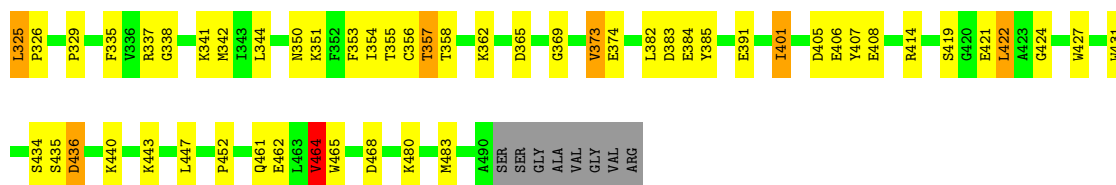
Chain CS: 35% 18% • 42%



• Molecule 23: mS29

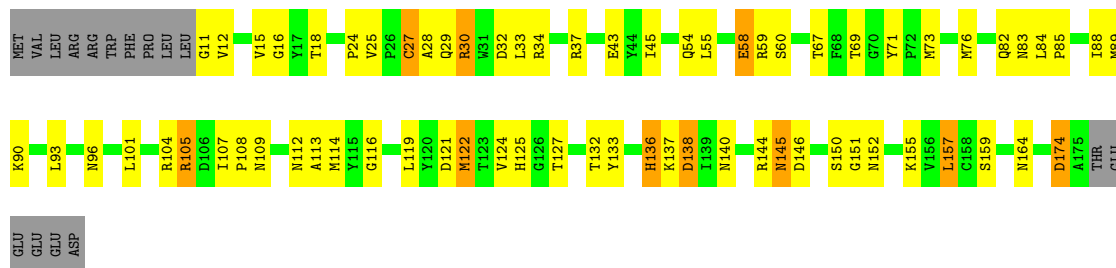
Chain Cg: 66% 27% • •





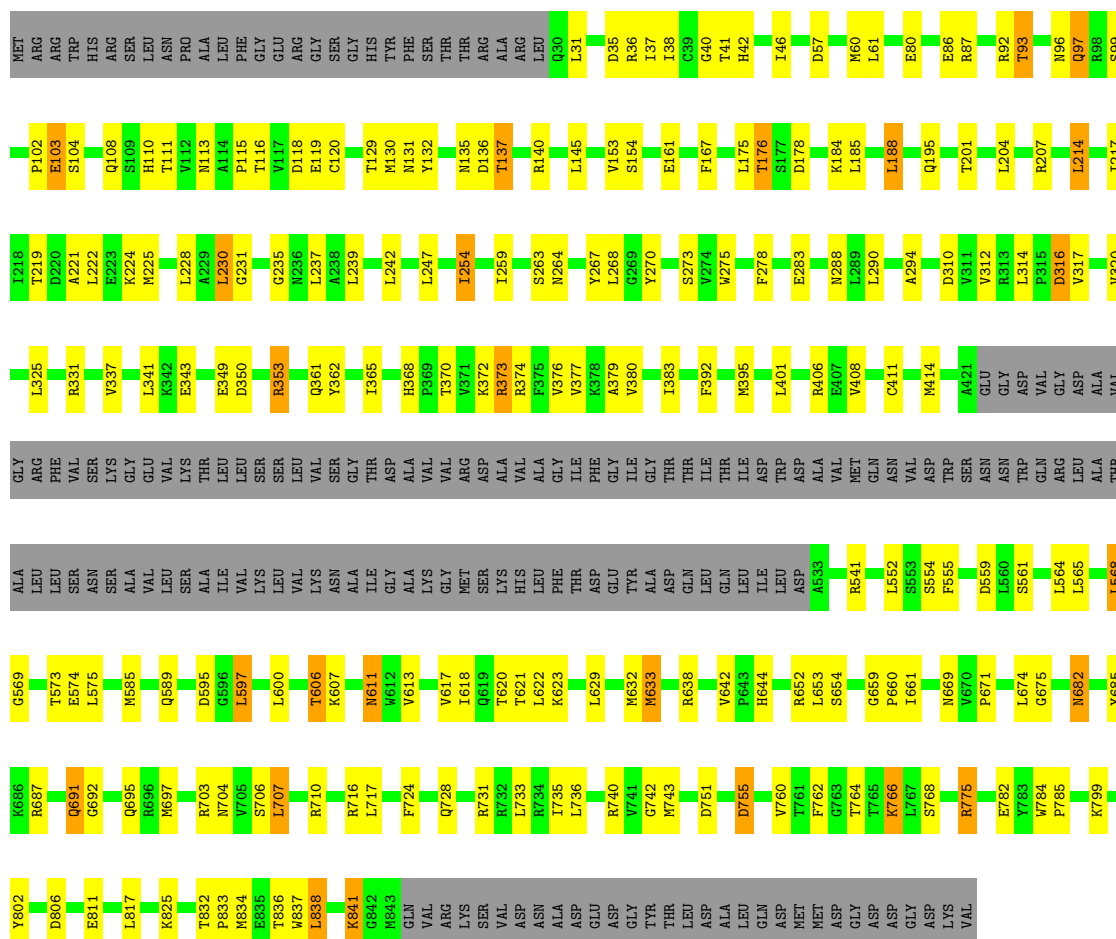
• Molecule 24: mS33

Chain Ci: 53% 33% 6% 9%



• Molecule 25: mS35

Chain Ck: 57% 21% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101308	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.587	Depositor
Minimum map value	-0.258	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, GTP, UTP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	DA	0.45	0/1010	0.90	5/1369 (0.4%)
2	DL	0.58	0/1185	1.01	5/1601 (0.3%)
3	DB	0.56	0/9369	0.98	30/12692 (0.2%)
4	DC	0.52	0/8952	0.93	23/12145 (0.2%)
5	DE	0.51	0/4955	0.97	17/6708 (0.3%)
6	DF	0.57	0/4856	0.96	13/6581 (0.2%)
7	DG	0.48	0/4674	0.92	6/6333 (0.1%)
8	DH	0.58	0/4684	0.96	16/6347 (0.3%)
9	DJ	0.57	1/2649 (0.0%)	0.97	6/3598 (0.2%)
10	DK	0.57	0/2045	0.92	2/2759 (0.1%)
11	DT	0.61	0/2133	1.03	7/2889 (0.2%)
12	DV	0.61	0/1382	1.06	5/1871 (0.3%)
13	DW	0.51	0/1407	0.95	4/1916 (0.2%)
14	DX	0.56	0/1231	1.02	9/1654 (0.5%)
15	DY	0.64	0/1334	0.98	3/1810 (0.2%)
16	CC	0.63	0/666	1.09	2/900 (0.2%)
17	CI	0.59	0/1783	1.00	2/2395 (0.1%)
18	CJ	0.67	3/6705 (0.0%)	1.06	49/9124 (0.5%)
19	CK	0.49	0/448	0.91	0/600
20	CN	0.63	0/1361	0.99	4/1840 (0.2%)
21	CR	0.55	0/361	1.18	5/490 (1.0%)
22	CS	0.55	0/1209	1.05	12/1626 (0.7%)
23	Cg	0.56	0/4025	1.00	15/5467 (0.3%)
24	Ci	0.67	0/1388	1.09	4/1878 (0.2%)
25	Ck	0.54	0/5696	0.94	6/7705 (0.1%)
26	CA	0.34	0/3392	0.52	0/5275
All	All	0.56	4/78900 (0.0%)	0.96	250/107573 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	DL	0	2
3	DB	0	2
4	DC	0	2
7	DG	0	2
9	DJ	0	1
11	DT	0	1
14	DX	0	1
18	CJ	0	1
23	Cg	0	1
24	Ci	0	1
25	Ck	0	1
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	CJ	424	HIS	CG-CD2	-12.76	1.21	1.35
18	CJ	424	HIS	CD2-NE2	9.05	1.47	1.37
18	CJ	424	HIS	CG-ND1	7.88	1.47	1.38
9	DJ	255	LYS	C-O	5.84	1.30	1.24

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DH	133	CYS	CA-C-N	-10.96	106.13	119.84
8	DH	133	CYS	C-N-CA	-10.96	106.13	119.84
5	DE	327	ASN	CA-C-N	-10.94	109.11	120.38
5	DE	327	ASN	C-N-CA	-10.94	109.11	120.38
18	CJ	783	ILE	CA-C-N	10.31	130.41	120.31
18	CJ	783	ILE	C-N-CA	10.31	130.41	120.31
23	Cg	16	ARG	CA-C-N	9.66	130.33	120.38
23	Cg	16	ARG	C-N-CA	9.66	130.33	120.38
25	Ck	687	ARG	N-CA-C	9.51	126.04	113.30
16	CC	10	VAL	N-CA-C	8.87	120.62	112.29
18	CJ	712	THR	CA-C-N	-8.68	109.00	119.84
18	CJ	712	THR	C-N-CA	-8.68	109.00	119.84
17	CI	65	MET	CA-C-N	8.60	128.18	119.24
17	CI	65	MET	C-N-CA	8.60	128.18	119.24
18	CJ	345	VAL	CA-C-N	8.42	128.00	119.24
18	CJ	345	VAL	C-N-CA	8.42	128.00	119.24
3	DB	944	HIS	N-CA-C	8.36	124.08	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DH	367	LEU	N-CA-C	-8.18	95.84	108.76
23	Cg	49	VAL	CA-C-N	-8.09	109.72	119.84
23	Cg	49	VAL	C-N-CA	-8.09	109.72	119.84
5	DE	739	PRO	CA-C-N	8.03	128.47	119.32
5	DE	739	PRO	C-N-CA	8.03	128.47	119.32
3	DB	554	GLU	CA-C-N	-8.02	111.74	119.76
3	DB	554	GLU	C-N-CA	-8.02	111.74	119.76
21	CR	285	GLY	N-CA-C	7.95	124.39	110.80
18	CJ	803	ILE	CA-C-N	-7.89	111.46	123.14
18	CJ	803	ILE	C-N-CA	-7.89	111.46	123.14
5	DE	591	LEU	CA-C-N	-7.89	110.53	120.23
5	DE	591	LEU	C-N-CA	-7.89	110.53	120.23
18	CJ	424	HIS	ND1-CE1-NE2	7.83	116.23	108.40
5	DE	613	ILE	N-CA-C	7.68	118.27	110.82
25	Ck	659	GLY	CA-C-N	-7.64	112.95	120.52
25	Ck	659	GLY	C-N-CA	-7.64	112.95	120.52
3	DB	672	VAL	N-CA-C	7.64	118.38	110.36
4	DC	601	GLU	N-CA-C	7.56	119.21	110.97
4	DC	699	VAL	CA-C-N	7.51	127.89	119.32
4	DC	699	VAL	C-N-CA	7.51	127.89	119.32
3	DB	1033	TYR	CA-C-N	-7.50	110.90	121.55
3	DB	1033	TYR	C-N-CA	-7.50	110.90	121.55
8	DH	239	SER	CA-C-N	7.38	127.54	120.31
8	DH	239	SER	C-N-CA	7.38	127.54	120.31
22	CS	130	SER	CA-C-N	7.37	127.64	119.90
22	CS	130	SER	C-N-CA	7.37	127.64	119.90
14	DX	78	GLU	CA-C-N	7.36	126.99	119.19
14	DX	78	GLU	C-N-CA	7.36	126.99	119.19
18	CJ	32	ALA	CA-C-N	7.34	129.01	119.84
18	CJ	32	ALA	C-N-CA	7.34	129.01	119.84
4	DC	776	ASN	N-CA-C	-7.34	103.47	113.30
11	DT	154	GLN	CA-C-N	-7.33	111.63	122.41
11	DT	154	GLN	C-N-CA	-7.33	111.63	122.41
14	DX	128	GLY	N-CA-C	7.27	127.17	112.34
3	DB	510	ASN	N-CA-C	7.25	120.99	112.72
1	DA	1314	GLY	N-CA-C	7.16	126.95	112.34
4	DC	598	ASP	CA-C-N	7.09	127.40	119.32
4	DC	598	ASP	C-N-CA	7.09	127.40	119.32
12	DV	122	ILE	CA-C-N	7.07	127.10	119.89
12	DV	122	ILE	C-N-CA	7.07	127.10	119.89
24	Ci	151	GLY	N-CA-C	-7.04	103.55	115.80
11	DT	154	GLN	N-CA-C	-7.01	99.90	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	DY	34	ASP	CA-C-N	6.94	127.23	119.32
15	DY	34	ASP	C-N-CA	6.94	127.23	119.32
3	DB	908	GLN	CA-C-N	6.93	127.51	119.47
3	DB	908	GLN	C-N-CA	6.93	127.51	119.47
18	CJ	424	HIS	CE1-NE2-CD2	-6.89	102.11	109.00
18	CJ	800	LEU	CA-C-N	-6.85	111.93	119.19
18	CJ	800	LEU	C-N-CA	-6.85	111.93	119.19
22	CS	55	ARG	N-CA-C	-6.83	99.83	110.14
7	DG	560	GLU	CA-C-N	6.82	128.36	119.84
7	DG	560	GLU	C-N-CA	6.82	128.36	119.84
4	DC	164	SER	CA-C-N	6.81	128.35	119.84
4	DC	164	SER	C-N-CA	6.81	128.35	119.84
18	CJ	52	PHE	CA-C-N	6.76	127.16	119.93
18	CJ	52	PHE	C-N-CA	6.76	127.16	119.93
23	Cg	17	PRO	CA-C-N	6.74	128.26	119.84
23	Cg	17	PRO	C-N-CA	6.74	128.26	119.84
15	DY	161	ARG	N-CA-C	6.74	118.70	111.36
3	DB	440	GLY	N-CA-C	6.70	122.57	113.99
2	DL	295	GLY	CA-C-N	6.65	126.24	119.19
2	DL	295	GLY	C-N-CA	6.65	126.24	119.19
4	DC	600	ASP	N-CA-C	6.63	121.11	112.89
3	DB	1166	VAL	N-CA-C	6.61	118.21	111.00
14	DX	164	THR	N-CA-C	6.54	120.72	112.87
3	DB	1079	TRP	N-CA-C	6.49	118.36	111.28
23	Cg	365	ASP	N-CA-C	6.48	121.24	112.88
23	Cg	102	PRO	CA-C-N	6.35	126.56	119.32
23	Cg	102	PRO	C-N-CA	6.35	126.56	119.32
18	CJ	58	GLY	CA-C-N	6.29	125.98	119.82
18	CJ	58	GLY	C-N-CA	6.29	125.98	119.82
4	DC	1143	VAL	CA-C-N	6.29	127.70	119.84
4	DC	1143	VAL	C-N-CA	6.29	127.70	119.84
6	DF	59	GLY	CA-C-N	6.29	127.70	119.84
6	DF	59	GLY	C-N-CA	6.29	127.70	119.84
12	DV	42	PHE	N-CA-C	-6.27	101.82	110.35
5	DE	432	GLU	N-CA-C	6.25	119.06	110.24
3	DB	1127	MET	CA-C-N	6.22	125.78	119.19
3	DB	1127	MET	C-N-CA	6.22	125.78	119.19
13	DW	51	GLY	CA-C-N	6.18	125.59	118.85
13	DW	51	GLY	C-N-CA	6.18	125.59	118.85
18	CJ	454	THR	CA-C-N	-6.15	112.15	119.84
18	CJ	454	THR	C-N-CA	-6.15	112.15	119.84
9	DJ	35	PRO	CA-C-O	-6.15	116.76	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	CJ	703	ALA	N-CA-C	6.15	118.77	111.33
22	CS	59	LYS	CA-C-N	-6.14	114.32	122.85
22	CS	59	LYS	C-N-CA	-6.14	114.32	122.85
18	CJ	240	GLY	N-CA-C	6.12	121.26	110.80
20	CN	108	VAL	CA-C-N	6.09	125.49	118.85
20	CN	108	VAL	C-N-CA	6.09	125.49	118.85
4	DC	845	ALA	N-CA-C	-6.08	97.86	110.80
6	DF	192	LEU	CA-C-N	6.06	125.76	119.82
6	DF	192	LEU	C-N-CA	6.06	125.76	119.82
5	DE	71	LEU	N-CA-C	-6.03	97.97	110.80
8	DH	135	ARG	N-CA-C	-6.02	106.27	113.97
18	CJ	398	PHE	N-CA-C	6.00	118.91	108.76
3	DB	735	VAL	N-CA-C	6.00	116.64	110.82
5	DE	479	PRO	CA-C-N	-5.99	113.18	122.16
5	DE	479	PRO	C-N-CA	-5.99	113.18	122.16
25	Ck	368	HIS	CA-C-N	5.97	125.67	119.05
25	Ck	368	HIS	C-N-CA	5.97	125.67	119.05
4	DC	1119	GLN	CA-C-N	5.95	125.92	120.03
4	DC	1119	GLN	C-N-CA	5.95	125.92	120.03
18	CJ	584	GLU	N-CA-C	5.93	118.25	111.02
18	CJ	429	CYS	N-CA-C	5.90	117.82	108.79
6	DF	569	GLN	CA-C-N	5.89	127.21	119.84
6	DF	569	GLN	C-N-CA	5.89	127.21	119.84
18	CJ	461	HIS	N-CA-C	5.89	119.78	112.59
18	CJ	26	GLY	CA-C-N	5.88	127.20	119.84
18	CJ	26	GLY	C-N-CA	5.88	127.20	119.84
23	Cg	464	VAL	N-CA-C	5.88	118.65	112.83
18	CJ	405	LEU	CA-C-N	5.87	125.98	119.87
18	CJ	405	LEU	C-N-CA	5.87	125.98	119.87
23	Cg	149	GLY	CA-C-N	5.86	126.67	120.11
23	Cg	149	GLY	C-N-CA	5.86	126.67	120.11
3	DB	382	GLY	CA-C-O	-5.86	118.41	122.22
4	DC	242	HIS	N-CA-C	-5.82	100.56	109.65
3	DB	471	TYR	N-CA-C	-5.82	101.00	110.20
10	DK	241	VAL	CB-CA-C	-5.82	104.43	111.88
22	CS	112	THR	N-CA-C	5.79	117.27	111.07
6	DF	128	HIS	N-CA-C	5.77	120.47	112.45
22	CS	68	ALA	CA-C-N	-5.76	113.08	119.19
22	CS	68	ALA	C-N-CA	-5.76	113.08	119.19
18	CJ	353	ASP	CA-C-N	5.72	125.34	119.56
18	CJ	353	ASP	C-N-CA	5.72	125.34	119.56
10	DK	241	VAL	N-CA-C	5.72	116.36	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	DC	88	LEU	N-CA-C	5.70	119.22	112.72
9	DJ	16	ASN	CA-C-N	5.70	125.38	119.56
9	DJ	16	ASN	C-N-CA	5.70	125.38	119.56
14	DX	102	MET	N-CA-C	5.69	120.36	112.45
20	CN	93	ASP	N-CA-C	5.69	118.26	110.24
18	CJ	544	THR	N-CA-C	5.68	116.40	108.00
8	DH	452	ARG	CA-C-N	5.67	125.69	119.90
8	DH	452	ARG	C-N-CA	5.67	125.69	119.90
18	CJ	210	TRP	N-CA-C	5.66	117.45	108.79
3	DB	1023	ARG	CA-C-N	5.64	125.59	119.78
3	DB	1023	ARG	C-N-CA	5.64	125.59	119.78
4	DC	1074	TYR	N-CA-C	5.64	118.16	110.55
8	DH	272	HIS	N-CA-C	5.63	119.46	112.59
21	CR	261	ILE	N-CA-C	-5.63	103.85	110.21
3	DB	622	ALA	N-CA-C	5.62	117.55	110.24
24	Ci	84	LEU	N-CA-C	5.62	116.97	109.83
4	DC	965	ASN	N-CA-C	5.62	118.25	111.40
7	DG	261	ARG	CA-C-N	5.61	125.45	119.28
7	DG	261	ARG	C-N-CA	5.61	125.45	119.28
21	CR	250	GLN	N-CA-C	5.61	120.40	113.50
14	DX	115	ARG	CA-C-N	-5.60	113.25	119.19
14	DX	115	ARG	C-N-CA	-5.60	113.25	119.19
16	CC	67	ASN	N-CA-C	5.58	120.21	113.17
4	DC	774	ASP	CA-C-N	-5.56	114.54	122.77
4	DC	774	ASP	C-N-CA	-5.56	114.54	122.77
6	DF	247	LEU	N-CA-C	-5.56	105.54	112.93
9	DJ	37	GLY	N-CA-C	-5.54	104.13	112.89
8	DH	148	ASP	CA-C-N	5.54	125.37	119.28
8	DH	148	ASP	C-N-CA	5.54	125.37	119.28
6	DF	242	VAL	CB-CA-C	-5.50	106.79	114.00
8	DH	307	ARG	N-CA-C	-5.49	101.92	110.10
14	DX	130	GLN	N-CA-C	5.49	118.02	111.71
18	CJ	544	THR	CB-CA-C	-5.49	108.66	116.34
22	CS	129	ASN	N-CA-C	-5.47	106.66	113.55
3	DB	472	GLY	CA-C-N	-5.43	118.04	123.04
3	DB	472	GLY	C-N-CA	-5.43	118.04	123.04
3	DB	891	GLN	CB-CA-C	-5.43	109.84	117.23
1	DA	1260	VAL	CA-C-N	5.42	126.62	119.84
1	DA	1260	VAL	C-N-CA	5.42	126.62	119.84
4	DC	462	THR	N-CA-C	-5.42	106.67	113.72
5	DE	447	ARG	CA-C-N	5.40	125.38	120.03
5	DE	447	ARG	C-N-CA	5.40	125.38	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DH	345	VAL	CB-CA-C	-5.40	104.17	112.05
8	DH	41	LYS	N-CA-C	-5.38	105.33	111.14
11	DT	210	GLY	CA-C-N	5.37	125.19	119.28
11	DT	210	GLY	C-N-CA	5.37	125.19	119.28
3	DB	626	LEU	N-CA-C	-5.35	100.45	109.07
4	DC	245	GLY	N-CA-C	5.35	120.71	110.86
3	DB	946	PRO	CA-C-N	-5.34	115.32	122.42
3	DB	946	PRO	C-N-CA	-5.34	115.32	122.42
2	DL	276	HIS	N-CA-C	5.33	119.77	113.16
1	DA	1250	ARG	CB-CA-C	-5.32	109.99	117.23
18	CJ	304	ARG	N-CA-C	-5.32	105.15	111.69
18	CJ	88	ARG	CA-C-N	5.30	125.28	120.03
18	CJ	88	ARG	C-N-CA	5.30	125.28	120.03
2	DL	21	VAL	CA-C-N	5.29	125.30	119.90
2	DL	21	VAL	C-N-CA	5.29	125.30	119.90
21	CR	280	ASN	CA-C-N	5.29	124.90	119.56
21	CR	280	ASN	C-N-CA	5.29	124.90	119.56
18	CJ	196	ALA	N-CA-C	5.29	116.73	110.97
18	CJ	485	GLU	N-CA-C	5.29	116.73	110.97
5	DE	239	TYR	CA-C-N	5.27	125.27	120.21
5	DE	239	TYR	C-N-CA	5.27	125.27	120.21
20	CN	38	ASP	N-CA-C	5.26	120.35	113.30
3	DB	1043	THR	CA-C-N	5.25	125.17	119.76
3	DB	1043	THR	C-N-CA	5.25	125.17	119.76
8	DH	81	LYS	CB-CA-C	-5.24	110.10	117.23
18	CJ	205	VAL	N-CA-C	5.23	115.89	110.82
9	DJ	156	LYS	CA-C-N	5.22	123.47	119.66
9	DJ	156	LYS	C-N-CA	5.22	123.47	119.66
18	CJ	158	THR	N-CA-C	5.21	117.65	110.35
22	CS	65	ASN	CA-C-N	5.21	125.51	119.93
22	CS	65	ASN	C-N-CA	5.21	125.51	119.93
18	CJ	346	PRO	N-CA-C	5.21	122.22	113.78
7	DG	496	ARG	N-CA-C	5.21	117.45	109.95
22	CS	61	THR	N-CA-C	-5.21	105.67	112.23
18	CJ	357	SER	N-CA-C	5.20	116.75	108.79
18	CJ	768	ASP	N-CA-C	5.18	116.85	109.14
18	CJ	56	ILE	N-CA-C	5.17	115.28	110.42
6	DF	3	VAL	N-CA-C	5.16	115.29	107.80
23	Cg	88	PHE	CA-C-N	-5.16	117.11	122.89
23	Cg	88	PHE	C-N-CA	-5.16	117.11	122.89
12	DV	109	ILE	CA-C-N	5.14	125.14	119.90
12	DV	109	ILE	C-N-CA	5.14	125.14	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Cg	369	GLY	N-CA-C	-5.14	103.83	112.77
13	DW	157	ASN	CA-C-N	5.14	125.18	119.32
13	DW	157	ASN	C-N-CA	5.14	125.18	119.32
8	DH	370	VAL	N-CA-C	5.13	115.56	110.23
11	DT	223	LEU	CA-C-N	-5.12	113.44	119.84
11	DT	223	LEU	C-N-CA	-5.12	113.44	119.84
4	DC	755	ASP	N-CA-C	5.12	116.75	108.26
24	Ci	108	PRO	CA-C-N	-5.10	115.86	123.11
24	Ci	108	PRO	C-N-CA	-5.10	115.86	123.11
6	DF	194	THR	N-CA-C	5.10	118.27	111.75
18	CJ	156	PRO	CA-C-N	5.10	126.21	119.84
18	CJ	156	PRO	C-N-CA	5.10	126.21	119.84
14	DX	39	GLY	N-CA-C	-5.08	104.81	111.37
3	DB	1082	LYS	N-CA-C	5.07	117.07	110.43
25	Ck	659	GLY	N-CA-C	-5.06	102.02	112.34
18	CJ	373	PHE	N-CA-C	5.06	116.76	109.07
1	DA	1311	SER	N-CA-C	5.05	119.59	113.38
6	DF	302	VAL	N-CA-C	5.04	115.70	110.82
3	DB	436	GLU	N-CA-C	5.03	116.45	111.07
6	DF	242	VAL	N-CA-C	5.03	118.38	112.35
5	DE	69	GLY	CA-C-N	-5.00	113.59	119.84
5	DE	69	GLY	C-N-CA	-5.00	113.59	119.84
7	DG	592	THR	N-CA-C	-5.00	106.77	112.92

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	CJ	100	ARG	Peptide
23	Cg	50	PRO	Peptide
24	Ci	150	SER	Peptide
25	Ck	230	LEU	Peptide
3	DB	383	ARG	Sidechain
3	DB	586	ARG	Sidechain
4	DC	497	PRO	Peptide
4	DC	775	ALA	Peptide
7	DG	184	ALA	Peptide
7	DG	592	THR	Peptide
9	DJ	35	PRO	Peptide
2	DL	269	MET	Peptide
2	DL	270	THR	Peptide
11	DT	43	ASP	Peptide

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Mol	Chain	Res	Type	Group
14	DX	127	MET	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DA	993	0	1016	21	0
2	DL	1153	0	1146	33	0
3	DB	9148	0	8834	228	0
4	DC	8748	0	8532	190	0
5	DE	4831	0	4789	110	0
6	DF	4747	0	4723	155	0
7	DG	4575	0	4490	150	0
8	DH	4578	0	4520	128	0
9	DJ	2572	0	2495	81	0
10	DK	2007	0	1998	46	0
11	DT	2058	0	1928	60	0
12	DV	1346	0	1335	47	0
13	DW	1359	0	1342	44	0
14	DX	1196	0	1189	41	0
15	DY	1293	0	1287	39	0
16	CC	646	0	679	19	0
17	CI	1754	0	1806	41	0
18	CJ	6516	0	6261	199	0
19	CK	438	0	438	13	0
20	CN	1322	0	1304	42	0
21	CR	353	0	334	13	0
22	CS	1175	0	1191	46	0
23	Cg	3904	0	3785	95	0
24	Ci	1348	0	1306	56	0
25	Ck	5596	0	5613	153	0
26	CA	3030	0	1513	52	0
27	UO	30	0	33	0	0
28	UP	42	0	44	0	0
29	CA	10	0	19	2	0
29	DL	10	0	19	0	0
30	DJ	29	0	11	5	0
31	Cg	32	0	12	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	CA	2	0	0	0	0
32	Cg	1	0	0	0	0
33	Cg	3	0	0	1	0
All	All	76845	0	73992	1698	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1698) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CJ:484:HIS:CD2	18:CJ:495:ARG:NH1	1.87	1.42
18:CJ:544:THR:CG2	18:CJ:552:ILE:HG12	1.53	1.36
18:CJ:544:THR:HG21	18:CJ:552:ILE:N	1.36	1.34
18:CJ:484:HIS:HD2	18:CJ:495:ARG:NH1	1.17	1.33
18:CJ:544:THR:HG22	18:CJ:552:ILE:CG1	1.68	1.23
18:CJ:484:HIS:CD2	18:CJ:495:ARG:HH12	1.48	1.20
3:DB:423:THR:HG23	10:DK:138:ALA:O	1.52	1.09
2:DL:271:PRO:O	2:DL:274:THR:HG23	1.51	1.09
3:DB:635:MET:HG3	25:Ck:373:ARG:HH11	1.16	1.06
6:DF:426:LEU:HB3	8:DH:200:THR:HG21	1.12	1.06
3:DB:423:THR:CG2	10:DK:138:ALA:O	2.04	1.06
23:Cg:109:PHE:HA	31:Cg:501:GTP:HN21	1.22	1.04
6:DF:426:LEU:O	8:DH:200:THR:HG22	1.57	1.04
13:DW:58:ARG:HG2	13:DW:58:ARG:HH11	1.21	1.02
9:DJ:308:ARG:HG3	9:DJ:308:ARG:HH11	1.21	1.01
6:DF:426:LEU:HB3	8:DH:200:THR:CG2	1.92	0.98
15:DY:148:ARG:NH1	26:CA:517:U:OP2	1.97	0.97
7:DG:196:ARG:NH1	7:DG:211:TYR:OH	1.98	0.97
18:CJ:544:THR:CG2	18:CJ:552:ILE:N	2.27	0.96
3:DB:511:ARG:HG3	3:DB:511:ARG:HH11	1.29	0.96
18:CJ:484:HIS:HD2	18:CJ:495:ARG:HH11	1.05	0.96
18:CJ:544:THR:HG21	18:CJ:551:ARG:C	1.90	0.95
6:DF:426:LEU:O	8:DH:200:THR:CG2	2.14	0.94
7:DG:300:ASP:OD2	17:CI:59:ARG:NH1	2.01	0.94
6:DF:216:LYS:NZ	18:CJ:472:SER:O	2.00	0.94
17:CI:293:ARG:NH2	17:CI:407:ARG:HH12	1.66	0.94
6:DF:426:LEU:CB	8:DH:200:THR:HG21	1.99	0.93
6:DF:57:ARG:HG2	6:DF:57:ARG:HH11	1.34	0.91
14:DX:50:ARG:NH1	22:CS:145:LYS:O	2.04	0.90
5:DE:144:PRO:HG2	5:DE:147:MET:HG3	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DF:589:GLN:HE21	8:DH:191:HIS:N	1.71	0.89
18:CJ:792:HIS:HD2	18:CJ:795:LYS:H	1.22	0.88
23:Cg:341:LYS:NZ	25:Ck:811:GLU:OE2	2.06	0.88
6:DF:188:ARG:NH1	30:DJ:401:UTP:O3G	2.07	0.87
7:DG:472:ARG:HH11	7:DG:472:ARG:HG2	1.40	0.87
6:DF:383:ASP:HB3	6:DF:468:MET:HE1	1.57	0.86
10:DK:254:GLU:HG3	10:DK:261:SER:HB3	1.56	0.86
3:DB:78:ARG:HG3	3:DB:78:ARG:HH11	1.40	0.85
2:DL:271:PRO:O	2:DL:274:THR:CG2	2.24	0.85
25:Ck:129:THR:HG22	25:Ck:131:ASN:H	1.41	0.85
13:DW:58:ARG:HG2	13:DW:58:ARG:NH1	1.91	0.84
22:CS:164:TYR:HB3	22:CS:170:LEU:HD13	1.58	0.84
7:DG:64:ARG:HH21	21:CR:249:GLN:HE22	1.25	0.84
3:DB:539:GLN:HG3	3:DB:585:MET:HE2	1.59	0.84
4:DC:155:VAL:HG13	4:DC:168:PHE:HE1	1.42	0.83
10:DK:238:ILE:HG21	10:DK:260:VAL:HG22	1.61	0.83
16:CC:44:LEU:HD13	16:CC:52:ILE:HG12	1.61	0.83
11:DT:14:THR:HG21	26:CA:438:U:O2	1.79	0.82
8:DH:80:ARG:HG2	8:DH:85:LEU:HG	1.60	0.82
3:DB:285:MET:HE1	25:Ck:37:ILE:HD11	1.62	0.81
9:DJ:31:HIS:HD2	9:DJ:33:ASN:H	1.29	0.81
12:DV:30:ASP:OD1	24:Ci:59:ARG:NH2	2.14	0.81
6:DF:38:GLY:H	6:DF:41:ASN:HD22	1.29	0.80
6:DF:425:ILE:HD13	8:DH:196:LEU:HD11	1.62	0.80
7:DG:476:GLN:HE22	7:DG:560:GLU:H	1.29	0.80
3:DB:635:MET:HG3	25:Ck:373:ARG:NH1	1.95	0.80
10:DK:252:ILE:HG22	10:DK:260:VAL:HG13	1.64	0.80
18:CJ:698:HIS:HB3	20:CN:65:LYS:HZ1	1.47	0.80
4:DC:119:THR:HG23	4:DC:132:SER:HB2	1.64	0.80
6:DF:426:LEU:H	8:DH:200:THR:HG23	1.47	0.79
8:DH:192:PHE:O	8:DH:196:LEU:HB2	1.82	0.79
3:DB:92:HIS:HD2	3:DB:94:ASP:H	1.28	0.79
5:DE:431:SER:O	5:DE:532:TYR:HB2	1.83	0.79
23:Cg:270:MET:HG2	23:Cg:338:GLY:HA3	1.63	0.79
3:DB:964:ARG:NH1	3:DB:1005:ILE:HD13	1.98	0.79
4:DC:844:ALA:HB1	5:DE:68:PRO:HB3	1.64	0.79
4:DC:1152:PRO:HG2	4:DC:1160:GLN:HE22	1.47	0.78
9:DJ:308:ARG:HH11	9:DJ:308:ARG:CG	1.96	0.78
3:DB:511:ARG:HH11	3:DB:511:ARG:CG	1.96	0.78
4:DC:155:VAL:HG13	4:DC:168:PHE:CE1	2.19	0.78
4:DC:240:VAL:HG23	4:DC:251:TRP:HZ3	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DB:236:ASP:HA	5:DE:587:MET:HE1	1.64	0.78
18:CJ:639:ARG:HH21	18:CJ:646:THR:HG22	1.48	0.78
3:DB:1068:GLY:HA2	25:Ck:660:PRO:HG3	1.66	0.78
23:Cg:109:PHE:HA	31:Cg:501:GTP:N2	1.99	0.77
7:DG:563:PHE:HA	7:DG:623:MET:HE1	1.65	0.77
6:DF:589:GLN:CB	8:DH:192:PHE:CE1	2.67	0.77
13:DW:37:MET:HG2	26:CA:519:U:H2'	1.66	0.77
18:CJ:544:THR:CG2	18:CJ:552:ILE:CG1	2.45	0.77
17:CI:326:ASN:ND2	17:CI:330:ASN:O	2.17	0.77
20:CN:104:THR:HG21	22:CS:48:ARG:HH22	1.51	0.76
3:DB:423:THR:HG21	10:DK:138:ALA:O	1.84	0.76
7:DG:390:GLY:O	7:DG:497:ARG:NH2	2.19	0.76
8:DH:269:ARG:NH1	18:CJ:288:GLN:OE1	2.19	0.75
3:DB:1053:ALA:HB2	8:DH:345:VAL:HG13	1.68	0.75
6:DF:548:ARG:NE	6:DF:574:GLU:OE2	2.20	0.75
21:CR:245:ALA:HA	21:CR:248:LYS:HD2	1.69	0.75
4:DC:441:VAL:HG11	4:DC:496:LYS:HD3	1.69	0.75
18:CJ:544:THR:HG21	18:CJ:552:ILE:CA	2.16	0.75
6:DF:373:ASP:N	6:DF:373:ASP:OD1	2.19	0.74
24:Ci:101:LEU:HD13	25:Ck:697:MET:HE1	1.68	0.74
1:DA:1312:TRP:CZ2	1:DA:1314:GLY:HA2	2.23	0.74
6:DF:29:ARG:H	9:DJ:314:GLN:HE22	1.36	0.74
23:Cg:289:ASN:HD21	23:Cg:358:THR:H	1.34	0.73
9:DJ:192:THR:HG21	9:DJ:222:GLU:HG2	1.69	0.73
25:Ck:832:THR:HG22	25:Ck:834:MET:H	1.54	0.73
7:DG:547:MET:HE1	7:DG:561:PRO:HB3	1.68	0.73
8:DH:85:LEU:HD12	8:DH:85:LEU:H	1.53	0.73
5:DE:182:ASP:OD1	5:DE:543:ARG:NH2	2.21	0.73
11:DT:9:GLN:O	26:CA:438:U:N3	2.17	0.73
25:Ck:331:ARG:NH2	25:Ck:595:ASP:OD1	2.21	0.73
3:DB:455:ARG:NH1	3:DB:461:GLN:O	2.22	0.73
4:DC:381:LEU:O	4:DC:385:THR:OG1	2.05	0.73
6:DF:589:GLN:HB2	8:DH:192:PHE:CD1	2.24	0.73
8:DH:19:THR:HG22	8:DH:21:LEU:H	1.53	0.72
9:DJ:209:ARG:NH2	30:DJ:401:UTP:O1B	2.22	0.72
25:Ck:617:VAL:HG21	25:Ck:638:ARG:HD2	1.70	0.72
3:DB:876:LEU:HD12	3:DB:877:PRO:HD2	1.72	0.72
15:DY:36:GLU:OE2	15:DY:40:ARG:NH1	2.21	0.72
15:DY:37:ARG:HH21	15:DY:106:GLN:HE22	1.36	0.72
13:DW:121:HIS:HD2	13:DW:123:ALA:H	1.34	0.72
17:CI:307:VAL:HG22	17:CI:322:LEU:HD22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CJ:793:HIS:CD2	18:CJ:794:GLU:HG2	2.23	0.72
14:DX:50:ARG:NH2	22:CS:122:PHE:O	2.22	0.72
4:DC:172:SER:HB2	4:DC:511:ARG:NH1	2.05	0.72
6:DF:589:GLN:NE2	8:DH:191:HIS:N	2.38	0.72
3:DB:801:LEU:HB2	3:DB:805:GLU:HB2	1.71	0.72
4:DC:574:GLN:HE21	4:DC:807:VAL:H	1.38	0.72
6:DF:576:SER:HB2	25:Ck:118:ASP:OD1	1.90	0.72
7:DG:366:ASP:HA	7:DG:370:ARG:HH12	1.54	0.72
3:DB:472:GLY:HA3	25:Ck:93:THR:O	1.90	0.71
3:DB:490:ARG:HB2	3:DB:962:MET:HE1	1.71	0.71
6:DF:53:ARG:HG2	6:DF:53:ARG:HH11	1.55	0.71
7:DG:22:GLN:HG2	25:Ck:102:PRO:HD3	1.71	0.71
24:Ci:145:ASN:HD21	24:Ci:152:ASN:HD21	1.36	0.71
3:DB:358:ASN:HB3	8:DH:542:LEU:HD21	1.72	0.71
2:DL:25:PRO:O	11:DT:202:LYS:NZ	2.24	0.71
9:DJ:308:ARG:HG3	9:DJ:308:ARG:NH1	1.95	0.71
7:DG:12:ASN:O	18:CJ:415:ARG:NH2	2.23	0.70
3:DB:110:ARG:NH2	3:DB:309:SER:O	2.24	0.70
3:DB:1164:ASP:HB3	13:DW:11:ALA:HB2	1.73	0.70
4:DC:327:GLU:OE2	4:DC:410:ARG:HD2	1.91	0.70
12:DV:31:HIS:H	12:DV:83:GLN:HE22	1.37	0.70
18:CJ:463:MET:HE1	24:Ci:85:PRO:HB2	1.72	0.70
9:DJ:242:LEU:HB3	9:DJ:294:MET:HE2	1.74	0.70
11:DT:164:GLY:O	11:DT:168:GLU:HB2	1.90	0.70
18:CJ:293:ASP:HB2	18:CJ:296:LEU:H	1.57	0.70
5:DE:467:MET:HE1	5:DE:486:ILE:HD13	1.72	0.70
3:DB:303:PRO:O	5:DE:489:ARG:NH2	2.25	0.70
12:DV:70:LYS:HD3	26:CA:513:U:H5'	1.74	0.69
4:DC:699:VAL:HB	4:DC:702:LEU:HD12	1.73	0.69
22:CS:31:LEU:HD12	22:CS:39:GLY:HA2	1.74	0.69
22:CS:48:ARG:HH11	22:CS:48:ARG:HG3	1.56	0.69
3:DB:478:ILE:HG22	25:Ck:46:ILE:HD11	1.74	0.69
7:DG:83:MET:HE3	7:DG:105:LEU:HD23	1.72	0.69
3:DB:550:LEU:HD13	3:DB:877:PRO:HB3	1.73	0.69
22:CS:106:TYR:HD2	22:CS:140:MET:HE1	1.57	0.69
4:DC:115:ASP:OD1	4:DC:116:TYR:N	2.24	0.69
6:DF:499:THR:HG22	8:DH:272:HIS:NE2	2.07	0.69
8:DH:193:VAL:N	8:DH:194:PRO:HD2	2.07	0.68
10:DK:119:ARG:NH2	10:DK:151:ASN:OD1	2.26	0.68
15:DY:37:ARG:NH2	15:DY:106:GLN:HE22	1.90	0.68
4:DC:240:VAL:HG23	4:DC:251:TRP:CZ3	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DH:14:TYR:OH	24:Ci:140:ASN:OD1	2.10	0.68
10:DK:254:GLU:CG	10:DK:261:SER:HB3	2.22	0.68
12:DV:123:PRO:O	12:DV:144:ARG:NH2	2.26	0.68
13:DW:89:ILE:HD13	15:DY:48:LEU:HD22	1.73	0.68
6:DF:548:ARG:HD2	25:Ck:116:THR:HG22	1.75	0.68
4:DC:340:PHE:HB3	4:DC:364:MET:HE1	1.74	0.68
23:Cg:301:HIS:HD2	23:Cg:303:ASP:H	1.40	0.68
18:CJ:712:THR:HG23	18:CJ:714:THR:H	1.58	0.68
3:DB:231:ASP:OD1	3:DB:232:ARG:N	2.27	0.68
3:DB:189:VAL:HG13	5:DE:471:ARG:HG2	1.75	0.67
8:DH:35:TYR:OH	9:DJ:46:ARG:NH2	2.27	0.67
4:DC:349:ASP:O	4:DC:353:LEU:N	2.28	0.67
7:DG:625:VAL:HG11	17:CI:35:GLY:HA3	1.76	0.67
25:Ck:682:ASN:HD22	25:Ck:682:ASN:H	1.42	0.67
5:DE:65:ILE:HD11	5:DE:83:LEU:HD23	1.76	0.67
18:CJ:544:THR:HG22	18:CJ:552:ILE:HG12	0.73	0.67
4:DC:77:ASP:H	4:DC:81:HIS:HD2	1.42	0.67
8:DH:421:THR:O	18:CJ:16:ARG:NH2	2.28	0.67
11:DT:176:ASP:OD1	11:DT:176:ASP:N	2.25	0.67
13:DW:168:MET:HE2	23:Cg:16:ARG:HH12	1.60	0.67
6:DF:288:MET:HE3	8:DH:363:PRO:HG3	1.77	0.67
9:DJ:261:PHE:O	9:DJ:305:ARG:NH2	2.28	0.67
15:DY:33:ALA:CB	15:DY:62:GLN:HG2	2.24	0.66
4:DC:862:PRO:HG2	4:DC:865:CYS:HB2	1.78	0.66
18:CJ:376:SER:HB2	26:CA:452:A:O2'	1.95	0.66
11:DT:183:LEU:HB2	11:DT:219:GLN:HE22	1.61	0.66
3:DB:881:ARG:HH11	3:DB:881:ARG:HG2	1.60	0.66
7:DG:77:CYS:O	7:DG:108:ARG:NH1	2.29	0.66
14:DX:89:ARG:HH11	14:DX:89:ARG:CG	2.08	0.66
18:CJ:548:ASP:OD2	18:CJ:553:ARG:NH2	2.29	0.66
22:CS:148:MET:HE2	22:CS:150:LEU:HB3	1.78	0.66
4:DC:87:MET:HE3	4:DC:90:GLY:HA2	1.78	0.66
11:DT:93:MET:HE1	11:DT:102:TRP:NE1	2.10	0.66
18:CJ:231:GLU:HG3	18:CJ:434:ILE:HD12	1.77	0.66
7:DG:190:GLU:HG3	19:CK:54:LEU:HD13	1.77	0.66
26:CA:449:G:O2'	26:CA:475:A:N6	2.29	0.66
4:DC:305:ARG:HH12	4:DC:359:GLU:CD	2.02	0.65
4:DC:349:ASP:HB2	4:DC:352:GLU:HB2	1.78	0.65
22:CS:100:VAL:HG21	22:CS:104:GLN:NE2	2.11	0.65
23:Cg:82:ASN:OD1	23:Cg:107:ARG:NH1	2.28	0.65
7:DG:192:MET:HG3	7:DG:214:TYR:CE2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CS:161:ARG:NH1	22:CS:170:LEU:HD23	2.10	0.65
24:CI:60:SER:HB2	24:CI:69:THR:HG22	1.78	0.65
9:DJ:232:ARG:HD3	26:CA:427:U:H3'	1.78	0.65
23:Cg:289:ASN:ND2	23:Cg:358:THR:H	1.93	0.65
7:DG:236:VAL:HG13	7:DG:258:VAL:HG21	1.78	0.65
18:CJ:541:LEU:O	18:CJ:544:THR:CG2	2.44	0.65
18:CJ:544:THR:HG21	18:CJ:552:ILE:H	1.50	0.65
3:DB:1030:ARG:HH11	3:DB:1030:ARG:CG	2.09	0.65
4:DC:871:GLN:HG3	5:DE:67:ASN:HD21	1.62	0.65
12:DV:31:HIS:CD2	12:DV:82:VAL:HG11	2.32	0.65
23:Cg:38:PRO:O	23:Cg:57:THR:OG1	2.13	0.65
5:DE:210:MET:HG3	5:DE:426:PHE:HZ	1.62	0.65
3:DB:276:VAL:O	3:DB:486:HIS:HE1	1.80	0.65
6:DF:425:ILE:HG21	8:DH:196:LEU:HD11	1.77	0.65
23:Cg:276:GLU:O	23:Cg:350:ASN:ND2	2.30	0.65
8:DH:253:SER:HA	8:DH:258:MET:HE1	1.77	0.65
4:DC:635:MET:O	4:DC:652:ARG:NH2	2.30	0.65
11:DT:16:HIS:HA	11:DT:28:GLU:OE2	1.97	0.64
6:DF:262:PHE:O	9:DJ:90:ARG:NH2	2.30	0.64
19:CK:26:ARG:HB2	26:CA:460:U:H5	1.63	0.64
3:DB:549:LEU:HD23	3:DB:554:GLU:HG2	1.78	0.64
18:CJ:436:ARG:NH2	25:Ck:671:PRO:HB2	2.12	0.64
3:DB:214:ARG:NE	5:DE:539:ARG:HH12	1.96	0.64
3:DB:1065:ASP:OD2	18:CJ:437:ARG:NH2	2.31	0.64
6:DF:27:ARG:NH1	26:CA:435:G:O2'	2.31	0.64
6:DF:57:ARG:HG2	6:DF:57:ARG:NH1	2.06	0.64
10:DK:36:ARG:NH1	10:DK:106:SER:HB3	2.12	0.64
8:DH:504:ARG:NH1	10:DK:287:ILE:HG23	2.12	0.64
25:Ck:644:HIS:HD2	25:Ck:669:ASN:H	1.46	0.64
7:DG:244:GLU:HG2	7:DG:251:ARG:HG3	1.80	0.64
7:DG:628:LEU:O	23:Cg:124:LYS:NZ	2.30	0.64
9:DJ:113:ASP:HB3	9:DJ:116:THR:HB	1.79	0.64
12:DV:107:ILE:HG12	18:CJ:754:VAL:HG22	1.79	0.64
6:DF:589:GLN:HB3	8:DH:192:PHE:CE1	2.33	0.64
13:DW:87:ASN:HD21	13:DW:158:PRO:HB3	1.63	0.64
3:DB:1133:PRO:HA	3:DB:1137:MET:HB2	1.80	0.63
8:DH:28:ASN:HD21	9:DJ:42:HIS:CE1	2.16	0.63
18:CJ:698:HIS:HB3	20:CN:65:LYS:NZ	2.13	0.63
3:DB:139:LEU:HD11	3:DB:219:GLU:HG2	1.79	0.63
25:Ck:167:PHE:HE2	25:Ck:235:GLY:HA2	1.63	0.63
4:DC:952:GLU:CD	4:DC:952:GLU:H	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:DG:401:CYS:N	7:DG:454:ASP:OD2	2.30	0.63
9:DJ:31:HIS:CD2	9:DJ:33:ASN:H	2.13	0.63
18:CJ:541:LEU:HD13	18:CJ:551:ARG:HE	1.63	0.63
18:CJ:713:PRO:HB3	26:CA:507:A:C2	2.33	0.63
6:DF:57:ARG:HH11	6:DF:57:ARG:CG	2.08	0.63
6:DF:5:GLY:HA3	24:Ci:159:SER:HB3	1.80	0.63
6:DF:358:MET:HG2	6:DF:368:ILE:HB	1.80	0.63
18:CJ:541:LEU:HA	18:CJ:552:ILE:HG13	1.80	0.63
23:Cg:316:THR:HG23	23:Cg:318:ILE:HG13	1.80	0.63
25:Ck:568:LEU:HD12	25:Ck:569:GLY:H	1.64	0.63
6:DF:426:LEU:N	8:DH:200:THR:HG23	2.13	0.63
14:DX:164:THR:HG22	14:DX:167:HIS:HB2	1.80	0.63
5:DE:147:MET:HE1	5:DE:567:HIS:CD2	2.34	0.63
7:DG:192:MET:HG3	7:DG:214:TYR:HE2	1.64	0.62
7:DG:215:LEU:HD22	7:DG:224:LEU:HD12	1.81	0.62
3:DB:975:LYS:HG2	7:DG:92:GLN:HE22	1.64	0.62
3:DB:1133:PRO:O	14:DX:115:ARG:NH1	2.32	0.62
5:DE:570:GLU:HA	5:DE:573:GLN:HB2	1.81	0.62
3:DB:885:PHE:HE2	3:DB:929:MET:HE2	1.63	0.62
9:DJ:132:ARG:NH1	9:DJ:171:LYS:O	2.31	0.62
3:DB:233:ASP:N	3:DB:233:ASP:OD1	2.33	0.62
3:DB:785:ASN:ND2	25:Ck:154:SER:OG	2.32	0.62
7:DG:324:LEU:HD23	7:DG:361:SER:HB2	1.79	0.62
4:DC:413:LEU:HD21	4:DC:422:VAL:HG21	1.82	0.62
5:DE:229:ARG:NH1	5:DE:255:PHE:CE1	2.68	0.62
6:DF:6:VAL:HG11	20:CN:10:MET:HE2	1.81	0.62
6:DF:425:ILE:HD13	8:DH:196:LEU:CD1	2.29	0.62
6:DF:589:GLN:OE1	8:DH:192:PHE:CZ	2.52	0.62
8:DH:253:SER:HB2	8:DH:287:GLY:HA3	1.81	0.62
9:DJ:22:MET:HG2	16:CC:67:ASN:HB2	1.81	0.62
4:DC:119:THR:HG21	4:DC:136:TRP:HE1	1.65	0.62
6:DF:589:GLN:HB2	8:DH:192:PHE:CE1	2.35	0.62
18:CJ:374:TRP:CZ3	20:CN:106:GLU:HB3	2.35	0.62
23:Cg:84:GLU:N	23:Cg:84:GLU:OE1	2.33	0.62
26:CA:518:G:H4'	26:CA:519:U:H5''	1.80	0.62
3:DB:560:THR:HG23	6:DF:548:ARG:NH1	2.14	0.62
3:DB:964:ARG:HH12	3:DB:1005:ILE:HD13	1.65	0.62
12:DV:42:PHE:CD2	12:DV:43:ASN:HB3	2.35	0.62
5:DE:246:ILE:HG13	5:DE:423:PHE:CG	2.34	0.62
9:DJ:71:MET:HE1	9:DJ:75:PHE:HB2	1.80	0.62
18:CJ:460:HIS:O	18:CJ:465:SER:OG	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DB:893:ILE:HG12	25:Ck:312:VAL:HB	1.80	0.61
7:DG:206:LEU:N	7:DG:234:GLU:OE2	2.31	0.61
18:CJ:275:ILE:HD13	18:CJ:412:PHE:HB2	1.81	0.61
25:Ck:728:GLN:HE22	25:Ck:731:ARG:HH11	1.47	0.61
3:DB:1107:THR:O	20:CN:70:LYS:HE3	2.00	0.61
18:CJ:385:LEU:HD11	22:CS:45:ARG:HD3	1.82	0.61
4:DC:46:ARG:HH11	4:DC:475:LEU:HB3	1.64	0.61
5:DE:543:ARG:HG2	5:DE:543:ARG:HH11	1.66	0.61
7:DG:624:ARG:HG2	12:DV:183:LEU:HD12	1.81	0.61
15:DY:33:ALA:HB2	15:DY:62:GLN:HG2	1.82	0.61
15:DY:39:VAL:HG21	23:Cg:461:GLN:HG2	1.81	0.61
18:CJ:281:VAL:HB	25:Ck:103:GLU:OE2	1.99	0.61
23:Cg:158:LEU:HD22	23:Cg:401:ILE:HD11	1.82	0.61
4:DC:1055:ARG:HA	4:DC:1055:ARG:HH11	1.65	0.61
7:DG:336:MET:HE2	7:DG:336:MET:HA	1.82	0.61
14:DX:89:ARG:NH1	14:DX:89:ARG:HG3	2.16	0.61
22:CS:48:ARG:HG3	22:CS:48:ARG:NH1	2.14	0.61
24:CI:33:LEU:HD11	25:Ck:785:PRO:HB3	1.81	0.61
5:DE:649:TYR:CG	5:DE:721:ASP:HB2	2.36	0.61
6:DF:125:TYR:H	6:DF:175:GLN:HE22	1.48	0.61
7:DG:472:ARG:HH11	7:DG:472:ARG:CG	2.11	0.61
24:CI:69:THR:HG23	24:CI:71:TYR:H	1.64	0.61
3:DB:488:ASN:OD1	3:DB:493:ARG:NH1	2.34	0.61
4:DC:1027:THR:O	4:DC:1027:THR:HG22	2.01	0.61
5:DE:319:ASN:OD1	5:DE:319:ASN:N	2.34	0.61
5:DE:610:LEU:HD22	5:DE:615:LEU:HD13	1.82	0.61
7:DG:346:ARG:HH21	7:DG:497:ARG:HD3	1.66	0.61
25:Ck:188:LEU:HD11	25:Ck:224:LYS:HB3	1.81	0.61
17:CI:62:GLU:OE2	19:CK:48:ARG:NH1	2.34	0.61
24:CI:133:TYR:CE2	24:CI:137:LYS:HE3	2.36	0.60
7:DG:117:VAL:HG13	7:DG:145:VAL:HG12	1.84	0.60
3:DB:190:HIS:HD2	3:DB:192:ILE:H	1.49	0.60
18:CJ:753:ASN:ND2	24:CI:16:GLY:O	2.32	0.60
5:DE:195:ILE:HG23	5:DE:198:CYS:SG	2.42	0.60
12:DV:100:LYS:HG3	18:CJ:773:GLU:HB3	1.82	0.60
15:DY:15:SER:HG	26:CA:518:G:H22	1.47	0.60
3:DB:823:PRO:HD2	3:DB:826:LEU:HG	1.83	0.60
4:DC:36:ASP:N	4:DC:36:ASP:OD1	2.34	0.60
4:DC:50:GLU:OE1	4:DC:405:ILE:HD11	2.01	0.60
6:DF:170:ARG:O	24:CI:104:ARG:NH2	2.34	0.60
8:DH:17:ILE:HD13	9:DJ:12:TYR:HE1	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:DT:33:HIS:CD2	11:DT:35:LYS:HD2	2.36	0.60
13:DW:63:THR:HG22	13:DW:65:ASP:H	1.66	0.60
13:DW:134:ALA:HB2	21:CR:286:LEU:HD22	1.82	0.60
18:CJ:54:MET:HE1	18:CJ:59:PRO:HA	1.84	0.60
3:DB:663:VAL:HG23	3:DB:665:ARG:HG3	1.83	0.60
3:DB:776:THR:HG22	3:DB:783:VAL:HG22	1.83	0.60
5:DE:451:THR:HB	5:DE:501:HIS:HD2	1.65	0.60
7:DG:118:ASP:OD1	25:Ck:406:ARG:NH2	2.35	0.60
8:DH:421:THR:HG21	8:DH:469:ASN:HD21	1.67	0.60
24:CI:109:ASN:HB2	24:CI:112:ASN:HD22	1.65	0.60
2:DL:302:PRO:HD2	17:CI:422:ARG:HH21	1.67	0.60
25:Ck:638:ARG:HG3	25:Ck:638:ARG:HH11	1.67	0.60
6:DF:121:LEU:HD22	6:DF:154:ASN:HA	1.83	0.60
3:DB:511:ARG:HG3	3:DB:511:ARG:NH1	2.06	0.60
4:DC:1088:PHE:CE1	10:DK:241:VAL:HG21	2.37	0.60
11:DT:104:PRO:HG2	11:DT:107:GLU:HG3	1.82	0.60
5:DE:604:ASP:OD1	5:DE:717:ARG:NH2	2.30	0.60
4:DC:200:VAL:HG13	4:DC:205:GLN:HB2	1.82	0.59
8:DH:520:GLY:HA2	11:DT:122:MET:HE3	1.84	0.59
11:DT:87:ARG:HD3	11:DT:139:HIS:CE1	2.36	0.59
18:CJ:441:HIS:HD2	25:Ck:768:SER:HB2	1.66	0.59
23:Cg:342:MET:HE3	23:Cg:351:LYS:HG2	1.84	0.59
4:DC:1143:VAL:HG12	4:DC:1144:PRO:HD2	1.83	0.59
5:DE:317:GLU:HG2	5:DE:318:PRO:HD2	1.83	0.59
6:DF:462:ARG:HH11	6:DF:474:GLN:NE2	2.01	0.59
11:DT:223:LEU:N	11:DT:229:GLU:OE1	2.31	0.59
14:DX:89:ARG:HH11	14:DX:89:ARG:HG3	1.67	0.59
19:CK:27:ARG:NH2	26:CA:465:U:OP1	2.36	0.59
25:Ck:130:MET:HE3	25:Ck:325:LEU:HD23	1.84	0.59
6:DF:343:GLU:HB3	6:DF:345:LEU:HG	1.84	0.59
8:DH:474:ASP:OD1	8:DH:474:ASP:N	2.33	0.59
3:DB:110:ARG:HH21	3:DB:116:GLY:HA2	1.66	0.59
4:DC:119:THR:HG21	4:DC:136:TRP:NE1	2.17	0.59
6:DF:93:PRO:HG2	22:CS:89:TYR:CD1	2.38	0.59
6:DF:188:ARG:HD3	30:DJ:401:UTP:H2'	1.85	0.59
18:CJ:261:ALA:O	18:CJ:265:CYS:HB2	2.03	0.59
3:DB:859:GLY:O	25:Ck:104:SER:HB2	2.02	0.59
8:DH:274:GLU:CD	8:DH:274:GLU:H	2.10	0.59
3:DB:940:GLN:OE1	3:DB:948:ARG:NH1	2.36	0.59
11:DT:109:GLU:CD	11:DT:109:GLU:H	2.11	0.59
20:CN:54:PRO:HB3	20:CN:60:VAL:HG13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DF:53:ARG:HG2	6:DF:53:ARG:NH1	2.15	0.59
18:CJ:730:TRP:CE2	18:CJ:731:MET:HG2	2.38	0.59
18:CJ:661:ARG:O	18:CJ:663:PRO:HD3	2.03	0.59
5:DE:732:ASP:OD1	5:DE:735:ARG:NH2	2.35	0.58
9:DJ:247:ASN:HD22	9:DJ:250:VAL:HG23	1.68	0.58
10:DK:62:PHE:CE1	10:DK:102:LYS:HD3	2.38	0.58
24:CI:107:ILE:HD11	24:CI:113:ALA:HB2	1.85	0.58
18:CJ:490:ASP:OD1	18:CJ:490:ASP:N	2.35	0.58
20:CN:108:VAL:HG21	20:CN:118:MET:HG3	1.83	0.58
21:CR:256:PRO:HA	21:CR:260:PRO:HB3	1.84	0.58
5:DE:697:THR:HG23	10:DK:59:TRP:HH2	1.66	0.58
7:DG:529:ASP:OD1	7:DG:529:ASP:N	2.36	0.58
3:DB:232:ARG:HG2	4:DC:953:MET:HE3	1.85	0.58
6:DF:156:ALA:O	26:CA:415:U:H3'	2.03	0.58
9:DJ:27:GLN:HG2	16:CC:66:ASN:HD22	1.69	0.58
4:DC:973:PRO:HB3	10:DK:244:LEU:HD21	1.84	0.58
18:CJ:698:HIS:CB	20:CN:65:LYS:HZ1	2.15	0.58
1:DA:1236:ILE:HG23	1:DA:1298:VAL:HG11	1.85	0.58
5:DE:184:PHE:O	5:DE:536:ARG:NH1	2.37	0.58
12:DV:179:LEU:HD22	23:Cg:117:LEU:HG	1.86	0.58
17:CI:54:SER:HB3	23:Cg:414:ARG:HH22	1.67	0.58
18:CJ:119:ARG:HG2	18:CJ:119:ARG:HH11	1.68	0.58
20:CN:158:ARG:NH1	20:CN:159:ASN:OD1	2.37	0.58
4:DC:455:TYR:CD1	4:DC:485:ILE:HD11	2.39	0.58
10:DK:2:SER:HA	11:DT:133:ASP:OD2	2.04	0.58
3:DB:514:ARG:HG3	3:DB:517:GLU:OE1	2.03	0.58
5:DE:147:MET:HE1	5:DE:567:HIS:CG	2.39	0.58
11:DT:44:ARG:HB2	11:DT:218:MET:HE2	1.86	0.58
6:DF:452:VAL:HG12	6:DF:453:MET:HE2	1.84	0.58
3:DB:546:ARG:HH21	3:DB:550:LEU:HD21	1.69	0.57
4:DC:305:ARG:NH1	4:DC:355:GLU:HG3	2.20	0.57
6:DF:187:ASN:HD22	6:DF:191:THR:HB	1.69	0.57
9:DJ:223:MET:HE1	9:DJ:233:VAL:HG21	1.85	0.57
11:DT:145:GLU:OE1	11:DT:149:TRP:NE1	2.36	0.57
18:CJ:345:VAL:HG22	18:CJ:346:PRO:HD2	1.85	0.57
25:Ck:135:ASN:ND2	25:Ck:137:THR:O	2.37	0.57
3:DB:519:PHE:HD2	3:DB:522:MET:HE2	1.67	0.57
7:DG:65:ASN:HD21	17:CI:294:ILE:H	1.52	0.57
7:DG:335:GLU:OE2	17:CI:17:ARG:NH2	2.33	0.57
11:DT:16:HIS:NE2	24:CI:138:ASP:OD1	2.37	0.57
20:CN:51:LEU:HD23	20:CN:55:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CI:34:ARG:NH1	24:CI:43:GLU:OE1	2.36	0.57
4:DC:219:LEU:HD11	4:DC:249:LYS:HA	1.86	0.57
7:DG:399:ARG:NH2	7:DG:457:ARG:HH12	2.03	0.57
12:DV:31:HIS:CE1	12:DV:48:HIS:HE1	2.23	0.57
6:DF:502:ARG:HG2	6:DF:519:TRP:O	2.05	0.57
17:CI:439:ARG:NH1	26:CA:496:U:O4	2.37	0.57
4:DC:149:ARG:HB3	4:DC:155:VAL:HG21	1.85	0.57
9:DJ:192:THR:HG21	9:DJ:222:GLU:CG	2.33	0.57
24:CI:83:ASN:ND2	26:CA:507:A:N3	2.52	0.57
2:DL:266:GLY:HA3	19:CK:22:PRO:HD3	1.86	0.57
5:DE:406:ASP:OD1	5:DE:406:ASP:N	2.26	0.57
7:DG:490:ARG:HD3	7:DG:571:VAL:HG11	1.85	0.57
3:DB:975:LYS:HG2	7:DG:92:GLN:NE2	2.19	0.57
7:DG:392:ARG:HG2	7:DG:392:ARG:HH11	1.69	0.57
10:DK:238:ILE:HG21	10:DK:260:VAL:CG2	2.31	0.57
15:DY:111:ARG:NH1	15:DY:125:THR:HG23	2.20	0.57
5:DE:539:ARG:HG2	5:DE:539:ARG:HH11	1.69	0.57
7:DG:394:PRO:O	7:DG:451:ARG:NH1	2.37	0.57
8:DH:17:ILE:HD13	9:DJ:12:TYR:CE1	2.39	0.57
8:DH:502:GLU:OE2	10:DK:301:ARG:HG3	2.04	0.56
9:DJ:291:ASN:HD22	9:DJ:294:MET:H	1.52	0.56
18:CJ:541:LEU:O	18:CJ:544:THR:HG23	2.05	0.56
20:CN:51:LEU:O	20:CN:68:GLN:NE2	2.38	0.56
23:Cg:155:LYS:HB3	23:Cg:356:CYS:SG	2.45	0.56
25:Ck:204:LEU:HD11	25:Ck:254:ILE:HG22	1.86	0.56
3:DB:386:ALA:O	3:DB:389:GLN:HG2	2.05	0.56
25:Ck:113:ASN:O	25:Ck:140:ARG:NH2	2.38	0.56
25:Ck:275:TRP:CD1	25:Ck:314:LEU:HD13	2.41	0.56
3:DB:968:VAL:HG13	7:DG:42:PRO:HG2	1.88	0.56
4:DC:77:ASP:H	4:DC:81:HIS:CD2	2.21	0.56
6:DF:426:LEU:CB	8:DH:200:THR:CG2	2.71	0.56
7:DG:77:CYS:HB2	7:DG:83:MET:HG3	1.87	0.56
7:DG:616:ARG:HG3	12:DV:183:LEU:HD11	1.88	0.56
19:CK:26:ARG:HB2	26:CA:460:U:C5	2.40	0.56
23:Cg:109:PHE:CA	31:Cg:501:GTP:HN21	2.08	0.56
7:DG:551:MET:SD	7:DG:561:PRO:HD3	2.46	0.56
8:DH:518:LYS:HG3	8:DH:523:ARG:NH1	2.20	0.56
23:Cg:406:GLU:OE2	23:Cg:406:GLU:N	2.35	0.56
4:DC:874:THR:HG22	4:DC:875:THR:H	1.70	0.56
22:CS:44:ARG:NH1	26:CA:493:U:O2'	2.38	0.56
18:CJ:230:PHE:CD2	25:Ck:710:ARG:HD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DF:502:ARG:HH21	6:DF:575:VAL:HG11	1.71	0.56
24:CI:24:PRO:O	24:CI:25:VAL:HG23	2.06	0.56
25:CK:724:PHE:O	25:CK:775:ARG:HD3	2.06	0.56
4:DC:594:GLU:HA	5:DE:412:GLU:OE2	2.06	0.56
8:DH:37:SER:O	9:DJ:49:ALA:HB1	2.06	0.56
6:DF:443:LEU:HD13	6:DF:452:VAL:HG11	1.88	0.56
18:CJ:384:GLU:HG3	26:CA:453:A:H4'	1.88	0.56
3:DB:1032:ASP:OD1	3:DB:1032:ASP:N	2.31	0.56
4:DC:78:PRO:O	4:DC:82:THR:OG1	2.23	0.56
4:DC:533:LEU:HD21	4:DC:1069:CYS:HA	1.87	0.56
5:DE:101:GLU:O	5:DE:105:ASN:ND2	2.38	0.56
8:DH:393:GLY:HA3	25:CK:691:GLN:HG2	1.88	0.56
4:DC:389:GLU:HG3	4:DC:496:LYS:NZ	2.21	0.55
6:DF:425:ILE:CD1	8:DH:196:LEU:HD11	2.36	0.55
6:DF:557:PRO:HB2	6:DF:563:SER:HB2	1.88	0.55
11:DT:52:ARG:NH1	11:DT:213:ASP:OD1	2.38	0.55
6:DF:92:MET:HE2	22:CS:104:GLN:HE22	1.71	0.55
4:DC:116:TYR:CE2	5:DE:572:VAL:HG11	2.41	0.55
7:DG:15:ARG:HG2	7:DG:15:ARG:HH11	1.72	0.55
8:DH:440:VAL:HG22	16:CC:77:THR:HG23	1.88	0.55
24:CI:34:ARG:NH2	24:CI:45:ILE:HG12	2.21	0.55
3:DB:153:HIS:HE1	3:DB:173:ARG:CZ	2.20	0.55
4:DC:243:TYR:O	4:DC:248:ARG:HB2	2.07	0.55
7:DG:399:ARG:HH21	7:DG:457:ARG:NH1	2.05	0.55
13:DW:50:LYS:HD3	13:DW:136:THR:HG21	1.89	0.55
20:CN:150:HIS:HD2	24:CI:67:THR:HG23	1.71	0.55
6:DF:394:GLU:OE2	6:DF:476:LEU:HB3	2.06	0.55
22:CS:62:HIS:O	22:CS:65:ASN:HB2	2.06	0.55
23:Cg:174:LEU:HD23	23:Cg:211:PHE:CE1	2.40	0.55
4:DC:1157:ALA:HA	8:DH:41:LYS:HZ1	1.71	0.55
5:DE:597:PHE:O	5:DE:601:ILE:HG22	2.06	0.55
6:DF:222:TYR:OH	6:DF:256:ASP:OD1	2.22	0.55
5:DE:618:ARG:NH1	5:DE:628:HIS:CE1	2.75	0.55
14:DX:88:ASP:OD1	14:DX:89:ARG:N	2.38	0.55
25:CK:621:THR:HG22	25:CK:623:LYS:HG3	1.89	0.55
25:CK:728:GLN:HG3	25:CK:784:TRP:CD2	2.42	0.55
6:DF:428:PRO:HB2	6:DF:493:MET:HE2	1.89	0.55
7:DG:186:ARG:NH1	7:DG:186:ARG:HG2	2.21	0.55
7:DG:204:SER:OG	7:DG:205:GLY:N	2.39	0.55
9:DJ:285:ARG:NH1	30:DJ:401:UTP:O2B	2.39	0.55
17:CI:32:LYS:O	17:CI:37:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:CR:244:THR:HG22	21:CR:246:GLU:H	1.72	0.55
3:DB:1012:THR:HG22	3:DB:1013:ARG:H	1.72	0.55
3:DB:1042:TYR:HA	18:CJ:263:ASP:OD1	2.07	0.55
4:DC:326:LYS:HG3	4:DC:346:ASP:OD2	2.06	0.55
7:DG:186:ARG:HG2	7:DG:186:ARG:HH11	1.71	0.55
9:DJ:87:PRO:HB3	9:DJ:92:LEU:HD12	1.87	0.55
10:DK:225:THR:HG22	10:DK:226:LEU:HD13	1.88	0.55
24:CI:101:LEU:HG	24:CI:105:ARG:HH11	1.71	0.55
4:DC:410:ARG:HE	4:DC:453:LEU:HD23	1.71	0.55
8:DH:277:THR:HG22	8:DH:278:VAL:H	1.71	0.55
9:DJ:322:SER:OG	11:DT:187:LYS:O	2.25	0.55
3:DB:1125:HIS:CG	3:DB:1126:PRO:HD2	2.42	0.54
7:DG:497:ARG:HG2	7:DG:497:ARG:HH11	1.72	0.54
13:DW:89:ILE:HG23	15:DY:109:PHE:HE2	1.72	0.54
13:DW:121:HIS:CD2	13:DW:123:ALA:H	2.21	0.54
18:CJ:760:MET:HE2	18:CJ:762:GLN:HG2	1.87	0.54
25:Ck:644:HIS:CD2	25:Ck:669:ASN:H	2.23	0.54
4:DC:302:ARG:HH11	4:DC:356:TRP:CD1	2.25	0.54
9:DJ:132:ARG:NH2	30:DJ:401:UTP:O2B	2.40	0.54
25:Ck:132:TYR:CZ	25:Ck:140:ARG:HG3	2.42	0.54
6:DF:589:GLN:CD	8:DH:192:PHE:CZ	2.84	0.54
25:Ck:119:GLU:OE1	25:Ck:132:TYR:OH	2.25	0.54
6:DF:521:THR:HG22	6:DF:523:LEU:H	1.71	0.54
7:DG:445:LEU:HD22	7:DG:531:ASP:HB3	1.89	0.54
11:DT:109:GLU:N	11:DT:109:GLU:OE1	2.39	0.54
18:CJ:54:MET:HE2	26:CA:463:A:N6	2.23	0.54
11:DT:65:VAL:HG13	11:DT:69:ASP:HB2	1.88	0.54
18:CJ:553:ARG:HH11	18:CJ:553:ARG:HG2	1.71	0.54
6:DF:55:ARG:HB2	6:DF:59:GLY:HA3	1.89	0.54
10:DK:21:SER:HB2	10:DK:231:SER:O	2.06	0.54
18:CJ:555:TRP:HA	18:CJ:583:LYS:HZ2	1.73	0.54
25:Ck:316:ASP:OD1	25:Ck:316:ASP:N	2.30	0.54
1:DA:1301:ASP:OD1	1:DA:1302:PHE:N	2.40	0.54
5:DE:299:LYS:HB2	5:DE:336:ILE:HD13	1.90	0.54
13:DW:42:SER:HB2	26:CA:519:U:OP1	2.08	0.54
18:CJ:800:LEU:HB2	18:CJ:803:ILE:HD12	1.89	0.54
23:Cg:435:SER:O	23:Cg:440:LYS:HE3	2.07	0.54
26:CA:461:A:C2	26:CA:463:A:H2'	2.43	0.54
4:DC:381:LEU:CD1	4:DC:385:THR:HG21	2.38	0.54
8:DH:504:ARG:HH12	10:DK:287:ILE:HG12	1.71	0.54
7:DG:186:ARG:HH12	7:DG:189:LYS:HD3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:DW:53:VAL:HG12	13:DW:54:GLU:O	2.08	0.54
18:CJ:553:ARG:O	18:CJ:583:LYS:HD2	2.08	0.54
3:DB:641:ARG:HD2	25:Ck:555:PHE:CD2	2.43	0.54
3:DB:1102:TYR:O	3:DB:1106:VAL:HG23	2.08	0.54
4:DC:1104:MET:HE1	8:DH:146:GLN:HE21	1.73	0.54
5:DE:199:SER:H	5:DE:202:HIS:HD2	1.56	0.54
17:CI:293:ARG:NH2	17:CI:407:ARG:NH1	2.47	0.54
18:CJ:555:TRP:HA	18:CJ:583:LYS:NZ	2.23	0.54
3:DB:388:VAL:HB	8:DH:509:TYR:HA	1.90	0.53
4:DC:56:ALA:HB2	10:DK:267:ARG:HD3	1.88	0.53
6:DF:371:ASN:HB2	6:DF:374:VAL:HG23	1.89	0.53
8:DH:26:PRO:HB3	9:DJ:17:PRO:HB2	1.90	0.53
18:CJ:585:SER:C	18:CJ:594:GLU:HB2	2.32	0.53
3:DB:917:LEU:HD13	3:DB:930:GLU:HB3	1.90	0.53
2:DL:91:PHE:CE1	2:DL:106:PHE:HB2	2.43	0.53
5:DE:174:VAL:HG11	5:DE:550:ALA:HB2	1.91	0.53
6:DF:84:PRO:HG2	6:DF:87:GLU:HB2	1.88	0.53
3:DB:78:ARG:HH11	3:DB:78:ARG:CG	2.17	0.53
11:DT:82:HIS:CD2	11:DT:128:PRO:HB3	2.43	0.53
16:CC:17:GLN:O	16:CC:19:TYR:N	2.41	0.53
18:CJ:233:THR:HG22	18:CJ:235:GLU:H	1.74	0.53
3:DB:517:GLU:HG2	3:DB:841:ARG:NH2	2.24	0.53
7:DG:80:LEU:N	7:DG:81:PRO:HD2	2.23	0.53
7:DG:530:PHE:HZ	7:DG:596:VAL:HG12	1.74	0.53
11:DT:162:TYR:CE2	11:DT:165:GLY:HA2	2.43	0.53
13:DW:140:TRP:HE3	13:DW:143:MET:HE3	1.73	0.53
14:DX:103:MET:HG2	14:DX:124:ILE:HG13	1.91	0.53
20:CN:93:ASP:OD1	20:CN:114:SER:N	2.41	0.53
23:Cg:233:THR:HG23	23:Cg:237:GLU:HB3	1.90	0.53
25:Ck:264:ASN:HD22	25:Ck:267:TYR:H	1.55	0.53
4:DC:229:THR:HG22	4:DC:232:GLN:H	1.72	0.53
18:CJ:572:CYS:SG	18:CJ:600:PRO:HA	2.48	0.53
22:CS:152:ASP:OD1	22:CS:152:ASP:N	2.34	0.53
1:DA:1244:LYS:NZ	1:DA:1296:GLU:HB3	2.23	0.53
4:DC:50:GLU:OE1	4:DC:405:ILE:CD1	2.57	0.53
7:DG:395:TRP:HA	7:DG:451:ARG:HH12	1.74	0.53
17:CI:439:ARG:NH2	26:CA:406:U:O2'	2.42	0.53
4:DC:1102:GLY:HA2	8:DH:59:MET:CE	2.39	0.53
6:DF:275:MET:O	6:DF:279:ILE:HG12	2.08	0.53
6:DF:383:ASP:O	6:DF:387:VAL:HG23	2.09	0.53
14:DX:136:ARG:HB3	14:DX:136:ARG:HH11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DB:881:ARG:HG2	3:DB:881:ARG:NH1	2.24	0.53
4:DC:119:THR:HG21	4:DC:136:TRP:CD1	2.44	0.53
4:DC:899:GLN:HG3	4:DC:933:ARG:HH22	1.74	0.53
6:DF:237:LEU:HB3	6:DF:253:ILE:HD13	1.91	0.53
15:DY:111:ARG:HH11	15:DY:125:THR:HG23	1.74	0.53
18:CJ:541:LEU:O	18:CJ:544:THR:HG22	2.08	0.53
3:DB:867:THR:HG21	18:CJ:343:VAL:HG21	1.89	0.53
4:DC:330:ARG:HB2	4:DC:344:MET:HE1	1.91	0.53
8:DH:175:ALA:HB1	8:DH:206:ILE:HD13	1.91	0.53
3:DB:580:PHE:HZ	3:DB:585:MET:CE	2.22	0.52
3:DB:815:ASP:OD2	6:DF:555:ARG:HA	2.09	0.52
7:DG:447:ALA:HA	7:DG:450:MET:HE2	1.91	0.52
8:DH:76:LEU:HD23	8:DH:93:LEU:HD22	1.91	0.52
11:DT:60:LEU:HD13	11:DT:149:TRP:HB3	1.91	0.52
15:DY:20:PRO:HG2	15:DY:23:SER:OG	2.10	0.52
15:DY:35:PRO:HB3	23:Cg:464:VAL:HG11	1.90	0.52
17:CI:303:THR:HB	17:CI:305:ILE:HG13	1.89	0.52
18:CJ:53:PRO:HG2	18:CJ:56:ILE:HD12	1.91	0.52
3:DB:78:ARG:HG3	3:DB:78:ARG:NH1	2.15	0.52
4:DC:393:THR:HG21	4:DC:457:LYS:HE3	1.89	0.52
4:DC:589:VAL:HG21	4:DC:604:VAL:O	2.10	0.52
4:DC:638:ASP:HB3	4:DC:652:ARG:HH22	1.73	0.52
13:DW:83:THR:HG21	13:DW:163:GLU:HG3	1.90	0.52
18:CJ:460:HIS:CE1	20:CN:57:LYS:HG3	2.44	0.52
4:DC:1008:GLY:O	10:DK:157:ALA:HB3	2.08	0.52
14:DX:85:LYS:HA	14:DX:87:PHE:H	1.73	0.52
7:DG:399:ARG:NH2	7:DG:457:ARG:NH1	2.57	0.52
6:DF:425:ILE:CD1	8:DH:196:LEU:CD1	2.87	0.52
3:DB:123:ILE:H	3:DB:123:ILE:HD12	1.73	0.52
3:DB:141:HIS:HA	4:DC:903:THR:HG21	1.92	0.52
4:DC:61:ILE:HB	4:DC:536:SER:HB2	1.91	0.52
4:DC:307:LEU:O	4:DC:310:ARG:HG2	2.10	0.52
4:DC:574:GLN:NE2	4:DC:807:VAL:H	2.07	0.52
18:CJ:441:HIS:CD2	25:Ck:768:SER:HB2	2.44	0.52
20:CN:76:TYR:HA	22:CS:86:GLU:OE2	2.10	0.52
23:Cg:61:PRO:HG2	23:Cg:79:CYS:SG	2.50	0.52
25:Ck:414:MET:SD	25:Ck:541:ARG:HG2	2.50	0.52
25:Ck:611:ASN:HD22	25:Ck:611:ASN:H	1.57	0.52
3:DB:522:MET:HB2	3:DB:526:PRO:HB3	1.91	0.52
5:DE:725:PRO:HG2	10:DK:146:TYR:CZ	2.45	0.52
6:DF:495:GLU:OE2	8:DH:243:SER:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DF:585:TYR:CD1	8:DH:195:TYR:CD1	2.97	0.52
10:DK:4:ARG:NH2	11:DT:131:SER:O	2.42	0.52
18:CJ:141:ASP:OD1	18:CJ:141:ASP:N	2.43	0.52
18:CJ:631:LEU:HD13	18:CJ:656:VAL:HG13	1.91	0.52
23:Cg:65:THR:HG22	23:Cg:67:THR:H	1.74	0.52
5:DE:229:ARG:NH1	5:DE:255:PHE:HE1	2.07	0.52
8:DH:156:LEU:HD13	8:DH:216:THR:HG23	1.91	0.52
2:DL:96:SER:OG	2:DL:98:ASP:OD1	2.26	0.52
2:DL:271:PRO:HG3	26:CA:456:A:H5"	1.92	0.52
3:DB:452:ARG:HG3	3:DB:462:ASP:OD1	2.09	0.52
3:DB:1030:ARG:CG	3:DB:1030:ARG:NH1	2.72	0.52
4:DC:1119:GLN:OE1	4:DC:1125:SER:OG	2.20	0.52
5:DE:570:GLU:HG3	8:DH:526:ASN:CG	2.34	0.52
7:DG:133:ARG:HG3	18:CJ:189:LEU:HD13	1.91	0.52
7:DG:447:ALA:O	7:DG:451:ARG:HD2	2.10	0.52
12:DV:31:HIS:HE1	12:DV:48:HIS:HE1	1.57	0.52
18:CJ:108:ASP:OD1	18:CJ:108:ASP:N	2.38	0.52
4:DC:946:GLU:HG2	4:DC:986:LEU:HD21	1.92	0.51
11:DT:55:ALA:HA	11:DT:58:HIS:CD2	2.46	0.51
14:DX:89:ARG:CG	14:DX:89:ARG:NH1	2.71	0.51
18:CJ:182:VAL:HG12	18:CJ:184:ARG:HG3	1.92	0.51
20:CN:150:HIS:CD2	24:CI:67:THR:HG23	2.45	0.51
25:Ck:132:TYR:CE2	25:Ck:140:ARG:HG3	2.45	0.51
3:DB:479:VAL:O	3:DB:483:VAL:HG12	2.10	0.51
3:DB:731:TYR:CE1	3:DB:820:GLU:HB2	2.45	0.51
6:DF:228:VAL:HG22	6:DF:261:LEU:HD22	1.91	0.51
8:DH:15:TYR:OH	16:CC:69:GLU:OE1	2.28	0.51
2:DL:104:ARG:NH1	18:CJ:48:ILE:HD12	2.25	0.51
2:DL:287:TRP:CD2	18:CJ:75:TYR:HA	2.45	0.51
4:DC:112:TYR:HB3	4:DC:960:VAL:HG12	1.93	0.51
4:DC:903:THR:HB	4:DC:906:GLN:HG3	1.92	0.51
4:DC:1028:THR:HG22	4:DC:1032:ASP:HB2	1.92	0.51
18:CJ:618:VAL:HG13	18:CJ:627:ILE:HD11	1.92	0.51
3:DB:308:PRO:HG3	5:DE:496:LEU:HD13	1.92	0.51
4:DC:46:ARG:NH1	4:DC:475:LEU:HB3	2.26	0.51
4:DC:295:VAL:HG21	4:DC:367:MET:HE3	1.93	0.51
4:DC:854:LEU:HD22	4:DC:859:LEU:HD12	1.92	0.51
5:DE:572:VAL:HA	5:DE:575:CYS:HB3	1.92	0.51
6:DF:119:HIS:CG	6:DF:120:ASP:H	2.29	0.51
7:DG:15:ARG:NH1	7:DG:18:TRP:CH2	2.78	0.51
7:DG:294:MET:SD	7:DG:310:LEU:HG	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Cg:85:LEU:HD22	23:Cg:107:ARG:HG2	1.92	0.51
23:Cg:325:LEU:HB3	23:Cg:326:PRO:HD2	1.90	0.51
3:DB:513:TYR:CE1	25:Ck:31:LEU:HD23	2.45	0.51
3:DB:1055:GLN:NE2	8:DH:33:VAL:H	2.09	0.51
11:DT:16:HIS:HD2	11:DT:28:GLU:OE1	1.93	0.51
12:DV:127:THR:HG23	25:Ck:742:GLY:HA2	1.92	0.51
22:CS:48:ARG:HH11	22:CS:48:ARG:CG	2.23	0.51
4:DC:381:LEU:HD12	4:DC:385:THR:HG21	1.92	0.51
5:DE:152:ALA:N	5:DE:157:ARG:HH11	2.09	0.51
7:DG:186:ARG:HD2	19:CK:54:LEU:HB3	1.93	0.51
7:DG:295:VAL:HG22	7:DG:336:MET:CE	2.40	0.51
9:DJ:22:MET:HE3	18:CJ:74:TRP:CH2	2.46	0.51
15:DY:62:GLN:OE1	15:DY:99:GLN:NE2	2.44	0.51
18:CJ:260:LEU:HD21	18:CJ:423:LEU:HD22	1.93	0.51
18:CJ:457:THR:HB	18:CJ:459:GLU:H	1.75	0.51
24:CI:28:ALA:HB3	25:Ck:785:PRO:HA	1.92	0.51
2:DL:278:ARG:NH1	2:DL:296:PRO:O	2.44	0.51
3:DB:641:ARG:HD2	25:Ck:555:PHE:CG	2.45	0.51
3:DB:861:GLU:HG2	3:DB:941:ARG:HA	1.93	0.51
3:DB:1051:GLN:NE2	9:DJ:42:HIS:H	2.09	0.51
6:DF:39:ARG:NH2	6:DF:163:ARG:HD3	2.25	0.51
7:DG:399:ARG:HG3	7:DG:411:TYR:CE1	2.46	0.51
11:DT:74:MET:HG3	11:DT:98:PRO:CG	2.40	0.51
15:DY:51:ASP:HB3	23:Cg:424:GLY:O	2.11	0.51
23:Cg:195:PRO:HD3	25:Ck:817:LEU:HD12	1.92	0.51
25:Ck:362:TYR:CD2	25:Ck:365:ILE:HB	2.46	0.51
3:DB:114:ASN:HD22	3:DB:686:GLN:HG2	1.75	0.51
4:DC:361:ASP:O	4:DC:365:LYS:HB2	2.10	0.51
25:Ck:188:LEU:HD21	25:Ck:224:LYS:HD3	1.91	0.51
25:Ck:728:GLN:HG3	25:Ck:784:TRP:CE2	2.46	0.51
3:DB:962:MET:HA	3:DB:962:MET:HE2	1.93	0.51
6:DF:502:ARG:HD2	6:DF:579:GLU:HG3	1.93	0.51
7:DG:334:MET:HE1	7:DG:384:VAL:O	2.10	0.51
9:DJ:69:PHE:CZ	9:DJ:71:MET:HG3	2.46	0.51
10:DK:273:LEU:HD11	11:DT:99:HIS:CE1	2.46	0.51
18:CJ:792:HIS:CD2	18:CJ:795:LYS:H	2.13	0.51
3:DB:281:GLN:HB3	3:DB:285:MET:HE3	1.93	0.51
6:DF:589:GLN:HB3	8:DH:192:PHE:HE1	1.74	0.51
11:DT:36:GLU:OE2	11:DT:36:GLU:HA	2.10	0.51
12:DV:31:HIS:HE1	12:DV:48:HIS:CE1	2.29	0.51
18:CJ:119:ARG:HG2	18:CJ:119:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CS:109:GLN:N	22:CS:109:GLN:OE1	2.44	0.51
3:DB:558:ASN:HB2	25:Ck:113:ASN:HB3	1.93	0.50
14:DX:57:ARG:NH2	22:CS:64:MET:HG3	2.25	0.50
23:Cg:260:ASP:OD1	25:Ck:825:LYS:HE2	2.10	0.50
23:Cg:294:GLU:HA	23:Cg:329:PRO:HA	1.93	0.50
3:DB:876:LEU:HD11	3:DB:949:THR:HG21	1.93	0.50
6:DF:349:ASP:OD1	6:DF:349:ASP:N	2.40	0.50
14:DX:64:SER:HB3	14:DX:163:TYR:H	1.75	0.50
2:DL:84:GLU:HA	2:DL:112:VAL:HG11	1.93	0.50
2:DL:270:THR:H	2:DL:271:PRO:HD2	1.77	0.50
4:DC:635:MET:HE2	4:DC:659:LEU:HD12	1.94	0.50
4:DC:934:ARG:HH11	4:DC:934:ARG:CG	2.25	0.50
6:DF:341:VAL:HG22	6:DF:346:LEU:HD11	1.92	0.50
7:DG:240:HIS:CG	7:DG:241:PRO:HD2	2.46	0.50
13:DW:58:ARG:HH11	13:DW:58:ARG:CG	2.05	0.50
24:CI:69:THR:HG21	24:CI:73:MET:HE3	1.91	0.50
3:DB:72:TRP:H	3:DB:72:TRP:CD1	2.29	0.50
3:DB:635:MET:HE1	25:Ck:374:ARG:HE	1.76	0.50
12:DV:25:SER:OG	12:DV:29:PHE:CZ	2.65	0.50
14:DX:31:LYS:HD3	14:DX:32:PRO:HD2	1.93	0.50
3:DB:975:LYS:HA	7:DG:92:GLN:HE22	1.76	0.50
4:DC:419:TYR:O	4:DC:422:VAL:HG12	2.11	0.50
5:DE:461:MET:SD	5:DE:461:MET:N	2.84	0.50
7:DG:248:LEU:HD11	7:DG:313:SER:HB2	1.93	0.50
18:CJ:372:GLU:HG2	18:CJ:391:HIS:CD2	2.47	0.50
23:Cg:205:ARG:HH21	23:Cg:259:ILE:HG12	1.77	0.50
25:Ck:80:GLU:O	25:Ck:92:ARG:NH1	2.45	0.50
4:DC:475:LEU:HB2	4:DC:476:PHE:CD2	2.46	0.50
6:DF:389:PRO:HA	6:DF:439:THR:HG21	1.94	0.50
7:DG:540:VAL:HG13	7:DG:569:LEU:HD22	1.94	0.50
8:DH:111:ASP:OD1	8:DH:170:ARG:NH2	2.45	0.50
17:CI:412:LYS:HD2	21:CR:253:PHE:HB2	1.92	0.50
4:DC:903:THR:HG22	4:DC:905:ALA:H	1.77	0.50
7:DG:99:VAL:HG22	7:DG:133:ARG:O	2.11	0.50
7:DG:245:ILE:HG22	7:DG:248:LEU:H	1.77	0.50
8:DH:14:TYR:OH	24:CI:136:HIS:HD2	1.95	0.50
8:DH:413:ASP:OD1	8:DH:413:ASP:N	2.37	0.50
13:DW:168:MET:CE	23:Cg:16:ARG:HH12	2.23	0.50
17:CI:313:ASP:C	17:CI:315:GLU:H	2.19	0.50
26:CA:460:U:O2	26:CA:461:A:N6	2.43	0.50
4:DC:121:LEU:H	4:DC:530:GLN:HE22	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:DX:48:LYS:O	14:DX:52:GLU:HG2	2.11	0.50
1:DA:1187:ASP:N	1:DA:1187:ASP:OD1	2.45	0.50
3:DB:194:GLN:HE22	5:DE:470:LYS:HB2	1.76	0.50
3:DB:519:PHE:CD2	3:DB:522:MET:HE2	2.46	0.50
6:DF:186:LEU:HD23	6:DF:193:PRO:HD3	1.94	0.50
6:DF:192:LEU:HD12	6:DF:264:VAL:HG13	1.93	0.50
8:DH:341:ASN:O	8:DH:344:VAL:HG23	2.12	0.50
9:DJ:71:MET:HG2	9:DJ:119:LEU:HD23	1.93	0.50
18:CJ:632:GLN:HB3	18:CJ:661:ARG:HD2	1.93	0.50
25:Ck:728:GLN:NE2	25:Ck:731:ARG:HH11	2.10	0.50
8:DH:193:VAL:N	8:DH:194:PRO:CD	2.74	0.49
9:DJ:101:ILE:HG23	9:DJ:139:LEU:HD11	1.93	0.49
13:DW:137:PRO:HA	13:DW:140:TRP:CD2	2.47	0.49
15:DY:37:ARG:HH21	15:DY:106:GLN:NE2	2.08	0.49
15:DY:58:THR:HG23	15:DY:99:GLN:HG2	1.94	0.49
4:DC:200:VAL:HG11	4:DC:206:PHE:HB2	1.94	0.49
13:DW:109:GLU:OE1	15:DY:96:ARG:NH1	2.42	0.49
14:DX:33:LYS:NZ	22:CS:32:LYS:HG2	2.27	0.49
21:CR:255:SER:HB2	21:CR:256:PRO:HD2	1.93	0.49
7:DG:173:MET:HE1	7:DG:209:THR:HG22	1.93	0.49
12:DV:25:SER:HG	12:DV:29:PHE:HZ	1.61	0.49
13:DW:44:ASN:O	13:DW:58:ARG:NH2	2.45	0.49
18:CJ:283:VAL:HG21	18:CJ:330:LEU:HD13	1.94	0.49
18:CJ:544:THR:CG2	18:CJ:552:ILE:H	2.15	0.49
18:CJ:552:ILE:HG22	18:CJ:557:GLU:CD	2.37	0.49
18:CJ:724:THR:HG21	23:Cg:302:PRO:HG3	1.94	0.49
6:DF:411:VAL:HG11	6:DF:586:TYR:CD2	2.47	0.49
7:DG:160:ARG:NH2	25:Ck:406:ARG:HE	2.09	0.49
7:DG:624:ARG:NH1	12:DV:181:LYS:O	2.44	0.49
18:CJ:151:ASN:HD21	18:CJ:209:GLN:HB3	1.77	0.49
24:Ci:34:ARG:HH21	24:Ci:45:ILE:HG12	1.77	0.49
3:DB:981:HIS:HD2	3:DB:983:LEU:HB2	1.78	0.49
3:DB:1047:TRP:CD2	9:DJ:41:PRO:HD3	2.48	0.49
4:DC:231:THR:HG21	4:DC:518:CYS:SG	2.53	0.49
6:DF:170:ARG:NH2	20:CN:33:GLU:OE1	2.45	0.49
8:DH:495:THR:HG22	8:DH:498:ASN:HD22	1.77	0.49
18:CJ:616:GLU:OE1	18:CJ:630:ARG:NH1	2.43	0.49
22:CS:118:ARG:HG2	22:CS:127:GLU:HG2	1.95	0.49
23:Cg:286:ASP:HA	23:Cg:356:CYS:HB3	1.93	0.49
24:Ci:27:CYS:SG	24:Ci:29:GLN:NE2	2.85	0.49
4:DC:1156:PRO:O	8:DH:41:LYS:NZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DF:532:LEU:HB2	6:DF:537:GLU:OE1	2.13	0.49
6:DF:543:HIS:HD2	8:DH:266:SER:OG	1.96	0.49
25:Ck:275:TRP:CG	25:Ck:314:LEU:HD13	2.47	0.49
3:DB:214:ARG:CZ	5:DE:539:ARG:HH12	2.24	0.49
7:DG:236:VAL:HG12	7:DG:237:PRO:HD2	1.93	0.49
8:DH:78:GLY:O	8:DH:81:LYS:HD2	2.13	0.49
8:DH:194:PRO:HG2	8:DH:195:TYR:CE2	2.48	0.49
14:DX:76:ARG:NH1	14:DX:146:PRO:HA	2.28	0.49
14:DX:136:ARG:HH11	14:DX:136:ARG:CG	2.25	0.49
23:Cg:283:ILE:HD11	23:Cg:342:MET:HE1	1.93	0.49
23:Cg:462:GLU:HA	23:Cg:465:TRP:NE1	2.28	0.49
25:Ck:606:THR:HG23	25:Ck:613:VAL:HG21	1.93	0.49
3:DB:285:MET:HE2	25:Ck:36:ARG:NH2	2.27	0.49
4:DC:218:TYR:CG	4:DC:256:ILE:HD11	2.47	0.49
6:DF:387:VAL:HG11	6:DF:475:TYR:HE2	1.77	0.49
6:DF:426:LEU:C	8:DH:200:THR:CG2	2.85	0.49
9:DJ:31:HIS:HD2	9:DJ:33:ASN:N	2.06	0.49
9:DJ:137:MET:HE2	9:DJ:169:CYS:SG	2.53	0.49
6:DF:56:TYR:OH	26:CA:485:U:H5'	2.12	0.49
7:DG:578:ASP:HA	7:DG:581:VAL:HG22	1.94	0.49
12:DV:31:HIS:NE2	12:DV:82:VAL:HG11	2.27	0.49
25:Ck:704:ASN:HB2	25:Ck:751:ASP:OD1	2.13	0.49
3:DB:1069:THR:HG21	25:Ck:764:THR:HG21	1.95	0.49
5:DE:729:ARG:HH22	25:Ck:92:ARG:NH1	2.10	0.49
7:DG:208:PRO:HG3	7:DG:282:ASP:OD1	2.12	0.49
7:DG:392:ARG:HH11	7:DG:392:ARG:CG	2.26	0.49
7:DG:399:ARG:HB2	7:DG:409:LYS:O	2.13	0.49
8:DH:518:LYS:HG3	8:DH:523:ARG:HH12	1.77	0.49
17:CI:420:ARG:O	19:CK:27:ARG:HB3	2.12	0.49
23:Cg:60:HIS:ND1	23:Cg:419:SER:HB2	2.28	0.49
23:Cg:102:PRO:HG2	23:Cg:105:HIS:HB2	1.95	0.49
25:Ck:37:ILE:HG22	25:Ck:38:ILE:HD12	1.94	0.49
25:Ck:414:MET:O	25:Ck:541:ARG:NH2	2.46	0.49
4:DC:211:LYS:NZ	4:DC:439:ALA:HA	2.28	0.48
11:DT:144:SER:OG	11:DT:161:ASN:ND2	2.46	0.48
12:DV:95:LEU:HD22	24:CI:55:LEU:HD23	1.94	0.48
12:DV:99:TRP:CE2	18:CJ:771:PRO:HG2	2.48	0.48
7:DG:46:TRP:CZ2	7:DG:93:ARG:HB2	2.48	0.48
3:DB:1080:ARG:NH1	6:DF:177:ASP:OD1	2.46	0.48
4:DC:282:GLY:O	4:DC:286:GLN:HG2	2.12	0.48
4:DC:666:GLU:OE1	4:DC:790:ARG:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DC:866:GLU:OE2	5:DE:202:HIS:HE1	1.96	0.48
11:DT:158:HIS:HB3	11:DT:160:TYR:HE1	1.77	0.48
12:DV:95:LEU:HD21	18:CJ:771:PRO:HB3	1.93	0.48
18:CJ:463:MET:HG2	24:CI:89:MET:HG3	1.95	0.48
25:Ck:411:CYS:HA	25:Ck:414:MET:HE2	1.96	0.48
2:DL:271:PRO:C	2:DL:274:THR:HG23	2.32	0.48
3:DB:684:GLN:HB2	3:DB:689:LEU:HD13	1.95	0.48
4:DC:107:SER:OG	4:DC:544:GLU:OE1	2.31	0.48
5:DE:543:ARG:HG2	5:DE:543:ARG:NH1	2.26	0.48
11:DT:87:ARG:HB2	11:DT:93:MET:HE2	1.94	0.48
18:CJ:206:PHE:CG	18:CJ:207:PRO:HA	2.48	0.48
25:Ck:372:LYS:NZ	25:Ck:559:ASP:OD1	2.35	0.48
3:DB:1109:TRP:CZ3	20:CN:66:MET:HG3	2.48	0.48
3:DB:1127:MET:HE3	3:DB:1144:LEU:HB3	1.94	0.48
6:DF:119:HIS:CG	6:DF:120:ASP:N	2.82	0.48
7:DG:199:LEU:HD12	7:DG:206:LEU:HD13	1.94	0.48
11:DT:44:ARG:H	11:DT:218:MET:HE1	1.79	0.48
12:DV:49:ASP:OD1	12:DV:50:ALA:N	2.46	0.48
17:CI:400:VAL:HG23	17:CI:410:LEU:HD12	1.96	0.48
26:CA:469:A:OP1	29:CA:703:SPD:N1	2.46	0.48
3:DB:722:ARG:NH2	3:DB:802:ASP:OD2	2.47	0.48
4:DC:909:ILE:HD13	4:DC:941:MET:HE2	1.94	0.48
4:DC:961:THR:HG21	5:DE:563:ASP:CG	2.39	0.48
5:DE:195:ILE:HG21	5:DE:203:LEU:HD11	1.93	0.48
8:DH:145:ALA:HA	8:DH:151:LEU:HD23	1.95	0.48
8:DH:257:ASN:ND2	8:DH:260:GLU:HG3	2.29	0.48
10:DK:99:ASP:C	10:DK:101:ASP:H	2.22	0.48
11:DT:74:MET:HG3	11:DT:98:PRO:HG3	1.94	0.48
17:CI:9:THR:HG22	17:CI:10:ALA:H	1.78	0.48
17:CI:320:THR:OG1	17:CI:375:GLU:OE1	2.28	0.48
3:DB:91:ALA:HB2	5:DE:529:ASP:O	2.13	0.48
3:DB:146:MET:HE1	3:DB:214:ARG:HB3	1.94	0.48
3:DB:910:PHE:CD2	18:CJ:112:ARG:HG2	2.48	0.48
3:DB:1030:ARG:NH1	3:DB:1030:ARG:HG2	2.28	0.48
6:DF:467:LEU:HB3	6:DF:475:TYR:HB2	1.95	0.48
17:CI:40:TRP:CE2	18:CJ:163:MET:HE2	2.49	0.48
3:DB:908:GLN:H	3:DB:908:GLN:NE2	2.12	0.48
3:DB:1160:LYS:O	14:DX:59:ARG:HD2	2.13	0.48
5:DE:539:ARG:HG2	5:DE:539:ARG:NH1	2.28	0.48
8:DH:480:ASP:OD1	18:CJ:16:ARG:NH1	2.46	0.48
8:DH:518:LYS:O	8:DH:523:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CJ:258:MET:HE2	18:CJ:259:LYS:HG2	1.95	0.48
5:DE:181:LEU:HD22	5:DE:538:VAL:HG21	1.96	0.48
7:DG:64:ARG:NH2	21:CR:249:GLN:HE22	2.04	0.48
7:DG:70:TYR:HB3	7:DG:90:MET:HE2	1.95	0.48
7:DG:214:TYR:C	7:DG:214:TYR:HD1	2.22	0.48
7:DG:296:ASP:OD2	17:CI:14:ARG:NH1	2.47	0.48
8:DH:55:ARG:HG2	8:DH:143:CYS:HA	1.95	0.48
14:DX:102:MET:HE2	14:DX:102:MET:HB3	1.70	0.48
16:CC:44:LEU:HD11	16:CC:50:ILE:HD12	1.96	0.48
22:CS:45:ARG:HB2	22:CS:48:ARG:HD2	1.94	0.48
23:Cg:40:LYS:NZ	23:Cg:57:THR:HA	2.29	0.48
23:Cg:139:THR:HG22	23:Cg:145:PHE:CZ	2.48	0.48
7:DG:46:TRP:HB3	7:DG:89:GLU:OE2	2.14	0.48
7:DG:229:HIS:CE1	7:DG:250:LEU:HD22	2.49	0.48
8:DH:1:MET:HB2	8:DH:1:MET:HE3	1.47	0.48
18:CJ:793:HIS:HB2	24:CI:90:LYS:O	2.14	0.48
23:Cg:159:MET:CG	23:Cg:356:CYS:HB2	2.44	0.48
25:Ck:392:PHE:CD1	25:Ck:408:VAL:HG11	2.48	0.48
1:DA:1244:LYS:NZ	1:DA:1298:VAL:HG23	2.29	0.47
4:DC:635:MET:HE3	4:DC:656:ILE:HG12	1.94	0.47
7:DG:497:ARG:HH11	7:DG:497:ARG:CG	2.26	0.47
14:DX:132:THR:HB	18:CJ:776:GLN:HB3	1.96	0.47
18:CJ:278:GLU:O	18:CJ:281:VAL:HG12	2.13	0.47
23:Cg:270:MET:HE1	23:Cg:335:PHE:CD1	2.49	0.47
1:DA:1262:PHE:HE1	1:DA:1305:PRO:HD3	1.80	0.47
3:DB:968:VAL:CG1	7:DG:42:PRO:HG2	2.43	0.47
6:DF:112:ARG:HH22	6:DF:118:THR:HG23	1.80	0.47
6:DF:268:GLY:HA3	6:DF:312:TRP:CG	2.49	0.47
11:DT:139:HIS:HB2	11:DT:176:ASP:OD1	2.13	0.47
12:DV:120:ARG:HH22	12:DV:131:GLN:HG2	1.79	0.47
13:DW:56:LEU:O	13:DW:58:ARG:NH1	2.43	0.47
25:Ck:176:THR:HG23	25:Ck:178:ASP:H	1.79	0.47
4:DC:430:ILE:HG23	4:DC:442:LEU:HD11	1.94	0.47
5:DE:581:THR:H	5:DE:585:ARG:HB2	1.79	0.47
6:DF:92:MET:HE2	22:CS:104:GLN:NE2	2.29	0.47
6:DF:426:LEU:CA	8:DH:200:THR:CG2	2.93	0.47
10:DK:237:PRO:HG2	10:DK:240:SER:HB2	1.95	0.47
13:DW:103:PRO:O	15:DY:90:GLN:NE2	2.48	0.47
18:CJ:484:HIS:HB2	18:CJ:487:GLU:HG3	1.95	0.47
20:CN:166:ILE:HD11	25:Ck:766:LYS:HB2	1.97	0.47
23:Cg:153:CYS:HA	23:Cg:452:PRO:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Ck:728:GLN:HE22	25:Ck:731:ARG:NH1	2.10	0.47
4:DC:263:GLN:HB3	4:DC:267:LYS:NZ	2.29	0.47
5:DE:503:ASP:OD1	5:DE:503:ASP:N	2.46	0.47
8:DH:309:TRP:HA	8:DH:310:PRO:C	2.39	0.47
18:CJ:130:ARG:NH1	25:Ck:710:ARG:HH21	2.12	0.47
22:CS:59:LYS:HE3	26:CA:411:A:OP1	2.14	0.47
3:DB:154:ARG:HA	3:DB:157:LEU:HB2	1.96	0.47
3:DB:209:GLN:NE2	5:DE:448:PRO:HG2	2.30	0.47
7:DG:372:LEU:O	7:DG:376:VAL:HG23	2.15	0.47
11:DT:183:LEU:H	11:DT:219:GLN:NE2	2.13	0.47
12:DV:70:LYS:HB3	26:CA:513:U:OP1	2.15	0.47
13:DW:61:ARG:NH1	23:Cg:374:GLU:OE2	2.47	0.47
15:DY:54:PRO:HB2	15:DY:102:GLU:HG2	1.97	0.47
18:CJ:83:HIS:CD2	18:CJ:86:ASP:O	2.67	0.47
25:Ck:817:LEU:HD22	25:Ck:836:THR:HG22	1.97	0.47
4:DC:582:ARG:O	4:DC:622:TYR:HA	2.15	0.47
5:DE:659:ARG:HD2	5:DE:659:ARG:HA	1.55	0.47
24:Ci:155:LYS:O	26:CA:439:U:O2'	2.32	0.47
25:Ck:201:THR:HG23	25:Ck:600:LEU:HD11	1.95	0.47
1:DA:1249:HIS:CE1	1:DA:1255:VAL:HG12	2.50	0.47
2:DL:54:GLY:HA3	16:CC:55:ILE:HG13	1.97	0.47
2:DL:294:LEU:HD11	20:CN:133:HIS:HB2	1.97	0.47
3:DB:548:ALA:HB1	3:DB:553:LEU:O	2.15	0.47
4:DC:801:HIS:CD2	4:DC:802:PRO:HD2	2.50	0.47
6:DF:516:ARG:HD2	6:DF:542:HIS:ND1	2.30	0.47
7:DG:472:ARG:CG	7:DG:472:ARG:NH1	2.75	0.47
8:DH:558:GLU:O	8:DH:565:ASN:ND2	2.48	0.47
9:DJ:31:HIS:CD2	9:DJ:33:ASN:HB2	2.50	0.47
10:DK:167:THR:HG22	10:DK:168:PRO:HD2	1.97	0.47
12:DV:25:SER:OG	12:DV:29:PHE:HZ	1.98	0.47
16:CC:65:ILE:HD13	18:CJ:75:TYR:HD2	1.79	0.47
24:Ci:30:ARG:HH11	24:Ci:30:ARG:HG3	1.79	0.47
3:DB:382:GLY:O	3:DB:396:ARG:NH2	2.32	0.47
4:DC:104:PRO:HG2	4:DC:112:TYR:CE1	2.50	0.47
10:DK:99:ASP:OD2	10:DK:102:LYS:HD2	2.14	0.47
16:CC:69:GLU:H	16:CC:69:GLU:HG2	1.58	0.47
18:CJ:712:THR:OG1	20:CN:52:ASP:HB2	2.14	0.47
25:Ck:167:PHE:CE2	25:Ck:235:GLY:HA2	2.46	0.47
1:DA:1203:CYS:HB3	3:DB:994:THR:HG23	1.97	0.47
3:DB:891:GLN:HG3	25:Ck:310:ASP:HA	1.96	0.47
4:DC:855:ARG:HH12	5:DE:202:HIS:CE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:DE:280:LEU:HD22	5:DE:413:GLU:OE2	2.15	0.47
6:DF:15:HIS:CE1	9:DJ:278:GLY:HA2	2.50	0.47
7:DG:334:MET:HE1	7:DG:388:TYR:N	2.30	0.47
18:CJ:59:PRO:HG3	26:CA:462:A:C8	2.49	0.47
18:CJ:376:SER:HB3	18:CJ:385:LEU:HD23	1.97	0.47
23:Cg:362:LYS:HG3	23:Cg:382:LEU:O	2.14	0.47
3:DB:78:ARG:NH1	5:DE:216:LEU:HD12	2.29	0.47
4:DC:696:VAL:HG13	4:DC:703:ALA:HB2	1.97	0.47
6:DF:38:GLY:H	6:DF:41:ASN:ND2	2.07	0.47
7:DG:577:LEU:HD21	7:DG:605:VAL:HG23	1.97	0.47
8:DH:348:LYS:O	8:DH:348:LYS:HG3	2.15	0.47
9:DJ:177:TRP:CZ2	9:DJ:178:ARG:HG2	2.50	0.47
10:DK:178:LYS:HB2	10:DK:256:GLY:O	2.14	0.47
11:DT:82:HIS:HD2	11:DT:128:PRO:HB3	1.80	0.47
18:CJ:94:ALA:HB2	18:CJ:101:PHE:HB3	1.95	0.47
18:CJ:160:GLU:HA	23:Cg:407:TYR:OH	2.15	0.47
18:CJ:555:TRP:HE1	18:CJ:581:GLN:HA	1.79	0.47
25:Ck:195:GLN:HB3	25:Ck:217:ILE:HD13	1.97	0.47
3:DB:78:ARG:CG	3:DB:78:ARG:NH1	2.76	0.46
6:DF:18:THR:HG21	9:DJ:274:SER:O	2.14	0.46
7:DG:214:TYR:C	7:DG:214:TYR:CD1	2.92	0.46
9:DJ:205:LYS:HD3	9:DJ:209:ARG:HH21	1.80	0.46
14:DX:94:GLY:HA2	23:Cg:187:TRP:CE2	2.50	0.46
18:CJ:632:GLN:HB2	18:CJ:661:ARG:HB2	1.96	0.46
23:Cg:112:ARG:HH21	23:Cg:154:GLY:HA3	1.81	0.46
3:DB:285:MET:HE2	25:Ck:36:ARG:HH21	1.80	0.46
3:DB:355:GLN:O	3:DB:359:ILE:HG13	2.15	0.46
4:DC:910:GLU:HG3	4:DC:937:LEU:HD11	1.96	0.46
5:DE:282:ALA:O	5:DE:403:PRO:HB3	2.15	0.46
6:DF:189:ASP:N	6:DF:189:ASP:OD1	2.48	0.46
11:DT:43:ASP:H	11:DT:218:MET:HE1	1.80	0.46
13:DW:102:MET:HE2	13:DW:102:MET:HB2	1.65	0.46
23:Cg:181:VAL:HG12	23:Cg:203:ALA:HB2	1.96	0.46
24:Ci:105:ARG:HD2	25:Ck:685:TYR:OH	2.16	0.46
25:Ck:838:LEU:HD23	25:Ck:838:LEU:HA	1.79	0.46
2:DL:51:PHE:HB3	18:CJ:29:PRO:HD2	1.98	0.46
3:DB:129:TYR:CD1	3:DB:129:TYR:C	2.94	0.46
3:DB:958:ASN:HD22	3:DB:959:PRO:HD2	1.80	0.46
6:DF:76:GLU:HB3	14:DX:38:VAL:HG21	1.98	0.46
13:DW:162:PRO:HB2	23:Cg:22:TYR:CE1	2.50	0.46
16:CC:70:TYR:CE2	16:CC:72:ILE:HB	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Cg:120:LEU:HD12	23:Cg:120:LEU:HA	1.78	0.46
25:Ck:115:PRO:HB2	25:Ck:120:CYS:SG	2.55	0.46
25:Ck:259:ILE:O	25:Ck:263:SER:HB3	2.15	0.46
25:Ck:353:ARG:HG2	25:Ck:353:ARG:HH11	1.79	0.46
3:DB:867:THR:HG22	3:DB:868:HIS:H	1.80	0.46
6:DF:421:ALA:HB1	6:DF:422:PRO:HD2	1.98	0.46
6:DF:502:ARG:HH11	6:DF:579:GLU:CD	2.23	0.46
7:DG:176:VAL:HG22	7:DG:188:LEU:HD11	1.96	0.46
9:DJ:22:MET:SD	16:CC:67:ASN:HB2	2.56	0.46
18:CJ:335:LEU:HD23	18:CJ:335:LEU:HA	1.79	0.46
3:DB:521:LEU:HD21	3:DB:662:ARG:NH1	2.30	0.46
3:DB:787:LEU:HB3	3:DB:788:PRO:HD2	1.98	0.46
3:DB:905:TYR:CD1	3:DB:918:VAL:HG22	2.50	0.46
10:DK:286:LEU:HA	10:DK:286:LEU:HD23	1.72	0.46
12:DV:66:VAL:HG13	12:DV:71:GLN:HG2	1.97	0.46
20:CN:165:ARG:O	25:Ck:740:ARG:NH1	2.49	0.46
5:DE:601:ILE:HD12	5:DE:638:LEU:HD23	1.98	0.46
8:DH:295:ASP:N	8:DH:295:ASP:OD1	2.48	0.46
15:DY:163:LYS:HB3	15:DY:163:LYS:HE2	1.71	0.46
17:CI:313:ASP:O	17:CI:315:GLU:N	2.48	0.46
18:CJ:381:SER:OG	18:CJ:384:GLU:HB3	2.16	0.46
18:CJ:463:MET:HE3	24:CI:89:MET:HG2	1.98	0.46
2:DL:61:VAL:HG21	18:CJ:29:PRO:HA	1.97	0.46
3:DB:671:VAL:HG11	3:DB:832:TYR:HB2	1.96	0.46
3:DB:983:LEU:HD22	7:DG:84:LEU:HD21	1.98	0.46
3:DB:1030:ARG:HH11	3:DB:1030:ARG:HG2	1.80	0.46
10:DK:220:PRO:HG2	10:DK:223:ALA:HB2	1.97	0.46
16:CC:16:LEU:HD13	16:CC:18:LYS:HE3	1.97	0.46
17:CI:435:LYS:HG2	17:CI:436:VAL:HG23	1.97	0.46
18:CJ:238:ILE:HD11	18:CJ:355:HIS:HA	1.98	0.46
23:Cg:427:TRP:CE2	23:Cg:434:SER:HB3	2.50	0.46
25:Ck:799:LYS:HG2	25:Ck:802:TYR:CE2	2.51	0.46
3:DB:569:HIS:CE1	3:DB:648:ARG:NH1	2.84	0.46
5:DE:186:ARG:HA	5:DE:186:ARG:NH1	2.31	0.46
7:DG:292:GLU:HA	7:DG:295:VAL:HG23	1.96	0.46
12:DV:177:MET:HB3	12:DV:183:LEU:HD22	1.98	0.46
18:CJ:484:HIS:CD2	18:CJ:495:ARG:HH11	1.95	0.46
18:CJ:769:GLN:HG3	24:CI:12:VAL:HG22	1.97	0.46
23:Cg:37:ILE:HD13	23:Cg:422:LEU:HG	1.97	0.46
25:Ck:288:ASN:O	25:Ck:294:ALA:HB1	2.16	0.46
1:DA:1225:HIS:CE1	1:DA:1310:LEU:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DB:1135:VAL:HG12	23:Cg:320:LEU:HD22	1.98	0.46
7:DG:117:VAL:HG13	7:DG:145:VAL:CG1	2.45	0.46
8:DH:133:CYS:HB3	8:DH:136:LEU:HB3	1.96	0.46
9:DJ:139:LEU:HD22	9:DJ:143:TYR:HE2	1.81	0.46
11:DT:111:ALA:HA	11:DT:114:LEU:HD22	1.98	0.46
17:CI:16:PHE:HA	17:CI:41:VAL:HG21	1.97	0.46
18:CJ:469:ASP:OD2	20:CN:56:SER:HB2	2.15	0.46
25:Ck:755:ASP:N	25:Ck:755:ASP:OD1	2.49	0.46
25:Ck:775:ARG:CB	25:Ck:775:ARG:HH11	2.29	0.46
3:DB:517:GLU:HG2	3:DB:841:ARG:HH22	1.79	0.46
3:DB:908:GLN:HA	3:DB:909:PRO:HD3	1.83	0.46
4:DC:203:MET:HA	4:DC:203:MET:HE3	1.97	0.46
6:DF:18:THR:CG2	9:DJ:274:SER:O	2.63	0.46
6:DF:279:ILE:HD12	6:DF:323:TYR:HB2	1.98	0.46
6:DF:502:ARG:HB2	6:DF:577:ALA:O	2.16	0.46
8:DH:17:ILE:HG12	24:CI:132:THR:CG2	2.46	0.46
9:DJ:230:LEU:HA	9:DJ:230:LEU:HD23	1.47	0.46
18:CJ:382:PHE:CD1	22:CS:48:ARG:HB2	2.50	0.46
24:CI:145:ASN:HD22	24:CI:145:ASN:HA	1.62	0.46
25:Ck:268:LEU:O	25:Ck:273:SER:HB2	2.15	0.46
1:DA:1235:GLY:HA3	1:DA:1264:LYS:HD3	1.98	0.45
2:DL:47:GLN:HG3	2:DL:48:LYS:H	1.81	0.45
3:DB:131:GLU:HG3	3:DB:228:THR:HG23	1.98	0.45
4:DC:753:LEU:HD22	4:DC:753:LEU:HA	1.83	0.45
8:DH:66:ARG:HE	8:DH:102:LEU:HD21	1.81	0.45
12:DV:114:VAL:HG11	12:DV:118:GLN:HB3	1.98	0.45
13:DW:60:VAL:CG1	15:DY:110:THR:HG21	2.46	0.45
25:Ck:153:VAL:HG21	25:Ck:247:LEU:HB3	1.97	0.45
2:DL:282:TRP:HZ3	18:CJ:33:PRO:HD3	1.82	0.45
3:DB:867:THR:HG22	3:DB:868:HIS:N	2.31	0.45
5:DE:524:PHE:CD1	5:DE:524:PHE:N	2.84	0.45
6:DF:486:LEU:HA	6:DF:486:LEU:HD23	1.73	0.45
7:DG:155:GLU:HB3	25:Ck:414:MET:HA	1.98	0.45
21:CR:265:ARG:HG2	21:CR:265:ARG:HH11	1.81	0.45
26:CA:504:U:H4'	26:CA:505:U:OP1	2.17	0.45
3:DB:92:HIS:CD2	3:DB:94:ASP:H	2.19	0.45
4:DC:517:LEU:HD23	4:DC:517:LEU:HA	1.80	0.45
5:DE:304:ASN:HB3	5:DE:306:VAL:H	1.81	0.45
13:DW:22:THR:HG21	22:CS:149:ASP:O	2.16	0.45
20:CN:166:ILE:HG23	25:Ck:762:PHE:HE2	1.82	0.45
25:Ck:379:ALA:HB3	25:Ck:565:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:CA:467:A:H2'	29:CA:703:SPD:H52	1.97	0.45
4:DC:396:ILE:HG23	4:DC:402:VAL:HG11	1.98	0.45
5:DE:49:MET:HE1	5:DE:91:GLY:HA2	1.97	0.45
7:DG:70:TYR:HB3	7:DG:90:MET:CE	2.46	0.45
18:CJ:250:GLU:HB3	18:CJ:398:PHE:CD1	2.52	0.45
25:Ck:621:THR:HG21	25:Ck:623:LYS:HE3	1.98	0.45
25:Ck:638:ARG:HG3	25:Ck:638:ARG:NH1	2.28	0.45
3:DB:544:ARG:NH1	3:DB:849:ASP:OD2	2.42	0.45
5:DE:648:GLU:HG3	5:DE:654:VAL:HG11	1.99	0.45
5:DE:704:LEU:HD12	5:DE:704:LEU:HA	1.66	0.45
6:DF:450:VAL:HG11	6:DF:486:LEU:HB3	1.99	0.45
7:DG:346:ARG:NH2	7:DG:497:ARG:HD3	2.32	0.45
12:DV:31:HIS:CD2	12:DV:82:VAL:CG1	3.00	0.45
14:DX:85:LYS:HB3	15:DY:163:LYS:HD3	1.98	0.45
14:DX:131:ILE:HB	18:CJ:776:GLN:OE1	2.17	0.45
15:DY:52:GLN:CD	15:DY:52:GLN:H	2.25	0.45
18:CJ:151:ASN:ND2	18:CJ:209:GLN:O	2.50	0.45
23:Cg:193:ILE:HD11	23:Cg:267:LYS:HD2	1.99	0.45
26:CA:508:A:H4'	26:CA:509:U:OP2	2.17	0.45
3:DB:513:TYR:H	3:DB:954:SER:HG	1.64	0.45
4:DC:1090:LYS:HA	4:DC:1090:LYS:HD3	1.79	0.45
5:DE:700:ASP:C	5:DE:700:ASP:OD1	2.59	0.45
6:DF:589:GLN:CD	8:DH:192:PHE:CE1	2.95	0.45
7:DG:333:LEU:O	7:DG:336:MET:HB2	2.17	0.45
8:DH:440:VAL:HG13	16:CC:62:PHE:CE2	2.52	0.45
9:DJ:22:MET:CG	16:CC:67:ASN:HB2	2.47	0.45
9:DJ:213:GLU:HB3	9:DJ:250:VAL:HG11	1.98	0.45
14:DX:43:HIS:CE1	22:CS:123:PRO:HB2	2.52	0.45
22:CS:122:PHE:CG	22:CS:123:PRO:HA	2.51	0.45
3:DB:281:GLN:CB	3:DB:285:MET:HE3	2.46	0.45
3:DB:572:ASP:OD2	3:DB:646:SER:HB2	2.16	0.45
4:DC:92:PHE:C	4:DC:94:ASN:H	2.24	0.45
6:DF:286:ARG:HA	6:DF:286:ARG:HD3	1.71	0.45
12:DV:124:GLU:O	12:DV:127:THR:HB	2.17	0.45
15:DY:71:CYS:O	21:CR:265:ARG:HD2	2.17	0.45
3:DB:339:ARG:HH21	8:DH:549:SER:HB3	1.82	0.45
3:DB:1032:ASP:HB3	3:DB:1036:MET:HE2	1.97	0.45
4:DC:605:GLU:CD	4:DC:605:GLU:H	2.25	0.45
4:DC:1157:ALA:HA	8:DH:41:LYS:NZ	2.32	0.45
7:DG:115:ILE:HG21	7:DG:120:VAL:HG23	1.99	0.45
8:DH:281:PHE:CD2	8:DH:304:LEU:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DH:452:ARG:HA	8:DH:453:PRO:HD3	1.85	0.45
14:DX:59:ARG:HG3	14:DX:60:ALA:N	2.32	0.45
15:DY:35:PRO:HA	23:Cg:464:VAL:HG11	1.98	0.45
15:DY:133:ASP:N	15:DY:133:ASP:OD1	2.50	0.45
25:Ck:373:ARG:HH21	25:Ck:554:SER:HA	1.81	0.45
3:DB:551:HIS:CD2	3:DB:574:ILE:HD13	2.52	0.45
3:DB:562:GLN:HE22	6:DF:571:LEU:HA	1.81	0.45
3:DB:881:ARG:NH1	25:Ck:110:HIS:HE1	2.15	0.45
4:DC:934:ARG:HH11	4:DC:934:ARG:HG2	1.82	0.45
7:DG:547:MET:HE3	7:DG:547:MET:HB3	1.64	0.45
18:CJ:118:MET:HE2	18:CJ:118:MET:HA	1.99	0.45
18:CJ:544:THR:CG2	18:CJ:551:ARG:C	2.76	0.45
23:Cg:35:GLY:HA3	23:Cg:431:TRP:NE1	2.31	0.45
24:Ci:122:MET:HE3	24:Ci:122:MET:HB3	1.58	0.45
3:DB:453:GLU:HB3	5:DE:712:MET:HE1	1.99	0.45
4:DC:29:TYR:OH	11:DT:45:HIS:HD2	2.00	0.45
4:DC:353:LEU:O	4:DC:357:GLN:HB2	2.17	0.45
4:DC:632:LEU:HD23	4:DC:632:LEU:HA	1.75	0.45
4:DC:704:HIS:NE2	10:DK:167:THR:HG21	2.32	0.45
5:DE:463:LEU:HD23	5:DE:486:ILE:HG23	1.99	0.45
6:DF:549:PHE:CD1	6:DF:577:ALA:HB2	2.52	0.45
7:DG:67:ALA:HB2	7:DG:96:LYS:O	2.17	0.45
7:DG:74:LEU:HD12	7:DG:74:LEU:HA	1.82	0.45
13:DW:16:PHE:CD1	14:DX:52:GLU:HB2	2.52	0.45
17:CI:65:MET:HA	17:CI:66:PRO:HD2	1.80	0.45
3:DB:388:VAL:HG21	8:DH:508:LEU:HB2	1.99	0.44
3:DB:532:GLU:H	3:DB:532:GLU:HG2	1.55	0.44
3:DB:800:GLN:HA	3:DB:805:GLU:O	2.16	0.44
4:DC:381:LEU:HD12	4:DC:385:THR:CG2	2.47	0.44
5:DE:147:MET:HE1	5:DE:567:HIS:CE1	2.52	0.44
6:DF:324:LEU:HD13	6:DF:332:GLU:HB2	1.98	0.44
8:DH:18:ARG:NH2	26:CA:449:G:N7	2.62	0.44
10:DK:254:GLU:HG3	10:DK:261:SER:CB	2.37	0.44
18:CJ:54:MET:HE2	26:CA:463:A:C6	2.53	0.44
18:CJ:258:MET:HE2	18:CJ:259:LYS:CG	2.47	0.44
20:CN:106:GLU:OE2	22:CS:48:ARG:NH2	2.50	0.44
25:Ck:682:ASN:H	25:Ck:682:ASN:ND2	2.13	0.44
3:DB:495:LEU:HD23	3:DB:589:ASP:OD1	2.18	0.44
3:DB:609:PRO:HB2	3:DB:614:VAL:HG23	1.99	0.44
4:DC:770:LEU:HD12	4:DC:771:PRO:HD2	2.00	0.44
6:DF:387:VAL:HG11	6:DF:475:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:DG:490:ARG:HD3	7:DG:571:VAL:CG1	2.47	0.44
18:CJ:668:GLU:HB3	18:CJ:671:LEU:HD22	1.99	0.44
22:CS:87:GLU:O	22:CS:104:GLN:HG3	2.17	0.44
2:DL:266:GLY:HA2	19:CK:22:PRO:HB3	1.99	0.44
3:DB:99:VAL:HG13	3:DB:103:TYR:CZ	2.52	0.44
3:DB:456:LEU:HA	3:DB:456:LEU:HD23	1.76	0.44
4:DC:151:SER:OG	4:DC:230:GLN:O	2.35	0.44
5:DE:80:LEU:HD12	5:DE:80:LEU:HA	1.64	0.44
7:DG:334:MET:HG3	7:DG:353:VAL:HG11	1.98	0.44
8:DH:99:GLN:HG2	8:DH:134:PRO:HD2	1.99	0.44
14:DX:138:LYS:HE2	15:DY:138:TYR:OH	2.17	0.44
18:CJ:130:ARG:HH12	25:Ck:710:ARG:HH21	1.65	0.44
22:CS:104:GLN:OE1	22:CS:110:HIS:HE1	1.99	0.44
23:Cg:155:LYS:HB2	31:Cg:501:GTP:O1B	2.17	0.44
23:Cg:436:ASP:OD1	23:Cg:436:ASP:C	2.61	0.44
25:Ck:633:MET:HB2	25:Ck:633:MET:HE2	1.66	0.44
3:DB:213:ASP:OD1	3:DB:213:ASP:N	2.40	0.44
3:DB:908:GLN:H	3:DB:908:GLN:HE21	1.65	0.44
4:DC:1159:ASP:OD1	4:DC:1159:ASP:N	2.48	0.44
5:DE:248:THR:O	5:DE:252:ASP:HB2	2.16	0.44
6:DF:257:GLY:C	6:DF:265:SER:HB2	2.42	0.44
9:DJ:35:PRO:O	9:DJ:37:GLY:N	2.50	0.44
10:DK:34:ASN:HA	10:DK:38:VAL:O	2.17	0.44
12:DV:131:GLN:HB3	12:DV:143:ILE:HD11	1.99	0.44
17:CI:324:ARG:HG2	17:CI:325:GLU:N	2.32	0.44
18:CJ:406:PRO:HG2	18:CJ:407:PHE:CD2	2.52	0.44
3:DB:192:ILE:HD11	3:DB:301:GLN:O	2.18	0.44
3:DB:831:ASN:ND2	3:DB:837:TYR:HD2	2.16	0.44
8:DH:500:VAL:HG13	8:DH:501:PRO:HD2	1.99	0.44
14:DX:109:LEU:HD23	14:DX:109:LEU:HA	1.70	0.44
23:Cg:462:GLU:O	23:Cg:462:GLU:HG2	2.17	0.44
25:Ck:362:TYR:HD2	25:Ck:365:ILE:HB	1.82	0.44
25:Ck:674:LEU:HD21	25:Ck:707:LEU:HG	2.00	0.44
3:DB:123:ILE:HG23	3:DB:128:GLU:HB3	2.00	0.44
4:DC:405:ILE:HG21	4:DC:460:SER:OG	2.18	0.44
4:DC:638:ASP:HB3	4:DC:652:ARG:NH2	2.32	0.44
4:DC:1119:GLN:HA	4:DC:1120:PRO:HD3	1.74	0.44
9:DJ:46:ARG:HA	9:DJ:46:ARG:HD3	1.71	0.44
12:DV:56:ARG:C	12:DV:58:ALA:N	2.74	0.44
22:CS:130:SER:HA	22:CS:131:PRO:HD3	1.80	0.44
23:Cg:183:THR:OG1	23:Cg:184:HIS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DB:885:PHE:CE2	3:DB:929:MET:HE2	2.50	0.44
3:DB:923:GLN:HE21	3:DB:923:GLN:HB3	1.60	0.44
3:DB:969:THR:HB	3:DB:1001:THR:HG21	1.98	0.44
4:DC:274:VAL:O	4:DC:278:GLN:HG3	2.18	0.44
4:DC:498:LEU:H	4:DC:498:LEU:HG	1.62	0.44
4:DC:653:LEU:HD12	4:DC:653:LEU:HA	1.75	0.44
7:DG:186:ARG:NH1	7:DG:189:LYS:HD3	2.33	0.44
7:DG:261:ARG:HA	7:DG:262:PRO:HD3	1.77	0.44
8:DH:20:ASN:OD1	9:DJ:10:VAL:N	2.50	0.44
9:DJ:71:MET:HB3	9:DJ:71:MET:HE2	1.62	0.44
9:DJ:180:LEU:HD23	9:DJ:180:LEU:HA	1.80	0.44
11:DT:92:LYS:HD2	11:DT:174:TYR:CD1	2.53	0.44
12:DV:101:GLN:HG3	23:Cg:385:TYR:O	2.18	0.44
13:DW:98:GLN:HE22	13:DW:154:HIS:CD2	2.36	0.44
15:DY:32:TRP:O	15:DY:37:ARG:NH1	2.47	0.44
15:DY:148:ARG:NH1	26:CA:517:U:P	2.91	0.44
18:CJ:713:PRO:HB3	26:CA:507:A:N1	2.33	0.44
20:CN:10:MET:HE3	26:CA:415:U:C6	2.53	0.44
25:Ck:35:ASP:O	25:Ck:40:GLY:N	2.50	0.44
25:Ck:841:LYS:HB3	25:Ck:841:LYS:HE2	1.73	0.44
1:DA:1277:LEU:HD23	1:DA:1277:LEU:HA	1.81	0.44
2:DL:28:ASN:ND2	18:CJ:15:TYR:O	2.49	0.44
3:DB:427:TRP:CH2	4:DC:1156:PRO:HB3	2.53	0.44
3:DB:852:TRP:HD1	3:DB:861:GLU:OE1	2.00	0.44
4:DC:977:ARG:HA	4:DC:977:ARG:HD3	1.79	0.44
5:DE:181:LEU:HD23	5:DE:181:LEU:HA	1.74	0.44
10:DK:172:LEU:HD12	10:DK:177:LYS:HD2	2.00	0.44
15:DY:33:ALA:O	15:DY:38:MET:HE2	2.17	0.44
15:DY:34:ASP:HA	15:DY:35:PRO:HD3	1.80	0.44
17:CI:58:GLU:OE1	23:Cg:436:ASP:HB2	2.18	0.44
24:CI:124:VAL:HG12	24:CI:125:HIS:CD2	2.53	0.44
25:Ck:184:LYS:HD3	25:Ck:228:LEU:HD21	1.99	0.44
25:Ck:343:GLU:HG2	25:Ck:589:GLN:HE22	1.82	0.44
2:DL:27:PRO:HB3	18:CJ:16:ARG:HG2	1.99	0.43
4:DC:389:GLU:HG3	4:DC:496:LYS:HZ1	1.83	0.43
4:DC:614:LEU:HB2	4:DC:817:ASP:HA	1.98	0.43
5:DE:725:PRO:HG2	10:DK:146:TYR:CE2	2.53	0.43
6:DF:321:LEU:HD23	6:DF:321:LEU:HA	1.83	0.43
8:DH:382:PHE:CD1	8:DH:382:PHE:N	2.84	0.43
3:DB:494:PRO:HB3	3:DB:955:ARG:HD2	2.00	0.43
3:DB:944:HIS:O	18:CJ:342:ASN:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DC:435:LEU:HD13	4:DC:442:LEU:HD23	1.99	0.43
5:DE:51:ARG:HA	5:DE:51:ARG:HD3	1.89	0.43
5:DE:570:GLU:OE1	8:DH:527:VAL:N	2.52	0.43
7:DG:71:ASN:ND2	7:DG:101:THR:OG1	2.39	0.43
7:DG:403:ASP:HB3	7:DG:409:LYS:NZ	2.32	0.43
8:DH:136:LEU:HD21	8:DH:159:GLU:HG2	2.00	0.43
11:DT:40:TRP:CH2	11:DT:214:ARG:HB3	2.53	0.43
13:DW:61:ARG:HG2	23:Cg:374:GLU:OE2	2.19	0.43
13:DW:92:LEU:HD23	13:DW:92:LEU:HA	1.80	0.43
20:CN:108:VAL:HA	20:CN:109:PRO:HD3	1.72	0.43
23:Cg:237:GLU:HG2	23:Cg:238:ARG:H	1.83	0.43
25:Ck:691:GLN:HG3	25:Ck:692:GLY:N	2.33	0.43
25:Ck:716:ARG:HA	25:Ck:716:ARG:HD3	1.80	0.43
3:DB:716:GLU:HG3	5:DE:474:LEU:HD21	2.00	0.43
4:DC:71:TRP:CE2	4:DC:544:GLU:HG3	2.52	0.43
4:DC:649:THR:HG22	4:DC:651:LYS:H	1.84	0.43
4:DC:960:VAL:HG21	5:DE:159:ALA:HB2	1.99	0.43
4:DC:1030:VAL:HG22	10:DK:98:LEU:HD21	1.99	0.43
6:DF:118:THR:O	6:DF:118:THR:HG22	2.17	0.43
7:DG:143:HIS:HA	7:DG:164:LEU:HD21	2.00	0.43
7:DG:155:GLU:HG2	25:Ck:414:MET:HG3	2.00	0.43
9:DJ:72:HIS:O	9:DJ:74:ALA:N	2.47	0.43
9:DJ:300:TRP:CE2	11:DT:224:PRO:HB3	2.53	0.43
15:DY:53:LEU:HA	15:DY:53:LEU:HD23	1.67	0.43
15:DY:64:ASP:CG	21:CR:269:SER:HB3	2.44	0.43
18:CJ:83:HIS:NE2	18:CJ:86:ASP:O	2.51	0.43
18:CJ:226:ARG:HD2	18:CJ:815:ASN:HD21	1.83	0.43
25:Ck:325:LEU:HD13	25:Ck:632:MET:HE2	1.99	0.43
3:DB:562:GLN:NE2	6:DF:571:LEU:HA	2.33	0.43
3:DB:586:ARG:HA	3:DB:586:ARG:HD3	1.85	0.43
4:DC:71:TRP:NE1	4:DC:544:GLU:HG3	2.33	0.43
4:DC:534:LEU:HD12	4:DC:534:LEU:HA	1.64	0.43
7:DG:175:GLU:OE2	7:DG:191:GLN:HG3	2.19	0.43
7:DG:392:ARG:CG	7:DG:392:ARG:NH1	2.81	0.43
13:DW:112:PHE:CD1	13:DW:113:PRO:HD2	2.54	0.43
24:Ci:93:LEU:HD23	24:Ci:93:LEU:HA	1.78	0.43
2:DL:44:LYS:O	2:DL:47:GLN:NE2	2.43	0.43
3:DB:983:LEU:HD23	3:DB:983:LEU:HA	1.80	0.43
3:DB:1132:ARG:HD3	18:CJ:709:GLU:OE2	2.19	0.43
4:DC:148:LEU:HD12	4:DC:148:LEU:HA	1.76	0.43
5:DE:406:ASP:HA	5:DE:409:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:DG:143:HIS:CE1	7:DG:202:LEU:HD13	2.53	0.43
9:DJ:87:PRO:O	9:DJ:123:LYS:HE3	2.19	0.43
9:DJ:192:THR:N	9:DJ:193:PRO:HD2	2.33	0.43
12:DV:133:THR:HB	12:DV:139:ASP:OD2	2.19	0.43
18:CJ:75:TYR:HE1	20:CN:123:ARG:O	2.00	0.43
18:CJ:388:SER:O	18:CJ:388:SER:OG	2.30	0.43
18:CJ:551:ARG:HB3	18:CJ:553:ARG:HH21	1.83	0.43
4:DC:219:LEU:HD23	4:DC:219:LEU:HA	1.86	0.43
4:DC:780:LEU:HD23	4:DC:780:LEU:HA	1.90	0.43
7:DG:236:VAL:HG11	7:DG:240:HIS:CG	2.54	0.43
7:DG:448:LEU:HD23	7:DG:448:LEU:HA	1.75	0.43
8:DH:405:ARG:HG3	8:DH:414:LEU:HD21	1.99	0.43
11:DT:140:ASN:HB2	11:DT:142:ILE:HD12	2.00	0.43
13:DW:85:GLU:H	13:DW:85:GLU:CD	2.26	0.43
14:DX:90:ILE:H	14:DX:90:ILE:HG13	1.52	0.43
18:CJ:758:TRP:CG	18:CJ:759:PRO:HA	2.53	0.43
20:CN:16:ASP:O	24:CI:133:TYR:HB3	2.19	0.43
23:Cg:112:ARG:HD2	23:Cg:408:GLU:OE2	2.18	0.43
25:Ck:674:LEU:CD2	25:Ck:707:LEU:HG	2.48	0.43
25:Ck:717:LEU:HD23	25:Ck:717:LEU:HA	1.74	0.43
3:DB:572:ASP:OD2	3:DB:648:ARG:HG2	2.18	0.43
6:DF:216:LYS:HB2	18:CJ:476:ASN:HB2	2.00	0.43
12:DV:129:ILE:HD13	18:CJ:138:PRO:HD3	2.00	0.43
17:CI:16:PHE:CE1	17:CI:38:LEU:HD13	2.53	0.43
18:CJ:575:HIS:O	18:CJ:579:THR:HG23	2.18	0.43
25:Ck:42:HIS:O	25:Ck:93:THR:HB	2.19	0.43
1:DA:1273:GLU:HG3	1:DA:1282:ILE:HD13	2.01	0.43
3:DB:589:ASP:OD1	3:DB:590:ASP:N	2.52	0.43
3:DB:983:LEU:HD11	7:DG:123:LEU:HD13	2.00	0.43
5:DE:77:PRO:HG3	8:DH:567:GLY:HA3	2.00	0.43
5:DE:162:LEU:HD12	5:DE:165:ARG:NH1	2.34	0.43
8:DH:252:LEU:HD23	8:DH:252:LEU:HA	1.82	0.43
12:DV:48:HIS:O	12:DV:61:ARG:NH1	2.51	0.43
12:DV:109:ILE:HA	12:DV:110:PRO:HD2	1.81	0.43
22:CS:75:MET:HE2	22:CS:75:MET:HB3	1.72	0.43
23:Cg:226:CYS:O	23:Cg:226:CYS:SG	2.77	0.43
25:Ck:145:LEU:HD23	25:Ck:145:LEU:HA	1.84	0.43
25:Ck:221:ALA:O	25:Ck:225:MET:HB2	2.19	0.43
3:DB:528:PHE:CE2	3:DB:529:LEU:HG	2.54	0.43
5:DE:344:ARG:O	5:DE:348:ILE:HG13	2.18	0.43
6:DF:132:LEU:HD12	6:DF:132:LEU:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:DG:99:VAL:HG23	18:CJ:187:GLY:HA2	2.01	0.43
7:DG:102:MET:HE1	7:DG:134:PRO:HA	2.00	0.43
9:DJ:206:SER:OG	9:DJ:207:ILE:N	2.52	0.43
16:CC:74:LEU:HB3	16:CC:77:THR:HB	2.01	0.43
18:CJ:485:GLU:HA	18:CJ:515:ALA:CB	2.49	0.43
18:CJ:720:THR:HA	18:CJ:721:PRO:HD3	1.88	0.43
18:CJ:768:ASP:OD1	18:CJ:769:GLN:N	2.45	0.43
18:CJ:797:LEU:HD12	18:CJ:797:LEU:HA	1.64	0.43
20:CN:55:LEU:HD23	20:CN:55:LEU:HA	1.88	0.43
23:Cg:342:MET:CE	23:Cg:351:LYS:HG2	2.48	0.43
2:DL:44:LYS:HB2	2:DL:44:LYS:HE3	1.83	0.43
3:DB:98:ASP:O	3:DB:103:TYR:N	2.52	0.43
4:DC:118:GLY:HA3	5:DE:150:ARG:HG2	2.00	0.43
4:DC:317:GLU:HG2	4:DC:320:ARG:HH12	1.84	0.43
5:DE:333:ASP:HA	5:DE:336:ILE:HD12	2.01	0.43
7:DG:381:ASP:O	7:DG:384:VAL:HG13	2.19	0.43
9:DJ:243:ASN:ND2	9:DJ:288:LEU:HD22	2.34	0.43
10:DK:177:LYS:NZ	10:DK:230:ASP:OD2	2.30	0.43
14:DX:78:GLU:HA	14:DX:79:PRO:HD3	1.66	0.43
14:DX:95:VAL:HG22	14:DX:127:MET:SD	2.59	0.43
17:CI:325:GLU:OE2	18:CJ:178:SER:HB2	2.19	0.43
18:CJ:293:ASP:OD1	18:CJ:293:ASP:N	2.52	0.43
18:CJ:688:GLU:OE1	20:CN:63:HIS:NE2	2.52	0.43
18:CJ:714:THR:OG1	20:CN:52:ASP:HB3	2.19	0.43
22:CS:116:LYS:HB3	22:CS:116:LYS:HE3	1.87	0.43
23:Cg:155:LYS:HE2	31:Cg:501:GTP:O1B	2.19	0.43
23:Cg:205:ARG:HD3	23:Cg:258:SER:HB3	2.01	0.43
24:CI:33:LEU:HD13	25:Ck:735:ILE:HG21	2.00	0.43
3:DB:975:LYS:CA	7:DG:92:GLN:HE22	2.31	0.42
4:DC:218:TYR:CD2	4:DC:256:ILE:HD11	2.53	0.42
4:DC:396:ILE:HD13	4:DC:457:LYS:HA	2.00	0.42
5:DE:163:LYS:HG2	5:DE:556:LEU:HD11	2.01	0.42
6:DF:88:LEU:HA	6:DF:88:LEU:HD12	1.73	0.42
6:DF:502:ARG:HH11	6:DF:579:GLU:CG	2.32	0.42
7:DG:318:ILE:HD12	7:DG:329:LEU:HD21	2.01	0.42
7:DG:497:ARG:CG	7:DG:497:ARG:NH1	2.80	0.42
9:DJ:31:HIS:HD2	9:DJ:33:ASN:HB2	1.84	0.42
12:DV:56:ARG:O	12:DV:58:ALA:N	2.51	0.42
22:CS:70:TYR:CE1	26:CA:505:U:H2'	2.54	0.42
24:CI:83:ASN:HD22	26:CA:507:A:H1'	1.84	0.42
25:Ck:96:ASN:OD1	25:Ck:97:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DB:333:ALA:HB1	5:DE:33:ILE:HD13	2.01	0.42
3:DB:413:PHE:HB2	11:DT:155:PHE:HB3	2.00	0.42
3:DB:891:GLN:HA	18:CJ:128:LYS:HE2	2.01	0.42
4:DC:56:ALA:HB2	10:DK:267:ARG:CD	2.49	0.42
4:DC:775:ALA:HA	4:DC:777:GLY:H	1.84	0.42
5:DE:193:ILE:HB	5:DE:426:PHE:HB3	2.01	0.42
6:DF:502:ARG:HD3	6:DF:577:ALA:C	2.44	0.42
7:DG:456:ARG:NH2	7:DG:546:ASP:OD2	2.52	0.42
8:DH:131:LEU:HD23	8:DH:131:LEU:HA	1.75	0.42
8:DH:195:TYR:CD2	8:DH:195:TYR:N	2.86	0.42
9:DJ:300:TRP:CZ2	11:DT:224:PRO:HB3	2.54	0.42
18:CJ:100:ARG:O	18:CJ:101:PHE:C	2.61	0.42
18:CJ:232:ASN:HB3	18:CJ:241:SER:O	2.19	0.42
18:CJ:257:VAL:HG13	18:CJ:399:ARG:HB2	2.01	0.42
31:Cg:501:GTP:H5'	31:Cg:501:GTP:H8	1.84	0.42
25:Ck:373:ARG:O	25:Ck:377:VAL:HG23	2.19	0.42
3:DB:92:HIS:HE1	5:DE:447:ARG:O	2.02	0.42
3:DB:463:LEU:HD23	3:DB:463:LEU:HA	1.85	0.42
3:DB:903:ILE:HD11	3:DB:921:ALA:HB2	2.02	0.42
3:DB:1056:PRO:HD3	8:DH:35:TYR:CE1	2.54	0.42
5:DE:71:LEU:HD23	5:DE:71:LEU:HA	1.84	0.42
6:DF:88:LEU:HD21	22:CS:97:LYS:HB2	2.01	0.42
8:DH:14:TYR:OH	24:CI:136:HIS:CD2	2.72	0.42
10:DK:25:GLU:OE2	10:DK:231:SER:HB2	2.20	0.42
23:Cg:284:VAL:HA	23:Cg:354:ILE:O	2.19	0.42
25:Ck:184:LYS:HD3	25:Ck:228:LEU:HD11	1.99	0.42
25:Ck:775:ARG:HH11	25:Ck:775:ARG:HB3	1.83	0.42
26:CA:414:A:O2'	26:CA:484:A:OP1	2.23	0.42
2:DL:304:MET:HE2	2:DL:304:MET:HB3	1.91	0.42
4:DC:242:HIS:N	4:DC:242:HIS:CD2	2.87	0.42
4:DC:327:GLU:CD	4:DC:410:ARG:HD2	2.44	0.42
7:DG:102:MET:HG3	7:DG:127:LEU:HD23	2.00	0.42
11:DT:88:THR:OG1	11:DT:106:ASP:OD1	2.29	0.42
1:DA:1216:LEU:HA	1:DA:1216:LEU:HD23	1.76	0.42
1:DA:1260:VAL:HA	1:DA:1261:PRO:HD3	1.66	0.42
3:DB:765:GLU:O	3:DB:769:VAL:HG23	2.20	0.42
4:DC:87:MET:HE2	4:DC:957:LYS:HA	2.01	0.42
4:DC:114:GLU:OE1	4:DC:118:GLY:HA2	2.19	0.42
5:DE:729:ARG:HH22	25:Ck:92:ARG:HH12	1.66	0.42
7:DG:206:LEU:HD12	7:DG:206:LEU:HA	1.93	0.42
13:DW:87:ASN:ND2	13:DW:158:PRO:HB3	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:DY:35:PRO:CB	23:Cg:464:VAL:HG11	2.49	0.42
15:DY:148:ARG:HD2	15:DY:148:ARG:HA	1.76	0.42
18:CJ:84:MET:H	18:CJ:84:MET:HG2	1.60	0.42
18:CJ:642:ASN:CG	18:CJ:654:VAL:HG12	2.44	0.42
18:CJ:770:THR:HB	24:CI:11:GLY:N	2.35	0.42
20:CN:38:ASP:OD1	20:CN:81:LEU:HD12	2.18	0.42
23:Cg:224:LEU:HD11	23:Cg:241:GLN:C	2.44	0.42
1:DA:1244:LYS:HZ2	1:DA:1298:VAL:HG23	1.85	0.42
2:DL:74:ARG:H	2:DL:74:ARG:HG2	1.61	0.42
3:DB:473:VAL:HA	3:DB:474:PRO:HD2	1.81	0.42
4:DC:934:ARG:CG	4:DC:934:ARG:NH1	2.83	0.42
4:DC:1102:GLY:HA2	8:DH:59:MET:HE3	2.01	0.42
6:DF:40:GLU:H	6:DF:40:GLU:HG2	1.63	0.42
7:DG:68:TYR:HE2	21:CR:250:GLN:OE1	2.03	0.42
7:DG:490:ARG:NH1	17:CI:4:LEU:HD11	2.34	0.42
9:DJ:22:MET:HE3	18:CJ:74:TRP:HH2	1.84	0.42
9:DJ:123:LYS:HA	9:DJ:123:LYS:HD2	1.61	0.42
11:DT:9:GLN:HB3	11:DT:10:ALA:H	1.68	0.42
12:DV:165:LEU:HD13	18:CJ:748:PRO:HB3	2.01	0.42
13:DW:140:TRP:CE3	13:DW:143:MET:HE3	2.54	0.42
14:DX:52:GLU:HG2	14:DX:52:GLU:H	1.74	0.42
17:CI:9:THR:HG22	17:CI:10:ALA:N	2.35	0.42
20:CN:115:TYR:CG	20:CN:116:TRP:N	2.87	0.42
22:CS:140:MET:H	22:CS:140:MET:HG2	1.62	0.42
23:Cg:114:GLU:CD	23:Cg:401:ILE:HG12	2.44	0.42
25:Ck:222:LEU:HD23	25:Ck:239:LEU:HD12	2.01	0.42
1:DA:1191:ILE:HD12	1:DA:1309:ILE:HG23	2.02	0.42
3:DB:206:LEU:HA	3:DB:206:LEU:HD23	1.79	0.42
4:DC:155:VAL:CG1	4:DC:168:PHE:HE1	2.23	0.42
4:DC:1112:ASP:O	8:DH:49:LEU:HD13	2.20	0.42
4:DC:1164:TRP:CG	4:DC:1165:SER:H	2.37	0.42
5:DE:433:ASN:HB3	5:DE:436:VAL:HG23	2.00	0.42
8:DH:76:LEU:HG	8:DH:85:LEU:CD2	2.50	0.42
10:DK:16:ARG:HA	10:DK:16:ARG:HD3	1.67	0.42
12:DV:51:ASN:HB3	23:Cg:373:VAL:HG11	2.01	0.42
19:CK:20:MET:HA	19:CK:20:MET:HE2	2.01	0.42
20:CN:127:LEU:HD23	20:CN:127:LEU:HA	1.74	0.42
20:CN:143:LEU:HD12	20:CN:143:LEU:HA	1.76	0.42
25:Ck:622:LEU:HD12	25:Ck:622:LEU:HA	1.74	0.42
3:DB:145:ARG:HD3	3:DB:145:ARG:HA	1.91	0.42
4:DC:88:LEU:HA	4:DC:88:LEU:HD23	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DC:91:LYS:HG3	5:DE:166:ARG:HD2	2.01	0.42
4:DC:299:LEU:HD12	4:DC:299:LEU:HA	1.88	0.42
4:DC:1082:ARG:NH2	11:DT:75:ARG:HD3	2.33	0.42
4:DC:1115:ARG:NH2	9:DJ:193:PRO:HD3	2.35	0.42
6:DF:13:ILE:H	6:DF:13:ILE:HG13	1.53	0.42
6:DF:43:THR:HG22	6:DF:44:ALA:H	1.84	0.42
7:DG:80:LEU:CD2	7:DG:115:ILE:HD11	2.50	0.42
7:DG:141:THR:O	7:DG:145:VAL:HG23	2.19	0.42
7:DG:496:ARG:NH2	17:CI:1:MET:HG2	2.35	0.42
13:DW:141:LEU:HD23	13:DW:141:LEU:HA	1.75	0.42
14:DX:35:ARG:HG2	14:DX:36:PRO:HD2	2.01	0.42
18:CJ:105:ASN:OD1	18:CJ:105:ASN:N	2.52	0.42
18:CJ:718:PRO:HA	18:CJ:719:PRO:HD3	1.92	0.42
23:Cg:443:LYS:HD3	23:Cg:465:TRP:CZ3	2.54	0.42
24:CI:116:GLY:HA3	26:CA:419:U:H5'	2.00	0.42
3:DB:255:LEU:HA	3:DB:255:LEU:HD23	1.80	0.42
3:DB:816:ARG:NH1	6:DF:571:LEU:HD11	2.34	0.42
3:DB:1039:ILE:HD11	16:CC:36:LEU:HD11	2.01	0.42
3:DB:1044:PRO:HG2	3:DB:1047:TRP:CD2	2.55	0.42
4:DC:46:ARG:HH21	4:DC:401:ARG:HD2	1.84	0.42
4:DC:1110:HIS:HD2	4:DC:1123:SER:HB2	1.85	0.42
5:DE:232:LEU:HD12	5:DE:420:VAL:HG13	2.01	0.42
5:DE:720:ASP:OD1	5:DE:720:ASP:C	2.63	0.42
6:DF:196:PHE:HD2	6:DF:198:HIS:CE1	2.38	0.42
7:DG:199:LEU:HD23	7:DG:199:LEU:HA	1.73	0.42
11:DT:183:LEU:H	11:DT:219:GLN:HE22	1.67	0.42
12:DV:94:THR:OG1	24:CI:58:GLU:OE2	2.31	0.42
18:CJ:613:SER:HA	18:CJ:666:LEU:HD13	2.02	0.42
23:Cg:190:PRO:O	25:Ck:833:PRO:HG3	2.20	0.42
25:Ck:349:GLU:O	25:Ck:349:GLU:HG2	2.19	0.42
1:DA:1203:CYS:CB	3:DB:994:THR:HG23	2.48	0.42
1:DA:1312:TRP:CE2	1:DA:1314:GLY:HA2	2.54	0.42
3:DB:118:VAL:HG21	3:DB:318:LEU:HD22	2.02	0.42
3:DB:120:TYR:O	3:DB:122:HIS:HD2	2.02	0.42
3:DB:511:ARG:CG	3:DB:511:ARG:NH1	2.66	0.42
3:DB:1145:LEU:HA	3:DB:1146:PRO:HD3	1.94	0.42
6:DF:489:ARG:O	6:DF:493:MET:HG2	2.20	0.42
7:DG:324:LEU:HD13	7:DG:373:TRP:CG	2.55	0.42
26:CA:409:A:O2'	26:CA:410:U:H5'	2.19	0.42
26:CA:441:G:O2'	26:CA:442:A:H5'	2.19	0.42
2:DL:77:LEU:HD23	2:DL:77:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DB:400:LYS:O	3:DB:402:THR:HG23	2.20	0.41
3:DB:562:GLN:HE21	6:DF:572:HIS:H	1.68	0.41
4:DC:147:ARG:HH11	4:DC:232:GLN:HB2	1.84	0.41
4:DC:166:GLU:H	4:DC:166:GLU:HG3	1.35	0.41
4:DC:302:ARG:HD3	4:DC:359:GLU:OE1	2.19	0.41
5:DE:405:ILE:HD13	5:DE:405:ILE:HA	1.74	0.41
6:DF:314:TYR:CZ	6:DF:318:MET:HG3	2.54	0.41
6:DF:460:ARG:HD3	6:DF:461:PHE:CE2	2.55	0.41
9:DJ:213:GLU:H	9:DJ:213:GLU:CD	2.28	0.41
11:DT:169:LEU:HD23	11:DT:169:LEU:HA	1.89	0.41
17:CI:353:MET:O	17:CI:392:ARG:HG3	2.20	0.41
18:CJ:297:LEU:HD12	18:CJ:319:VAL:HG21	2.01	0.41
18:CJ:618:VAL:HG23	18:CJ:652:ASP:O	2.19	0.41
18:CJ:790:MET:HE2	18:CJ:790:MET:HB3	1.78	0.41
5:DE:72:ARG:HB3	5:DE:194:HIS:HB2	2.02	0.41
6:DF:353:ARG:HH12	6:DF:380:LEU:HD21	1.85	0.41
6:DF:426:LEU:CA	8:DH:200:THR:HG23	2.50	0.41
12:DV:93:GLN:OE1	12:DV:96:ARG:NH1	2.52	0.41
12:DV:131:GLN:HE21	12:DV:131:GLN:HB2	1.61	0.41
18:CJ:755:ASN:ND2	18:CJ:757:LEU:O	2.53	0.41
23:Cg:148:ASP:OD1	23:Cg:357:THR:HG21	2.20	0.41
24:CI:96:ASN:HD21	25:Ck:697:MET:HA	1.84	0.41
25:Ck:230:LEU:HD23	25:Ck:230:LEU:HA	1.78	0.41
2:DL:270:THR:N	2:DL:271:PRO:HD2	2.35	0.41
3:DB:585:MET:HE2	3:DB:585:MET:HB2	1.76	0.41
3:DB:1100:LEU:HD23	3:DB:1100:LEU:HA	1.76	0.41
8:DH:46:LEU:HD12	8:DH:46:LEU:HA	1.59	0.41
8:DH:269:ARG:HD2	18:CJ:288:GLN:OE1	2.20	0.41
8:DH:396:VAL:CG2	26:CA:420:A:H5"	2.50	0.41
9:DJ:173:ASP:OD1	9:DJ:206:SER:HB2	2.20	0.41
9:DJ:304:ILE:HD12	11:DT:42:PHE:HD2	1.84	0.41
11:DT:105:ARG:NH1	11:DT:146:GLN:HB3	2.34	0.41
12:DV:51:ASN:OD1	15:DY:11:THR:HB	2.20	0.41
18:CJ:485:GLU:HA	18:CJ:515:ALA:HB2	2.01	0.41
24:CI:88:ILE:HG22	24:CI:89:MET:HE2	2.02	0.41
25:Ck:361:GLN:H	25:Ck:361:GLN:HG3	1.62	0.41
3:DB:255:LEU:HD13	3:DB:403:ASN:OD1	2.20	0.41
3:DB:898:GLN:HE21	25:Ck:270:TYR:HB2	1.85	0.41
4:DC:888:LEU:HD23	4:DC:888:LEU:HA	1.83	0.41
6:DF:54:GLY:CA	6:DF:156:ALA:HB3	2.51	0.41
6:DF:310:LEU:HD23	9:DJ:73:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DH:292:ARG:HH12	8:DH:330:THR:CG2	2.33	0.41
10:DK:32:ILE:HG13	10:DK:41:VAL:HG22	2.01	0.41
10:DK:273:LEU:HD12	10:DK:273:LEU:HA	1.73	0.41
13:DW:98:GLN:HE22	13:DW:154:HIS:HD2	1.68	0.41
13:DW:128:LEU:HD23	13:DW:128:LEU:HA	1.82	0.41
18:CJ:103:PRO:HB2	18:CJ:104:PHE:CD1	2.55	0.41
18:CJ:762:GLN:HB3	24:CI:15:VAL:HG21	2.03	0.41
23:Cg:405:ASP:OD1	23:Cg:405:ASP:C	2.63	0.41
24:CI:157:LEU:HD12	24:CI:157:LEU:HA	1.77	0.41
25:Ck:383:ILE:HG21	25:Ck:392:PHE:CE2	2.55	0.41
1:DA:1280:GLU:O	1:DA:1284:VAL:HG23	2.20	0.41
2:DL:46:LYS:HB3	26:CA:469:A:C2	2.56	0.41
2:DL:273:THR:CG2	2:DL:276:HIS:HB2	2.50	0.41
3:DB:383:ARG:HA	3:DB:396:ARG:HH12	1.85	0.41
3:DB:623:SER:HA	3:DB:656:LEU:HD22	2.02	0.41
3:DB:795:VAL:HA	3:DB:796:PRO:HD3	1.93	0.41
4:DC:57:GLU:H	4:DC:57:GLU:HG3	1.66	0.41
4:DC:868:GLU:OE2	4:DC:893:PHE:CZ	2.73	0.41
4:DC:881:MET:HB3	4:DC:881:MET:HE3	1.72	0.41
6:DF:94:ASP:OD1	6:DF:94:ASP:C	2.64	0.41
6:DF:125:TYR:H	6:DF:175:GLN:NE2	2.15	0.41
6:DF:332:GLU:CD	6:DF:332:GLU:H	2.27	0.41
7:DG:293:ARG:HE	7:DG:299:PHE:HE1	1.67	0.41
8:DH:69:VAL:HG22	8:DH:96:ARG:HH11	1.85	0.41
8:DH:214:LEU:HD23	8:DH:214:LEU:HA	1.80	0.41
9:DJ:51:PRO:HG2	9:DJ:53:GLN:NE2	2.34	0.41
10:DK:130:LEU:HD23	10:DK:130:LEU:HA	1.80	0.41
14:DX:46:ALA:HA	22:CS:148:MET:HE1	2.03	0.41
17:CI:38:LEU:HD12	17:CI:38:LEU:HA	1.90	0.41
17:CI:295:ASP:OD2	18:CJ:100:ARG:NH2	2.54	0.41
17:CI:361:ALA:HB1	17:CI:406:THR:OG1	2.21	0.41
18:CJ:154:THR:HG21	18:CJ:201:ALA:O	2.19	0.41
22:CS:106:TYR:HD2	22:CS:140:MET:CE	2.30	0.41
23:Cg:153:CYS:HA	23:Cg:452:PRO:HD2	2.02	0.41
23:Cg:483:MET:HE2	23:Cg:483:MET:HB3	1.89	0.41
24:CI:69:THR:HG21	24:CI:73:MET:SD	2.61	0.41
25:Ck:552:LEU:HB3	25:Ck:561:SER:OG	2.20	0.41
25:Ck:597:LEU:HD23	25:Ck:597:LEU:HA	1.92	0.41
25:Ck:817:LEU:HD23	25:Ck:817:LEU:HA	1.80	0.41
3:DB:302:LEU:HD23	3:DB:302:LEU:HA	1.72	0.41
3:DB:539:GLN:HG3	3:DB:585:MET:CE	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DB:1101:GLN:HB2	18:CJ:680:LEU:HD22	2.02	0.41
4:DC:912:LEU:HD23	4:DC:912:LEU:HA	1.92	0.41
4:DC:953:MET:HE2	4:DC:953:MET:HB3	1.94	0.41
6:DF:125:TYR:N	6:DF:175:GLN:HE22	2.16	0.41
7:DG:66:LEU:HD23	7:DG:66:LEU:HA	1.74	0.41
9:DJ:136:ALA:HB3	9:DJ:168:TYR:CZ	2.55	0.41
18:CJ:432:HIS:HB3	18:CJ:817:PRO:HB3	2.03	0.41
19:CK:18:ALA:HB2	26:CA:527:A:N6	2.34	0.41
25:Ck:175:LEU:HD23	25:Ck:175:LEU:HA	1.91	0.41
6:DF:476:LEU:HD12	6:DF:476:LEU:HA	1.81	0.41
6:DF:533:LEU:HA	6:DF:533:LEU:HD23	1.73	0.41
7:DG:117:VAL:HG21	7:DG:149:SER:HB2	2.01	0.41
16:CC:50:ILE:HG13	16:CC:51:HIS:N	2.30	0.41
17:CI:65:MET:HE2	17:CI:65:MET:HB3	1.78	0.41
17:CI:351:MET:HB2	23:Cg:447:LEU:CD2	2.51	0.41
18:CJ:731:MET:HE1	18:CJ:744:ILE:HD12	2.01	0.41
18:CJ:731:MET:HE2	18:CJ:731:MET:HB3	1.77	0.41
18:CJ:804:ASN:OD1	20:CN:152:TRP:HD1	2.04	0.41
20:CN:66:MET:HE2	20:CN:66:MET:HB2	1.61	0.41
23:Cg:270:MET:HG2	23:Cg:338:GLY:CA	2.42	0.41
24:CI:37:ARG:HG3	25:Ck:736:LEU:O	2.21	0.41
3:DB:326:THR:HA	3:DB:327:PRO:HD3	1.91	0.41
4:DC:437:LEU:HD22	4:DC:437:LEU:HA	1.83	0.41
4:DC:553:ALA:HA	4:DC:556:GLN:NE2	2.36	0.41
4:DC:844:ALA:CB	5:DE:68:PRO:HB3	2.43	0.41
5:DE:212:LEU:HD23	5:DE:212:LEU:HA	1.86	0.41
5:DE:708:LEU:HA	5:DE:708:LEU:HD23	1.81	0.41
6:DF:16:GLU:H	6:DF:16:GLU:HG3	1.58	0.41
6:DF:540:VAL:HG12	6:DF:541:PHE:N	2.36	0.41
7:DG:124:PHE:CD1	7:DG:142:LEU:HD21	2.56	0.41
11:DT:15:ARG:NH2	24:CI:174:ASP:OD2	2.54	0.41
18:CJ:416:MET:HE2	18:CJ:416:MET:HB3	1.94	0.41
20:CN:165:ARG:HH11	25:Ck:751:ASP:CG	2.28	0.41
21:CR:248:LYS:HB2	21:CR:252:GLN:NE2	2.35	0.41
23:Cg:195:PRO:HA	25:Ck:837:TRP:CE2	2.56	0.41
25:Ck:60:MET:HG3	25:Ck:61:LEU:HG	2.03	0.41
2:DL:269:MET:HE2	2:DL:272:HIS:HD2	1.85	0.41
3:DB:428:ASN:HA	3:DB:429:PRO:HD2	1.92	0.41
3:DB:462:ASP:HB3	3:DB:465:GLU:HG3	2.02	0.41
4:DC:78:PRO:HG2	4:DC:708:TYR:CE2	2.55	0.41
4:DC:242:HIS:CE1	4:DC:464:THR:HB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DC:635:MET:CE	4:DC:659:LEU:HD12	2.51	0.41
4:DC:968:THR:HG22	4:DC:970:GLN:H	1.86	0.41
4:DC:1098:THR:HG22	4:DC:1103:PHE:HA	2.03	0.41
6:DF:192:LEU:C	6:DF:194:THR:H	2.27	0.41
6:DF:200:ALA:N	6:DF:201:PRO:HD2	2.36	0.41
6:DF:313:ARG:HD2	6:DF:339:TYR:OH	2.20	0.41
6:DF:502:ARG:HH21	6:DF:575:VAL:CG1	2.34	0.41
7:DG:256:ALA:HB1	7:DG:261:ARG:NH2	2.36	0.41
8:DH:151:LEU:HD12	8:DH:151:LEU:HA	1.90	0.41
9:DJ:220:LEU:HD23	9:DJ:220:LEU:HA	1.92	0.41
9:DJ:300:TRP:CH2	9:DJ:304:ILE:HG13	2.56	0.41
11:DT:199:LYS:HA	11:DT:199:LYS:HD3	1.71	0.41
13:DW:10:THR:HG23	22:CS:132:SER:HB2	2.03	0.41
18:CJ:130:ARG:O	18:CJ:130:ARG:HG3	2.20	0.41
18:CJ:433:THR:O	25:Ck:675:GLY:HA2	2.20	0.41
22:CS:145:LYS:HA	22:CS:146:PRO:HD3	1.87	0.41
23:Cg:144:GLY:HA3	23:Cg:353:PHE:O	2.21	0.41
31:Cg:501:GTP:O2A	33:Cg:601:HOH:O	2.22	0.41
25:Ck:214:LEU:HD23	25:Ck:214:LEU:HA	1.83	0.41
25:Ck:395:MET:HE2	25:Ck:564:LEU:HD23	2.03	0.41
25:Ck:585:MET:HE2	25:Ck:585:MET:HB3	1.95	0.41
3:DB:768:ALA:HB1	3:DB:774:ASN:HD21	1.86	0.41
3:DB:969:THR:CB	3:DB:1001:THR:HG21	2.51	0.41
3:DB:990:ARG:O	3:DB:993:ASP:HB2	2.21	0.41
7:DG:164:LEU:HA	7:DG:164:LEU:HD12	1.81	0.41
7:DG:393:ASN:HA	7:DG:394:PRO:HD3	1.93	0.41
7:DG:569:LEU:HD23	7:DG:569:LEU:HA	1.87	0.41
9:DJ:27:GLN:HE21	16:CC:66:ASN:ND2	2.19	0.41
11:DT:158:HIS:HB3	11:DT:160:TYR:CE1	2.55	0.41
23:Cg:46:LYS:C	23:Cg:48:GLY:H	2.29	0.41
23:Cg:356:CYS:SG	23:Cg:357:THR:N	2.94	0.41
26:CA:445:C:C2	26:CA:480:C:H5	2.39	0.41
4:DC:866:GLU:OE1	5:DE:70:PRO:HD2	2.21	0.40
5:DE:292:TYR:O	5:DE:295:TYR:HB3	2.20	0.40
6:DF:311:ILE:HA	6:DF:311:ILE:HD13	1.80	0.40
8:DH:268:LEU:HD12	8:DH:268:LEU:HA	1.76	0.40
8:DH:327:HIS:CD2	8:DH:346:GLU:HG2	2.56	0.40
9:DJ:92:LEU:HD21	9:DJ:130:PHE:CD2	2.56	0.40
10:DK:222:LEU:HD22	10:DK:226:LEU:HD22	2.01	0.40
14:DX:127:MET:HE3	14:DX:127:MET:HB3	1.82	0.40
18:CJ:134:GLN:HE21	18:CJ:134:GLN:HB2	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CJ:749:ALA:HA	18:CJ:750:PRO:HD2	1.87	0.40
24:CI:121:ASP:HB3	24:CI:127:THR:O	2.21	0.40
25:CK:314:LEU:HD23	25:CK:314:LEU:HA	1.90	0.40
3:DB:414:GLN:HA	4:DC:1141:GLN:HE22	1.85	0.40
3:DB:867:THR:HG21	18:CJ:343:VAL:CG2	2.52	0.40
3:DB:1158:LYS:HE3	14:DX:159:ASP:OD2	2.21	0.40
4:DC:496:LYS:CG	4:DC:497:PRO:HD2	2.51	0.40
4:DC:854:LEU:HD23	4:DC:854:LEU:HA	1.92	0.40
6:DF:208:ARG:HD2	18:CJ:563:ASP:O	2.21	0.40
7:DG:184:ALA:O	19:CK:51:ASN:ND2	2.55	0.40
7:DG:326:THR:HG22	7:DG:329:LEU:H	1.85	0.40
7:DG:577:LEU:O	7:DG:581:VAL:HG13	2.20	0.40
8:DH:282:ASN:ND2	8:DH:315:LEU:HD23	2.37	0.40
9:DJ:291:ASN:ND2	9:DJ:294:MET:HB2	2.36	0.40
11:DT:210:GLY:HA3	11:DT:211:PRO:HD2	1.91	0.40
13:DW:55:TRP:CD1	13:DW:136:THR:HG22	2.57	0.40
18:CJ:83:HIS:O	18:CJ:84:MET:C	2.62	0.40
18:CJ:704:GLU:H	18:CJ:704:GLU:HG3	1.51	0.40
23:Cg:231:LEU:N	23:Cg:239:GLN:HE22	2.19	0.40
24:CI:30:ARG:HH11	24:CI:30:ARG:CG	2.34	0.40
7:DG:136:LEU:HD12	7:DG:136:LEU:HA	1.82	0.40
7:DG:626:LEU:HD12	7:DG:626:LEU:HA	1.83	0.40
8:DH:119:LEU:HD22	8:DH:123:HIS:HB3	2.02	0.40
9:DJ:270:ARG:HH11	9:DJ:270:ARG:HD2	1.78	0.40
12:DV:143:ILE:H	12:DV:143:ILE:HG13	1.56	0.40
14:DX:64:SER:HA	14:DX:162:VAL:HG22	2.04	0.40
14:DX:136:ARG:HA	14:DX:136:ARG:HD2	2.01	0.40
18:CJ:457:THR:H	18:CJ:460:HIS:HD2	1.69	0.40
22:CS:103:ARG:HD2	26:CA:488:A:C4	2.57	0.40
23:Cg:110:LEU:HD21	23:Cg:408:GLU:HB3	2.04	0.40
23:Cg:383:ASP:O	23:Cg:384:GLU:OE2	2.40	0.40
1:DA:1244:LYS:HZ3	1:DA:1296:GLU:HB3	1.85	0.40
2:DL:69:GLU:HB2	2:DL:73:SER:OG	2.22	0.40
3:DB:557:ALA:O	6:DF:512:ASN:ND2	2.54	0.40
3:DB:608:LEU:HD23	3:DB:608:LEU:HA	1.93	0.40
3:DB:720:LYS:HE3	3:DB:720:LYS:HB2	1.77	0.40
4:DC:86:THR:OG1	4:DC:959:VAL:HG21	2.22	0.40
5:DE:203:LEU:HD12	5:DE:422:LEU:HD12	2.02	0.40
5:DE:206:LEU:HA	5:DE:206:LEU:HD23	1.83	0.40
5:DE:601:ILE:HG21	5:DE:601:ILE:HD13	1.77	0.40
5:DE:610:LEU:HA	5:DE:610:LEU:HD23	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DF:125:TYR:OH	6:DF:140:HIS:HE1	2.04	0.40
6:DF:502:ARG:HD3	6:DF:577:ALA:O	2.22	0.40
7:DG:524:PHE:HZ	7:DG:582:VAL:HG11	1.86	0.40
12:DV:167:PRO:HA	12:DV:168:PRO:HD3	1.91	0.40
15:DY:84:LYS:HB3	15:DY:84:LYS:HE2	1.88	0.40
17:CI:431:LEU:HD23	17:CI:431:LEU:HA	1.82	0.40
18:CJ:723:GLU:HG2	18:CJ:724:THR:H	1.87	0.40
19:CK:54:LEU:HD23	19:CK:54:LEU:HA	1.89	0.40
20:CN:72:THR:HG21	22:CS:83:PHE:CE2	2.56	0.40
25:Ck:275:TRP:O	25:Ck:278:PHE:HB3	2.22	0.40
3:DB:495:LEU:HG	3:DB:589:ASP:OD2	2.22	0.40
4:DC:85:PRO:HD2	4:DC:912:LEU:HD23	2.03	0.40
4:DC:270:LEU:HA	4:DC:270:LEU:HD23	1.83	0.40
4:DC:317:GLU:HG2	4:DC:320:ARG:NH1	2.35	0.40
5:DE:240:PRO:HD3	8:DH:563:HIS:NE2	2.36	0.40
6:DF:102:LEU:HD23	6:DF:102:LEU:HA	1.91	0.40
7:DG:38:ARG:HB3	18:CJ:88:ARG:NH1	2.36	0.40
9:DJ:21:PRO:HG2	18:CJ:74:TRP:CZ2	2.56	0.40
9:DJ:92:LEU:HD12	9:DJ:92:LEU:HA	1.88	0.40
9:DJ:258:LEU:HD12	9:DJ:258:LEU:HA	1.90	0.40
11:DT:87:ARG:NH1	11:DT:93:MET:HB2	2.36	0.40
13:DW:12:THR:HA	13:DW:13:PRO:HD3	1.77	0.40
13:DW:74:THR:HG22	23:Cg:98:PHE:HE2	1.87	0.40
18:CJ:132:ASN:O	25:Ck:743:MET:HG3	2.22	0.40
18:CJ:671:LEU:HD12	18:CJ:671:LEU:HA	1.89	0.40
20:CN:153:ASN:HD22	20:CN:153:ASN:HA	1.61	0.40
22:CS:42:LEU:HD13	26:CA:411:A:C4	2.56	0.40
25:Ck:119:GLU:OE1	25:Ck:140:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DA	129/1788 (7%)	126 (98%)	3 (2%)	0	100	100
2	DL	139/307 (45%)	130 (94%)	9 (6%)	0	100	100
3	DB	1109/1181 (94%)	1078 (97%)	29 (3%)	2 (0%)	43	71
4	DC	1087/1165 (93%)	1052 (97%)	34 (3%)	1 (0%)	48	76
5	DE	576/747 (77%)	564 (98%)	11 (2%)	1 (0%)	43	71
6	DF	586/666 (88%)	569 (97%)	16 (3%)	1 (0%)	43	71
7	DG	558/631 (88%)	543 (97%)	14 (2%)	1 (0%)	43	71
8	DH	560/581 (96%)	540 (96%)	20 (4%)	0	100	100
9	DJ	313/396 (79%)	304 (97%)	8 (3%)	1 (0%)	36	64
10	DK	249/324 (77%)	240 (96%)	9 (4%)	0	100	100
11	DT	237/247 (96%)	233 (98%)	4 (2%)	0	100	100
12	DV	158/183 (86%)	151 (96%)	6 (4%)	1 (1%)	21	49
13	DW	159/179 (89%)	153 (96%)	6 (4%)	0	100	100
14	DX	139/169 (82%)	133 (96%)	6 (4%)	0	100	100
15	DY	152/163 (93%)	148 (97%)	4 (3%)	0	100	100
16	CC	72/74 (97%)	68 (94%)	3 (4%)	1 (1%)	9	31
17	CI	218/443 (49%)	210 (96%)	8 (4%)	0	100	100
18	CJ	796/817 (97%)	765 (96%)	30 (4%)	1 (0%)	48	76
19	CK	50/326 (15%)	47 (94%)	3 (6%)	0	100	100
20	CN	155/166 (93%)	150 (97%)	5 (3%)	0	100	100
21	CR	42/320 (13%)	40 (95%)	2 (5%)	0	100	100
22	CS	140/244 (57%)	135 (96%)	5 (4%)	0	100	100
23	Cg	480/498 (96%)	461 (96%)	19 (4%)	0	100	100
24	Ci	163/181 (90%)	155 (95%)	8 (5%)	0	100	100
25	Ck	699/874 (80%)	671 (96%)	26 (4%)	2 (0%)	36	64
All	All	8966/12670 (71%)	8666 (97%)	288 (3%)	12 (0%)	49	76

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	DJ	36	GLN
12	DV	57	THR
18	CJ	799	ASP
3	DB	1033	TYR

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Mol	Chain	Res	Type
25	Ck	231	GLY
25	Ck	653	LEU
5	DE	71	LEU
4	DC	441	VAL
16	CC	18	LYS
7	DG	48	VAL
6	DF	184	VAL
3	DB	946	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DA	111/1514 (7%)	100 (90%)	11 (10%)	7	27
2	DL	123/263 (47%)	114 (93%)	9 (7%)	13	38
3	DB	976/1030 (95%)	855 (88%)	121 (12%)	4	18
4	DC	927/985 (94%)	803 (87%)	124 (13%)	4	15
5	DE	519/644 (81%)	454 (88%)	65 (12%)	4	17
6	DF	500/560 (89%)	433 (87%)	67 (13%)	4	15
7	DG	490/543 (90%)	427 (87%)	63 (13%)	4	16
8	DH	493/504 (98%)	427 (87%)	66 (13%)	4	15
9	DJ	275/347 (79%)	236 (86%)	39 (14%)	3	13
10	DK	209/261 (80%)	184 (88%)	25 (12%)	5	19
11	DT	220/228 (96%)	194 (88%)	26 (12%)	5	20
12	DV	145/165 (88%)	124 (86%)	21 (14%)	3	13
13	DW	148/163 (91%)	136 (92%)	12 (8%)	11	34
14	DX	124/149 (83%)	109 (88%)	15 (12%)	5	18
15	DY	137/146 (94%)	115 (84%)	22 (16%)	2	10
16	CC	73/73 (100%)	58 (80%)	15 (20%)	1	5
17	CI	186/370 (50%)	161 (87%)	25 (13%)	4	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	CJ	709/723 (98%)	616 (87%)	93 (13%)	4	16
19	CK	47/283 (17%)	39 (83%)	8 (17%)	2	9
20	CN	142/150 (95%)	122 (86%)	20 (14%)	3	13
21	CR	41/279 (15%)	32 (78%)	9 (22%)	1	4
22	CS	126/220 (57%)	108 (86%)	18 (14%)	3	13
23	Cg	424/437 (97%)	374 (88%)	50 (12%)	5	20
24	Ci	144/160 (90%)	124 (86%)	20 (14%)	3	14
25	Ck	608/747 (81%)	541 (89%)	67 (11%)	6	23
All	All	7897/10944 (72%)	6886 (87%)	1011 (13%)	6	16

All (1011) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DA	1187	ASP
1	DA	1191	ILE
1	DA	1208	THR
1	DA	1220	VAL
1	DA	1240	LEU
1	DA	1253	VAL
1	DA	1263	VAL
1	DA	1268	LEU
1	DA	1271	LEU
1	DA	1278	THR
1	DA	1292	CYS
2	DL	28	ASN
2	DL	39	THR
2	DL	68	LEU
2	DL	102	SER
2	DL	267	HIS
2	DL	268	VAL
2	DL	269	MET
2	DL	270	THR
2	DL	286	THR
3	DB	99	VAL
3	DB	118	VAL
3	DB	129	TYR
3	DB	137	VAL
3	DB	146	MET
3	DB	173	ARG

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Mol	Chain	Res	Type
3	DB	183	VAL
3	DB	186	SER
3	DB	189	VAL
3	DB	192	ILE
3	DB	204	SER
3	DB	213	ASP
3	DB	217	ILE
3	DB	221	HIS
3	DB	233	ASP
3	DB	249	SER
3	DB	295	THR
3	DB	321	SER
3	DB	339	ARG
3	DB	341	THR
3	DB	343	VAL
3	DB	357	ILE
3	DB	365	THR
3	DB	368	GLU
3	DB	383	ARG
3	DB	388	VAL
3	DB	394	ASP
3	DB	397	THR
3	DB	416	ASN
3	DB	424	ASP
3	DB	433	ARG
3	DB	435	THR
3	DB	439	VAL
3	DB	445	ASN
3	DB	448	ASP
3	DB	450	MET
3	DB	454	ASP
3	DB	479	VAL
3	DB	490	ARG
3	DB	507	LEU
3	DB	511	ARG
3	DB	514	ARG
3	DB	521	LEU
3	DB	522	MET
3	DB	532	GLU
3	DB	539	GLN
3	DB	550	LEU
3	DB	553	LEU

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Mol	Chain	Res	Type
3	DB	554	GLU
3	DB	564	ARG
3	DB	572	ASP
3	DB	574	ILE
3	DB	584	GLU
3	DB	585	MET
3	DB	587	VAL
3	DB	590	ASP
3	DB	592	MET
3	DB	597	GLU
3	DB	637	THR
3	DB	671	VAL
3	DB	686	GLN
3	DB	689	LEU
3	DB	693	SER
3	DB	719	MET
3	DB	720	LYS
3	DB	743	VAL
3	DB	744	VAL
3	DB	755	LEU
3	DB	756	THR
3	DB	757	VAL
3	DB	758	SER
3	DB	774	ASN
3	DB	776	THR
3	DB	785	ASN
3	DB	790	SER
3	DB	793	ARG
3	DB	810	THR
3	DB	815	ASP
3	DB	820	GLU
3	DB	830	LEU
3	DB	831	ASN
3	DB	834	ILE
3	DB	849	ASP
3	DB	850	SER
3	DB	878	VAL
3	DB	901	VAL
3	DB	908	GLN
3	DB	920	VAL
3	DB	923	GLN
3	DB	937	MET

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Mol	Chain	Res	Type
3	DB	941	ARG
3	DB	950	VAL
3	DB	958	ASN
3	DB	964	ARG
3	DB	968	VAL
3	DB	969	THR
3	DB	984	ASP
3	DB	995	VAL
3	DB	1002	THR
3	DB	1009	ASP
3	DB	1012	THR
3	DB	1013	ARG
3	DB	1020	ASP
3	DB	1026	SER
3	DB	1028	SER
3	DB	1030	ARG
3	DB	1034	ILE
3	DB	1067	ILE
3	DB	1069	THR
3	DB	1080	ARG
3	DB	1104	ASP
3	DB	1110	LYS
3	DB	1117	THR
3	DB	1142	VAL
3	DB	1153	ASP
3	DB	1156	THR
3	DB	1165	SER
3	DB	1168	ASP
3	DB	1172	LYS
3	DB	1173	THR
3	DB	1181	LEU
4	DC	30	THR
4	DC	36	ASP
4	DC	46	ARG
4	DC	57	GLU
4	DC	58	VAL
4	DC	82	THR
4	DC	86	THR
4	DC	87	MET
4	DC	93	ARG
4	DC	106	SER
4	DC	108	SER

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Mol	Chain	Res	Type
4	DC	114	GLU
4	DC	119	THR
4	DC	131	GLU
4	DC	148	LEU
4	DC	154	THR
4	DC	155	VAL
4	DC	162	ILE
4	DC	166	GLU
4	DC	227	GLN
4	DC	231	THR
4	DC	240	VAL
4	DC	268	ASP
4	DC	271	SER
4	DC	279	GLU
4	DC	299	LEU
4	DC	313	THR
4	DC	365	LYS
4	DC	371	ILE
4	DC	374	LEU
4	DC	379	LEU
4	DC	386	MET
4	DC	423	ILE
4	DC	432	ARG
4	DC	435	LEU
4	DC	437	LEU
4	DC	442	LEU
4	DC	464	THR
4	DC	467	THR
4	DC	471	ARG
4	DC	474	LEU
4	DC	475	LEU
4	DC	491	LEU
4	DC	498	LEU
4	DC	503	ASP
4	DC	506	SER
4	DC	511	ARG
4	DC	513	SER
4	DC	519	SER
4	DC	525	THR
4	DC	533	LEU
4	DC	534	LEU
4	DC	540	LEU

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Mol	Chain	Res	Type
4	DC	544	GLU
4	DC	545	ASP
4	DC	569	LEU
4	DC	595	SER
4	DC	604	VAL
4	DC	609	VAL
4	DC	611	MET
4	DC	618	ARG
4	DC	620	VAL
4	DC	632	LEU
4	DC	652	ARG
4	DC	659	LEU
4	DC	669	LEU
4	DC	705	LEU
4	DC	710	THR
4	DC	749	GLU
4	DC	752	VAL
4	DC	753	LEU
4	DC	755	ASP
4	DC	756	ASP
4	DC	757	ARG
4	DC	766	VAL
4	DC	774	ASP
4	DC	794	LEU
4	DC	799	ASN
4	DC	807	VAL
4	DC	817	ASP
4	DC	839	VAL
4	DC	865	CYS
4	DC	871	GLN
4	DC	873	VAL
4	DC	881	MET
4	DC	885	LEU
4	DC	894	HIS
4	DC	919	VAL
4	DC	928	GLU
4	DC	931	THR
4	DC	934	ARG
4	DC	952	GLU
4	DC	953	MET
4	DC	954	LEU
4	DC	960	VAL

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Mol	Chain	Res	Type
4	DC	961	THR
4	DC	963	SER
4	DC	970	GLN
4	DC	984	THR
4	DC	985	VAL
4	DC	987	THR
4	DC	1000	LEU
4	DC	1006	VAL
4	DC	1009	THR
4	DC	1019	THR
4	DC	1023	ASN
4	DC	1025	THR
4	DC	1055	ARG
4	DC	1062	GLN
4	DC	1063	SER
4	DC	1071	VAL
4	DC	1076	PHE
4	DC	1104	MET
4	DC	1121	THR
4	DC	1125	SER
4	DC	1128	ARG
4	DC	1132	THR
4	DC	1133	THR
4	DC	1143	VAL
4	DC	1151	THR
4	DC	1153	LEU
4	DC	1159	ASP
4	DC	1161	LYS
4	DC	1163	GLU
5	DE	46	SER
5	DE	51	ARG
5	DE	54	ARG
5	DE	65	ILE
5	DE	80	LEU
5	DE	147	MET
5	DE	149	LEU
5	DE	154	SER
5	DE	178	GLN
5	DE	196	ASP
5	DE	203	LEU
5	DE	204	VAL
5	DE	212	LEU

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Mol	Chain	Res	Type
5	DE	229	ARG
5	DE	246	ILE
5	DE	280	LEU
5	DE	286	THR
5	DE	299	LYS
5	DE	319	ASN
5	DE	333	ASP
5	DE	335	GLU
5	DE	343	LEU
5	DE	398	LEU
5	DE	405	ILE
5	DE	406	ASP
5	DE	408	LEU
5	DE	418	LEU
5	DE	429	ILE
5	DE	445	LEU
5	DE	451	THR
5	DE	466	VAL
5	DE	482	THR
5	DE	484	THR
5	DE	486	ILE
5	DE	497	GLN
5	DE	503	ASP
5	DE	529	ASP
5	DE	538	VAL
5	DE	545	ARG
5	DE	554	LEU
5	DE	561	THR
5	DE	566	ARG
5	DE	570	GLU
5	DE	572	VAL
5	DE	573	GLN
5	DE	575	CYS
5	DE	586	THR
5	DE	587	MET
5	DE	591	LEU
5	DE	600	ILE
5	DE	601	ILE
5	DE	602	LYS
5	DE	604	ASP
5	DE	607	ILE
5	DE	610	LEU

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Mol	Chain	Res	Type
5	DE	615	LEU
5	DE	651	ASN
5	DE	659	ARG
5	DE	678	THR
5	DE	698	GLN
5	DE	704	LEU
5	DE	717	ARG
5	DE	718	SER
5	DE	721	ASP
5	DE	726	THR
6	DF	8	SER
6	DF	13	ILE
6	DF	15	HIS
6	DF	19	THR
6	DF	22	LEU
6	DF	27	ARG
6	DF	33	GLN
6	DF	39	ARG
6	DF	40	GLU
6	DF	50	LEU
6	DF	53	ARG
6	DF	57	ARG
6	DF	69	THR
6	DF	72	THR
6	DF	85	ARG
6	DF	87	GLU
6	DF	95	ILE
6	DF	110	ASN
6	DF	137	VAL
6	DF	144	THR
6	DF	154	ASN
6	DF	157	THR
6	DF	170	ARG
6	DF	182	ARG
6	DF	188	ARG
6	DF	189	ASP
6	DF	192	LEU
6	DF	194	THR
6	DF	202	LEU
6	DF	238	THR
6	DF	246	LYS
6	DF	255	GLU

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Mol	Chain	Res	Type
6	DF	258	ASP
6	DF	259	SER
6	DF	264	VAL
6	DF	274	LEU
6	DF	294	MET
6	DF	297	ARG
6	DF	307	GLU
6	DF	321	LEU
6	DF	326	ASP
6	DF	331	GLU
6	DF	332	GLU
6	DF	343	GLU
6	DF	362	ILE
6	DF	370	LEU
6	DF	373	ASP
6	DF	394	GLU
6	DF	395	LEU
6	DF	402	THR
6	DF	403	LEU
6	DF	437	GLU
6	DF	439	THR
6	DF	450	VAL
6	DF	452	VAL
6	DF	476	LEU
6	DF	491	ARG
6	DF	502	ARG
6	DF	512	ASN
6	DF	516	ARG
6	DF	550	VAL
6	DF	553	THR
6	DF	568	LEU
6	DF	573	THR
6	DF	575	VAL
6	DF	584	LEU
6	DF	591	HIS
7	DG	36	THR
7	DG	56	ARG
7	DG	57	GLU
7	DG	62	SER
7	DG	74	LEU
7	DG	78	HIS
7	DG	84	LEU

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Mol	Chain	Res	Type
7	DG	93	ARG
7	DG	95	VAL
7	DG	115	ILE
7	DG	125	ASP
7	DG	127	LEU
7	DG	130	LEU
7	DG	141	THR
7	DG	142	LEU
7	DG	147	SER
7	DG	149	SER
7	DG	155	GLU
7	DG	162	LEU
7	DG	165	VAL
7	DG	176	VAL
7	DG	179	LEU
7	DG	186	ARG
7	DG	200	GLN
7	DG	206	LEU
7	DG	210	VAL
7	DG	220	THR
7	DG	236	VAL
7	DG	296	ASP
7	DG	298	ASP
7	DG	305	VAL
7	DG	318	ILE
7	DG	326	THR
7	DG	332	GLN
7	DG	334	MET
7	DG	336	MET
7	DG	365	GLN
7	DG	366	ASP
7	DG	367	SER
7	DG	370	ARG
7	DG	377	GLU
7	DG	384	VAL
7	DG	392	ARG
7	DG	405	GLN
7	DG	444	THR
7	DG	448	LEU
7	DG	457	ARG
7	DG	466	VAL
7	DG	472	ARG

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Mol	Chain	Res	Type
7	DG	473	CYS
7	DG	494	THR
7	DG	496	ARG
7	DG	497	ARG
7	DG	529	ASP
7	DG	547	MET
7	DG	557	GLN
7	DG	577	LEU
7	DG	582	VAL
7	DG	608	ARG
7	DG	615	SER
7	DG	616	ARG
7	DG	623	MET
7	DG	626	LEU
8	DH	1	MET
8	DH	4	GLN
8	DH	6	VAL
8	DH	9	THR
8	DH	40	THR
8	DH	46	LEU
8	DH	47	ILE
8	DH	51	ARG
8	DH	74	GLU
8	DH	76	LEU
8	DH	79	ASP
8	DH	81	LYS
8	DH	82	GLN
8	DH	83	GLU
8	DH	84	SER
8	DH	85	LEU
8	DH	102	LEU
8	DH	105	GLN
8	DH	135	ARG
8	DH	167	GLU
8	DH	174	LEU
8	DH	181	VAL
8	DH	195	TYR
8	DH	206	ILE
8	DH	236	MET
8	DH	257	ASN
8	DH	258	MET
8	DH	268	LEU

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Mol	Chain	Res	Type
8	DH	273	SER
8	DH	297	CYS
8	DH	311	ARG
8	DH	318	GLU
8	DH	323	SER
8	DH	344	VAL
8	DH	345	VAL
8	DH	346	GLU
8	DH	348	LYS
8	DH	350	VAL
8	DH	354	LEU
8	DH	359	GLU
8	DH	360	LEU
8	DH	364	ARG
8	DH	369	ARG
8	DH	375	VAL
8	DH	380	ARG
8	DH	382	PHE
8	DH	386	ARG
8	DH	396	VAL
8	DH	411	LEU
8	DH	414	LEU
8	DH	421	THR
8	DH	428	ARG
8	DH	450	ASN
8	DH	452	ARG
8	DH	460	LEU
8	DH	474	ASP
8	DH	476	VAL
8	DH	486	THR
8	DH	495	THR
8	DH	499	GLU
8	DH	503	THR
8	DH	515	ASP
8	DH	523	ARG
8	DH	554	ARG
8	DH	557	VAL
8	DH	562	THR
9	DJ	16	ASN
9	DJ	19	THR
9	DJ	38	MET
9	DJ	46	ARG

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Mol	Chain	Res	Type
9	DJ	54	SER
9	DJ	55	ASN
9	DJ	59	VAL
9	DJ	71	MET
9	DJ	76	SER
9	DJ	91	THR
9	DJ	92	LEU
9	DJ	100	VAL
9	DJ	107	LEU
9	DJ	110	LEU
9	DJ	119	LEU
9	DJ	123	LYS
9	DJ	137	MET
9	DJ	149	THR
9	DJ	151	GLU
9	DJ	164	SER
9	DJ	166	LEU
9	DJ	178	ARG
9	DJ	180	LEU
9	DJ	182	ASP
9	DJ	206	SER
9	DJ	210	MET
9	DJ	212	ASP
9	DJ	226	VAL
9	DJ	234	GLU
9	DJ	236	ARG
9	DJ	246	THR
9	DJ	258	LEU
9	DJ	266	VAL
9	DJ	271	THR
9	DJ	291	ASN
9	DJ	302	SER
9	DJ	305	ARG
9	DJ	308	ARG
9	DJ	323	THR
10	DK	2	SER
10	DK	6	THR
10	DK	18	LEU
10	DK	34	ASN
10	DK	36	ARG
10	DK	54	THR
10	DK	111	LEU

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Mol	Chain	Res	Type
10	DK	115	THR
10	DK	116	ARG
10	DK	134	THR
10	DK	167	THR
10	DK	172	LEU
10	DK	173	VAL
10	DK	225	THR
10	DK	226	LEU
10	DK	238	ILE
10	DK	240	SER
10	DK	250	VAL
10	DK	263	GLU
10	DK	265	VAL
10	DK	270	LEU
10	DK	273	LEU
10	DK	275	ARG
10	DK	282	GLU
10	DK	294	SER
11	DT	12	ARG
11	DT	14	THR
11	DT	35	LYS
11	DT	52	ARG
11	DT	88	THR
11	DT	90	THR
11	DT	91	GLN
11	DT	103	LEU
11	DT	105	ARG
11	DT	106	ASP
11	DT	114	LEU
11	DT	122	MET
11	DT	131	SER
11	DT	137	LEU
11	DT	163	ARG
11	DT	166	THR
11	DT	168	GLU
11	DT	176	ASP
11	DT	177	MET
11	DT	179	VAL
11	DT	181	ASP
11	DT	195	VAL
11	DT	202	LYS
11	DT	205	VAL

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Mol	Chain	Res	Type
11	DT	209	THR
11	DT	241	ASN
12	DV	26	THR
12	DV	39	ARG
12	DV	41	THR
12	DV	43	ASN
12	DV	56	ARG
12	DV	63	ILE
12	DV	68	ILE
12	DV	71	GLN
12	DV	77	LYS
12	DV	114	VAL
12	DV	118	GLN
12	DV	127	THR
12	DV	131	GLN
12	DV	134	ASP
12	DV	140	PHE
12	DV	143	ILE
12	DV	151	GLU
12	DV	178	THR
12	DV	179	LEU
12	DV	180	ASP
12	DV	183	LEU
13	DW	10	THR
13	DW	12	THR
13	DW	22	THR
13	DW	37	MET
13	DW	58	ARG
13	DW	60	VAL
13	DW	70	LEU
13	DW	74	THR
13	DW	83	THR
13	DW	128	LEU
13	DW	133	LYS
13	DW	163	GLU
14	DX	34	LYS
14	DX	57	ARG
14	DX	72	SER
14	DX	76	ARG
14	DX	78	GLU
14	DX	89	ARG
14	DX	90	ILE

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Mol	Chain	Res	Type
14	DX	98	LEU
14	DX	124	ILE
14	DX	131	ILE
14	DX	132	THR
14	DX	136	ARG
14	DX	162	VAL
14	DX	164	THR
14	DX	168	ASN
15	DY	11	THR
15	DY	14	THR
15	DY	15	SER
15	DY	23	SER
15	DY	39	VAL
15	DY	43	LEU
15	DY	47	THR
15	DY	50	VAL
15	DY	52	GLN
15	DY	64	ASP
15	DY	65	LEU
15	DY	77	VAL
15	DY	79	ASP
15	DY	81	THR
15	DY	84	LYS
15	DY	87	ARG
15	DY	93	THR
15	DY	113	VAL
15	DY	124	THR
15	DY	128	GLN
15	DY	141	VAL
15	DY	163	LYS
16	CC	4	MET
16	CC	7	ILE
16	CC	10	VAL
16	CC	14	THR
16	CC	20	THR
16	CC	21	PHE
16	CC	22	LYS
16	CC	45	ILE
16	CC	46	TRP
16	CC	47	LEU
16	CC	50	ILE
16	CC	55	ILE

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Mol	Chain	Res	Type
16	CC	69	GLU
16	CC	72	ILE
16	CC	76	SER
17	CI	2	GLN
17	CI	9	THR
17	CI	18	LEU
17	CI	33	SER
17	CI	34	ASP
17	CI	38	LEU
17	CI	43	SER
17	CI	57	GLU
17	CI	59	ARG
17	CI	65	MET
17	CI	290	ILE
17	CI	303	THR
17	CI	309	ARG
17	CI	311	CYS
17	CI	324	ARG
17	CI	330	ASN
17	CI	332	ILE
17	CI	338	LYS
17	CI	343	VAL
17	CI	356	MET
17	CI	372	ILE
17	CI	406	THR
17	CI	415	LEU
17	CI	420	ARG
17	CI	439	ARG
18	CJ	17	MET
18	CJ	20	GLN
18	CJ	23	LYS
18	CJ	34	GLN
18	CJ	43	GLU
18	CJ	50	ASP
18	CJ	65	VAL
18	CJ	68	ASP
18	CJ	77	CYS
18	CJ	78	THR
18	CJ	84	MET
18	CJ	93	SER
18	CJ	105	ASN
18	CJ	106	GLU

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Mol	Chain	Res	Type
18	CJ	110	LYS
18	CJ	118	MET
18	CJ	141	ASP
18	CJ	149	GLU
18	CJ	158	THR
18	CJ	162	ILE
18	CJ	186	VAL
18	CJ	202	ASP
18	CJ	204	SER
18	CJ	212	THR
18	CJ	257	VAL
18	CJ	273	ARG
18	CJ	279	LYS
18	CJ	286	LEU
18	CJ	287	LEU
18	CJ	293	ASP
18	CJ	311	LEU
18	CJ	313	GLU
18	CJ	325	SER
18	CJ	328	ARG
18	CJ	330	LEU
18	CJ	345	VAL
18	CJ	346	PRO
18	CJ	370	MET
18	CJ	372	GLU
18	CJ	380	THR
18	CJ	396	LYS
18	CJ	399	ARG
18	CJ	401	ILE
18	CJ	403	CYS
18	CJ	409	SER
18	CJ	413	GLU
18	CJ	434	ILE
18	CJ	456	THR
18	CJ	457	THR
18	CJ	480	THR
18	CJ	481	ASP
18	CJ	490	ASP
18	CJ	498	CYS
18	CJ	500	VAL
18	CJ	517	VAL
18	CJ	519	ILE

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Mol	Chain	Res	Type
18	CJ	523	VAL
18	CJ	526	THR
18	CJ	530	THR
18	CJ	542	LYS
18	CJ	543	THR
18	CJ	547	LYS
18	CJ	552	ILE
18	CJ	556	GLU
18	CJ	565	THR
18	CJ	569	LEU
18	CJ	585	SER
18	CJ	605	THR
18	CJ	618	VAL
18	CJ	629	ARG
18	CJ	633	CYS
18	CJ	648	VAL
18	CJ	654	VAL
18	CJ	667	VAL
18	CJ	671	LEU
18	CJ	684	THR
18	CJ	687	GLU
18	CJ	704	GLU
18	CJ	714	THR
18	CJ	720	THR
18	CJ	724	THR
18	CJ	727	THR
18	CJ	731	MET
18	CJ	757	LEU
18	CJ	762	GLN
18	CJ	769	GLN
18	CJ	770	THR
18	CJ	773	GLU
18	CJ	781	HIS
18	CJ	796	ASP
18	CJ	797	LEU
18	CJ	798	GLN
18	CJ	803	ILE
19	CK	15	ARG
19	CK	23	ASP
19	CK	32	LEU
19	CK	33	LYS
19	CK	40	GLN

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Mol	Chain	Res	Type
19	CK	47	ILE
19	CK	48	ARG
19	CK	56	GLN
20	CN	22	THR
20	CN	27	GLU
20	CN	30	LEU
20	CN	41	LEU
20	CN	43	SER
20	CN	49	SER
20	CN	57	LYS
20	CN	60	VAL
20	CN	66	MET
20	CN	70	LYS
20	CN	72	THR
20	CN	77	ASN
20	CN	81	LEU
20	CN	83	LYS
20	CN	105	ARG
20	CN	111	VAL
20	CN	118	MET
20	CN	127	LEU
20	CN	135	THR
20	CN	158	ARG
21	CR	243	THR
21	CR	248	LYS
21	CR	250	GLN
21	CR	267	ASN
21	CR	269	SER
21	CR	274	VAL
21	CR	280	ASN
21	CR	282	THR
21	CR	286	LEU
22	CS	32	LYS
22	CS	33	ILE
22	CS	45	ARG
22	CS	47	GLN
22	CS	48	ARG
22	CS	59	LYS
22	CS	64	MET
22	CS	75	MET
22	CS	76	THR
22	CS	86	GLU

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Mol	Chain	Res	Type
22	CS	95	THR
22	CS	105	VAL
22	CS	107	THR
22	CS	119	VAL
22	CS	121	SER
22	CS	125	ILE
22	CS	140	MET
22	CS	152	ASP
23	Cg	20	THR
23	Cg	27	GLU
23	Cg	56	ARG
23	Cg	57	THR
23	Cg	73	ASP
23	Cg	76	SER
23	Cg	77	MET
23	Cg	87	GLN
23	Cg	107	ARG
23	Cg	112	ARG
23	Cg	114	GLU
23	Cg	117	LEU
23	Cg	120	LEU
23	Cg	127	HIS
23	Cg	143	THR
23	Cg	153	CYS
23	Cg	170	ASN
23	Cg	173	THR
23	Cg	194	LEU
23	Cg	213	VAL
23	Cg	221	SER
23	Cg	224	LEU
23	Cg	225	ARG
23	Cg	226	CYS
23	Cg	227	THR
23	Cg	230	ASP
23	Cg	233	THR
23	Cg	254	VAL
23	Cg	262	GLN
23	Cg	290	LEU
23	Cg	296	HIS
23	Cg	308	LEU
23	Cg	310	SER
23	Cg	316	THR

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Mol	Chain	Res	Type
23	Cg	318	ILE
23	Cg	319	ASP
23	Cg	325	LEU
23	Cg	337	ARG
23	Cg	344	LEU
23	Cg	355	THR
23	Cg	357	THR
23	Cg	373	VAL
23	Cg	391	GLU
23	Cg	401	ILE
23	Cg	421	GLU
23	Cg	422	LEU
23	Cg	436	ASP
23	Cg	464	VAL
23	Cg	468	ASP
23	Cg	480	LYS
24	Ci	18	THR
24	Ci	27	CYS
24	Ci	30	ARG
24	Ci	32	ASP
24	Ci	54	GLN
24	Ci	58	GLU
24	Ci	76	MET
24	Ci	82	GLN
24	Ci	105	ARG
24	Ci	114	MET
24	Ci	119	LEU
24	Ci	122	MET
24	Ci	136	HIS
24	Ci	138	ASP
24	Ci	144	ARG
24	Ci	145	ASN
24	Ci	146	ASP
24	Ci	157	LEU
24	Ci	164	ASN
24	Ci	174	ASP
25	Ck	41	THR
25	Ck	57	ASP
25	Ck	86	GLU
25	Ck	87	ARG
25	Ck	93	THR
25	Ck	97	GLN

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Mol	Chain	Res	Type
25	Ck	99	SER
25	Ck	103	GLU
25	Ck	108	GLN
25	Ck	111	THR
25	Ck	136	ASP
25	Ck	137	THR
25	Ck	161	GLU
25	Ck	176	THR
25	Ck	185	LEU
25	Ck	188	LEU
25	Ck	207	ARG
25	Ck	214	LEU
25	Ck	219	THR
25	Ck	237	LEU
25	Ck	242	LEU
25	Ck	254	ILE
25	Ck	283	GLU
25	Ck	290	LEU
25	Ck	316	ASP
25	Ck	317	VAL
25	Ck	320	VAL
25	Ck	337	VAL
25	Ck	341	LEU
25	Ck	350	ASP
25	Ck	353	ARG
25	Ck	370	THR
25	Ck	373	ARG
25	Ck	376	VAL
25	Ck	380	VAL
25	Ck	401	LEU
25	Ck	568	LEU
25	Ck	573	THR
25	Ck	574	GLU
25	Ck	575	LEU
25	Ck	597	LEU
25	Ck	606	THR
25	Ck	607	LYS
25	Ck	611	ASN
25	Ck	618	ILE
25	Ck	620	THR
25	Ck	629	LEU
25	Ck	633	MET

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Mol	Chain	Res	Type
25	Ck	642	VAL
25	Ck	652	ARG
25	Ck	654	SER
25	Ck	661	ILE
25	Ck	682	ASN
25	Ck	691	GLN
25	Ck	695	GLN
25	Ck	703	ARG
25	Ck	706	SER
25	Ck	707	LEU
25	Ck	733	LEU
25	Ck	755	ASP
25	Ck	760	VAL
25	Ck	766	LYS
25	Ck	775	ARG
25	Ck	782	GLU
25	Ck	806	ASP
25	Ck	838	LEU
25	Ck	841	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (234) such sidechains are listed below:

Mol	Chain	Res	Type
1	DA	1225	HIS
1	DA	1258	ASN
2	DL	116	ASN
3	DB	90	GLN
3	DB	92	HIS
3	DB	106	GLN
3	DB	122	HIS
3	DB	134	HIS
3	DB	153	HIS
3	DB	194	GLN
3	DB	209	GLN
3	DB	395	GLN
3	DB	401	HIS
3	DB	414	GLN
3	DB	461	GLN
3	DB	486	HIS
3	DB	539	GLN
3	DB	551	HIS
3	DB	562	GLN

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Mol	Chain	Res	Type
3	DB	569	HIS
3	DB	630	HIS
3	DB	682	HIS
3	DB	686	GLN
3	DB	691	HIS
3	DB	703	HIS
3	DB	737	HIS
3	DB	748	HIS
3	DB	774	ASN
3	DB	785	ASN
3	DB	800	GLN
3	DB	828	HIS
3	DB	836	ASN
3	DB	908	GLN
3	DB	923	GLN
3	DB	958	ASN
3	DB	981	HIS
3	DB	1004	GLN
3	DB	1051	GLN
3	DB	1055	GLN
3	DB	1113	GLN
3	DB	1124	HIS
4	DC	81	HIS
4	DC	128	HIS
4	DC	242	HIS
4	DC	263	GLN
4	DC	360	HIS
4	DC	368	ASN
4	DC	445	HIS
4	DC	574	GLN
4	DC	797	ASN
4	DC	920	HIS
4	DC	943	HIS
4	DC	970	GLN
4	DC	1110	HIS
4	DC	1141	GLN
4	DC	1160	GLN
5	DE	38	GLN
5	DE	40	ASN
5	DE	67	ASN
5	DE	84	HIS
5	DE	105	ASN

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Mol	Chain	Res	Type
5	DE	202	HIS
5	DE	327	ASN
5	DE	414	ASN
5	DE	442	HIS
5	DE	465	ASN
5	DE	501	HIS
5	DE	628	HIS
5	DE	658	ASN
5	DE	671	ASN
5	DE	698	GLN
5	DE	699	ASN
6	DF	41	ASN
6	DF	62	ASN
6	DF	140	HIS
6	DF	175	GLN
6	DF	187	ASN
6	DF	198	HIS
6	DF	214	HIS
6	DF	283	HIS
6	DF	474	GLN
6	DF	520	GLN
6	DF	543	HIS
6	DF	556	HIS
6	DF	572	HIS
7	DG	23	HIS
7	DG	65	ASN
7	DG	71	ASN
7	DG	92	GLN
7	DG	143	HIS
7	DG	170	ASN
7	DG	191	GLN
7	DG	200	GLN
7	DG	201	GLN
7	DG	229	HIS
7	DG	230	ASN
7	DG	240	HIS
7	DG	365	GLN
7	DG	405	GLN
7	DG	476	GLN
7	DG	477	GLN
8	DH	4	GLN
8	DH	28	ASN

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Mol	Chain	Res	Type
8	DH	45	HIS
8	DH	100	HIS
8	DH	123	HIS
8	DH	138	GLN
8	DH	146	GLN
8	DH	166	GLN
8	DH	257	ASN
8	DH	302	GLN
8	DH	327	HIS
8	DH	437	GLN
8	DH	469	ASN
8	DH	490	HIS
8	DH	498	ASN
8	DH	526	ASN
9	DJ	27	GLN
9	DJ	31	HIS
9	DJ	33	ASN
9	DJ	42	HIS
9	DJ	55	ASN
9	DJ	82	GLN
9	DJ	190	ASN
9	DJ	199	GLN
9	DJ	227	GLN
9	DJ	247	ASN
9	DJ	291	ASN
9	DJ	293	ASN
9	DJ	301	HIS
9	DJ	314	GLN
10	DK	132	HIS
10	DK	171	GLN
10	DK	175	HIS
11	DT	45	HIS
11	DT	58	HIS
11	DT	64	GLN
11	DT	72	HIS
11	DT	82	HIS
11	DT	91	GLN
11	DT	139	HIS
11	DT	140	ASN
11	DT	161	ASN
11	DT	219	GLN
12	DV	31	HIS

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Mol	Chain	Res	Type
12	DV	40	HIS
12	DV	48	HIS
12	DV	71	GLN
12	DV	83	GLN
12	DV	131	GLN
12	DV	145	ASN
13	DW	87	ASN
13	DW	99	HIS
13	DW	121	HIS
13	DW	135	ASN
13	DW	154	HIS
14	DX	43	HIS
14	DX	58	HIS
14	DX	130	GLN
14	DX	167	HIS
14	DX	168	ASN
15	DY	99	GLN
15	DY	106	GLN
16	CC	25	HIS
16	CC	48	ASN
16	CC	51	HIS
17	CI	397	ASN
18	CJ	82	HIS
18	CJ	134	GLN
18	CJ	232	ASN
18	CJ	441	HIS
18	CJ	450	HIS
18	CJ	460	HIS
18	CJ	476	ASN
18	CJ	484	HIS
18	CJ	619	HIS
18	CJ	621	ASN
18	CJ	711	HIS
18	CJ	755	ASN
18	CJ	761	GLN
18	CJ	769	GLN
18	CJ	781	HIS
18	CJ	792	HIS
18	CJ	793	HIS
18	CJ	815	ASN
19	CK	56	GLN
20	CN	50	GLN

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Mol	Chain	Res	Type
20	CN	142	HIS
20	CN	150	HIS
20	CN	153	ASN
21	CR	249	GLN
22	CS	110	HIS
22	CS	135	ASN
23	Cg	164	HIS
23	Cg	170	ASN
23	Cg	184	HIS
23	Cg	239	GLN
23	Cg	262	GLN
23	Cg	289	ASN
23	Cg	296	HIS
23	Cg	301	HIS
23	Cg	323	GLN
23	Cg	418	ASN
23	Cg	458	HIS
24	Ci	19	HIS
24	Ci	29	GLN
24	Ci	83	ASN
24	Ci	95	ASN
24	Ci	96	ASN
24	Ci	109	ASN
24	Ci	112	ASN
24	Ci	125	HIS
24	Ci	136	HIS
24	Ci	143	GLN
24	Ci	145	ASN
25	Ck	49	HIS
25	Ck	95	HIS
25	Ck	97	GLN
25	Ck	110	HIS
25	Ck	113	ASN
25	Ck	131	ASN
25	Ck	134	HIS
25	Ck	236	ASN
25	Ck	264	ASN
25	Ck	589	GLN
25	Ck	611	ASN
25	Ck	634	HIS
25	Ck	644	HIS
25	Ck	679	GLN

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Mol	Chain	Res	Type
25	Ck	682	ASN
25	Ck	691	GLN
25	Ck	695	GLN
25	Ck	723	GLN
25	Ck	728	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	CA	142/611 (23%)	85 (59%)	2 (1%)

All (85) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	CA	397	U
26	CA	398	U
26	CA	399	A
26	CA	400	U
26	CA	401	A
26	CA	406	U
26	CA	407	U
26	CA	408	C
26	CA	410	U
26	CA	411	A
26	CA	413	A
26	CA	414	A
26	CA	415	U
26	CA	418	A
26	CA	419	U
26	CA	421	G
26	CA	423	A
26	CA	426	A
26	CA	427	U
26	CA	428	A
26	CA	430	U
26	CA	431	U
26	CA	433	U
26	CA	434	A
26	CA	435	G
26	CA	438	U
26	CA	441	G

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Mol	Chain	Res	Type
26	CA	442	A
26	CA	444	A
26	CA	445	C
26	CA	446	C
26	CA	448	U
26	CA	449	G
26	CA	450	A
26	CA	451	U
26	CA	452	A
26	CA	453	A
26	CA	455	G
26	CA	457	U
26	CA	458	U
26	CA	459	A
26	CA	460	U
26	CA	461	A
26	CA	462	A
26	CA	463	A
26	CA	464	U
26	CA	467	A
26	CA	468	A
26	CA	469	A
26	CA	470	G
26	CA	471	U
26	CA	472	G
26	CA	476	A
26	CA	478	A
26	CA	480	C
26	CA	481	A
26	CA	482	U
26	CA	483	A
26	CA	484	A
26	CA	485	U
26	CA	486	C
26	CA	487	A
26	CA	489	A
26	CA	491	U
26	CA	494	A
26	CA	495	U
26	CA	496	U
26	CA	497	A
26	CA	498	U

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Mol	Chain	Res	Type
26	CA	500	U
26	CA	502	U
26	CA	505	U
26	CA	507	A
26	CA	509	U
26	CA	510	A
26	CA	513	U
26	CA	514	A
26	CA	517	U
26	CA	518	G
26	CA	519	U
26	CA	520	A
26	CA	532	A
26	CA	535	U
26	CA	536	U
26	CA	537	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	CA	512	G
26	CA	527	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
31	GTP	Cg	501	32	33,34,34	0.94	1 (3%)	50,54,54	1.91	15 (30%)
29	SPD	DL	401	-	9,9,9	0.39	0	8,8,8	1.04	0
29	SPD	CA	703	-	9,9,9	0.39	0	8,8,8	0.58	0
30	UTP	DJ	401	-	29,30,30	1.74	8 (27%)	43,47,47	1.87	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GTP	Cg	501	32	-	5/22/38/38	0/3/3/3
29	SPD	DL	401	-	-	2/7/7/7	-
29	SPD	CA	703	-	-	5/7/7/7	-
30	UTP	DJ	401	-	-	13/22/38/38	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	DJ	401	UTP	PB-O3A	5.31	1.65	1.59
30	DJ	401	UTP	PA-O3A	2.44	1.62	1.59
30	DJ	401	UTP	PG-O3G	-2.28	1.46	1.54
30	DJ	401	UTP	PB-O3B	2.18	1.61	1.59
30	DJ	401	UTP	C6-C5	2.18	1.40	1.35
30	DJ	401	UTP	PA-O5'	2.18	1.67	1.59
30	DJ	401	UTP	C1'-N1	2.15	1.53	1.47
30	DJ	401	UTP	PG-O1G	-2.09	1.47	1.54
31	Cg	501	GTP	O4'-C4'	-2.07	1.40	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Cg	501	GTP	C5-C4-N3	-5.01	120.42	128.39
31	Cg	501	GTP	O3G-PG-O3B	4.60	120.05	104.64
31	Cg	501	GTP	C2-N1-C6	-4.30	117.31	125.11
30	DJ	401	UTP	C4-N3-C2	-4.27	121.31	126.61
30	DJ	401	UTP	N3-C2-N1	4.16	120.31	114.89
30	DJ	401	UTP	C1'-N1-C2	4.08	124.92	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Cg	501	GTP	C2-N3-C4	3.73	118.72	112.30
30	DJ	401	UTP	O4-C4-C5	-3.43	119.25	125.16
30	DJ	401	UTP	C5-C4-N3	3.42	119.59	114.80
31	Cg	501	GTP	C2'-C1'-N9	-2.87	105.27	113.25
31	Cg	501	GTP	O2A-PA-O3A	2.83	114.93	107.27
30	DJ	401	UTP	C2'-C1'-N1	2.75	120.90	113.25
31	Cg	501	GTP	O6-C6-C5	-2.71	119.38	126.53
31	Cg	501	GTP	N9-C4-N3	2.65	131.26	125.95
31	Cg	501	GTP	O3B-PB-O1B	-2.63	102.80	110.70
31	Cg	501	GTP	N2-C2-N3	-2.61	114.57	119.67
30	DJ	401	UTP	O1B-PB-O3A	2.61	114.32	107.27
31	Cg	501	GTP	O2B-PB-O3B	2.53	114.12	107.27
30	DJ	401	UTP	O4'-C4'-C3'	-2.48	100.23	105.15
30	DJ	401	UTP	C6-N1-C2	-2.44	118.03	121.00
31	Cg	501	GTP	C4-C5-N7	-2.33	106.98	110.67
31	Cg	501	GTP	N2-C2-N1	2.22	121.44	116.76
30	DJ	401	UTP	O3B-PG-O2G	-2.15	99.70	111.04
31	Cg	501	GTP	C8-N7-C5	2.10	108.00	104.26
31	Cg	501	GTP	N9-C8-N7	-2.00	109.69	113.40

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	DJ	401	UTP	C5'-O5'-PA-O1A
30	DJ	401	UTP	C5'-O5'-PA-O2A
30	DJ	401	UTP	O4'-C4'-C5'-O5'
31	Cg	501	GTP	PB-O3B-PG-O3G
29	CA	703	SPD	N6-C7-C8-C9
29	CA	703	SPD	C3-C4-C5-N6
30	DJ	401	UTP	C3'-C4'-C5'-O5'
29	CA	703	SPD	C2-C3-C4-C5
29	DL	401	SPD	C4-C5-N6-C7
30	DJ	401	UTP	PB-O3B-PG-O2G
31	Cg	501	GTP	PB-O3B-PG-O2G
29	CA	703	SPD	C4-C5-N6-C7
29	DL	401	SPD	C2-C3-C4-C5
30	DJ	401	UTP	C5'-O5'-PA-O3A
30	DJ	401	UTP	O4'-C1'-N1-C2
30	DJ	401	UTP	O4'-C1'-N1-C6
30	DJ	401	UTP	PA-O3A-PB-O2B
31	Cg	501	GTP	PG-O3B-PB-O2B

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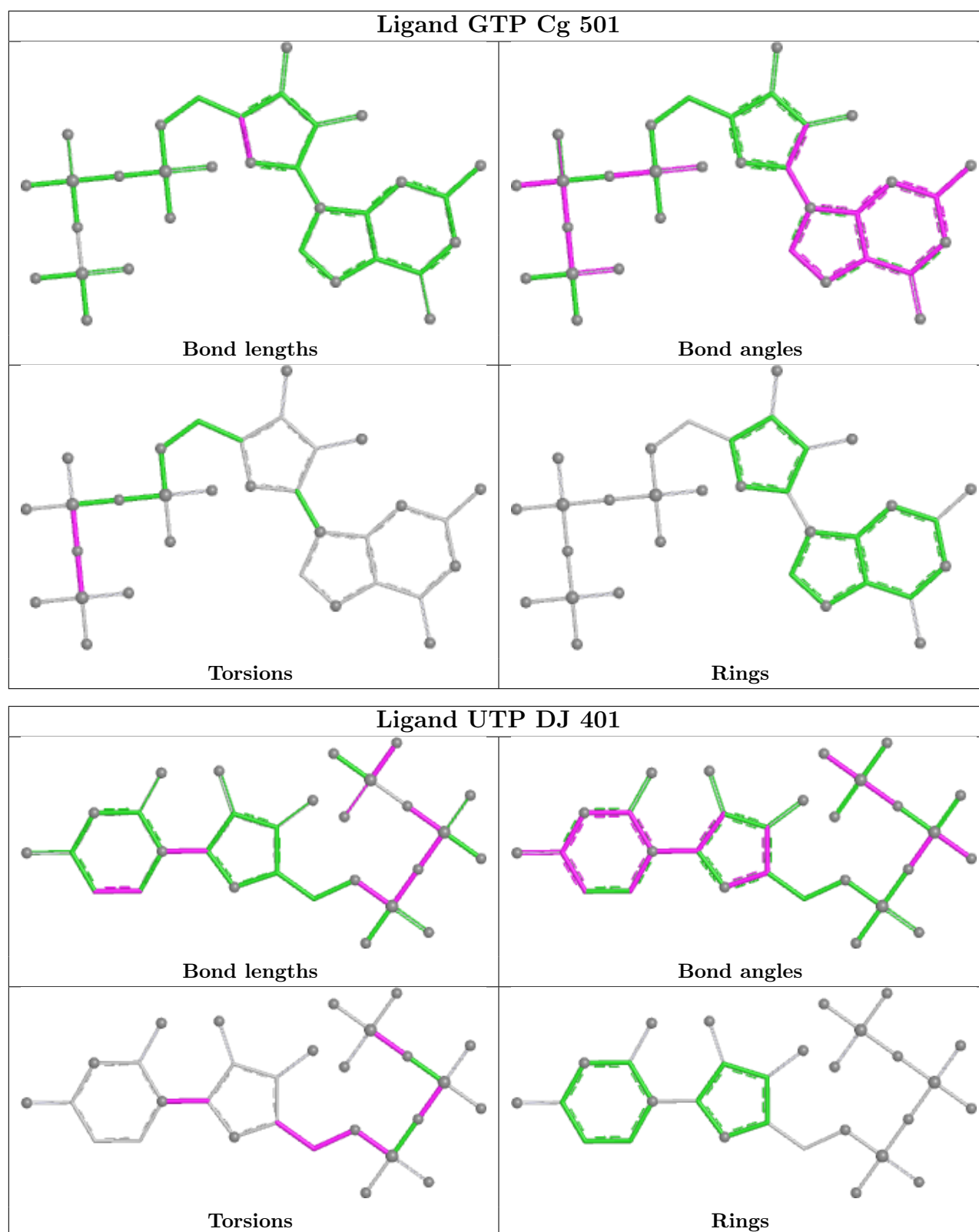
Mol	Chain	Res	Type	Atoms
30	DJ	401	UTP	C2'-C1'-N1-C6
30	DJ	401	UTP	C2'-C1'-N1-C2
31	Cg	501	GTP	PB-O3B-PG-O1G
30	DJ	401	UTP	PA-O3A-PB-O1B
31	Cg	501	GTP	PG-O3B-PB-O1B
30	DJ	401	UTP	C4'-C5'-O5'-PA
29	CA	703	SPD	C7-C8-C9-N10

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	Cg	501	GTP	7	0
29	CA	703	SPD	2	0
30	DJ	401	UTP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

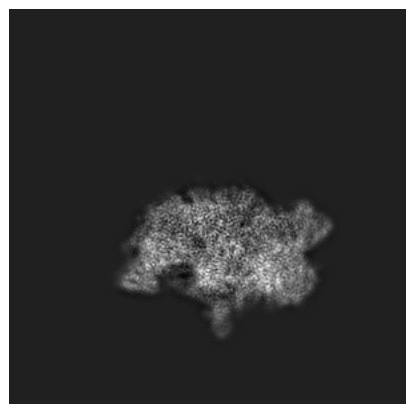
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0233. These allow visual inspection of the internal detail of the map and identification of artifacts.

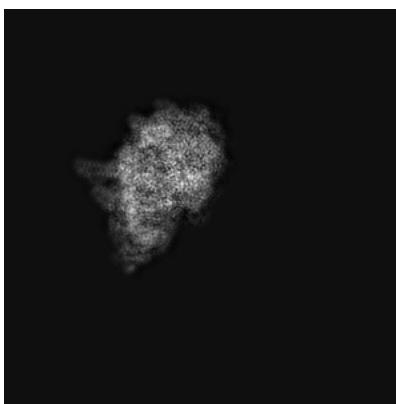
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

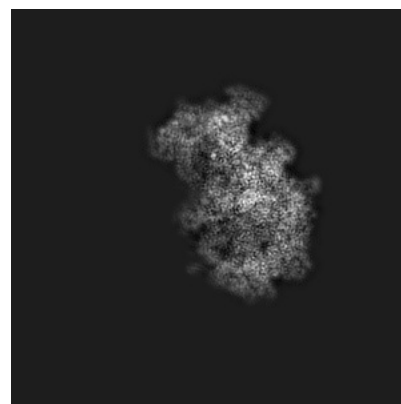
6.1.1 Primary map



X

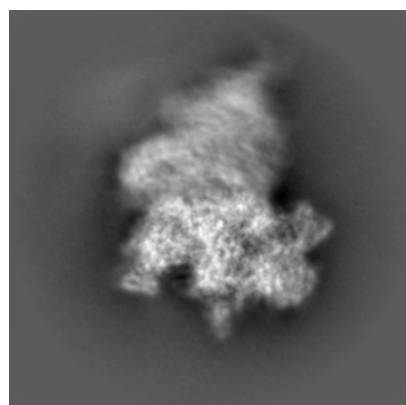


Y

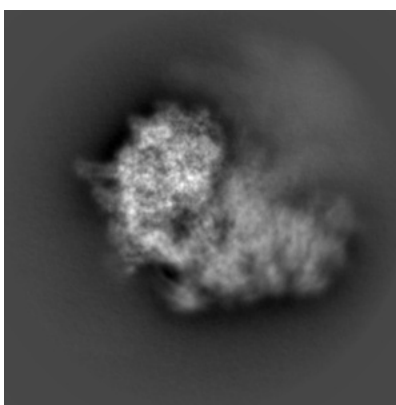


Z

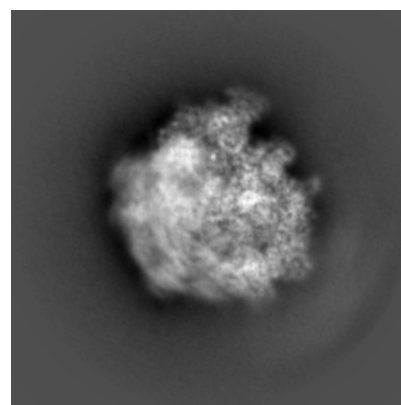
6.1.2 Raw map



X



Y

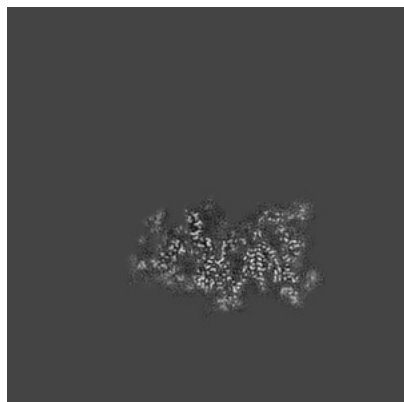


Z

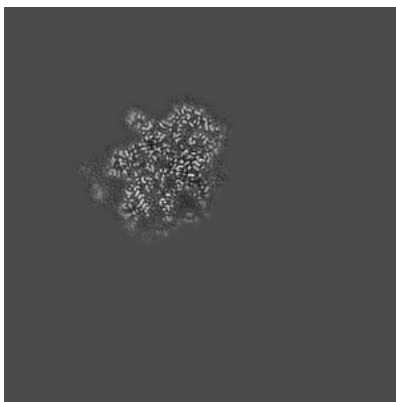
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

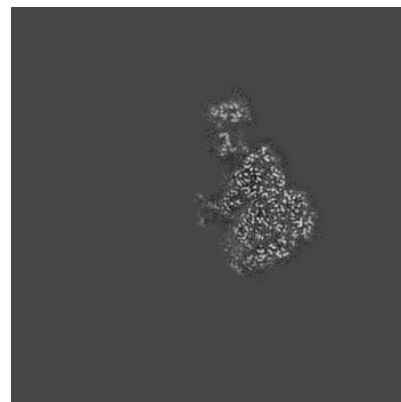
6.2.1 Primary map



X Index: 160

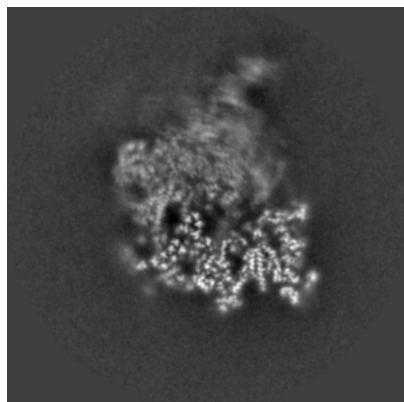


Y Index: 160

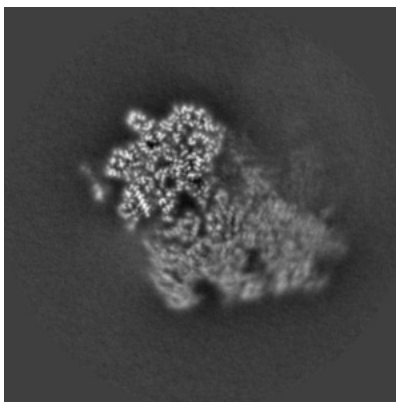


Z Index: 160

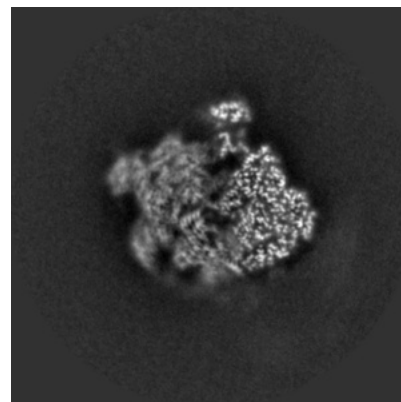
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

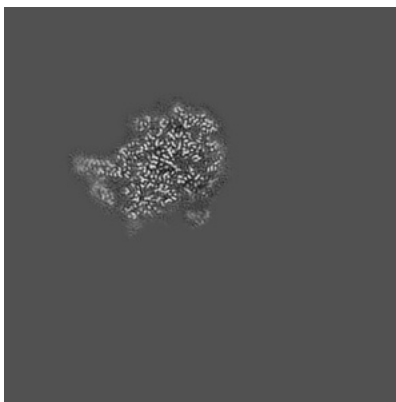
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

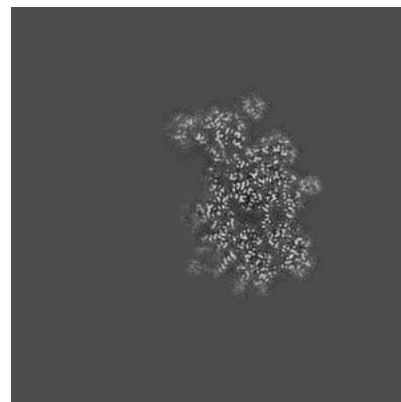
6.3.1 Primary map



X Index: 187

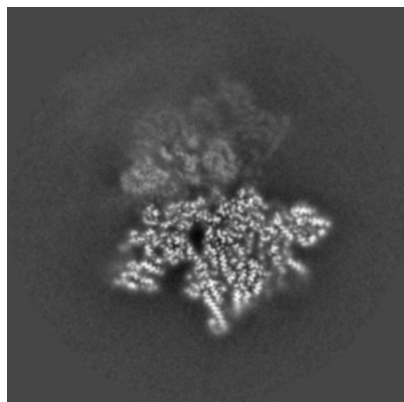


Y Index: 167

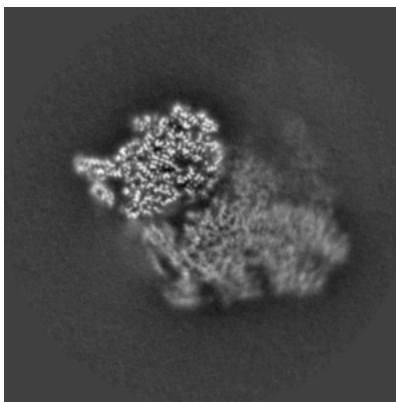


Z Index: 131

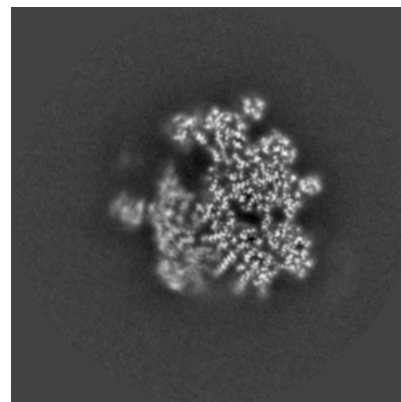
6.3.2 Raw map



X Index: 187



Y Index: 167

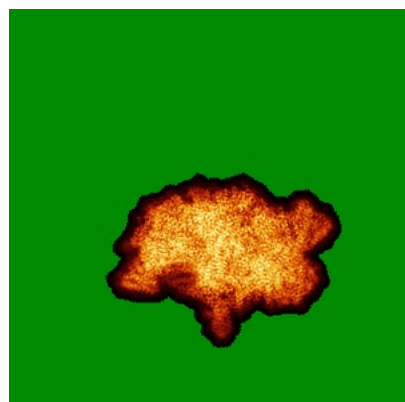


Z Index: 131

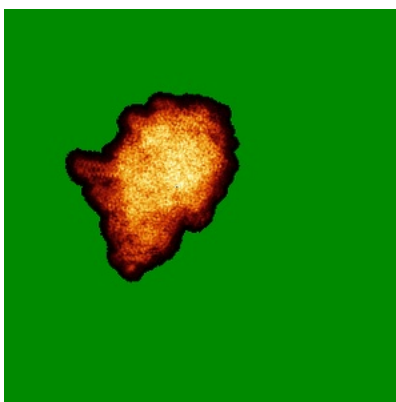
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

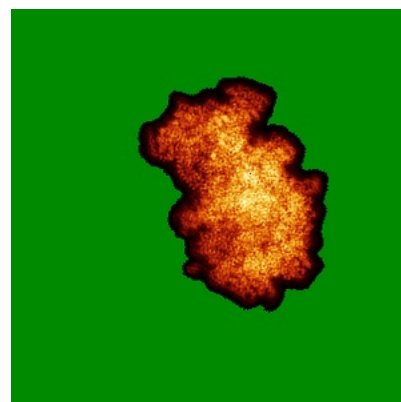
6.4.1 Primary map



X



Y

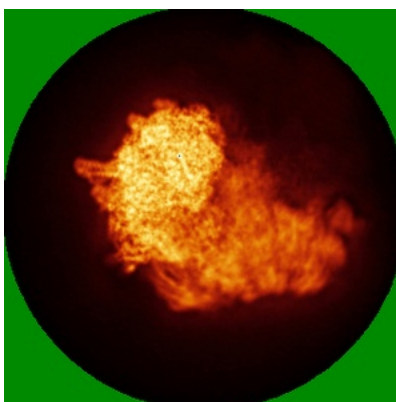


Z

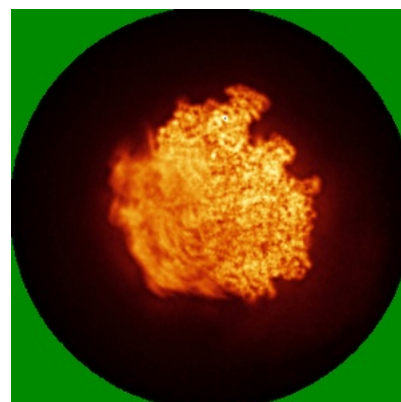
6.4.2 Raw map



X



Y

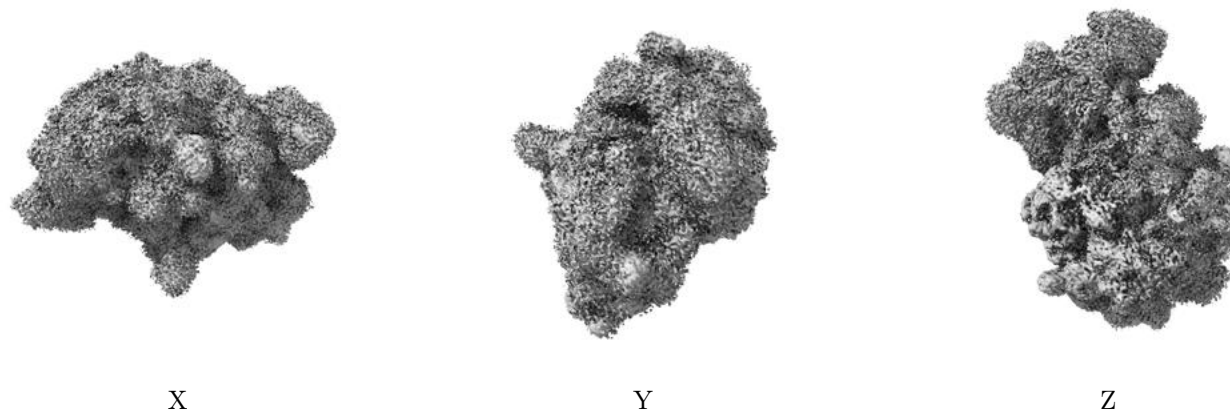


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

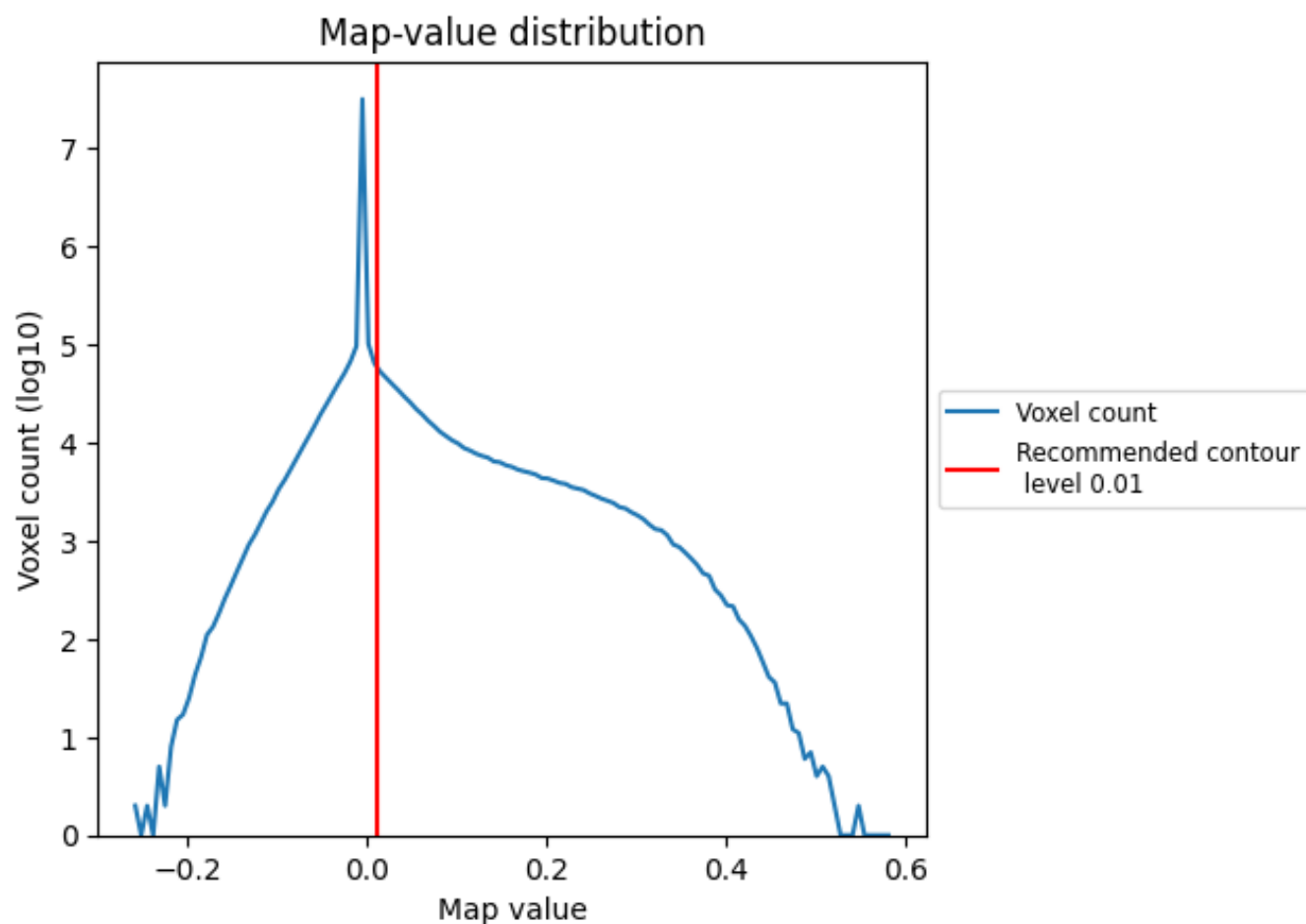
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

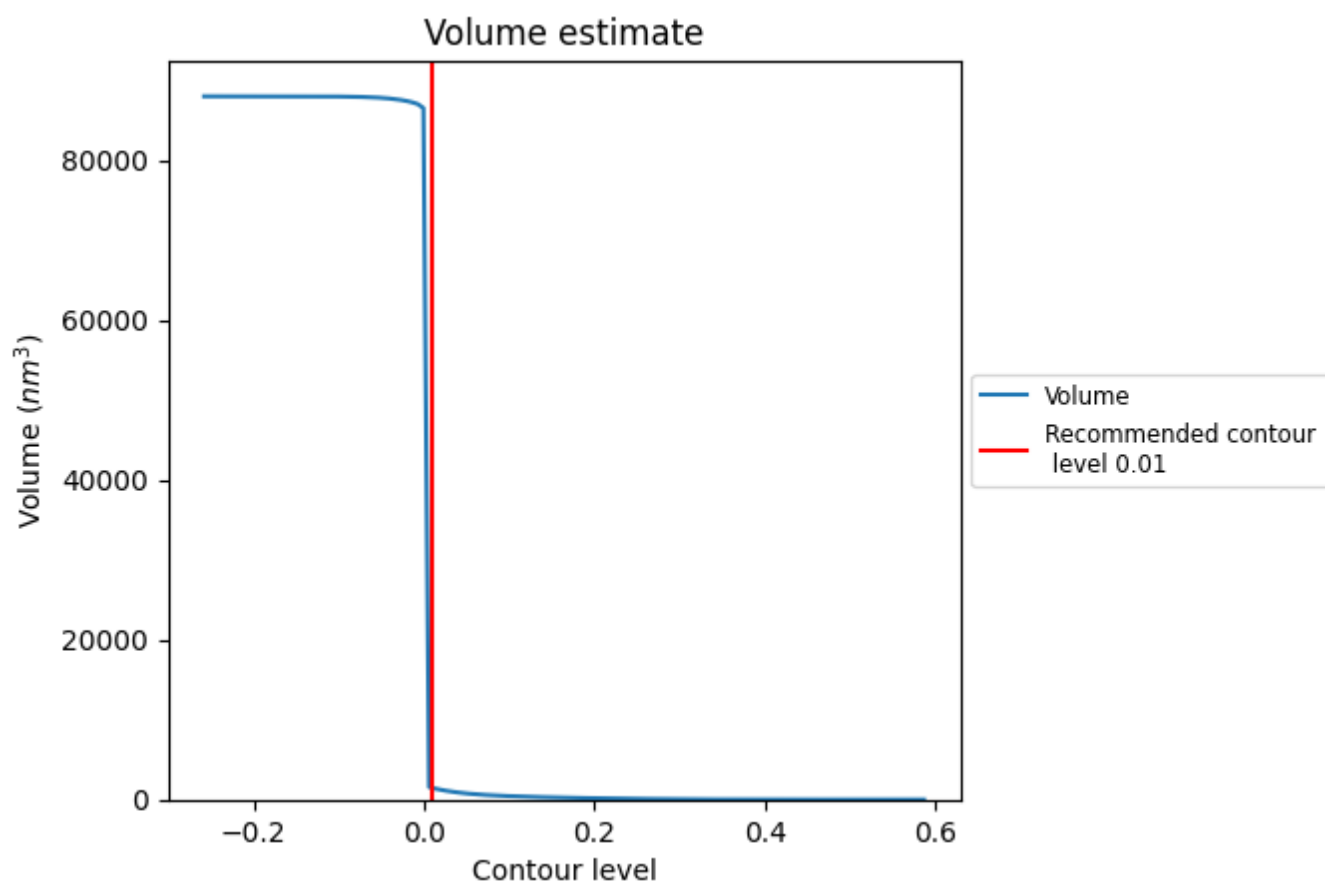
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

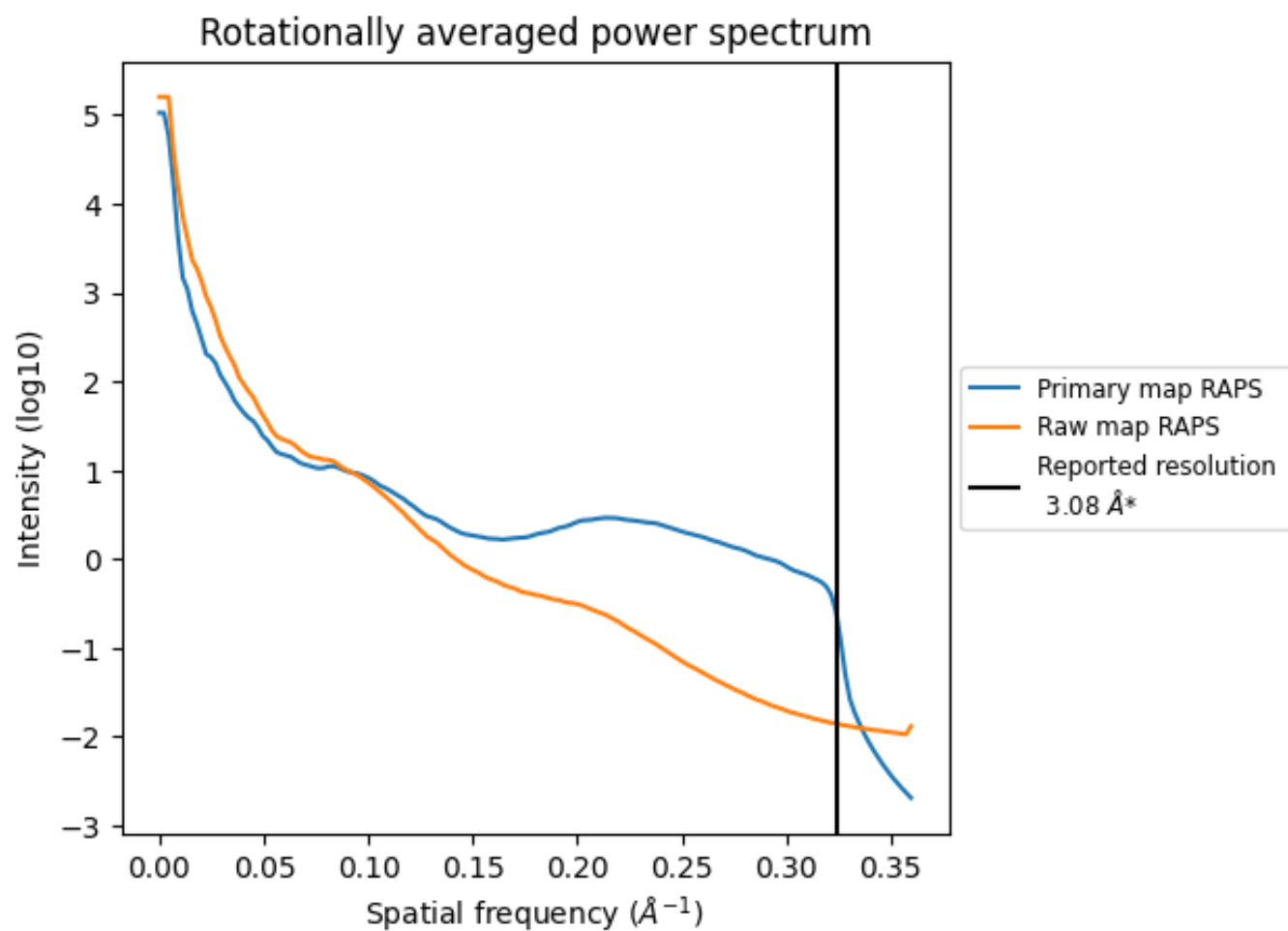
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1453 nm^3 ; this corresponds to an approximate mass of 1312 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

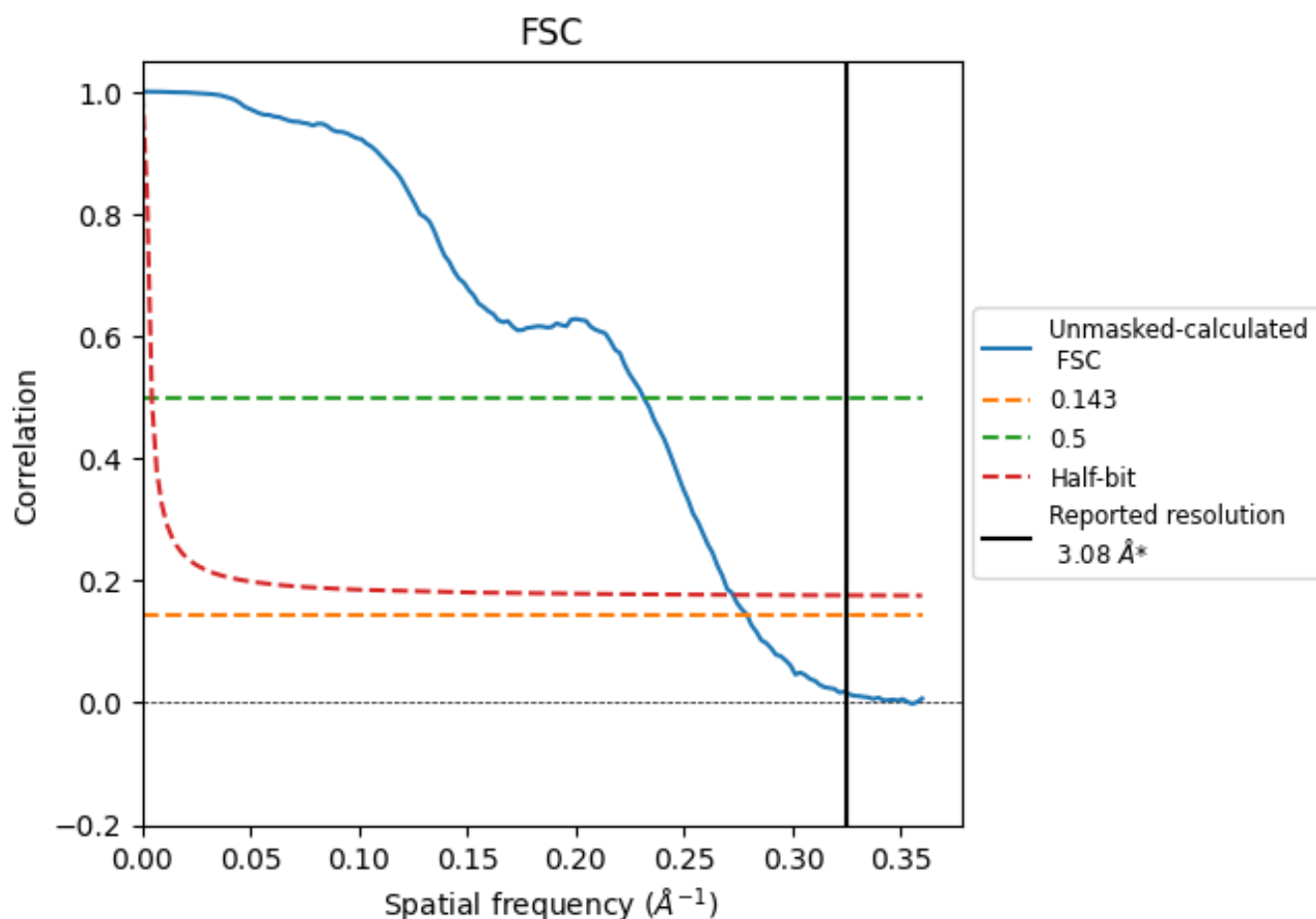


*Reported resolution corresponds to spatial frequency of $0.325 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.325 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

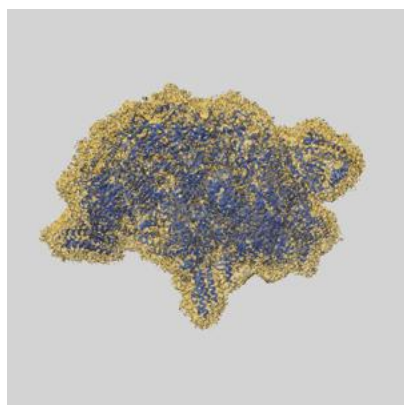
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	4.33	3.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.58 differs from the reported value 3.08 by more than 10 %

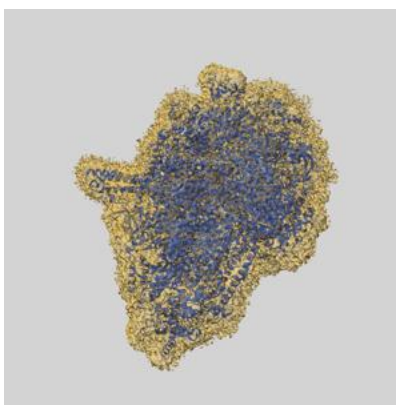
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0233 and PDB model 6HIZ. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

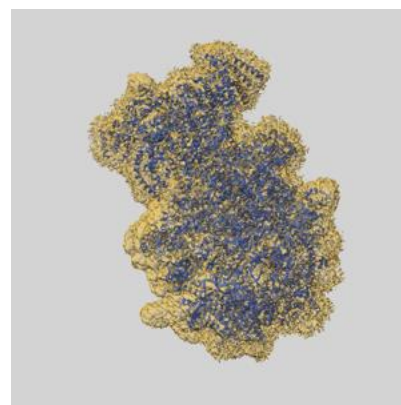
9.1 Map-model overlay [i](#)



X



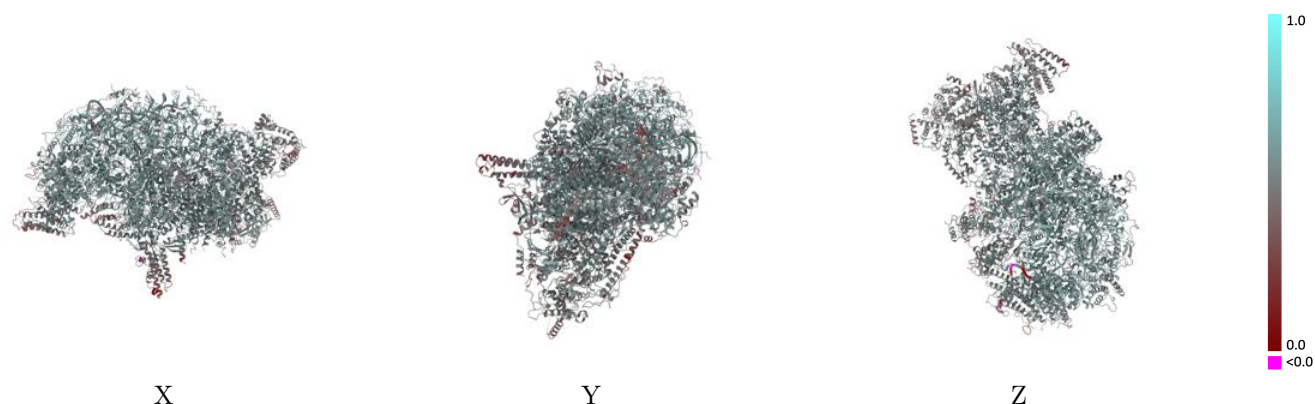
Y



Z

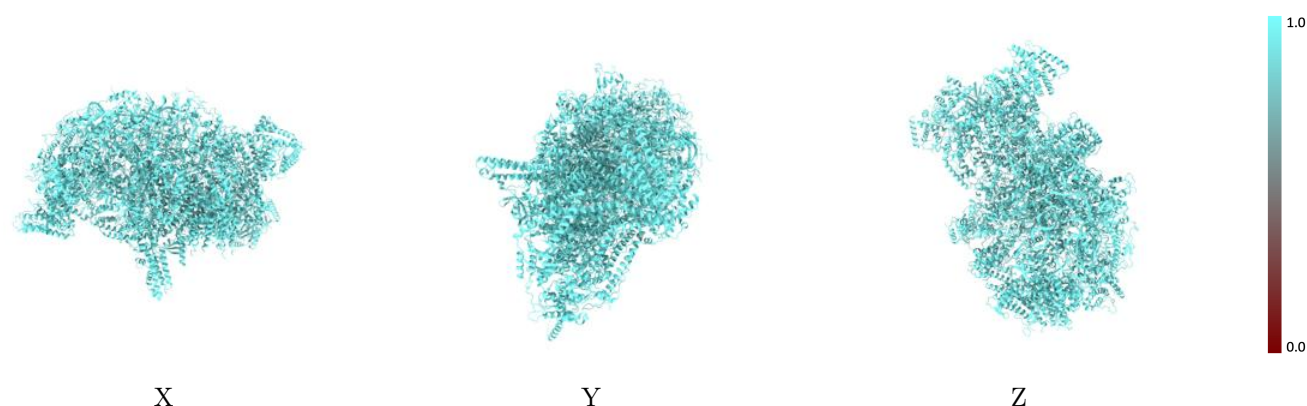
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



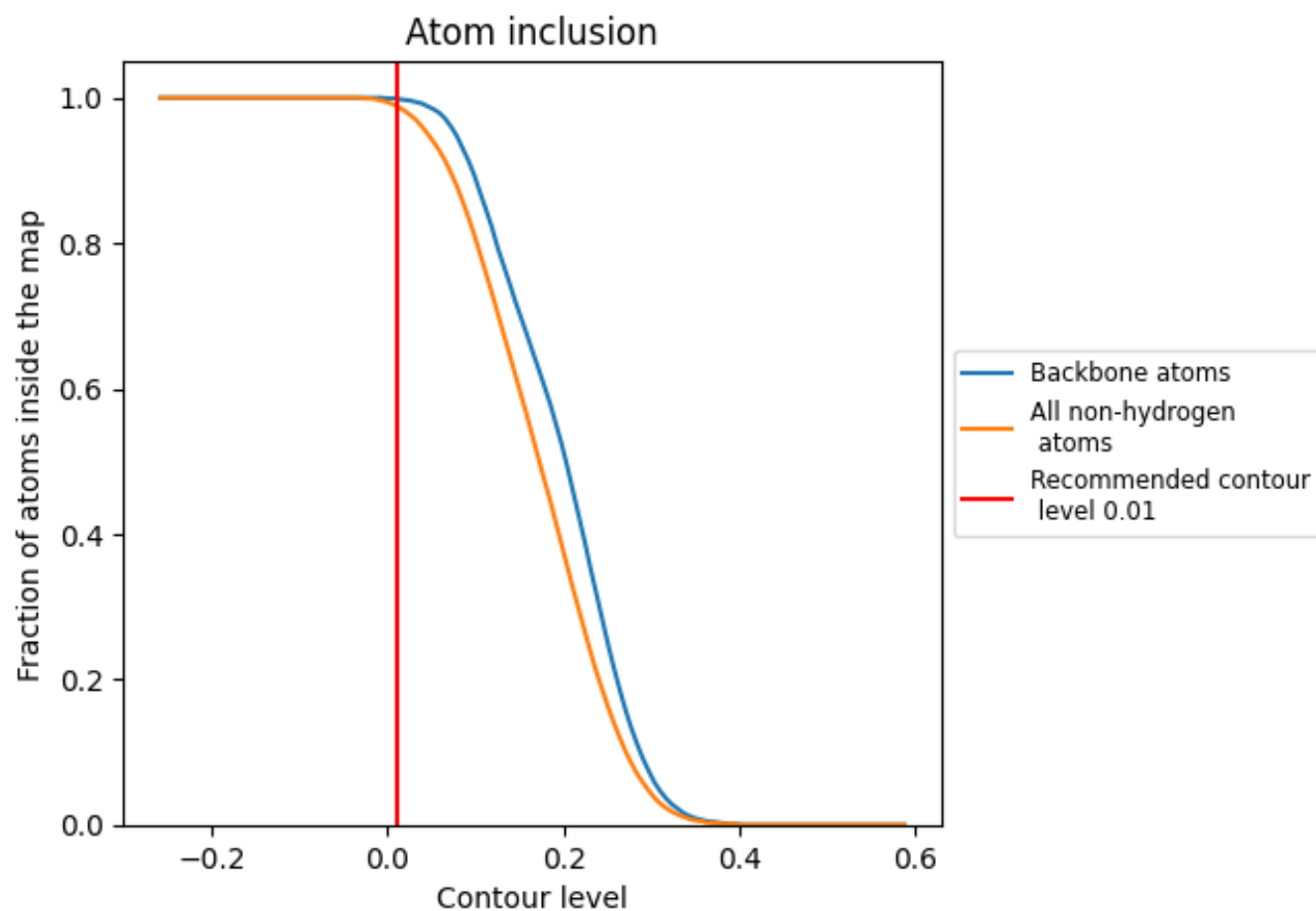
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9890	 0.5340
CA	 0.9940	 0.5550
CC	 0.9720	 0.5570
CI	 0.9860	 0.5660
CJ	 0.9880	 0.5560
CK	 0.9980	 0.5570
CN	 0.9940	 0.5830
CR	 0.9800	 0.5220
CS	 0.9940	 0.5730
Cg	 0.9940	 0.5550
Ci	 0.9890	 0.5670
Ck	 0.9860	 0.5040
DA	 0.9770	 0.4800
DB	 0.9830	 0.5310
DC	 0.9920	 0.4960
DE	 0.9930	 0.5000
DF	 0.9930	 0.5530
DG	 0.9910	 0.5060
DH	 0.9870	 0.5440
DJ	 0.9920	 0.5570
DK	 0.9890	 0.5270
DL	 0.9540	 0.5040
DT	 0.9930	 0.5690
DV	 0.9920	 0.5670
DW	 0.9900	 0.5550
DX	 0.9900	 0.5560
DY	 0.9950	 0.5700
UO	 1.0000	 0.5160
UP	 1.0000	 0.4590

