



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:15 PM UTC

PDB ID : 5YBB / pdb_00005ybb
Title : Structural basis underlying complex assembly and conformational transition of the type I R-M system
Authors : Liu, Y.P.; Tang, Q.; Zhang, J.Z.; Tian, L.F.; Gao, P.; Yan, X.X.
Deposited on : 2017-09-04
Resolution : 3.20 Å (reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

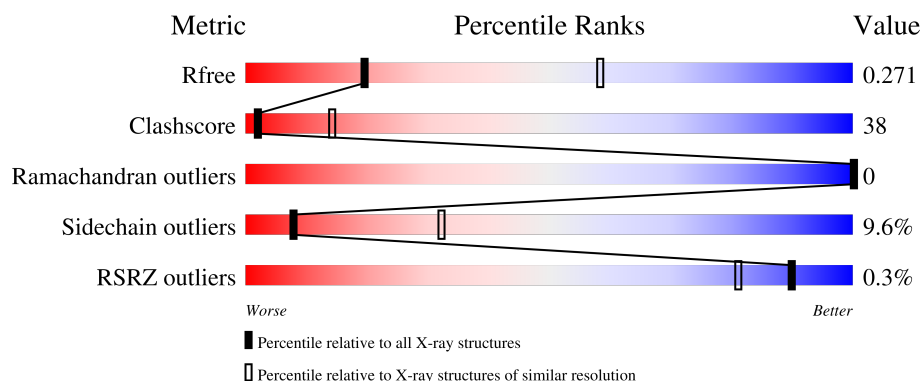
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	507	
1	B	507	
1	C	507	
1	E	507	
2	D	398	

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Mol	Chain	Length	Quality of chain
2	G	398	
3	H	22	
4	I	22	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SAM	A	601	-	-	X	-
5	SAM	B	601	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15456 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Type I restriction-modification system methyltransferase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3934	2513	686	719	16			
1	C	30	Total	C	N	O	S	0	0	0
			229	145	35	48	1			
1	B	487	Total	C	N	O	S	0	0	0
			3934	2513	686	719	16			
1	E	30	Total	C	N	O	S	0	0	0
			229	145	35	48	1			

- Molecule 2 is a protein called Restriction endonuclease S subunits.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	390	Total	C	N	O	S	0	0	0
			3090	1971	549	558	12			
2	G	390	Total	C	N	O	S	0	0	0
			3090	1971	549	558	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	-	expression tag	UNP Q8R9Q6
G	1	VAL	-	expression tag	UNP Q8R9Q6

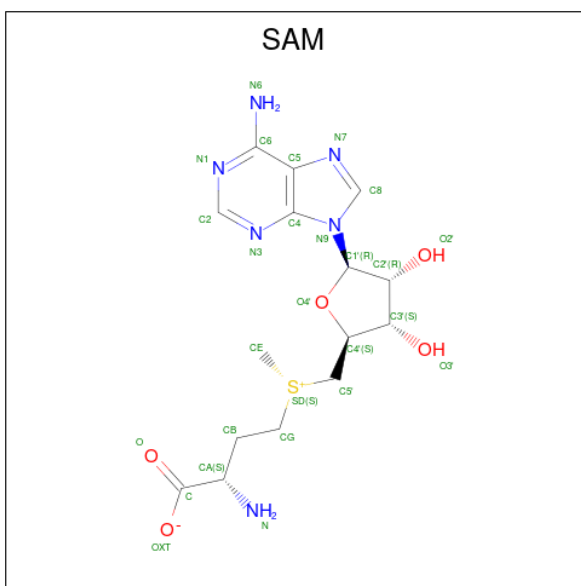
- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	22	Total	C	N	O	P	0	0	0
			454	215	88	130	21			

- Molecule 4 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	22	Total	C	N	O	P	0	0	0
			442	211	80	130	21			

- Molecule 5 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).

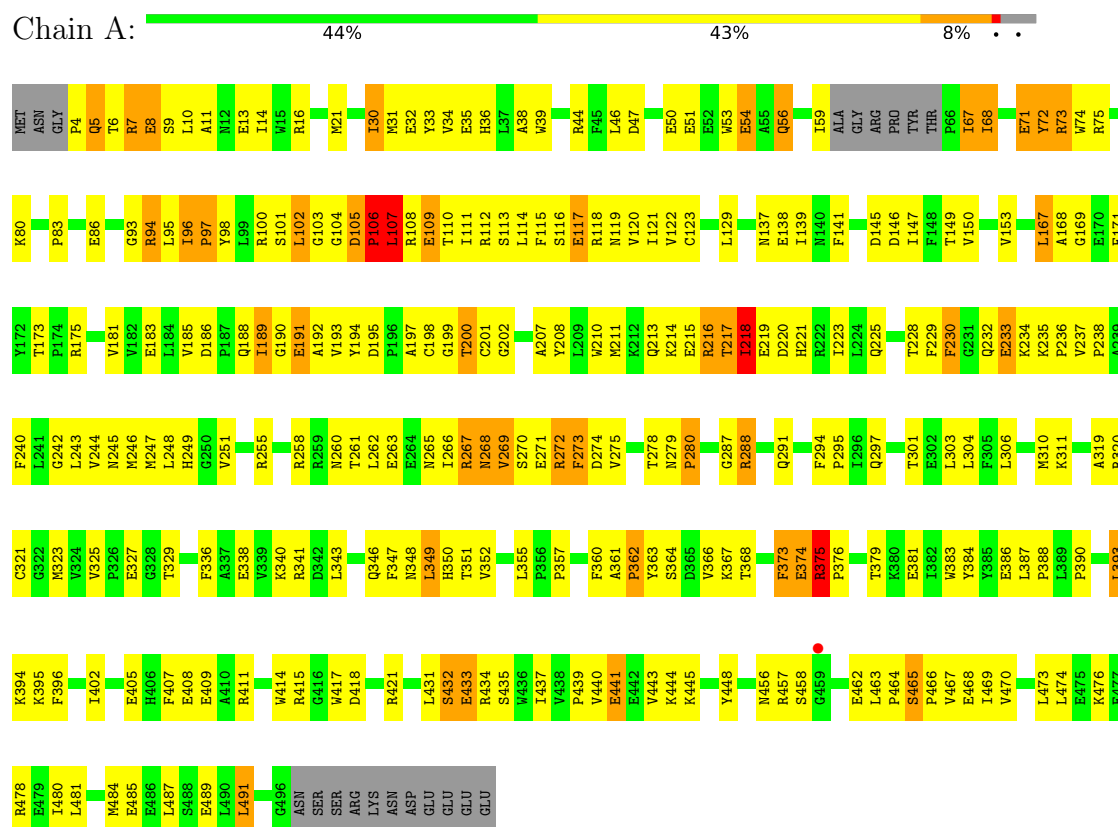


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 27	C 15	N 6	O 5	S 1	0	0
5	B	1	Total 27	C 15	N 6	O 5	S 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Type I restriction-modification system methyltransferase subunit



- Molecule 1: Type I restriction-modification system methyltransferase subunit



M484	ARG	ALA	THR	LEU	VAL
	LYS	PRO	GLU	GLY	VAL
L487	GLY	TYR	LEU	LEU	GLU
	LEU	SER	LEU	VAL	LEU
L490	GLY	ASP	PHE	ASN	VAL
L491	PRO	VAL	LEU	MET	ASP
E492	VAL	LYS	GLN	PRO	PRO
M493	GLU	THR	HIS	LEU	GLN
E494	ALA	ALA	ILE	HIS	GLY
	CYS	LEU	MET	GLY	GLY
	GLY	ILE	LYS	VAL	GLU
	LEU	PHE	LYS	THR	ALA
ASN	SER	GLU	LEU	VAL	VAL
SER	GLU	PHE	LEU	PRO	VAL
SER	ARG	GLU	LYS	ARG	ASP
ARG	SER	ARG	PRO	ARG	PRO
LYS	TRP	PRO	ARG	VAL	VAL
ASN	ILE	GLY	ASP	MET	ALA
ASP	VAL	PRO	GLY	ARG	CYS
GLU	PRO	THR	ALA	ARG	GLY
GLU	VAL	LYS	ARG	ASN	THR
GLU	GLU	GLU	CYS	THR	CYS
GLU	GLU	ILE	GLY	LEU	GLY
	VAL	TRP	MET	GLU	PHE
	LYS	TYR	VAL	LEU	LEU
	LYS	TYR	VAL	ASN	VAL
	ARG	LEU	PRO	ILE	GLU
	GLY	GLU	GLU	ARG	ALA
	TYR	PRO	GLY	ASN	TYR
	ASP	LEU	THR	VAL	LEU
	LEU	PRO	LEU	SER	TRP
	THR	GLU	PHE	GLU	MET
	ALA	GLY	ARG	ARG	LYS
	ARG	LEU	GLY	PHE	GLN
	ASN	LYS	GLY	ASP	LYS
	PRO	PHE	ALA	VAL	GLU
	ASN	GLU	PHE	VAL	ARG
	ARG	SER	ALA	VAL	THR
	GLY	LYS	GLU	THR	ILE
	GLY	GLY	VAL	ASN	GLU
	GLY	ASN	LYS	PRO	ASP
	GLU	ILE	ARG	PRO	HIS
	LEU	GLN	ASP	PHE	ARG
	PRO	ASP	LEU	GLY	ILE
	PRO	GLU	LEU	GLY	LEU
	P465	GLU	GLN	THR	GLU
	P466	HIS	GLN	GLU	GLN
	P467	PHE	PHE	GLY	ARG
	P468	GLU	ASN	ARG	THR
	I469	GLU	LEU	HIS	PHE
	P470	ALA	HIS	ILE	PHE
	A471	ARG	VAL	GLN	GLY
		LYS	VAL	GLN	GLN
	K476	LEU	VAL	ASN	GLU
	E477	TRP	SER	PHE	LYS
	R478	ARG	LEU	PRO	LYS
	E479	GLY	PRO	ILE	PRO
	I480	TRP	PRO	GLN	VAL
	L481	ASP	GLY	SER	PRO
	P482	ALA	THR	ASN	ALA
	I483	TYR	THR	ALA	THR

- Molecule 1: Type I restriction-modification system methyltransferase subunit

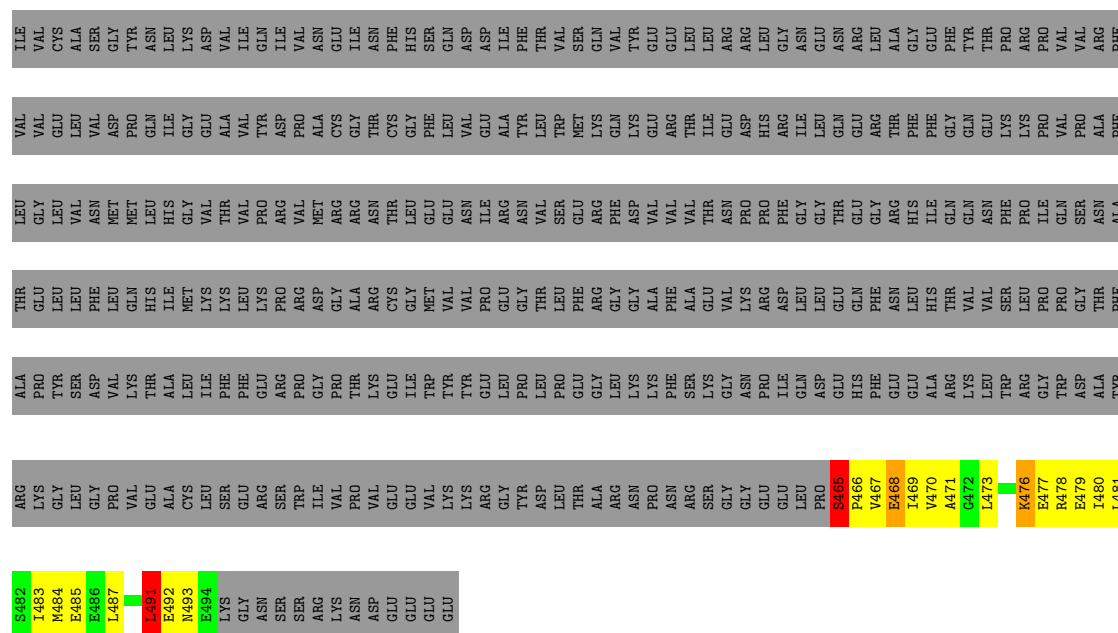
Chain B: 44% 42% 9% ..

L481	F396	A319	G242	R175	Met
M484 E485	I402	R320	L243	L181	Asn
	F407	G322	N245	L182	Gly
	E408	M323	M246	G83	Q5
	E409	M324	M247	L95	T6
L490	E409	V325	L248	L185	R7
E492	A410	R411	H249	P97	E8
M493	K412		G250	L187	S9
G496	K412	T329	V251	G188	L99
	L413		T252	L189	A11
	M414	F336	V253	G190	N12
	R415	A337		L191	M11
ASN	G416	E338	V256	A192	E13
SER	M417	V339	M257	L193	R16
SER	ARG	K340	R258	L194	A17
LYS	D418	R441	R259	D195	L107
ASN	R421	T342	N260	P196	R108
ASN		L343	T261	L197	E109
ASP	S432		L262	C198	T110
GLU	R433	F347	R263	G199	I111
GLU	R434	N348	E264	T200	I112
GLU	S435	L349	N265	C201	M31
	S436	H350	L266	G202	E32
	E437	T351	R267		S113
	V438	V352	N268		L114
	P439	V353	V269	A207	F115
	V440	R354	S270	E208	E35
	E441	L355	E271	L209	H36
	E442		R272	M211	L37
	V443		F273	K212	E38
	K444	G358	D274	L212	A38
	R445	A361	V275	C123	W39
	G447	P362		E215	
	Y448	S364	T278	R216	R44
		D365	N279	T217	F45
	N454	V366	P280	L218	L46
	P455		F281	E219	
	M456	L370	R282	D220	E50
	R457		G283	H221	E51
	S458	F373	E286	R222	E52
		R374	G287	L223	W53
		R375	R288	G225	E54
		P376	H289	L224	A55
		T379	L290	E226	Q56
		K380	Q291	F141	
				D145	
	E461		F294		L159
	L463	W383	P295	R227	ALA
	P464	S384	L296	T228	Gly
	S465	V385	Q297	F148	ARG
	P466			T149	PRO
	V467			V150	TYR
	E468			S151	THR
	L469			L152	
	V470			V153	P66
					L67
					I68
	L473	L387	L303	R235	D89
	L474	P388	L304	P236	S70
	K476	E391	K311	P238	E71
			K312	A239	Y72
			L313	E169	R73
			K314	F240	L74
			L315		
			K354		
			L355		

- Molecule 1: Type I restriction-modification system methyltransferase subunit

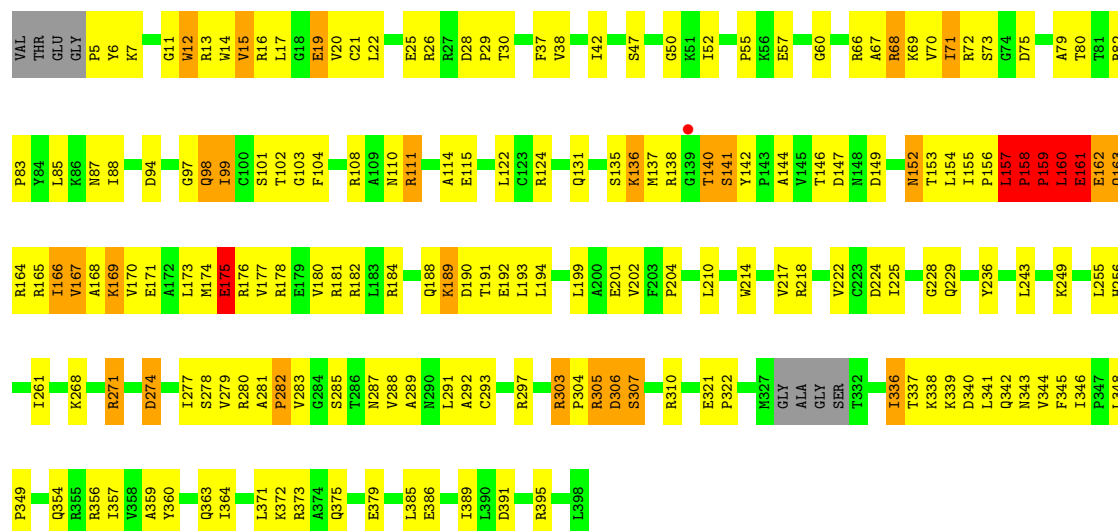
Chain E: 94%

[illegible]



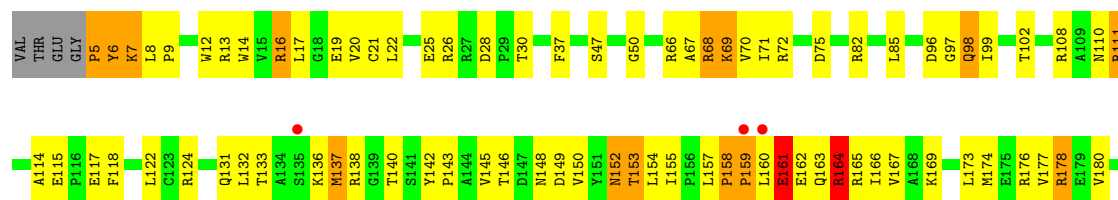
• Molecule 2: Restriction endonuclease S subunits

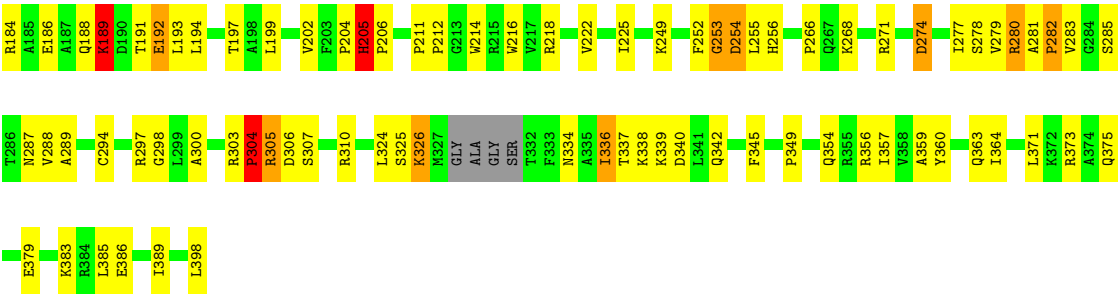
Chain D: 52% 38% 7% ..



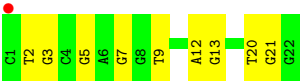
• Molecule 2: Restriction endonuclease S subunits

Chain G: 58% 33% 6% ..





● Molecule 3: DNA



● Molecule 4: DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	121.60Å 121.60Å 280.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.00 – 3.20 47.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.3 (47.00-3.20) 95.4 (47.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.236 , 0.272 0.246 , 0.271	Depositor DCC
R_{free} test set	3039 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	96.9	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 76.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15456	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SAM

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	A	0.76	5/4031 (0.1%)	1.27	45/5466 (0.8%)
1	B	0.72	5/4031 (0.1%)	1.14	35/5466 (0.6%)
1	C	0.83	1/229 (0.4%)	1.32	4/308 (1.3%)
1	E	0.97	0/229	1.41	5/308 (1.6%)
2	D	0.77	3/3165 (0.1%)	1.32	34/4307 (0.8%)
2	G	0.65	4/3165 (0.1%)	1.15	26/4307 (0.6%)
3	H	0.22	0/510	0.36	0/787
4	I	0.26	0/494	0.42	0/759
All	All	0.71	18/15854 (0.1%)	1.19	149/21708 (0.7%)

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
1	A	0	2
1	B	0	2
1	E	0	1
2	D	0	4
2	G	0	3
All	All	0	12

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	158	PRO	N-CD	-19.06	1.21	1.47
1	A	106	PRO	N-CD	7.78	1.58	1.47
1	B	463	LEU	C-N	5.71	1.40	1.33
1	A	280	PRO	C-N	5.57	1.40	1.33
1	B	464	PRO	N-CD	5.40	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362	PRO	N-CD	5.38	1.55	1.47
1	B	362	PRO	N-CD	5.31	1.55	1.47
2	D	282	PRO	N-CD	5.30	1.55	1.47
1	C	465	SER	C-N	5.28	1.40	1.34
2	G	204	PRO	C-O	-5.26	1.18	1.23
2	G	282	PRO	N-CD	5.26	1.55	1.47
2	G	304	PRO	N-CD	5.21	1.55	1.47
1	B	106	PRO	N-CD	5.19	1.55	1.47
1	B	466	PRO	N-CD	5.14	1.54	1.47
1	A	105	ASP	C-N	5.12	1.40	1.34
1	A	97	PRO	N-CD	5.12	1.54	1.47
2	G	303	ARG	C-N	5.08	1.40	1.33
2	D	159	PRO	N-CD	5.05	1.54	1.47

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	158	PRO	N-CA-C	30.75	148.22	110.70
1	A	106	PRO	N-CA-C	22.92	146.25	113.47
2	D	141	SER	N-CA-CB	-18.70	83.27	110.56
1	A	268	ASN	N-CA-C	-18.57	78.76	109.96
1	A	107	LEU	N-CA-C	-15.82	77.09	110.80
2	D	158	PRO	CB-CA-C	-12.56	95.59	110.92
1	A	375	ARG	CB-CA-C	-12.22	94.54	111.41
2	D	158	PRO	CA-N-CD	11.88	128.63	112.00
2	G	161	GLU	CB-CA-C	-11.58	91.92	111.26
1	B	283	GLY	N-CA-C	11.57	129.30	114.25
2	D	161	GLU	CB-CA-C	-11.22	88.10	110.42
2	D	159	PRO	CB-CA-C	-10.77	93.80	111.56
2	G	5	PRO	CB-CA-C	10.75	130.52	110.10
2	D	159	PRO	N-CA-C	10.22	133.52	112.47
1	B	119	ASN	N-CA-C	9.99	123.51	111.02
2	D	303	ARG	CB-CA-C	-9.76	97.06	110.13
2	D	163	GLN	N-CA-C	-9.51	100.90	111.07
2	D	158	PRO	N-CA-CB	-9.47	93.90	103.08
1	A	107	LEU	N-CA-CB	9.32	126.24	110.49
2	D	140	THR	N-CA-C	-9.13	97.75	110.35
1	A	269	VAL	N-CA-CB	-8.67	96.92	111.23
1	A	106	PRO	CB-CA-C	-8.47	99.59	113.06
2	D	141	SER	N-CA-C	8.37	123.21	112.92
1	B	200	THR	CB-CA-C	-8.32	106.97	116.54
1	A	361	ALA	C-N-CD	8.26	138.77	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	LEU	CB-CA-C	8.22	126.78	110.42
1	B	361	ALA	C-N-CD	8.16	138.54	120.60
2	G	281	ALA	C-N-CD	8.11	138.45	120.60
2	D	281	ALA	C-N-CD	8.06	138.32	120.60
2	G	5	PRO	CA-C-N	8.04	136.03	122.20
2	G	5	PRO	C-N-CA	8.04	136.03	122.20
1	A	200	THR	CB-CA-C	-7.96	107.39	116.54
1	A	288	ARG	CB-CA-C	-7.81	106.61	117.23
2	D	160	LEU	CB-CA-C	-7.74	96.42	109.50
2	G	253	GLY	N-CA-C	-7.62	100.99	112.41
2	G	162	GLU	N-CA-C	-7.60	101.89	113.89
2	G	6	TYR	N-CA-C	-7.52	98.97	108.45
2	D	161	GLU	CA-C-N	7.41	137.43	121.64
2	D	161	GLU	C-N-CA	7.41	137.43	121.64
1	A	230	PHE	N-CA-C	-7.30	96.42	108.76
1	A	95	LEU	N-CA-C	7.28	119.00	111.14
2	D	274	ASP	N-CA-C	-7.15	101.09	110.53
1	B	54	GLU	N-CA-C	-7.07	103.00	111.69
2	G	158	PRO	N-CA-C	7.06	119.32	110.70
2	G	7	LYS	N-CA-C	-7.03	98.33	109.23
1	B	282	PHE	N-CA-C	-7.03	103.70	111.36
2	D	82	ARG	CA-C-N	-6.93	111.18	119.84
2	D	82	ARG	C-N-CA	-6.93	111.18	119.84
1	B	230	PHE	N-CA-C	-6.93	97.05	108.76
2	G	98	GLN	CA-C-N	-6.93	114.16	123.10
2	G	98	GLN	C-N-CA	-6.93	114.16	123.10
1	E	491	LEU	N-CA-C	6.85	121.66	113.16
1	B	463	LEU	CA-C-N	-6.83	113.26	120.03
1	B	463	LEU	C-N-CA	-6.83	113.26	120.03
1	A	120	VAL	N-CA-C	-6.83	99.87	108.89
1	B	10	LEU	N-CA-C	6.75	118.72	111.36
1	A	232	GLN	N-CA-C	6.63	119.15	109.07
2	G	82	ARG	CA-C-N	-6.63	111.56	119.84
2	G	82	ARG	C-N-CA	-6.63	111.56	119.84
2	G	303	ARG	CA-C-N	-6.54	112.93	119.99
2	G	303	ARG	C-N-CA	-6.54	112.93	119.99
1	E	491	LEU	CA-C-N	-6.50	112.78	122.39
1	E	491	LEU	C-N-CA	-6.50	112.78	122.39
1	B	232	GLN	N-CA-C	6.40	118.80	109.07
1	C	465	SER	CA-C-N	-6.39	112.32	118.97
1	C	465	SER	C-N-CA	-6.39	112.32	118.97
2	G	324	LEU	N-CA-C	-6.35	104.40	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	HIS	N-CA-C	6.33	118.25	111.36
1	A	54	GLU	N-CA-C	-6.28	103.97	111.69
2	G	274	ASP	N-CA-C	-6.27	102.25	110.53
2	D	140	THR	CB-CA-C	-6.23	97.81	111.71
2	D	157	LEU	C-N-CD	-6.20	99.59	125.00
1	A	280	PRO	CA-C-N	-6.19	113.18	120.11
1	A	280	PRO	C-N-CA	-6.19	113.18	120.11
1	B	249	HIS	N-CA-C	6.17	118.01	111.28
1	B	109	GLU	N-CA-C	-6.05	104.69	111.28
2	G	6	TYR	CB-CA-C	6.05	126.87	113.02
2	D	157	LEU	CB-CA-C	-6.04	100.52	110.55
1	E	465	SER	CA-C-N	-5.97	112.43	119.05
1	E	465	SER	C-N-CA	-5.97	112.43	119.05
1	B	118	ARG	N-CA-C	5.89	118.36	110.35
1	A	287	GLY	N-CA-C	5.87	122.00	112.61
2	G	205	HIS	CA-C-N	5.87	125.81	119.76
2	G	205	HIS	C-N-CA	5.87	125.81	119.76
2	D	167	VAL	N-CA-C	-5.84	104.66	110.62
1	A	117	GLU	N-CA-C	5.83	118.72	109.50
1	B	271	GLU	CA-C-N	5.79	132.13	121.70
1	B	271	GLU	C-N-CA	5.79	132.13	121.70
1	B	214	LYS	N-CA-C	5.78	120.03	112.92
2	D	287	ASN	N-CA-C	-5.77	99.96	108.79
1	A	105	ASP	CA-C-N	-5.75	112.99	118.97
1	A	105	ASP	C-N-CA	-5.75	112.99	118.97
1	B	273	PHE	N-CA-C	5.71	118.38	109.52
2	D	304	PRO	CA-N-CD	-5.70	104.02	112.00
1	B	454	ASN	CA-C-N	-5.70	112.73	119.05
1	B	454	ASN	C-N-CA	-5.70	112.73	119.05
1	A	269	VAL	CA-C-N	5.68	132.39	121.54
1	A	269	VAL	C-N-CA	5.68	132.39	121.54
2	G	153	THR	N-CA-C	5.66	117.91	109.59
1	C	491	LEU	CA-C-N	-5.64	114.04	122.39
1	C	491	LEU	C-N-CA	-5.64	114.04	122.39
2	D	159	PRO	CA-N-CD	-5.61	104.14	112.00
2	D	171	GLU	CA-C-N	5.59	128.02	120.65
2	D	171	GLU	C-N-CA	5.59	128.02	120.65
1	A	109	GLU	N-CA-C	-5.56	105.22	111.28
1	B	230	PHE	CA-C-N	5.55	131.32	121.05
1	B	230	PHE	C-N-CA	5.55	131.32	121.05
2	G	164	ARG	N-CA-C	-5.51	106.32	113.16
1	A	465	SER	CA-C-N	-5.51	112.94	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	SER	C-N-CA	-5.51	112.94	119.05
1	A	355	LEU	CA-C-N	5.50	126.05	120.38
1	A	355	LEU	C-N-CA	5.50	126.05	120.38
2	D	159	PRO	CA-C-N	-5.46	113.36	122.64
2	D	159	PRO	C-N-CA	-5.46	113.36	122.64
2	G	189	LYS	N-CA-C	-5.40	105.29	111.07
1	A	218	ILE	CB-CA-C	-5.39	104.86	112.14
1	B	105	ASP	CA-C-N	-5.39	113.07	119.05
1	B	105	ASP	C-N-CA	-5.39	113.07	119.05
2	D	189	LYS	N-CA-C	-5.39	105.10	110.97
1	A	96	ILE	CA-C-N	-5.38	113.08	119.05
1	A	96	ILE	C-N-CA	-5.38	113.08	119.05
1	A	191	GLU	N-CA-C	-5.38	100.25	109.24
1	A	432	SER	N-CA-C	-5.38	101.12	109.24
1	B	373	PHE	CA-C-N	-5.37	113.46	122.92
1	B	373	PHE	C-N-CA	-5.37	113.46	122.92
1	A	217	THR	N-CA-C	5.37	117.35	109.24
1	A	230	PHE	CA-C-N	5.37	130.98	121.05
1	A	230	PHE	C-N-CA	5.37	130.98	121.05
1	A	107	LEU	CA-C-N	5.36	131.78	121.54
1	A	107	LEU	C-N-CA	5.36	131.78	121.54
1	A	116	SER	N-CA-C	5.34	117.86	111.71
1	B	355	LEU	CA-C-N	5.25	125.79	120.38
1	B	355	LEU	C-N-CA	5.25	125.79	120.38
2	D	136	LYS	CA-CB-CG	5.23	124.55	114.10
1	A	234	LYS	N-CA-C	5.23	117.78	111.40
1	B	465	SER	CA-C-N	-5.20	113.27	119.05
1	B	465	SER	C-N-CA	-5.20	113.27	119.05
1	B	288	ARG	CB-CA-C	-5.17	110.19	117.23
2	G	152	ASN	N-CA-C	5.15	119.66	113.17
1	B	278	THR	N-CA-C	5.14	116.88	109.07
2	G	98	GLN	N-CA-C	5.13	116.61	108.96
1	A	233	GLU	N-CA-C	5.12	117.77	109.06
2	D	175	GLU	N-CA-C	-5.10	105.61	111.07
1	B	112	ARG	N-CA-C	-5.10	105.72	111.28
1	B	263	GLU	CA-CB-CG	5.05	124.21	114.10
2	D	98	GLN	N-CA-C	5.05	116.75	109.07
1	B	67	ILE	CB-CA-C	-5.04	105.27	112.22
1	A	373	PHE	CA-C-N	-5.04	114.03	123.05
1	A	373	PHE	C-N-CA	-5.04	114.03	123.05

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	LEU	Peptide
1	A	375	ARG	Peptide
1	B	268	ASN	Peptide
1	B	282	PHE	Peptide
2	D	158	PRO	Peptide
2	D	159	PRO	Peptide
2	D	160	LEU	Peptide
2	D	161	GLU	Peptide
1	E	491	LEU	Peptide
2	G	159	PRO	Peptide
2	G	161	GLU	Peptide
2	G	5	PRO	Peptide

5.2 Too-close contacts [i](#)

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	A	3934	0	3858	370	0
1	B	3934	0	3857	315	1
1	C	229	0	233	28	0
1	E	229	0	233	25	0
2	D	3090	0	3103	271	1
2	G	3090	0	3106	162	2
3	H	454	0	248	5	1
4	I	442	0	248	4	1
5	A	27	0	22	10	0
5	B	27	0	22	9	0
All	All	15456	0	14930	1151	3

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 38.

All (1151) 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)
1:B:50:GLU:CG	1:B:67:ILE:HD11	1.19	1.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:PHE:CD2	2:D:99:ILE:HD11	1.30	1.63
1:B:50:GLU:HG3	1:B:67:ILE:CD1	1.10	1.54
1:A:68:ILE:HG21	1:A:98:TYR:CE1	1.47	1.49
2:D:391:ASP:CG	2:D:395:ARG:HH22	1.18	1.47
2:D:37:PHE:CE2	2:D:99:ILE:HD11	1.51	1.45
1:A:68:ILE:HG22	1:A:98:TYR:CZ	1.50	1.43
1:A:68:ILE:CG2	1:A:98:TYR:CE1	2.04	1.41
2:D:137:MET:CG	2:D:140:THR:OG1	1.67	1.40
1:A:68:ILE:CG2	1:A:98:TYR:OH	1.69	1.40
2:D:37:PHE:CD2	2:D:99:ILE:CD1	2.06	1.36
1:A:68:ILE:CG2	1:A:98:TYR:CZ	2.09	1.36
2:D:391:ASP:CG	2:D:395:ARG:NH2	1.89	1.30
2:D:157:LEU:O	2:D:157:LEU:CD2	1.81	1.27
1:A:100:ARG:O	1:A:112:ARG:HD3	1.33	1.26
2:G:161:GLU:CD	2:G:161:GLU:O	1.79	1.25
1:A:50:GLU:HG3	1:A:67:ILE:CD1	1.69	1.22
2:D:38:VAL:HG22	2:D:98:GLN:OE1	1.36	1.20
1:A:409:GLU:OE2	1:A:434:ARG:NH1	1.77	1.17
1:B:409:GLU:OE2	1:B:434:ARG:NH1	1.76	1.16
2:D:38:VAL:CG2	2:D:98:GLN:OE1	1.95	1.15
2:D:163:GLN:O	2:D:166:ILE:N	1.77	1.15
2:D:160:LEU:HA	2:D:161:GLU:HB2	1.19	1.15
2:D:162:GLU:O	2:D:165:ARG:HB2	1.41	1.15
2:D:160:LEU:CA	2:D:161:GLU:HB2	1.77	1.14
1:A:107:LEU:CA	1:A:110:THR:HG23	1.75	1.14
2:D:157:LEU:O	2:D:157:LEU:HD23	0.97	1.14
1:B:193:VAL:O	1:B:230:PHE:O	1.65	1.14
2:D:163:GLN:CA	2:D:166:ILE:HG23	1.77	1.13
1:A:266:ILE:HD11	1:A:295:PRO:CD	1.79	1.12
1:A:191:GLU:HB3	1:A:274:ASP:HB2	1.32	1.12
1:A:107:LEU:HA	1:A:110:THR:CG2	1.80	1.12
2:D:71:ILE:HG12	2:D:98:GLN:O	1.50	1.12
1:A:7:ARG:HG3	1:A:149:THR:HG23	1.28	1.12
1:A:100:ARG:O	1:A:112:ARG:CD	1.97	1.11
1:A:169:GLY:HA2	1:A:363:TYR:HB2	1.22	1.10
1:A:7:ARG:HG2	1:A:11:ALA:HB2	1.24	1.10
2:D:391:ASP:OD1	2:D:395:ARG:NH2	1.82	1.10
1:A:50:GLU:HG3	1:A:67:ILE:HD12	1.16	1.09
1:A:7:ARG:HG2	1:A:11:ALA:CB	1.80	1.09
1:A:107:LEU:O	1:A:110:THR:HG23	1.52	1.09
1:B:50:GLU:HG3	1:B:67:ILE:CG1	1.82	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:MET:HG2	2:D:140:THR:CB	1.83	1.09
1:A:102:LEU:HD22	1:A:108:ARG:HB3	1.32	1.08
1:B:271:GLU:HB3	1:B:272:ARG:HA	1.34	1.08
1:A:107:LEU:C	1:A:110:THR:HG23	1.78	1.07
1:A:266:ILE:HD11	1:A:295:PRO:HD2	1.35	1.07
1:B:432:SER:N	1:B:435:SER:OG	1.88	1.07
1:B:433:GLU:OE1	1:B:433:GLU:N	1.88	1.06
2:D:163:GLN:HA	2:D:166:ILE:CG2	1.84	1.06
2:D:157:LEU:HG	2:D:164:ARG:NH1	1.71	1.05
1:A:433:GLU:N	1:A:433:GLU:OE1	1.88	1.05
1:A:72:TYR:HE2	1:A:98:TYR:HB2	1.21	1.05
1:B:99:LEU:HA	1:B:102:LEU:CD2	1.87	1.04
1:A:104:GLY:C	1:A:106:PRO:HD2	1.83	1.04
2:D:160:LEU:HB3	2:D:161:GLU:C	1.81	1.03
1:B:68:ILE:CD1	1:B:73:ARG:HG2	1.87	1.03
1:A:193:VAL:O	1:A:230:PHE:O	1.75	1.03
1:C:466:PRO:HG3	2:D:201:GLU:OE2	1.54	1.03
2:D:37:PHE:CE2	2:D:99:ILE:CD1	2.34	1.03
1:A:68:ILE:HG22	1:A:98:TYR:OH	0.86	1.03
2:D:162:GLU:O	2:D:165:ARG:CB	2.06	1.03
1:B:218:ILE:H	1:B:218:ILE:HD12	1.19	1.02
1:A:72:TYR:CD2	1:A:98:TYR:CG	2.48	1.01
1:A:191:GLU:HB3	1:A:274:ASP:CB	1.89	1.01
2:D:163:GLN:HA	2:D:166:ILE:HG23	1.02	1.01
1:A:216:ARG:CG	1:A:217:THR:HG23	1.89	1.01
1:B:215:GLU:OE1	1:B:216:ARG:N	1.92	1.01
2:D:137:MET:HG2	2:D:140:THR:OG1	0.83	1.00
2:G:6:TYR:HB3	2:G:14:TRP:HZ2	1.21	1.00
1:A:107:LEU:CA	1:A:110:THR:CG2	2.38	1.00
2:D:161:GLU:O	2:D:161:GLU:OE1	1.77	1.00
2:D:114:ALA:HA	2:D:164:ARG:HH22	1.24	1.00
1:A:7:ARG:HA	1:A:149:THR:HG21	1.44	1.00
1:B:5:GLN:NE2	1:B:7:ARG:HB2	1.77	1.00
1:A:107:LEU:HA	1:A:110:THR:HG21	1.39	0.99
2:D:69:LYS:O	2:D:99:ILE:HA	1.60	0.99
2:D:391:ASP:OD2	2:D:395:ARG:NH2	1.94	0.99
1:A:7:ARG:CG	1:A:11:ALA:HB2	1.91	0.99
1:B:348:ASN:O	1:B:374:GLU:N	1.94	0.98
1:A:169:GLY:HA2	1:A:363:TYR:CB	1.93	0.97
1:A:268:ASN:C	1:A:268:ASN:OD1	2.06	0.97
1:A:7:ARG:HA	1:A:149:THR:CG2	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97:GLY:O	2:D:98:GLN:HG2	1.63	0.96
1:A:216:ARG:HG3	1:A:217:THR:HG23	1.47	0.96
1:A:267:ARG:HH11	1:A:267:ARG:HG2	1.31	0.96
1:A:68:ILE:CG2	1:A:98:TYR:HE1	1.61	0.95
1:B:50:GLU:CD	1:B:67:ILE:HD11	1.90	0.95
1:B:102:LEU:HB2	1:B:112:ARG:HG2	1.48	0.95
1:B:105:ASP:OD1	1:B:108:ARG:HG3	1.64	0.94
1:A:67:ILE:HD13	1:A:67:ILE:H	1.28	0.94
1:B:191:GLU:HB3	1:B:274:ASP:CB	1.97	0.94
2:G:67:ALA:O	2:G:68:ARG:NH1	2.01	0.94
1:B:169:GLY:HA2	1:B:363:TYR:HB2	1.49	0.94
2:D:114:ALA:HA	2:D:164:ARG:NH2	1.81	0.93
1:B:432:SER:O	1:B:435:SER:N	1.99	0.93
1:A:217:THR:OG1	1:A:220:ASP:OD1	1.85	0.93
2:D:136:LYS:HD2	2:D:137:MET:H	1.30	0.93
1:B:432:SER:OG	1:B:433:GLU:OE1	1.85	0.93
1:A:6:THR:HA	1:A:8:GLU:HG3	1.50	0.93
1:B:5:GLN:NE2	1:B:7:ARG:CB	2.31	0.93
2:D:140:THR:HG22	2:D:141:SER:N	1.83	0.92
1:B:271:GLU:HB3	1:B:272:ARG:CA	1.98	0.92
1:A:67:ILE:C	1:A:68:ILE:HD13	1.94	0.92
2:G:6:TYR:CB	2:G:14:TRP:HZ2	1.82	0.92
2:D:67:ALA:O	2:D:68:ARG:NH1	2.02	0.92
1:A:268:ASN:OD1	1:A:268:ASN:O	1.88	0.91
2:G:6:TYR:HB3	2:G:14:TRP:CZ2	2.04	0.91
1:A:464:PRO:HG2	1:A:469:ILE:HD11	1.52	0.91
2:D:157:LEU:HG	2:D:164:ARG:HH11	1.25	0.91
2:D:164:ARG:HG2	2:D:164:ARG:HH21	1.34	0.91
2:D:160:LEU:HB3	2:D:161:GLU:HB3	1.53	0.91
2:D:160:LEU:HB3	2:D:161:GLU:CB	2.01	0.90
2:D:68:ARG:HH11	2:D:68:ARG:HG2	1.37	0.90
1:A:269:VAL:HG23	1:A:270:SER:H	1.35	0.90
1:A:13:GLU:O	1:A:16:ARG:N	2.05	0.90
2:D:160:LEU:O	2:D:163:GLN:HG2	1.70	0.89
1:A:169:GLY:CA	1:A:363:TYR:HB2	2.01	0.89
1:A:102:LEU:HD12	1:A:102:LEU:H	1.36	0.89
2:G:161:GLU:O	2:G:161:GLU:OE1	1.90	0.89
2:D:37:PHE:HD2	2:D:99:ILE:HD11	1.38	0.88
2:D:160:LEU:CA	2:D:161:GLU:CB	2.49	0.88
2:D:162:GLU:O	2:D:165:ARG:N	2.06	0.88
1:A:72:TYR:CD2	1:A:98:TYR:CD2	2.62	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:PRO:O	1:C:469:ILE:HG22	1.74	0.88
2:D:140:THR:HG22	2:D:141:SER:H	1.38	0.88
1:B:217:THR:HG23	1:B:220:ASP:CG	1.98	0.88
2:D:184:ARG:HH21	2:D:375:GLN:HB3	1.39	0.88
2:D:160:LEU:HB3	2:D:162:GLU:N	1.89	0.88
1:A:72:TYR:CE2	1:A:98:TYR:HB2	2.08	0.87
2:D:224:ASP:HB3	2:D:305:ARG:NH2	1.90	0.87
1:A:72:TYR:CE2	1:A:98:TYR:CD2	2.62	0.87
1:A:266:ILE:HD11	1:A:295:PRO:HD3	1.55	0.87
1:A:68:ILE:HG22	1:A:98:TYR:HH	1.07	0.87
2:D:137:MET:CB	2:D:140:THR:OG1	2.21	0.87
1:A:50:GLU:CG	1:A:67:ILE:HD12	2.03	0.86
2:D:222:VAL:O	2:D:305:ARG:HB2	1.75	0.86
1:A:216:ARG:HG2	1:A:217:THR:N	1.88	0.86
1:A:67:ILE:HG12	1:A:68:ILE:H	1.37	0.86
1:A:6:THR:CA	1:A:8:GLU:HG3	2.05	0.85
1:A:117:GLU:OE1	1:A:118:ARG:NH1	2.09	0.85
1:A:106:PRO:HG2	1:A:108:ARG:HG3	1.56	0.85
1:B:68:ILE:HD11	1:B:73:ARG:HG2	1.56	0.85
2:G:6:TYR:CB	2:G:14:TRP:CZ2	2.58	0.85
2:D:165:ARG:HH11	2:D:165:ARG:HG3	1.41	0.85
1:E:466:PRO:O	1:E:469:ILE:HG22	1.75	0.84
1:A:7:ARG:HG3	1:A:149:THR:CG2	2.07	0.84
1:B:219:GLU:N	1:B:219:GLU:OE2	2.09	0.84
1:B:35:GLU:HG3	1:B:121:ILE:HG13	1.57	0.84
1:B:191:GLU:HB3	1:B:274:ASP:CG	2.01	0.84
2:G:159:PRO:HA	2:G:161:GLU:N	1.92	0.84
1:A:72:TYR:CE2	1:A:98:TYR:CB	2.60	0.84
1:A:72:TYR:HD2	1:A:98:TYR:CG	1.92	0.84
1:A:216:ARG:HD3	1:A:220:ASP:OD2	1.76	0.84
1:B:170:GLU:HG2	1:B:363:TYR:CE1	2.11	0.84
2:D:160:LEU:CB	2:D:161:GLU:CB	2.55	0.84
2:D:131:GLN:NE2	2:D:154:LEU:O	2.11	0.84
2:G:131:GLN:NE2	2:G:154:LEU:O	2.11	0.84
1:A:102:LEU:HD22	1:A:108:ARG:CB	2.06	0.84
1:A:68:ILE:HG21	1:A:98:TYR:HE1	0.94	0.83
1:A:218:ILE:HD12	1:A:218:ILE:H	1.43	0.83
2:D:37:PHE:CD2	2:D:99:ILE:HD13	2.13	0.83
2:G:7:LYS:O	2:G:8:LEU:HD23	1.79	0.82
2:G:6:TYR:CD2	2:G:8:LEU:HD21	2.13	0.82
2:G:136:LYS:HG3	2:G:137:MET:N	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PRO:O	1:B:109:GLU:HB2	1.79	0.82
1:B:235:LYS:HD2	1:B:236:PRO:HD2	1.60	0.82
2:G:69:LYS:O	2:G:99:ILE:HA	1.80	0.82
2:D:67:ALA:O	2:D:68:ARG:HG2	1.80	0.81
1:B:68:ILE:HD12	1:B:68:ILE:O	1.80	0.81
1:A:72:TYR:HE2	1:A:98:TYR:CB	1.92	0.81
1:B:110:THR:O	1:B:113:SER:OG	1.98	0.81
1:A:102:LEU:CD1	1:A:103:GLY:H	1.94	0.81
1:A:201:CYS:SG	1:A:202:GLY:N	2.54	0.81
1:B:102:LEU:HB2	1:B:112:ARG:CG	2.11	0.81
1:A:67:ILE:HG12	1:A:68:ILE:N	1.94	0.81
1:A:432:SER:OG	1:A:433:GLU:OE1	1.97	0.81
1:B:50:GLU:CG	1:B:67:ILE:CD1	2.05	0.81
2:D:162:GLU:O	2:D:165:ARG:CA	2.29	0.80
1:A:5:GLN:NE2	1:A:7:ARG:H	1.79	0.80
2:D:137:MET:HG3	2:D:140:THR:H	1.45	0.80
1:A:260:ASN:OD1	5:A:601:SAM:N6	2.14	0.80
2:D:164:ARG:O	2:D:167:VAL:HG12	1.80	0.80
1:B:375:ARG:HG2	1:B:375:ARG:O	1.80	0.79
1:A:216:ARG:HG2	1:A:217:THR:HG23	1.62	0.79
2:D:162:GLU:OE2	2:D:165:ARG:NH1	2.15	0.79
1:B:10:LEU:HD12	1:B:10:LEU:O	1.82	0.79
1:B:272:ARG:HH11	1:B:272:ARG:HG2	1.46	0.79
1:B:201:CYS:SG	1:B:202:GLY:N	2.54	0.79
1:B:218:ILE:HB	1:B:219:GLU:OE2	1.83	0.79
2:D:71:ILE:N	2:D:98:GLN:O	2.13	0.79
2:D:136:LYS:CD	2:D:137:MET:H	1.95	0.79
2:G:184:ARG:HH21	2:G:375:GLN:HB3	1.46	0.79
1:A:107:LEU:O	1:A:110:THR:CG2	2.31	0.79
2:G:192:GLU:OE1	2:G:193:LEU:N	2.16	0.78
2:G:280:ARG:HH22	2:G:297:ARG:NH1	1.80	0.78
2:G:280:ARG:NH2	2:G:297:ARG:NH1	2.31	0.78
1:B:217:THR:HG23	1:B:220:ASP:OD1	1.83	0.78
1:B:270:SER:O	1:B:272:ARG:HG3	1.83	0.78
2:D:72:ARG:HG2	2:D:72:ARG:HH11	1.46	0.78
1:B:199:GLY:H	5:B:601:SAM:HA	1.47	0.78
2:G:132:LEU:O	2:G:136:LYS:HG2	1.84	0.78
1:A:67:ILE:HA	1:A:108:ARG:NH1	1.99	0.77
2:D:66:ARG:O	2:D:102:THR:HG23	1.84	0.77
2:D:17:LEU:HD13	2:D:155:ILE:HD13	1.66	0.77
1:B:272:ARG:HG2	1:B:272:ARG:NH1	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:TYR:CE2	1:A:98:TYR:CG	2.72	0.77
1:B:199:GLY:N	5:B:601:SAM:HA	2.00	0.77
1:A:199:GLY:H	5:A:601:SAM:HA	1.50	0.77
1:B:457:ARG:HG2	1:B:458:SER:N	2.00	0.77
1:A:272:ARG:HG2	1:A:272:ARG:HH11	1.49	0.77
2:D:157:LEU:CG	2:D:164:ARG:NH1	2.48	0.77
1:B:99:LEU:HA	1:B:102:LEU:HD21	1.66	0.77
1:A:71:GLU:HB3	1:A:72:TYR:CD1	2.19	0.76
1:A:112:ARG:O	1:A:113:SER:C	2.27	0.76
1:A:183:GLU:OE2	1:A:415:ARG:NH2	2.18	0.76
2:G:249:LYS:HD3	2:G:282:PRO:HG3	1.67	0.76
2:D:137:MET:CG	2:D:140:THR:CB	2.53	0.76
1:B:442:GLU:HA	1:B:445:LYS:HG3	1.68	0.76
1:A:10:LEU:HD12	1:A:10:LEU:O	1.84	0.75
1:A:347:PHE:HE1	1:A:375:ARG:HD2	1.50	0.75
2:G:71:ILE:HG12	2:G:98:GLN:O	1.87	0.75
2:G:16:ARG:O	2:G:19:GLU:HG3	1.87	0.75
1:A:35:GLU:HG3	1:A:121:ILE:HG13	1.68	0.75
1:B:170:GLU:HG2	1:B:363:TYR:HE1	1.51	0.75
1:A:5:GLN:HE21	1:A:7:ARG:H	1.31	0.75
2:D:157:LEU:O	2:D:157:LEU:CG	2.32	0.75
1:B:166:ARG:HA	1:B:362:PRO:HG2	1.69	0.75
1:A:267:ARG:HG2	1:A:267:ARG:NH1	1.99	0.74
2:D:114:ALA:CA	2:D:164:ARG:HH22	1.99	0.74
2:G:68:ARG:NH1	2:G:68:ARG:HG2	2.02	0.74
2:D:12:TRP:HE3	2:D:12:TRP:N	1.85	0.74
2:D:163:GLN:C	2:D:166:ILE:H	1.95	0.74
2:D:166:ILE:O	2:D:169:LYS:N	2.19	0.74
1:A:68:ILE:HD13	1:A:68:ILE:N	2.03	0.74
2:D:68:ARG:NH1	2:D:68:ARG:HG2	2.00	0.74
2:D:72:ARG:HG2	2:D:72:ARG:NH1	2.01	0.74
1:A:265:ASN:HD21	1:A:267:ARG:HD2	1.50	0.74
2:G:6:TYR:HD2	2:G:8:LEU:HD21	1.50	0.74
1:A:67:ILE:CD1	1:A:67:ILE:H	2.01	0.74
1:A:364:SER:OG	1:A:366:VAL:HG23	1.88	0.74
1:A:484:MET:HE3	2:D:371:LEU:HD11	1.69	0.74
2:D:271:ARG:HG2	2:D:274:ASP:OD2	1.88	0.74
1:A:347:PHE:CE1	1:A:375:ARG:HD2	2.22	0.74
2:D:160:LEU:HD13	2:D:161:GLU:HB3	1.71	0.73
1:B:50:GLU:CG	1:B:67:ILE:CG1	2.54	0.73
1:A:53:TRP:HD1	1:A:56:GLN:HE21	1.33	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ARG:O	1:A:97:PRO:HG2	1.88	0.73
1:C:467:VAL:O	1:C:470:VAL:HG12	1.88	0.73
1:B:53:TRP:HA	1:B:56:GLN:HG3	1.71	0.73
1:B:191:GLU:CB	1:B:274:ASP:HB2	2.18	0.73
2:G:68:ARG:HG2	2:G:68:ARG:HH11	1.54	0.73
2:D:160:LEU:CB	2:D:162:GLU:H	2.01	0.72
2:D:162:GLU:HA	2:D:165:ARG:HG2	1.71	0.72
2:D:339:LYS:O	2:D:343:ASN:ND2	2.21	0.72
2:G:379:GLU:OE2	2:G:383:LYS:NZ	2.19	0.72
1:A:100:ARG:O	1:A:112:ARG:HD2	1.89	0.72
2:D:11:GLY:O	2:D:159:PRO:CD	2.38	0.72
2:D:137:MET:HG3	2:D:140:THR:N	2.04	0.72
1:B:112:ARG:O	1:B:116:SER:HB2	1.88	0.72
2:G:6:TYR:HD2	2:G:8:LEU:CD2	2.01	0.72
1:A:218:ILE:HD12	1:A:218:ILE:N	2.03	0.72
1:A:106:PRO:CG	1:A:108:ARG:HG3	2.20	0.72
1:A:230:PHE:CB	1:A:273:PHE:HE2	2.03	0.72
1:B:68:ILE:HD11	1:B:73:ARG:CG	2.20	0.72
2:D:140:THR:CG2	2:D:141:SER:N	2.53	0.72
2:D:160:LEU:CB	2:D:161:GLU:HB3	2.19	0.72
1:A:272:ARG:HG2	1:A:272:ARG:NH1	2.01	0.72
1:E:465:SER:HA	1:E:468:GLU:OE2	1.89	0.72
2:G:115:GLU:O	2:G:164:ARG:NH1	2.22	0.72
1:A:199:GLY:N	5:A:601:SAM:HA	2.04	0.71
1:B:107:LEU:C	1:B:107:LEU:HD12	2.15	0.71
1:A:102:LEU:HD12	1:A:102:LEU:N	2.04	0.71
1:A:386:GLU:OE1	1:A:457:ARG:NH1	2.23	0.71
2:G:71:ILE:N	2:G:98:GLN:O	2.22	0.71
1:A:169:GLY:HA2	1:A:363:TYR:CG	2.26	0.71
1:B:349:LEU:HA	1:B:373:PHE:HA	1.72	0.71
1:A:349:LEU:C	1:A:349:LEU:HD12	2.15	0.71
1:B:183:GLU:OE2	1:B:415:ARG:NH2	2.23	0.71
1:A:67:ILE:HD13	1:A:67:ILE:N	2.04	0.71
2:D:111:ARG:NH1	2:D:115:GLU:OE2	2.23	0.70
2:D:12:TRP:HA	2:D:159:PRO:HD3	1.74	0.70
1:B:139:ILE:HD13	1:B:150:VAL:HG21	1.73	0.70
2:G:283:VAL:CG2	2:G:325:SER:HA	2.20	0.70
1:A:6:THR:C	1:A:8:GLU:HG3	2.16	0.70
1:A:381:GLU:HG3	1:A:439:PRO:HA	1.71	0.70
1:A:186:ASP:OD1	1:A:188:GLN:NE2	2.25	0.70
1:B:349:LEU:HD12	1:B:349:LEU:C	2.15	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:280:ARG:HG3	2:G:298:GLY:HA2	1.71	0.70
2:G:26:ARG:HB2	2:G:68:ARG:O	1.92	0.70
2:D:166:ILE:HD12	2:D:166:ILE:C	2.17	0.69
2:G:326:LYS:HG3	2:G:334:ASN:HD21	1.57	0.69
1:A:104:GLY:C	1:A:106:PRO:CD	2.61	0.69
2:D:163:GLN:O	2:D:164:ARG:C	2.33	0.69
1:A:107:LEU:O	1:A:109:GLU:N	2.24	0.69
1:A:216:ARG:HD3	1:A:220:ASP:CG	2.17	0.69
1:A:269:VAL:HG23	1:A:270:SER:N	2.06	0.69
1:B:266:ILE:HD13	1:B:311:LYS:HD3	1.74	0.69
2:G:280:ARG:HH22	2:G:297:ARG:HH12	1.38	0.69
2:D:140:THR:CG2	2:D:141:SER:H	2.05	0.69
1:B:260:ASN:O	1:B:263:GLU:HB2	1.92	0.69
1:A:441:GLU:O	1:A:445:LYS:HD2	1.93	0.69
2:D:16:ARG:O	2:D:19:GLU:HG3	1.92	0.69
1:A:113:SER:O	1:A:258:ARG:NH2	2.26	0.69
2:D:271:ARG:N	2:D:274:ASP:OD2	2.26	0.69
1:A:102:LEU:HD13	1:A:103:GLY:H	1.58	0.69
1:B:220:ASP:OD1	1:B:220:ASP:N	2.25	0.69
2:G:205:HIS:C	2:G:205:HIS:CD2	2.71	0.69
2:G:214:TRP:CE2	2:G:349:PRO:HB3	2.28	0.69
1:A:102:LEU:HD21	1:A:108:ARG:O	1.92	0.69
1:B:271:GLU:HG2	1:B:273:PHE:HE1	1.58	0.69
1:B:457:ARG:HG3	1:B:457:ARG:HH21	1.57	0.69
1:A:6:THR:O	1:A:8:GLU:HB2	1.92	0.68
1:A:348:ASN:O	1:A:374:GLU:N	2.23	0.68
2:D:5:PRO:HG2	2:D:14:TRP:CE2	2.28	0.68
1:A:191:GLU:CB	1:A:274:ASP:HB2	2.19	0.68
1:B:5:GLN:HE21	1:B:7:ARG:N	1.91	0.68
2:D:28:ASP:OD1	2:D:30:THR:OG1	2.11	0.68
1:A:72:TYR:OH	1:A:94:ARG:NH1	2.27	0.68
1:A:107:LEU:HD12	1:A:108:ARG:N	2.09	0.68
1:A:216:ARG:NH1	1:A:220:ASP:OD2	2.18	0.68
1:A:265:ASN:ND2	1:A:267:ARG:HD2	2.08	0.68
1:A:7:ARG:CG	1:A:149:THR:HG23	2.15	0.68
1:B:5:GLN:HE22	1:B:7:ARG:CB	2.06	0.68
2:G:161:GLU:O	2:G:161:GLU:CG	2.35	0.68
2:D:97:GLY:C	2:D:98:GLN:HG2	2.20	0.67
2:D:214:TRP:CE2	2:D:349:PRO:HB3	2.28	0.67
1:B:260:ASN:OD1	5:B:601:SAM:N6	2.26	0.67
1:A:267:ARG:HA	1:A:311:LYS:HZ2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLU:OE1	2:D:373:ARG:NH1	2.27	0.67
1:A:347:PHE:O	1:A:379:THR:OG1	2.11	0.67
1:B:117:GLU:HA	1:B:117:GLU:OE1	1.94	0.67
1:E:468:GLU:O	1:E:471:ALA:HB3	1.95	0.67
1:B:118:ARG:HG2	1:B:118:ARG:HH11	1.59	0.67
1:A:7:ARG:HA	1:A:149:THR:HG23	1.76	0.67
1:B:68:ILE:HD12	1:B:68:ILE:C	2.18	0.67
2:D:280:ARG:C	2:D:283:VAL:HG12	2.19	0.67
1:B:191:GLU:HB3	1:B:274:ASP:HB2	1.72	0.67
2:D:38:VAL:HG23	2:D:98:GLN:OE1	1.92	0.67
2:D:306:ASP:OD1	2:D:306:ASP:N	2.28	0.67
2:D:67:ALA:C	2:D:68:ARG:HG2	2.19	0.67
2:D:11:GLY:C	2:D:159:PRO:HD2	2.20	0.67
2:D:12:TRP:N	2:D:12:TRP:CE3	2.62	0.67
2:G:70:VAL:HA	2:G:98:GLN:O	1.93	0.67
2:G:174:MET:HE1	2:G:386:GLU:HG3	1.77	0.66
1:A:112:ARG:O	1:A:114:LEU:N	2.28	0.66
2:D:136:LYS:HD2	2:D:137:MET:N	2.07	0.66
1:A:433:GLU:O	1:A:456:ASN:OD1	2.13	0.66
1:B:461:GLU:HB3	1:B:463:LEU:CD1	2.26	0.66
1:E:487:LEU:HD21	2:G:177:VAL:HG22	1.76	0.66
2:D:160:LEU:HB3	2:D:162:GLU:H	1.56	0.66
1:A:230:PHE:HB2	1:A:273:PHE:CE2	2.31	0.66
2:G:283:VAL:HG23	2:G:325:SER:HA	1.78	0.66
2:D:157:LEU:CG	2:D:164:ARG:HH11	2.05	0.66
1:A:201:CYS:HB3	1:A:245:ASN:HD22	1.60	0.65
1:A:367:LYS:NZ	1:A:462:GLU:HG3	2.10	0.65
1:A:102:LEU:HD12	1:A:103:GLY:H	1.61	0.65
2:D:174:MET:O	2:D:178:ARG:HG2	1.97	0.65
1:B:50:GLU:CB	1:B:67:ILE:HD11	2.19	0.65
1:B:347:PHE:O	1:B:379:THR:OG1	2.14	0.65
1:A:221:HIS:CE1	1:A:225:GLN:NE2	2.65	0.65
2:G:160:LEU:O	2:G:161:GLU:HB3	1.95	0.65
2:G:279:VAL:HG21	2:G:300:ALA:HB2	1.79	0.65
1:A:230:PHE:HB2	1:A:273:PHE:HE2	1.62	0.65
2:D:25:GLU:HG3	2:D:70:VAL:HB	1.79	0.65
1:B:270:SER:OG	1:B:271:GLU:N	2.29	0.65
1:A:139:ILE:HD13	1:A:150:VAL:HG21	1.78	0.65
1:A:118:ARG:HG3	1:A:119:ASN:H	1.60	0.64
1:C:491:LEU:HD21	2:D:173:LEU:HD11	1.78	0.64
1:C:480:ILE:HG23	2:D:180:VAL:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ASN:N	1:B:374:GLU:O	2.30	0.64
1:B:347:PHE:CD1	1:B:375:ARG:HB2	2.33	0.64
1:B:5:GLN:HE21	1:B:7:ARG:H	1.44	0.64
1:B:186:ASP:OD1	1:B:188:GLN:NE2	2.31	0.64
1:B:218:ILE:HD12	1:B:218:ILE:N	2.03	0.64
2:G:188:GLN:O	2:G:191:THR:HG22	1.98	0.64
1:A:106:PRO:HG2	1:A:108:ARG:CG	2.28	0.64
2:D:167:VAL:O	2:D:168:ALA:C	2.39	0.64
2:D:164:ARG:NH2	2:D:164:ARG:HG2	2.02	0.64
1:B:183:GLU:HG3	1:B:210:TRP:CH2	2.33	0.63
1:B:243:LEU:O	1:B:247:MET:HG3	1.98	0.63
2:D:158:PRO:O	2:D:160:LEU:O	2.16	0.63
2:G:47:SER:OG	2:G:85:LEU:O	2.16	0.63
1:A:194:TYR:HA	1:A:230:PHE:O	1.99	0.63
1:B:118:ARG:HH11	1:B:118:ARG:CG	2.12	0.63
1:B:201:CYS:HB3	1:B:245:ASN:HD22	1.63	0.63
2:D:188:GLN:O	2:D:191:THR:HG22	1.98	0.63
3:H:12:DA:H2"	3:H:13:DG:H5"	1.80	0.63
1:A:93:GLY:O	1:A:97:PRO:HG3	1.99	0.63
2:D:166:ILE:HD12	2:D:167:VAL:N	2.14	0.63
1:B:217:THR:HG23	1:B:220:ASP:OD2	1.98	0.63
2:G:47:SER:O	2:G:124:ARG:NH2	2.31	0.63
2:D:160:LEU:CD1	2:D:161:GLU:HB3	2.29	0.63
1:B:457:ARG:HG3	1:B:457:ARG:NH2	2.12	0.63
2:D:135:SER:OG	2:D:136:LYS:N	2.32	0.63
1:E:480:ILE:HG23	2:G:180:VAL:HG13	1.79	0.63
2:D:165:ARG:HG3	2:D:165:ARG:NH1	2.14	0.62
2:D:165:ARG:O	2:D:168:ALA:HB3	1.98	0.62
1:B:5:GLN:NE2	1:B:7:ARG:CA	2.62	0.62
1:B:271:GLU:CB	1:B:272:ARG:HA	2.20	0.62
1:B:118:ARG:HB3	1:B:118:ARG:NH1	2.14	0.62
1:E:467:VAL:O	1:E:470:VAL:HG12	2.00	0.62
1:B:432:SER:N	1:B:435:SER:HG	1.93	0.62
1:A:267:ARG:HA	1:A:311:LYS:NZ	2.14	0.62
2:D:71:ILE:CG1	2:D:98:GLN:O	2.38	0.62
1:E:479:GLU:O	1:E:483:ILE:HG12	1.98	0.62
2:G:118:PHE:CZ	2:G:158:PRO:HG3	2.34	0.62
1:A:484:MET:SD	1:C:477:GLU:HG3	2.39	0.62
2:D:202:VAL:HG21	2:D:357:ILE:HG21	1.82	0.62
2:G:157:LEU:HG	2:G:159:PRO:HD3	1.80	0.62
1:A:433:GLU:H	1:A:433:GLU:CD	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:PHE:HB2	1:B:273:PHE:CE2	2.34	0.62
2:G:249:LYS:HD3	2:G:282:PRO:CG	2.30	0.61
1:C:465:SER:HB3	1:C:468:GLU:OE2	1.99	0.61
2:G:115:GLU:OE2	2:G:117:GLU:HG3	2.00	0.61
1:A:191:GLU:HB3	1:A:274:ASP:CG	2.26	0.61
1:B:338:GLU:OE1	2:G:373:ARG:NH1	2.32	0.61
2:G:161:GLU:CD	2:G:161:GLU:C	2.66	0.61
2:D:146:THR:HG22	2:D:149:ASP:OD2	2.01	0.61
2:D:160:LEU:HB3	2:D:161:GLU:CA	2.29	0.61
1:B:484:MET:SD	1:E:477:GLU:HG3	2.40	0.61
1:B:107:LEU:O	1:B:110:THR:N	2.32	0.61
2:G:17:LEU:HD23	2:G:150:VAL:O	1.99	0.61
1:C:492:GLU:HA	1:C:493:ASN:HB2	1.82	0.61
1:B:100:ARG:O	1:B:112:ARG:NH1	2.33	0.61
2:G:271:ARG:N	2:G:274:ASP:OD2	2.34	0.61
2:D:249:LYS:HD3	2:D:282:PRO:HG3	1.82	0.61
1:E:470:VAL:HG13	1:E:471:ALA:N	2.15	0.61
1:A:72:TYR:CD2	1:A:98:TYR:CB	2.83	0.60
1:B:464:PRO:HG2	1:B:469:ILE:HD11	1.83	0.60
1:A:243:LEU:O	1:A:247:MET:HG2	2.00	0.60
2:D:279:VAL:HG22	2:D:279:VAL:O	2.00	0.60
1:B:279:ASN:O	5:B:601:SAM:HG1	2.01	0.60
1:B:350:HIS:HD2	1:B:374:GLU:HB2	1.66	0.60
2:G:280:ARG:NH2	2:G:297:ARG:HH12	1.97	0.60
2:G:28:ASP:OD1	2:G:30:THR:OG1	2.12	0.60
1:A:216:ARG:HG2	1:A:217:THR:H	1.64	0.60
1:B:222:ARG:NH2	1:B:227:ARG:HH22	1.99	0.60
2:G:161:GLU:OE1	2:G:161:GLU:C	2.44	0.60
1:A:272:ARG:HH11	1:A:272:ARG:CG	2.14	0.60
2:D:137:MET:CB	2:D:140:THR:CB	2.79	0.60
2:D:175:GLU:HA	2:D:178:ARG:HE	1.67	0.60
1:A:7:ARG:CB	1:A:11:ALA:HB2	2.32	0.60
1:A:141:PHE:HA	1:A:147:ILE:HD11	1.82	0.60
1:A:340:LYS:NZ	1:A:448:TYR:O	2.23	0.60
1:B:230:PHE:CD2	1:B:273:PHE:HE2	2.20	0.60
2:G:186:GLU:HA	2:G:189:LYS:HE3	1.84	0.60
2:D:47:SER:OG	2:D:85:LEU:O	2.20	0.60
1:B:439:PRO:HB2	1:B:441:GLU:OE1	2.02	0.60
2:D:47:SER:O	2:D:124:ARG:NH2	2.34	0.59
2:D:66:ARG:NH2	3:H:7:DG:O6	2.36	0.59
2:G:6:TYR:CD2	2:G:8:LEU:CD2	2.81	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLU:OE1	5:A:601:SAM:H1'	2.02	0.59
1:A:266:ILE:CD1	1:A:295:PRO:HD2	2.22	0.59
1:A:271:GLU:HG2	1:A:273:PHE:HE1	1.68	0.59
1:B:351:THR:HG21	1:B:414:TRP:HE1	1.67	0.59
1:B:484:MET:HE3	2:G:371:LEU:HD11	1.84	0.59
1:A:6:THR:O	1:A:6:THR:HG22	2.01	0.59
1:A:186:ASP:HA	1:A:210:TRP:CZ3	2.37	0.59
1:A:405:GLU:O	1:A:408:GLU:HG2	2.02	0.59
1:B:99:LEU:HA	1:B:102:LEU:HD23	1.79	0.59
1:B:418:ASP:OD1	1:B:421:ARG:NH2	2.35	0.59
1:A:71:GLU:HB3	1:A:72:TYR:HD1	1.63	0.59
1:A:418:ASP:OD1	1:A:421:ARG:NH2	2.36	0.59
1:C:465:SER:HA	1:C:468:GLU:OE2	2.02	0.59
2:D:15:VAL:HG21	2:D:157:LEU:HD13	1.84	0.59
2:D:26:ARG:HB2	2:D:68:ARG:O	2.03	0.59
1:B:141:PHE:HA	1:B:147:ILE:HD11	1.85	0.59
1:E:492:GLU:HA	1:E:493:ASN:C	2.28	0.59
1:B:407:PHE:O	1:B:411:ARG:HG3	2.03	0.59
1:A:112:ARG:O	1:A:115:PHE:N	2.36	0.58
1:C:490:LEU:O	1:C:493:ASN:ND2	2.36	0.58
1:B:5:GLN:NE2	1:B:7:ARG:N	2.50	0.58
1:B:71:GLU:HG2	1:B:72:TYR:CE1	2.37	0.58
2:G:279:VAL:HG12	2:G:279:VAL:O	2.04	0.58
1:A:186:ASP:CG	1:A:210:TRP:HH2	2.11	0.58
1:B:271:GLU:HG2	1:B:273:PHE:CE1	2.38	0.58
2:G:71:ILE:O	2:G:97:GLY:N	2.36	0.58
2:G:115:GLU:H	2:G:164:ARG:HH11	1.49	0.58
1:B:46:LEU:HD11	1:B:111:ILE:CD1	2.34	0.58
2:G:122:LEU:HD21	2:G:155:ILE:HB	1.85	0.58
2:D:162:GLU:HA	2:D:165:ARG:CG	2.33	0.58
1:B:197:ALA:HB1	5:B:601:SAM:O4'	2.03	0.58
2:G:176:ARG:HG3	2:G:176:ARG:HH11	1.69	0.58
1:A:102:LEU:HD22	1:A:108:ARG:CA	2.33	0.58
1:A:350:HIS:O	1:A:351:THR:CG2	2.51	0.58
2:D:69:LYS:HD2	2:D:102:THR:HA	1.86	0.58
1:A:112:ARG:C	1:A:114:LEU:N	2.59	0.58
2:D:136:LYS:CG	2:D:137:MET:H	2.17	0.58
1:A:102:LEU:HD11	1:A:108:ARG:O	2.03	0.58
1:C:479:GLU:O	1:C:483:ILE:HG12	2.03	0.58
2:D:11:GLY:C	2:D:159:PRO:CD	2.76	0.58
2:D:72:ARG:NH1	2:D:97:GLY:CA	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:GLU:O	1:B:489:GLU:HG3	2.04	0.58
2:G:115:GLU:N	2:G:164:ARG:HH11	2.01	0.58
2:D:163:GLN:C	2:D:165:ARG:N	2.61	0.58
2:D:122:LEU:HD21	2:D:155:ILE:HB	1.86	0.57
1:B:272:ARG:HH11	1:B:272:ARG:CG	2.17	0.57
1:B:340:LYS:NZ	1:B:448:TYR:O	2.25	0.57
1:B:375:ARG:O	1:B:375:ARG:CG	2.50	0.57
2:G:66:ARG:NH2	4:I:6:DG:O6	2.36	0.57
1:B:175:ARG:NH2	1:B:201:CYS:SG	2.75	0.57
1:B:269:VAL:O	1:B:270:SER:HB3	2.03	0.57
1:B:470:VAL:O	1:B:474:LEU:HG	2.04	0.57
1:A:440:VAL:O	1:A:443:VAL:HG12	2.04	0.57
2:D:146:THR:OG1	4:I:13:DA:OP1	2.18	0.57
1:B:343:LEU:HD23	1:B:347:PHE:HB2	1.87	0.57
1:B:455:PRO:HB2	1:B:456:ASN:ND2	2.19	0.57
2:D:163:GLN:C	2:D:166:ILE:HG23	2.29	0.57
1:B:99:LEU:CA	1:B:102:LEU:CD2	2.73	0.57
2:D:371:LEU:O	2:D:375:GLN:HG2	2.05	0.57
1:B:225:GLN:HE22	1:B:251:VAL:HA	1.69	0.57
1:B:461:GLU:HB3	1:B:463:LEU:HD11	1.86	0.57
1:A:5:GLN:NE2	1:A:7:ARG:HB2	2.19	0.57
1:B:350:HIS:ND1	1:B:351:THR:HG23	2.20	0.57
2:G:161:GLU:HA	2:G:164:ARG:HG3	1.86	0.57
1:A:271:GLU:C	1:A:272:ARG:HG3	2.29	0.57
1:A:405:GLU:O	1:A:408:GLU:N	2.38	0.57
1:B:222:ARG:HH21	1:B:227:ARG:HH22	1.51	0.57
2:D:5:PRO:HG2	2:D:14:TRP:CZ2	2.39	0.56
2:D:149:ASP:O	2:D:153:THR:HG23	2.04	0.56
2:D:349:PRO:HG2	2:D:354:GLN:HG2	1.87	0.56
1:B:383:TRP:HB2	1:B:417:TRP:CE2	2.40	0.56
1:B:440:VAL:O	1:B:443:VAL:HG12	2.04	0.56
2:G:371:LEU:O	2:G:375:GLN:HG2	2.05	0.56
1:A:7:ARG:HG2	1:A:11:ALA:HB1	1.78	0.56
2:D:165:ARG:HH11	2:D:165:ARG:CG	2.15	0.56
2:D:277:ILE:O	2:D:277:ILE:HG23	2.03	0.56
1:B:70:SER:O	1:B:73:ARG:HG3	2.05	0.56
1:B:474:LEU:HD22	1:E:485:GLU:OE2	2.05	0.56
1:A:36:HIS:ND1	1:A:121:ILE:O	2.34	0.56
2:D:37:PHE:CG	2:D:99:ILE:CD1	2.83	0.56
1:A:72:TYR:HD1	1:A:72:TYR:N	2.03	0.56
1:B:273:PHE:CD1	1:B:273:PHE:N	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:MET:HB2	2:D:140:THR:OG1	2.06	0.56
2:G:50:GLY:N	2:G:124:ARG:HH21	2.04	0.56
1:A:72:TYR:CD1	1:A:72:TYR:N	2.72	0.56
1:A:104:GLY:O	1:A:106:PRO:HD2	2.06	0.56
2:D:280:ARG:CA	2:D:283:VAL:HG12	2.35	0.56
2:G:137:MET:HB2	2:G:140:THR:OG1	2.06	0.56
1:A:5:GLN:NE2	1:A:7:ARG:N	2.52	0.56
1:B:71:GLU:HG2	1:B:72:TYR:CD1	2.40	0.56
1:B:191:GLU:HB2	1:B:274:ASP:HB2	1.86	0.56
1:B:347:PHE:CE1	1:B:375:ARG:HB2	2.40	0.56
1:A:102:LEU:CD2	1:A:108:ARG:O	2.53	0.56
1:A:467:VAL:HA	1:A:470:VAL:HG22	1.87	0.56
1:B:218:ILE:H	1:B:218:ILE:CD1	1.96	0.56
1:B:266:ILE:HD11	1:B:295:PRO:HD3	1.87	0.56
2:G:278:SER:OG	2:G:282:PRO:O	2.20	0.56
1:A:102:LEU:CD1	1:A:103:GLY:N	2.66	0.55
1:A:207:ALA:O	1:A:211:MET:HG3	2.05	0.55
2:G:68:ARG:HH11	2:G:68:ARG:CG	2.17	0.55
1:C:487:LEU:HD21	2:D:177:VAL:HG22	1.87	0.55
1:A:272:ARG:C	1:A:273:PHE:CD1	2.85	0.55
2:D:162:GLU:C	2:D:165:ARG:H	2.14	0.55
1:B:192:ALA:N	1:B:274:ASP:OD1	2.40	0.55
1:A:175:ARG:NH2	1:A:201:CYS:SG	2.78	0.55
1:C:466:PRO:CG	2:D:201:GLU:OE2	2.44	0.55
2:D:137:MET:HG2	2:D:140:THR:CA	2.36	0.55
2:G:288:VAL:HG12	2:G:289:ALA:N	2.21	0.55
1:A:118:ARG:CG	1:A:119:ASN:H	2.18	0.55
1:A:173:THR:HB	5:A:601:SAM:O	2.06	0.55
1:A:407:PHE:O	1:A:411:ARG:HG3	2.06	0.55
1:A:273:PHE:CD1	1:A:273:PHE:N	2.73	0.55
1:A:288:ARG:O	1:A:291:GLN:HB2	2.06	0.55
1:A:351:THR:HG21	1:A:414:TRP:HE1	1.71	0.55
2:G:133:THR:HA	2:G:136:LYS:HE2	1.89	0.55
1:B:72:TYR:CD1	1:B:72:TYR:N	2.72	0.55
1:B:233:GLU:OE1	5:B:601:SAM:HI'	2.06	0.55
3:H:2:DT:H2''	3:H:3:DG:C8	2.42	0.55
1:A:102:LEU:HD13	1:A:103:GLY:N	2.22	0.55
1:A:229:PHE:C	1:A:230:PHE:HD1	2.15	0.55
2:D:204:PRO:HG3	2:D:210:LEU:HD22	1.88	0.54
2:G:159:PRO:HA	2:G:161:GLU:H	1.69	0.54
2:G:202:VAL:HG21	2:G:357:ILE:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLN:HE22	1:A:7:ARG:CB	2.21	0.54
1:A:467:VAL:O	1:A:468:GLU:C	2.48	0.54
2:D:282:PRO:O	2:D:282:PRO:HG2	2.07	0.54
1:B:167:LEU:HD12	1:B:170:GLU:HG3	1.87	0.54
2:G:174:MET:O	2:G:178:ARG:HG3	2.07	0.54
1:A:13:GLU:O	1:A:14:ILE:C	2.50	0.54
1:B:123:CYS:HB2	1:B:129:LEU:HB2	1.89	0.54
1:A:44:ARG:HE	1:A:137:ASN:HA	1.73	0.54
1:A:98:TYR:CD1	1:A:98:TYR:C	2.85	0.54
1:B:200:THR:OG1	1:B:201:CYS:N	2.40	0.54
2:G:148:ASN:O	2:G:152:ASN:ND2	2.35	0.54
1:A:466:PRO:O	1:A:469:ILE:HB	2.08	0.54
2:D:224:ASP:HB3	2:D:305:ARG:HH21	1.71	0.54
1:B:5:GLN:HE22	1:B:7:ARG:CG	2.20	0.54
1:B:68:ILE:HD13	1:B:73:ARG:HG2	1.86	0.54
1:E:487:LEU:O	1:E:491:LEU:HD13	2.08	0.54
2:G:277:ILE:HG23	2:G:277:ILE:O	2.08	0.54
2:G:349:PRO:HG2	2:G:354:GLN:HG2	1.89	0.54
2:D:360:TYR:CZ	2:D:364:ILE:HD11	2.43	0.54
1:A:71:GLU:HB3	1:A:72:TYR:CE1	2.44	0.54
2:D:20:VAL:O	2:D:21:CYS:SG	2.65	0.54
1:B:192:ALA:CB	1:B:273:PHE:HD2	2.21	0.54
1:B:208:TYR:HA	1:B:229:PHE:HZ	1.74	0.54
1:B:268:ASN:OD1	1:B:268:ASN:N	2.41	0.54
2:G:360:TYR:CZ	2:G:364:ILE:HD11	2.42	0.54
1:A:13:GLU:OE2	1:A:16:ARG:NH1	2.41	0.53
2:G:205:HIS:CD2	2:G:206:PRO:O	2.61	0.53
1:A:457:ARG:CG	1:A:458:SER:H	2.21	0.53
1:B:473:LEU:HB3	1:E:484:MET:SD	2.48	0.53
1:A:200:THR:OG1	1:A:201:CYS:N	2.42	0.53
2:D:228:GLY:H	2:D:268:LYS:HD3	1.73	0.53
1:B:117:GLU:CD	1:B:118:ARG:H	2.17	0.53
1:B:191:GLU:CB	1:B:274:ASP:CB	2.74	0.53
2:G:165:ARG:HA	2:G:167:VAL:HG12	1.91	0.53
2:D:137:MET:CG	2:D:140:THR:N	2.71	0.53
1:B:223:ILE:HG22	1:B:228:THR:HG23	1.91	0.53
2:D:13:ARG:HH21	2:D:14:TRP:H	1.57	0.53
1:B:5:GLN:NE2	1:B:7:ARG:CG	2.72	0.53
1:B:7:ARG:HG2	1:B:11:ALA:HB2	1.89	0.53
1:B:319:ALA:HB3	1:B:375:ARG:HB3	1.89	0.53
1:A:5:GLN:O	1:A:6:THR:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HG23	1:A:98:TYR:OH	1.93	0.53
1:A:364:SER:HG	1:A:366:VAL:HG23	1.74	0.53
1:A:390:PRO:HB2	1:A:393:LEU:HD12	1.91	0.53
2:D:15:VAL:CG2	2:D:157:LEU:HB3	2.38	0.53
2:D:50:GLY:N	2:D:124:ARG:HH21	2.07	0.53
2:G:17:LEU:HD13	2:G:155:ILE:HD13	1.90	0.53
1:A:73:ARG:HH11	1:A:75:ARG:NH2	2.07	0.53
2:D:160:LEU:HB2	2:D:162:GLU:H	1.74	0.53
2:D:188:GLN:NE2	2:D:379:GLU:OE1	2.34	0.53
2:G:282:PRO:O	2:G:282:PRO:HG2	2.08	0.53
1:B:46:LEU:HD11	1:B:111:ILE:HD11	1.91	0.53
1:E:481:LEU:O	1:E:485:GLU:HG2	2.08	0.53
1:A:260:ASN:O	1:A:263:GLU:HG2	2.08	0.53
2:D:160:LEU:O	2:D:163:GLN:NE2	2.41	0.53
1:B:230:PHE:CB	1:B:273:PHE:CE2	2.92	0.53
2:G:20:VAL:HG11	2:G:114:ALA:CB	2.39	0.53
1:A:68:ILE:HG23	1:A:98:TYR:CE1	2.32	0.52
1:B:5:GLN:HE21	1:B:5:GLN:C	2.18	0.52
1:B:72:TYR:N	1:B:72:TYR:HD1	2.07	0.52
1:A:105:ASP:N	1:A:106:PRO:CD	2.73	0.52
1:A:279:ASN:O	5:A:601:SAM:HG1	2.10	0.52
2:D:391:ASP:OD1	2:D:395:ARG:CZ	2.55	0.52
1:B:5:GLN:HE22	1:B:7:ARG:CA	2.23	0.52
1:B:351:THR:HG21	1:B:414:TRP:NE1	2.25	0.52
2:G:146:THR:HG22	2:G:149:ASP:OD2	2.10	0.52
1:A:181:VAL:O	1:A:185:VAL:HG23	2.10	0.52
1:A:465:SER:HB3	1:A:468:GLU:OE1	2.09	0.52
1:B:194:TYR:HA	1:B:230:PHE:O	2.10	0.52
2:G:20:VAL:O	2:G:21:CYS:SG	2.67	0.52
1:A:4:PRO:HB3	1:A:145:ASP:HA	1.91	0.52
1:A:343:LEU:HD23	1:A:347:PHE:HB2	1.90	0.52
1:A:5:GLN:OE1	1:A:7:ARG:HD2	2.09	0.52
1:A:476:LYS:O	1:A:480:ILE:HG13	2.08	0.52
1:B:457:ARG:HG2	1:B:458:SER:H	1.73	0.52
2:G:199:LEU:HA	2:G:202:VAL:HG12	1.92	0.52
1:A:347:PHE:CE1	1:A:375:ARG:CD	2.92	0.52
2:D:176:ARG:HG3	2:D:176:ARG:HH11	1.74	0.52
1:B:36:HIS:ND1	1:B:121:ILE:O	2.38	0.51
2:D:37:PHE:CG	2:D:99:ILE:HD13	2.44	0.51
1:B:169:GLY:HA2	1:B:363:TYR:CB	2.33	0.51
1:A:5:GLN:NE2	1:A:5:GLN:CA	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:VAL:HG13	1:C:471:ALA:N	2.24	0.51
2:G:306:ASP:OD1	2:G:307:SER:N	2.43	0.51
1:A:467:VAL:O	1:A:470:VAL:HG22	2.10	0.51
1:A:102:LEU:CD1	1:A:108:ARG:O	2.58	0.51
1:B:5:GLN:NE2	1:B:7:ARG:HG3	2.25	0.51
1:B:98:TYR:O	1:B:102:LEU:HD22	2.10	0.51
2:D:16:ARG:HB2	2:D:19:GLU:CG	2.40	0.51
1:B:275:VAL:HG22	1:B:320:ARG:NH1	2.24	0.51
1:B:461:GLU:HA	1:B:462:GLU:OE2	2.10	0.51
2:G:37:PHE:CE2	2:G:99:ILE:HD11	2.46	0.51
1:A:473:LEU:HB3	1:C:484:MET:CE	2.41	0.51
1:B:106:PRO:O	1:B:109:GLU:CB	2.57	0.51
1:B:106:PRO:O	1:B:109:GLU:N	2.44	0.51
1:A:71:GLU:C	1:A:72:TYR:HD1	2.19	0.51
1:A:107:LEU:C	1:A:110:THR:CG2	2.68	0.51
1:A:457:ARG:CG	1:A:458:SER:N	2.73	0.51
1:A:485:GLU:O	1:A:489:GLU:HG3	2.10	0.51
1:B:207:ALA:O	1:B:211:MET:HG3	2.10	0.51
1:A:383:TRP:HB2	1:A:417:TRP:CE2	2.45	0.51
1:B:341:ARG:HG3	1:B:448:TYR:OH	2.11	0.51
2:G:66:ARG:O	2:G:102:THR:HG23	2.11	0.51
2:G:205:HIS:C	2:G:205:HIS:HD2	2.18	0.51
1:A:192:ALA:HB1	1:A:273:PHE:HD2	1.76	0.51
1:A:230:PHE:CB	1:A:273:PHE:CE2	2.89	0.51
2:D:229:GLN:HA	2:D:297:ARG:HG2	1.93	0.51
1:B:10:LEU:HD12	1:B:10:LEU:C	2.35	0.50
2:G:266:PRO:HB3	2:G:294:CYS:HB2	1.92	0.50
1:A:223:ILE:HG22	1:A:228:THR:HG23	1.94	0.50
1:A:225:GLN:HG2	1:A:251:VAL:HG12	1.92	0.50
1:A:265:ASN:HD21	1:A:267:ARG:CD	2.21	0.50
2:D:163:GLN:O	2:D:165:ARG:N	2.44	0.50
2:D:174:MET:HE1	2:D:386:GLU:HG3	1.93	0.50
1:B:272:ARG:HB3	1:B:312:LYS:O	2.10	0.50
1:B:303:LEU:HD12	1:B:336:PHE:CD1	2.47	0.50
1:B:476:LYS:O	1:B:480:ILE:HG13	2.12	0.50
2:G:115:GLU:H	2:G:164:ARG:NH1	2.09	0.50
1:E:465:SER:N	1:E:466:PRO:CD	2.73	0.50
2:G:280:ARG:NH2	2:G:297:ARG:HH11	2.09	0.50
1:A:46:LEU:HD11	1:A:111:ILE:HD11	1.94	0.50
1:B:229:PHE:C	1:B:230:PHE:HD1	2.19	0.50
2:G:136:LYS:CG	2:G:137:MET:N	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:ARG:NH2	2:D:14:TRP:O	2.44	0.50
2:D:385:LEU:O	2:D:389:ILE:HG12	2.11	0.50
1:B:191:GLU:HA	1:B:274:ASP:OD1	2.11	0.50
1:B:230:PHE:CB	1:B:273:PHE:HE2	2.23	0.50
2:D:164:ARG:H	2:D:164:ARG:HD2	1.75	0.50
1:A:72:TYR:HD2	1:A:98:TYR:CD1	2.29	0.50
2:D:173:LEU:HD13	2:D:389:ILE:HD12	1.93	0.50
2:G:191:THR:HA	2:G:194:LEU:HD13	1.94	0.50
2:G:326:LYS:CG	2:G:334:ASN:HD21	2.24	0.50
1:C:465:SER:CB	1:C:468:GLU:HG3	2.42	0.50
2:D:11:GLY:O	2:D:159:PRO:HD3	2.10	0.50
1:B:168:ALA:HA	1:B:169:GLY:C	2.36	0.50
1:A:457:ARG:HG2	1:A:458:SER:N	2.26	0.49
2:D:161:GLU:H	2:D:164:ARG:HD3	1.77	0.49
2:G:385:LEU:O	2:G:389:ILE:HG12	2.12	0.49
2:D:163:GLN:NE2	2:D:163:GLN:N	2.60	0.49
2:D:249:LYS:HD3	2:D:282:PRO:CG	2.41	0.49
1:B:68:ILE:CD1	1:B:68:ILE:C	2.86	0.49
1:B:464:PRO:CG	1:B:469:ILE:HD11	2.42	0.49
1:B:30:ILE:HA	1:B:33:TYR:CD2	2.46	0.49
2:G:72:ARG:HA	2:G:97:GLY:H	1.77	0.49
1:A:123:CYS:HB2	1:A:129:LEU:HB2	1.93	0.49
1:A:341:ARG:HG3	1:A:448:TYR:OH	2.11	0.49
1:B:16:ARG:O	1:B:20:ILE:HG13	2.13	0.49
1:B:242:GLY:O	1:B:246:MET:HG3	2.11	0.49
2:D:160:LEU:CB	2:D:161:GLU:HB2	2.27	0.49
2:G:13:ARG:HH21	2:G:13:ARG:HG3	1.76	0.49
1:A:199:GLY:H	5:A:601:SAM:HG2	1.77	0.49
2:D:161:GLU:C	2:D:161:GLU:OE1	2.55	0.49
1:A:481:LEU:HD11	1:C:481:LEU:HD13	1.94	0.49
1:B:265:ASN:HD21	1:B:267:ARG:HH11	1.61	0.49
1:B:465:SER:OG	1:B:467:VAL:HG22	2.12	0.49
2:G:6:TYR:HB2	2:G:14:TRP:CZ2	2.44	0.49
2:G:6:TYR:CG	2:G:14:TRP:HZ2	2.28	0.49
1:A:67:ILE:HA	1:A:108:ARG:HH12	1.77	0.49
2:D:160:LEU:O	2:D:163:GLN:CG	2.54	0.49
2:D:166:ILE:HD12	2:D:167:VAL:CA	2.43	0.49
2:G:253:GLY:O	2:G:287:ASN:ND2	2.45	0.49
1:A:208:TYR:HA	1:A:229:PHE:HZ	1.78	0.49
1:B:5:GLN:HE21	1:B:7:ARG:HB2	1.71	0.49
1:B:72:TYR:HE2	1:B:94:ARG:O	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:GLU:H	1:B:215:GLU:CD	2.19	0.49
1:B:280:PRO:HG3	1:B:323:MET:HE3	1.95	0.49
1:A:6:THR:C	1:A:8:GLU:CG	2.86	0.48
1:B:5:GLN:HE22	1:B:7:ARG:HG3	1.77	0.48
2:G:158:PRO:HG2	2:G:164:ARG:HD2	1.94	0.48
2:G:222:VAL:O	2:G:305:ARG:CB	2.61	0.48
2:G:254:ASP:OD1	2:G:254:ASP:N	2.36	0.48
1:A:44:ARG:NE	1:A:137:ASN:HA	2.28	0.48
2:D:162:GLU:O	2:D:163:GLN:C	2.51	0.48
2:D:191:THR:HA	2:D:194:LEU:HD13	1.95	0.48
1:B:433:GLU:H	1:B:433:GLU:CD	1.96	0.48
2:G:66:ARG:NH2	4:I:5:DT:C7	2.76	0.48
2:D:15:VAL:HG22	2:D:157:LEU:HB3	1.95	0.48
1:B:31:MET:O	1:B:35:GLU:HG2	2.13	0.48
2:G:115:GLU:N	2:G:164:ARG:NH1	2.61	0.48
1:A:5:GLN:HE21	1:A:5:GLN:C	2.20	0.48
1:A:13:GLU:O	1:A:16:ARG:HB3	2.13	0.48
2:D:166:ILE:HD12	2:D:167:VAL:HA	1.96	0.48
1:B:463:LEU:HD12	1:B:463:LEU:N	2.29	0.48
1:A:102:LEU:H	1:A:102:LEU:CD1	2.10	0.48
1:A:186:ASP:HA	1:A:210:TRP:CH2	2.48	0.48
1:A:351:THR:HG21	1:A:414:TRP:NE1	2.28	0.48
1:B:183:GLU:HG3	1:B:210:TRP:HH2	1.76	0.48
1:A:6:THR:O	1:A:7:ARG:C	2.55	0.48
1:A:7:ARG:CG	1:A:149:THR:CG2	2.84	0.48
1:A:175:ARG:NH1	1:A:201:CYS:SG	2.87	0.48
1:A:266:ILE:C	1:A:268:ASN:O	2.56	0.48
2:G:304:PRO:O	2:G:304:PRO:HG2	2.12	0.48
2:G:338:LYS:O	2:G:342:GLN:HG3	2.13	0.48
1:A:32:GLU:N	1:A:32:GLU:OE1	2.44	0.48
1:A:107:LEU:HD12	1:A:108:ARG:CA	2.43	0.48
1:A:350:HIS:ND1	1:A:351:THR:HG23	2.28	0.48
1:A:357:PRO:HD3	1:A:367:LYS:HD3	1.95	0.48
2:D:72:ARG:HG2	2:D:97:GLY:H	1.79	0.48
1:B:200:THR:HA	1:B:238:PRO:O	2.13	0.48
2:D:190:ASP:HA	2:D:193:LEU:HD13	1.96	0.48
1:B:7:ARG:HA	1:B:149:THR:CG2	2.44	0.48
1:B:118:ARG:HB3	1:B:118:ARG:CZ	2.44	0.48
1:B:321:CYS:HB3	1:B:373:PHE:CZ	2.49	0.48
1:B:456:ASN:ND2	1:B:456:ASN:N	2.60	0.48
2:G:149:ASP:O	2:G:153:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:PRO:HA	2:D:160:LEU:C	2.39	0.48
1:B:192:ALA:HB1	1:B:273:PHE:HD2	1.79	0.48
1:A:168:ALA:HA	1:A:169:GLY:C	2.38	0.47
2:D:184:ARG:NH2	2:D:375:GLN:HB3	2.16	0.47
2:D:307:SER:O	2:D:348:LEU:HD11	2.14	0.47
1:B:148:PHE:O	1:B:151:SER:OG	2.23	0.47
1:E:465:SER:O	1:E:468:GLU:HG2	2.14	0.47
1:A:44:ARG:HG2	1:A:44:ARG:HH11	1.79	0.47
1:A:51:GLU:O	1:A:54:GLU:HG2	2.14	0.47
2:D:158:PRO:O	2:D:160:LEU:C	2.57	0.47
1:B:32:GLU:OE1	1:B:32:GLU:N	2.45	0.47
1:B:350:HIS:CD2	1:B:374:GLU:HB2	2.49	0.47
1:A:271:GLU:HG2	1:A:273:PHE:CE1	2.47	0.47
1:A:303:LEU:HD12	1:A:336:PHE:CD1	2.49	0.47
2:D:158:PRO:O	2:D:163:GLN:HG2	2.15	0.47
1:B:72:TYR:OH	1:B:94:ARG:NH1	2.47	0.47
2:G:279:VAL:HG13	2:G:336:ILE:HB	1.96	0.47
1:A:275:VAL:HG22	1:A:320:ARG:NH1	2.30	0.47
2:D:68:ARG:NH1	2:D:68:ARG:CG	2.72	0.47
1:B:102:LEU:CB	1:B:112:ARG:CG	2.89	0.47
1:B:169:GLY:CA	1:B:363:TYR:HB2	2.34	0.47
1:B:364:SER:OG	1:B:366:VAL:HG23	2.15	0.47
2:G:25:GLU:HG3	2:G:70:VAL:HB	1.96	0.47
2:G:146:THR:HG22	2:G:149:ASP:CG	2.39	0.47
1:B:7:ARG:HA	1:B:149:THR:HG23	1.96	0.47
1:B:219:GLU:O	1:B:223:ILE:HG13	2.14	0.47
2:G:9:PRO:HB2	2:G:12:TRP:CE3	2.50	0.47
1:A:267:ARG:NH1	1:A:267:ARG:CG	2.73	0.47
1:C:468:GLU:H	1:C:468:GLU:HG2	1.51	0.47
1:B:5:GLN:NE2	1:B:5:GLN:C	2.73	0.47
1:B:44:ARG:HH11	1:B:44:ARG:HG2	1.79	0.47
1:B:235:LYS:CD	1:B:236:PRO:HD2	2.39	0.47
1:B:457:ARG:HD3	1:B:458:SER:O	2.14	0.47
2:G:222:VAL:O	2:G:305:ARG:HB2	2.14	0.47
2:D:218:ARG:HG3	2:D:345:PHE:CE1	2.50	0.47
1:B:294:PHE:CE1	1:B:304:LEU:HD13	2.50	0.47
2:G:6:TYR:CG	2:G:14:TRP:CZ2	3.03	0.47
2:G:349:PRO:HG2	2:G:354:GLN:CG	2.45	0.47
1:A:7:ARG:CG	1:A:11:ALA:CB	2.65	0.47
2:D:163:GLN:NE2	2:D:163:GLN:H	2.13	0.47
1:A:396:PHE:CE2	1:A:402:ILE:HD12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:SER:O	1:A:435:SER:N	2.43	0.47
1:A:197:ALA:HB1	5:A:601:SAM:O4'	2.14	0.47
1:C:466:PRO:HG2	1:C:467:VAL:H	1.80	0.47
2:D:173:LEU:O	2:D:177:VAL:HG23	2.15	0.47
1:B:296:ILE:HG23	2:G:373:ARG:NH1	2.30	0.47
2:G:193:LEU:O	2:G:197:THR:HG23	2.15	0.47
1:A:350:HIS:CD2	1:A:374:GLU:HB2	2.50	0.46
2:D:163:GLN:N	2:D:163:GLN:CD	2.73	0.46
2:D:165:ARG:NH1	2:D:165:ARG:CG	2.73	0.46
2:D:224:ASP:OD1	2:D:224:ASP:N	2.48	0.46
1:B:191:GLU:CA	1:B:274:ASP:OD1	2.63	0.46
1:B:489:GLU:O	1:B:493:ASN:HB2	2.15	0.46
1:A:375:ARG:CG	1:A:375:ARG:O	2.62	0.46
1:B:72:TYR:CD2	1:B:98:TYR:CG	3.03	0.46
1:B:181:VAL:O	1:B:185:VAL:HG23	2.15	0.46
1:B:199:GLY:CA	5:B:601:SAM:HA	2.44	0.46
1:B:215:GLU:CD	1:B:215:GLU:N	2.73	0.46
1:B:274:ASP:OD2	1:B:314:LYS:HE3	2.15	0.46
1:B:396:PHE:CE2	1:B:402:ILE:HD12	2.49	0.46
1:E:470:VAL:CG1	1:E:471:ALA:N	2.79	0.46
2:G:218:ARG:HG3	2:G:345:PHE:CE1	2.51	0.46
1:B:230:PHE:CG	1:B:273:PHE:HE2	2.33	0.46
1:B:348:ASN:O	1:B:374:GLU:O	2.34	0.46
2:G:136:LYS:HG3	2:G:137:MET:O	2.15	0.46
2:D:162:GLU:CD	2:D:165:ARG:NH1	2.74	0.46
1:A:189:ILE:HA	1:A:190:GLY:HA2	1.64	0.46
1:A:367:LYS:HB2	1:A:367:LYS:HE2	1.57	0.46
1:B:275:VAL:HG22	1:B:320:ARG:HH11	1.80	0.46
1:A:278:THR:OG1	1:A:280:PRO:HD3	2.15	0.46
1:C:491:LEU:HD23	1:C:491:LEU:HA	1.55	0.46
1:B:364:SER:O	1:B:365:ASP:HB2	2.16	0.46
2:G:71:ILE:O	2:G:98:GLN:N	2.46	0.46
2:G:206:PRO:HA	2:G:216:TRP:CH2	2.51	0.46
2:D:167:VAL:CG1	2:D:168:ALA:N	2.78	0.46
1:B:17:ALA:O	1:B:21:MET:HG3	2.16	0.46
1:E:473:LEU:HA	1:E:476:LYS:HG3	1.98	0.46
2:G:136:LYS:HG3	2:G:137:MET:H	1.78	0.46
4:I:19:DC:H2''	4:I:20:DA:C8	2.50	0.46
2:D:157:LEU:HA	2:D:158:PRO:HD2	1.22	0.46
1:B:52:GLU:O	1:B:55:ALA:HB3	2.16	0.46
3:H:20:DT:H2''	3:H:21:DG:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:160:LEU:N	2:D:160:LEU:HD23	2.31	0.46
1:B:175:ARG:NH1	1:B:201:CYS:SG	2.88	0.46
1:B:463:LEU:CD1	1:B:463:LEU:N	2.78	0.46
1:A:96:ILE:N	1:A:97:PRO:HD2	2.31	0.45
1:A:195:ASP:OD1	1:A:278:THR:OG1	2.29	0.45
2:D:137:MET:HB3	2:D:140:THR:HB	1.98	0.45
2:D:166:ILE:C	2:D:166:ILE:CD1	2.85	0.45
1:B:118:ARG:CG	1:B:118:ARG:NH1	2.73	0.45
1:B:474:LEU:CD2	1:E:484:MET:HG2	2.46	0.45
2:D:22:LEU:HG	2:D:110:ASN:HB3	1.96	0.45
1:B:99:LEU:HD23	1:B:102:LEU:HD21	1.98	0.45
1:B:442:GLU:O	1:B:446:ARG:HG3	2.16	0.45
2:G:136:LYS:HD3	2:G:145:VAL:CG1	2.46	0.45
1:A:266:ILE:O	1:A:268:ASN:O	2.34	0.45
1:A:348:ASN:O	1:A:374:GLU:O	2.35	0.45
1:A:350:HIS:O	1:A:351:THR:HG22	2.16	0.45
1:A:350:HIS:HD2	1:A:374:GLU:HB2	1.81	0.45
1:B:99:LEU:O	1:B:102:LEU:HD23	2.16	0.45
1:B:353:VAL:HB	1:B:370:LEU:HB2	1.97	0.45
2:G:288:VAL:CG1	2:G:289:ALA:N	2.79	0.45
1:A:440:VAL:O	1:A:444:LYS:HG3	2.17	0.45
2:D:71:ILE:O	2:D:72:ARG:HG3	2.16	0.45
2:D:164:ARG:H	2:D:164:ARG:CD	2.30	0.45
1:B:46:LEU:HD11	1:B:111:ILE:HD13	1.99	0.45
1:E:469:ILE:HG23	1:E:470:VAL:N	2.31	0.45
1:A:200:THR:HA	1:A:238:PRO:O	2.16	0.45
1:A:247:MET:HE2	1:A:247:MET:HB3	1.82	0.45
1:A:465:SER:CB	1:A:468:GLU:OE1	2.65	0.45
2:D:137:MET:CB	2:D:140:THR:HB	2.47	0.45
2:G:184:ARG:O	2:G:188:GLN:HG3	2.17	0.45
1:A:235:LYS:HD3	1:A:236:PRO:HD2	1.99	0.45
2:D:236:TYR:HB3	2:D:261:ILE:HD11	1.97	0.45
2:G:72:ARG:NH1	2:G:96:ASP:OD1	2.49	0.45
1:A:476:LYS:HE3	1:A:476:LYS:HB2	1.78	0.45
2:D:142:TYR:CE2	2:D:144:ALA:HB3	2.52	0.45
1:B:287:GLY:HA2	1:B:291:GLN:OE1	2.15	0.45
1:B:364:SER:OG	1:B:366:VAL:HB	2.16	0.45
1:A:53:TRP:CD1	1:A:56:GLN:HE21	2.22	0.45
1:A:215:GLU:OE2	1:A:221:HIS:CD2	2.70	0.45
1:A:463:LEU:HD22	1:A:464:PRO:HD3	1.99	0.45
1:A:478:ARG:HG2	1:C:481:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:ARG:HD2	2:D:164:ARG:N	2.32	0.45
1:B:51:GLU:O	1:B:54:GLU:HG2	2.17	0.45
1:B:461:GLU:C	1:B:462:GLU:CD	2.85	0.45
2:G:71:ILE:HG12	2:G:98:GLN:C	2.39	0.45
1:A:221:HIS:HE1	1:A:225:GLN:NE2	2.14	0.45
2:D:338:LYS:O	2:D:342:GLN:HG3	2.17	0.45
1:B:107:LEU:O	1:B:108:ARG:C	2.60	0.45
1:B:117:GLU:HG3	1:B:236:PRO:HG2	1.99	0.45
1:A:13:GLU:HG3	1:A:138:GLU:OE2	2.17	0.44
1:A:215:GLU:OE2	1:A:221:HIS:HD2	1.99	0.44
1:B:233:GLU:CD	5:B:601:SAM:HI'	2.43	0.44
1:A:294:PHE:CE1	1:A:304:LEU:HD13	2.52	0.44
1:A:321:CYS:HB3	1:A:373:PHE:CZ	2.52	0.44
1:A:395:LYS:HG3	1:A:396:PHE:O	2.17	0.44
1:A:439:PRO:HB2	1:A:441:GLU:OE2	2.16	0.44
2:D:166:ILE:O	2:D:169:LYS:HB3	2.17	0.44
2:G:118:PHE:CD1	2:G:164:ARG:NH2	2.85	0.44
2:G:186:GLU:HA	2:G:189:LYS:HG3	1.99	0.44
1:A:13:GLU:O	1:A:16:ARG:CB	2.65	0.44
1:B:265:ASN:O	1:B:268:ASN:OD1	2.35	0.44
1:A:30:ILE:HA	1:A:33:TYR:CD2	2.52	0.44
2:G:137:MET:HA	2:G:140:THR:HG23	1.98	0.44
1:A:31:MET:O	1:A:35:GLU:HG2	2.17	0.44
1:A:67:ILE:CB	1:A:68:ILE:HD13	2.47	0.44
1:B:476:LYS:HE2	1:B:476:LYS:HB2	1.78	0.44
2:G:22:LEU:HG	2:G:110:ASN:HB3	1.98	0.44
1:A:280:PRO:HG2	1:A:323:MET:HE3	2.00	0.44
1:A:348:ASN:N	1:A:374:GLU:O	2.48	0.44
1:C:487:LEU:HD12	1:C:487:LEU:HA	1.82	0.44
2:D:71:ILE:O	2:D:97:GLY:N	2.51	0.44
2:D:97:GLY:C	2:D:98:GLN:CG	2.89	0.44
1:B:112:ARG:HB3	1:B:112:ARG:CZ	2.48	0.44
1:A:5:GLN:NE2	1:A:5:GLN:C	2.76	0.44
1:C:480:ILE:O	1:C:484:MET:HG2	2.18	0.44
1:B:118:ARG:NH1	1:B:118:ARG:CB	2.81	0.44
2:G:136:LYS:HD3	2:G:145:VAL:HG11	2.00	0.44
2:G:337:THR:H	2:G:340:ASP:HB2	1.82	0.44
1:A:218:ILE:H	1:A:218:ILE:CD1	2.09	0.44
1:B:71:GLU:CG	1:B:72:TYR:CE1	3.00	0.44
1:B:225:GLN:NE2	1:B:251:VAL:HA	2.32	0.44
1:B:467:VAL:O	1:B:470:VAL:HG22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:26:ARG:CB	2:G:68:ARG:O	2.65	0.44
2:G:142:TYR:HA	2:G:143:PRO:HD3	1.86	0.44
1:B:107:LEU:HD12	1:B:107:LEU:O	2.18	0.44
1:B:266:ILE:CD1	1:B:295:PRO:HD3	2.48	0.44
1:A:107:LEU:C	1:A:109:GLU:N	2.69	0.43
1:A:375:ARG:O	1:A:375:ARG:HG2	2.18	0.43
2:D:16:ARG:O	2:D:19:GLU:CG	2.64	0.43
1:B:396:PHE:HE2	1:B:402:ILE:HD12	1.83	0.43
1:B:440:VAL:O	1:B:444:LYS:HG3	2.18	0.43
1:A:74:TRP:HZ2	1:A:137:ASN:HB3	1.82	0.43
2:D:70:VAL:O	2:D:108:ARG:NH2	2.51	0.43
2:D:80:THR:HG21	2:D:147:ASP:OD1	2.18	0.43
2:D:164:ARG:NH2	2:D:164:ARG:CG	2.73	0.43
2:D:191:THR:HG21	2:D:375:GLN:NE2	2.33	0.43
1:B:71:GLU:OE1	1:B:72:TYR:CE1	2.70	0.43
1:B:244:VAL:O	1:B:248:LEU:HB2	2.18	0.43
1:B:411:ARG:O	1:B:415:ARG:HG2	2.17	0.43
1:B:481:LEU:HD11	1:E:481:LEU:HD13	1.99	0.43
2:D:14:TRP:CZ3	2:D:156:PRO:HB3	2.53	0.43
2:D:101:SER:O	2:D:104:PHE:HD1	2.00	0.43
2:D:146:THR:HG22	2:D:149:ASP:CG	2.42	0.43
1:A:36:HIS:HA	1:A:39:TRP:CD1	2.54	0.43
1:A:104:GLY:CA	1:A:106:PRO:HD2	2.44	0.43
1:B:195:ASP:HB3	1:B:198:CYS:HB3	2.00	0.43
1:B:350:HIS:O	1:B:351:THR:CG2	2.67	0.43
2:G:326:LYS:O	2:G:334:ASN:ND2	2.51	0.43
1:A:31:MET:O	1:A:34:VAL:HG12	2.18	0.43
1:A:31:MET:HB3	1:A:32:GLU:OE1	2.17	0.43
1:A:146:ASP:O	1:A:150:VAL:HG23	2.19	0.43
1:A:325:VAL:HB	1:A:329:THR:OG1	2.17	0.43
2:D:184:ARG:HE	2:D:375:GLN:CB	2.31	0.43
1:B:93:GLY:O	1:B:97:PRO:HG3	2.18	0.43
1:B:348:ASN:HB3	1:B:376:PRO:HD2	2.00	0.43
2:G:20:VAL:HG11	2:G:114:ALA:HB2	1.98	0.43
2:G:176:ARG:O	2:G:180:VAL:HG23	2.18	0.43
1:A:240:PHE:O	1:A:244:VAL:HG23	2.18	0.43
2:D:140:THR:HG22	2:D:141:SER:OG	2.18	0.43
2:D:279:VAL:CG2	2:D:336:ILE:O	2.66	0.43
2:D:341:LEU:O	2:D:344:VAL:HG22	2.19	0.43
1:A:201:CYS:HB3	1:A:245:ASN:ND2	2.31	0.43
2:D:217:VAL:HG13	2:D:346:ILE:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:255:LEU:HG	2:D:256:HIS:ND1	2.34	0.43
2:G:136:LYS:CG	2:G:137:MET:H	2.29	0.43
2:G:279:VAL:CG1	2:G:336:ILE:O	2.66	0.43
1:A:68:ILE:N	1:A:68:ILE:CD1	2.73	0.43
1:A:223:ILE:O	1:A:228:THR:HG23	2.18	0.43
2:D:16:ARG:NE	2:D:152:ASN:OD1	2.52	0.43
2:D:184:ARG:O	2:D:188:GLN:HG3	2.18	0.43
2:D:303:ARG:HE	2:D:303:ARG:HB2	1.57	0.43
1:B:325:VAL:HB	1:B:329:THR:OG1	2.19	0.43
1:B:408:GLU:O	1:B:411:ARG:HB2	2.19	0.43
1:B:481:LEU:O	1:B:485:GLU:HG3	2.19	0.43
2:D:72:ARG:O	2:D:73:SER:C	2.61	0.43
1:B:349:LEU:HA	1:B:373:PHE:CA	2.43	0.43
1:A:107:LEU:HD12	1:A:108:ARG:HA	2.01	0.43
1:A:167:LEU:HD23	1:A:167:LEU:HA	1.77	0.43
2:D:255:LEU:HG	2:D:256:HIS:CE1	2.54	0.43
1:B:102:LEU:N	1:B:112:ARG:HD2	2.33	0.43
1:B:191:GLU:OE2	1:B:320:ARG:NH1	2.44	0.43
2:G:189:LYS:O	2:G:192:GLU:OE1	2.37	0.43
1:A:47:ASP:OD1	1:A:75:ARG:NE	2.52	0.42
1:A:319:ALA:HB3	1:A:375:ARG:HB3	2.01	0.42
1:A:463:LEU:HD23	1:A:463:LEU:HA	1.87	0.42
1:B:240:PHE:O	1:B:244:VAL:HG23	2.18	0.42
1:A:5:GLN:HB3	1:A:6:THR:H	1.61	0.42
1:A:387:LEU:HG	1:A:388:PRO:HD2	2.02	0.42
2:D:149:ASP:O	2:D:152:ASN:N	2.48	0.42
1:A:195:ASP:HB3	1:A:198:CYS:HB3	2.02	0.42
1:A:269:VAL:CG2	1:A:270:SER:N	2.75	0.42
2:D:243:LEU:HB3	2:D:293:CYS:HA	2.01	0.42
1:B:31:MET:HB3	1:B:32:GLU:OE1	2.20	0.42
1:B:196:PRO:HD2	1:B:278:THR:OG1	2.20	0.42
1:A:10:LEU:O	1:A:14:ILE:HG12	2.20	0.42
1:A:118:ARG:CG	1:A:119:ASN:N	2.83	0.42
1:A:405:GLU:C	1:A:408:GLU:H	2.28	0.42
2:D:136:LYS:CG	2:D:137:MET:N	2.80	0.42
2:G:118:PHE:HB3	2:G:164:ARG:NH1	2.35	0.42
1:A:53:TRP:HD1	1:A:56:GLN:NE2	2.07	0.42
1:A:149:THR:O	1:A:153:VAL:HG23	2.19	0.42
1:A:360:PHE:CE2	1:A:368:THR:HG21	2.54	0.42
1:A:431:LEU:HA	1:A:435:SER:OG	2.20	0.42
2:D:189:LYS:HE3	2:D:189:LYS:HB2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:PRO:HG2	2:D:354:GLN:CG	2.49	0.42
1:B:236:PRO:HG3	1:B:258:ARG:CZ	2.49	0.42
1:A:36:HIS:CE1	1:A:122:VAL:HA	2.54	0.42
2:D:37:PHE:HE1	2:D:60:GLY:HA2	1.85	0.42
1:A:244:VAL:O	1:A:248:LEU:HB2	2.20	0.42
1:A:265:ASN:O	1:A:268:ASN:O	2.38	0.42
2:D:5:PRO:HG2	2:D:14:TRP:NE1	2.34	0.42
1:A:199:GLY:O	5:A:601:SAM:OXT	2.37	0.42
1:A:262:LEU:HD11	1:A:301:THR:HG23	2.01	0.42
1:A:327:GLU:HG3	1:A:367:LYS:O	2.19	0.42
1:B:4:PRO:HB3	1:B:145:ASP:HA	2.01	0.42
1:B:7:ARG:O	1:B:11:ALA:N	2.37	0.42
1:A:102:LEU:CD2	1:A:108:ARG:CA	2.98	0.42
1:C:465:SER:O	1:C:468:GLU:HG3	2.18	0.42
2:D:52:ILE:CG2	2:D:55:PRO:HG3	2.50	0.42
2:D:80:THR:HG23	2:D:103:GLY:O	2.20	0.42
2:D:224:ASP:OD1	2:D:303:ARG:O	2.37	0.42
1:B:387:LEU:HG	1:B:388:PRO:HD2	2.02	0.42
1:B:474:LEU:HD23	1:E:484:MET:HG2	2.01	0.42
5:B:601:SAM:H8	5:B:601:SAM:H2'	1.91	0.42
2:G:359:ALA:O	2:G:363:GLN:HG3	2.19	0.42
1:A:21:MET:SD	1:A:33:TYR:HA	2.60	0.42
1:A:208:TYR:HB2	1:A:229:PHE:CZ	2.55	0.42
1:C:492:GLU:HA	1:C:493:ASN:C	2.44	0.42
2:D:167:VAL:O	2:D:170:VAL:N	2.52	0.42
2:G:20:VAL:HG11	2:G:114:ALA:HB3	2.01	0.42
1:A:487:LEU:O	1:A:491:LEU:HG	2.19	0.41
2:D:6:TYR:CD1	2:D:7:LYS:O	2.73	0.41
2:D:192:GLU:CD	2:D:372:LYS:HE3	2.45	0.41
1:B:118:ARG:CZ	1:B:118:ARG:CB	2.98	0.41
1:B:236:PRO:HG3	1:B:258:ARG:NH1	2.34	0.41
1:B:252:THR:HG22	1:B:253:VAL:HG23	2.02	0.41
1:B:262:LEU:HD12	1:B:286:GLU:HG3	2.02	0.41
2:G:163:GLN:O	2:G:166:ILE:HG23	2.19	0.41
1:A:102:LEU:HD21	1:A:111:ILE:HB	2.03	0.41
1:C:476:LYS:O	1:C:480:ILE:HG13	2.20	0.41
2:D:137:MET:CG	2:D:140:THR:H	2.20	0.41
1:B:13:GLU:O	1:B:16:ARG:N	2.54	0.41
1:B:474:LEU:HD22	1:E:485:GLU:CD	2.44	0.41
1:E:466:PRO:HG2	1:E:467:VAL:H	1.85	0.41
2:G:252:PHE:HB3	2:G:287:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LEU:HA	1:A:373:PHE:HA	2.02	0.41
2:D:37:PHE:HD2	2:D:99:ILE:CD1	2.07	0.41
2:D:87:ASN:C	2:D:88:ILE:HG13	2.44	0.41
2:D:154:LEU:HA	2:D:154:LEU:HD23	1.83	0.41
1:B:189:ILE:HA	1:B:190:GLY:HA2	1.65	0.41
1:B:311:LYS:HE2	1:B:311:LYS:HB3	1.82	0.41
1:A:275:VAL:HG22	1:A:320:ARG:HH11	1.86	0.41
2:D:321:GLU:N	2:D:322:PRO:HD2	2.36	0.41
1:A:5:GLN:NE2	1:A:7:ARG:CB	2.81	0.41
1:A:111:ILE:O	1:A:112:ARG:C	2.59	0.41
1:A:457:ARG:HG2	1:A:458:SER:H	1.84	0.41
2:D:79:ALA:O	2:D:83:PRO:HB3	2.21	0.41
1:B:278:THR:HG23	1:B:280:PRO:HD3	2.03	0.41
2:G:111:ARG:NH1	2:G:115:GLU:HG2	2.34	0.41
1:A:39:TRP:HA	1:A:240:PHE:HZ	1.85	0.41
1:A:83:PRO:HG2	1:A:86:GLU:HB2	2.01	0.41
2:D:199:LEU:HA	2:D:202:VAL:HG12	2.01	0.41
2:D:224:ASP:HB3	2:D:305:ARG:HH22	1.78	0.41
2:D:291:LEU:HD23	2:D:292:ALA:N	2.36	0.41
2:D:359:ALA:O	2:D:363:GLN:HG3	2.20	0.41
1:B:39:TRP:HA	1:B:240:PHE:HZ	1.85	0.41
1:B:45:PHE:HE2	1:B:248:LEU:HD13	1.85	0.41
2:G:255:LEU:HG	2:G:256:HIS:ND1	2.34	0.41
1:A:6:THR:HA	1:A:8:GLU:CG	2.34	0.41
1:A:473:LEU:HB3	1:C:484:MET:HE1	2.03	0.41
1:B:266:ILE:CG1	1:B:295:PRO:HD3	2.51	0.41
1:B:282:PHE:N	1:B:282:PHE:CD1	2.89	0.41
1:A:102:LEU:HD12	1:A:103:GLY:N	2.33	0.41
1:A:348:ASN:HB3	1:A:376:PRO:HD2	2.01	0.41
1:A:367:LYS:HZ1	1:A:462:GLU:HG3	1.84	0.41
2:D:66:ARG:O	2:D:102:THR:CG2	2.63	0.41
2:D:375:GLN:HG2	2:D:375:GLN:H	1.71	0.41
1:B:47:ASP:OD2	1:B:74:TRP:N	2.52	0.41
1:B:130:LYS:O	1:B:134:GLN:HG2	2.21	0.41
2:G:75:ASP:OD2	2:G:108:ARG:NH2	2.43	0.41
2:G:169:LYS:HD3	2:G:398:LEU:HG	2.03	0.41
2:G:211:PRO:HA	2:G:212:PRO:HD3	1.94	0.41
1:A:31:MET:HE1	1:A:171:PHE:HZ	1.86	0.41
1:A:67:ILE:HB	1:A:68:ILE:HD13	2.03	0.41
1:A:352:VAL:HG11	1:A:384:TYR:CZ	2.56	0.41
2:D:28:ASP:HA	2:D:29:PRO:HD2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:ARG:CZ	2:D:97:GLY:HA2	2.51	0.41
2:D:176:ARG:O	2:D:180:VAL:HG23	2.21	0.41
2:D:337:THR:H	2:D:340:ASP:HB2	1.85	0.41
1:B:31:MET:HE1	1:B:171:PHE:HZ	1.86	0.41
1:B:31:MET:HG3	1:B:35:GLU:OE1	2.21	0.41
1:B:208:TYR:OH	1:B:212:LYS:NZ	2.54	0.41
1:B:210:TRP:O	1:B:213:GLN:N	2.53	0.41
1:B:383:TRP:CH2	1:B:385:TYR:HB2	2.56	0.41
2:G:173:LEU:O	2:G:177:VAL:HG23	2.21	0.41
2:G:184:ARG:NH2	2:G:375:GLN:HB3	2.24	0.41
1:A:38:ALA:HB1	1:A:244:VAL:HG21	2.03	0.41
1:C:470:VAL:CG1	1:C:471:ALA:N	2.84	0.41
1:B:6:THR:O	1:B:6:THR:OG1	2.37	0.41
1:B:348:ASN:O	1:B:374:GLU:CA	2.68	0.41
1:A:242:GLY:O	1:A:246:MET:HG3	2.21	0.40
1:B:457:ARG:O	1:B:458:SER:C	2.63	0.40
2:G:96:ASP:O	2:G:98:GLN:HG2	2.21	0.40
1:A:265:ASN:CG	1:A:267:ARG:HD2	2.45	0.40
1:A:306:LEU:O	1:A:310:MET:HG3	2.22	0.40
2:D:75:ASP:OD1	2:D:108:ARG:HG3	2.21	0.40
2:D:288:VAL:HG12	2:D:289:ALA:N	2.35	0.40
1:B:358:GLY:HA2	1:B:365:ASP:HA	2.02	0.40
2:G:67:ALA:C	2:G:68:ARG:HH11	2.28	0.40
1:A:94:ARG:C	1:A:97:PRO:HD2	2.46	0.40
2:D:42:ILE:HB	3:H:5:DG:H3'	2.04	0.40
2:D:165:ARG:HD3	2:D:165:ARG:HA	1.85	0.40
1:B:31:MET:O	1:B:34:VAL:HG12	2.21	0.40
1:B:37:LEU:HD12	1:B:37:LEU:HA	1.84	0.40
1:B:68:ILE:HD11	1:B:73:ARG:CB	2.51	0.40
1:B:108:ARG:O	1:B:112:ARG:HG3	2.21	0.40
1:B:149:THR:O	1:B:153:VAL:HG23	2.21	0.40
2:G:67:ALA:C	2:G:68:ARG:NH1	2.73	0.40
1:A:233:GLU:O	1:A:258:ARG:HA	2.21	0.40
1:A:396:PHE:HE2	1:A:402:ILE:HD12	1.85	0.40
1:A:470:VAL:O	1:A:474:LEU:HG	2.22	0.40
1:B:96:ILE:N	1:B:97:PRO:HD2	2.36	0.40
1:B:189:ILE:CG2	1:B:211:MET:HE3	2.51	0.40
1:B:223:ILE:O	1:B:228:THR:HG23	2.21	0.40
1:A:5:GLN:HE21	1:A:6:THR:N	2.18	0.40
1:A:96:ILE:N	1:A:97:PRO:CD	2.84	0.40
1:A:233:GLU:CD	5:A:601:SAM:H1'	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LYS:HG3	1:B:238:PRO:HD2	2.03	0.40
1:B:466:PRO:HB2	1:E:491:LEU:HD23	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:271:ARG:NH1	1:B:85:ASP:OD2[2_764]	1.87	0.33
2:G:339:LYS:NZ	3:H:9:DT:OP1[3_645]	2.06	0.14
2:G:268:LYS:NZ	4:I:16:DT:OP2[3_645]	2.19	0.01

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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	483/507 (95%)	460 (95%)	23 (5%)	0	100	100
1	B	483/507 (95%)	465 (96%)	18 (4%)	0	100	100
1	C	28/507 (6%)	26 (93%)	2 (7%)	0	100	100
1	E	28/507 (6%)	27 (96%)	1 (4%)	0	100	100
2	D	386/398 (97%)	368 (95%)	18 (5%)	0	100	100
2	G	386/398 (97%)	372 (96%)	14 (4%)	0	100	100
All	All	1794/2824 (64%)	1718 (96%)	76 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	420/445 (94%)	378 (90%)	42 (10%)	7	30
1	B	420/445 (94%)	373 (89%)	47 (11%)	6	25
1	C	26/445 (6%)	21 (81%)	5 (19%)	1	8
1	E	26/445 (6%)	22 (85%)	4 (15%)	2	14
2	D	333/340 (98%)	303 (91%)	30 (9%)	9	34
2	G	333/340 (98%)	312 (94%)	21 (6%)	16	48
All	All	1558/2460 (63%)	1409 (90%)	149 (10%)	8	32

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	7	ARG
1	A	8	GLU
1	A	9	SER
1	A	30	ILE
1	A	56	GLN
1	A	59	ILE
1	A	67	ILE
1	A	68	ILE
1	A	71	GLU
1	A	72	TYR
1	A	73	ARG
1	A	80	LYS
1	A	94	ARG
1	A	101	SER
1	A	102	LEU
1	A	106	PRO
1	A	107	LEU
1	A	167	LEU
1	A	189	ILE
1	A	213	GLN
1	A	214	LYS
1	A	216	ARG
1	A	218	ILE
1	A	219	GLU
1	A	237	VAL
1	A	255	ARG

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Mol	Chain	Res	Type
1	A	261	THR
1	A	267	ARG
1	A	272	ARG
1	A	273	PHE
1	A	297	GLN
1	A	346	GLN
1	A	349	LEU
1	A	362	PRO
1	A	374	GLU
1	A	393	LEU
1	A	394	LYS
1	A	433	GLU
1	A	437	ILE
1	A	441	GLU
1	A	491	LEU
1	C	465	SER
1	C	468	GLU
1	C	469	ILE
1	C	478	ARG
1	C	484	MET
2	D	12	TRP
2	D	15	VAL
2	D	19	GLU
2	D	57	GLU
2	D	68	ARG
2	D	71	ILE
2	D	94	ASP
2	D	99	ILE
2	D	111	ARG
2	D	138	ARG
2	D	152	ASN
2	D	157	LEU
2	D	160	LEU
2	D	161	GLU
2	D	162	GLU
2	D	166	ILE
2	D	169	LYS
2	D	175	GLU
2	D	181	ARG
2	D	182	ARG
2	D	225	ILE
2	D	271	ARG

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Mol	Chain	Res	Type
2	D	278	SER
2	D	285	SER
2	D	305	ARG
2	D	306	ASP
2	D	307	SER
2	D	310	ARG
2	D	336	ILE
2	D	356	ARG
1	B	6	THR
1	B	7	ARG
1	B	8	GLU
1	B	30	ILE
1	B	56	GLN
1	B	67	ILE
1	B	72	TYR
1	B	101	SER
1	B	107	LEU
1	B	110	THR
1	B	114	LEU
1	B	117	GLU
1	B	118	ARG
1	B	189	ILE
1	B	191	GLU
1	B	213	GLN
1	B	215	GLU
1	B	216	ARG
1	B	217	THR
1	B	218	ILE
1	B	219	GLU
1	B	220	ASP
1	B	230	PHE
1	B	237	VAL
1	B	248	LEU
1	B	253	VAL
1	B	256	VAL
1	B	271	GLU
1	B	272	ARG
1	B	274	ASP
1	B	289	HIS
1	B	297	GLN
1	B	349	LEU
1	B	362	PRO

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Mol	Chain	Res	Type
1	B	374	GLU
1	B	380	LYS
1	B	391	GLU
1	B	394	LYS
1	B	412	LYS
1	B	433	GLU
1	B	437	ILE
1	B	456	ASN
1	B	457	ARG
1	B	461	GLU
1	B	462	GLU
1	B	476	LYS
1	B	491	LEU
1	E	465	SER
1	E	468	GLU
1	E	476	LYS
1	E	478	ARG
2	G	16	ARG
2	G	68	ARG
2	G	69	LYS
2	G	111	ARG
2	G	137	MET
2	G	138	ARG
2	G	164	ARG
2	G	178	ARG
2	G	189	LYS
2	G	192	GLU
2	G	205	HIS
2	G	225	ILE
2	G	254	ASP
2	G	280	ARG
2	G	285	SER
2	G	304	PRO
2	G	305	ARG
2	G	310	ARG
2	G	326	LYS
2	G	336	ILE
2	G	356	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	12	ASN
1	A	221	HIS
1	A	225	GLN
1	A	456	ASN
1	B	5	GLN
1	B	56	GLN
1	B	213	GLN
1	B	225	GLN
1	B	456	ASN
2	G	121	HIS
2	G	205	HIS
2	G	334	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

2 ligands are modelled in this entry.

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
5	SAM	B	601	-	27,29,29	1.48	7 (25%)	34,42,42	2.06	9 (26%)
5	SAM	A	601	-	27,29,29	1.48	6 (22%)	34,42,42	2.02	10 (29%)

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
5	SAM	B	601	-	-	9/17/33/33	0/3/3/3
5	SAM	A	601	-	-	8/17/33/33	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	SAM	C5-C4	3.98	1.46	1.39
5	B	601	SAM	C5-C4	3.83	1.45	1.39
5	B	601	SAM	C5-N7	-2.82	1.33	1.39
5	A	601	SAM	C5-N7	-2.73	1.34	1.39
5	A	601	SAM	C4-N9	-2.43	1.32	1.37
5	B	601	SAM	C4-N9	-2.32	1.32	1.37
5	B	601	SAM	C5-C6	2.28	1.47	1.41
5	A	601	SAM	C5-C6	2.27	1.47	1.41
5	B	601	SAM	OXT-C	-2.14	1.23	1.30
5	B	601	SAM	CE-SD	-2.11	1.65	1.78
5	A	601	SAM	C8-N9	-2.07	1.34	1.37
5	B	601	SAM	C8-N9	-2.02	1.34	1.37
5	A	601	SAM	CE-SD	-2.02	1.66	1.78

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	SAM	C5-C4-N3	-6.10	118.32	126.72
5	A	601	SAM	C5-C4-N3	-5.76	118.78	126.72
5	B	601	SAM	N3-C4-N9	4.78	135.29	127.17
5	A	601	SAM	N3-C4-N9	4.43	134.69	127.17
5	B	601	SAM	C2-N3-C4	3.94	121.45	111.83
5	A	601	SAM	C2-N3-C4	3.65	120.75	111.83
5	A	601	SAM	C4-C5-N7	-3.56	106.52	110.58
5	B	601	SAM	N3-C2-N1	-3.34	123.53	128.58
5	B	601	SAM	C4-C5-N7	-3.32	106.78	110.58
5	A	601	SAM	N3-C2-N1	-3.21	123.72	128.58
5	A	601	SAM	C4-N9-C8	2.68	108.55	105.74
5	B	601	SAM	CG-SD-C5'	2.66	109.94	103.43
5	B	601	SAM	C4-N9-C8	2.57	108.44	105.74
5	A	601	SAM	C5-N7-C8	2.52	107.41	103.45
5	B	601	SAM	C5-N7-C8	2.45	107.30	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	SAM	CG-SD-C5'	2.19	108.80	103.43
5	A	601	SAM	C6-C5-N7	2.10	136.14	132.09
5	A	601	SAM	N9-C8-N7	-2.07	111.00	113.94
5	B	601	SAM	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	SAM	O-C-CA-N
5	A	601	SAM	O4'-C4'-C5'-SD
5	A	601	SAM	C3'-C4'-C5'-SD
5	B	601	SAM	CA-CB-CG-SD
5	A	601	SAM	OXT-C-CA-N
5	B	601	SAM	OXT-C-CA-CB
5	A	601	SAM	C2'-C1'-N9-C8
5	B	601	SAM	C2'-C1'-N9-C8
5	A	601	SAM	CA-CB-CG-SD
5	A	601	SAM	OXT-C-CA-CB
5	B	601	SAM	O4'-C4'-C5'-SD
5	B	601	SAM	C3'-C4'-C5'-SD
5	A	601	SAM	O-C-CA-CB
5	B	601	SAM	O-C-CA-CB
5	B	601	SAM	C2'-C1'-N9-C4
5	B	601	SAM	O4'-C1'-N9-C8
5	B	601	SAM	OXT-C-CA-N

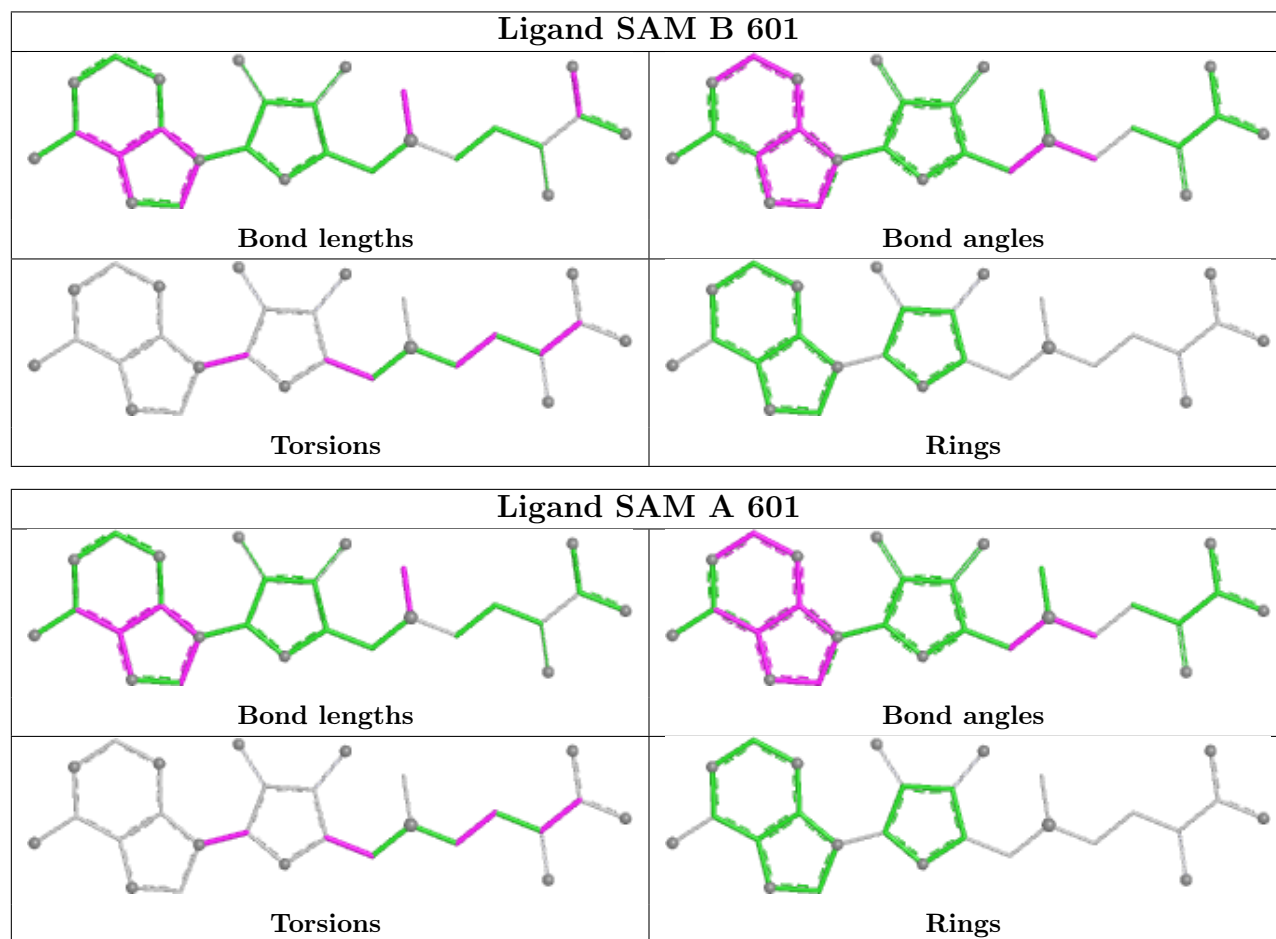
There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	SAM	9	0
5	A	601	SAM	10	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/507 (96%)	-0.76	1 (0%) 91 85	42, 94, 167, 229	0
1	B	487/507 (96%)	-0.74	0 100 100	45, 97, 167, 238	0
1	C	30/507 (5%)	-0.62	0 100 100	87, 117, 154, 217	0
1	E	30/507 (5%)	-0.51	0 100 100	90, 117, 169, 233	0
2	D	390/398 (97%)	-0.73	1 (0%) 90 81	63, 94, 164, 235	0
2	G	390/398 (97%)	-0.65	3 (0%) 82 67	59, 95, 154, 218	0
3	H	22/22 (100%)	0.01	1 (4%) 38 24	84, 100, 183, 220	0
4	I	22/22 (100%)	-0.22	0 100 100	78, 92, 170, 237	0
All	All	1858/2868 (64%)	-0.70	6 (0%) 90 81	42, 96, 167, 238	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	135	SER	4.6
2	G	159	PRO	2.5
2	G	160	LEU	2.4
3	H	1	DC	2.3
1	A	459	GLY	2.3
2	D	139	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

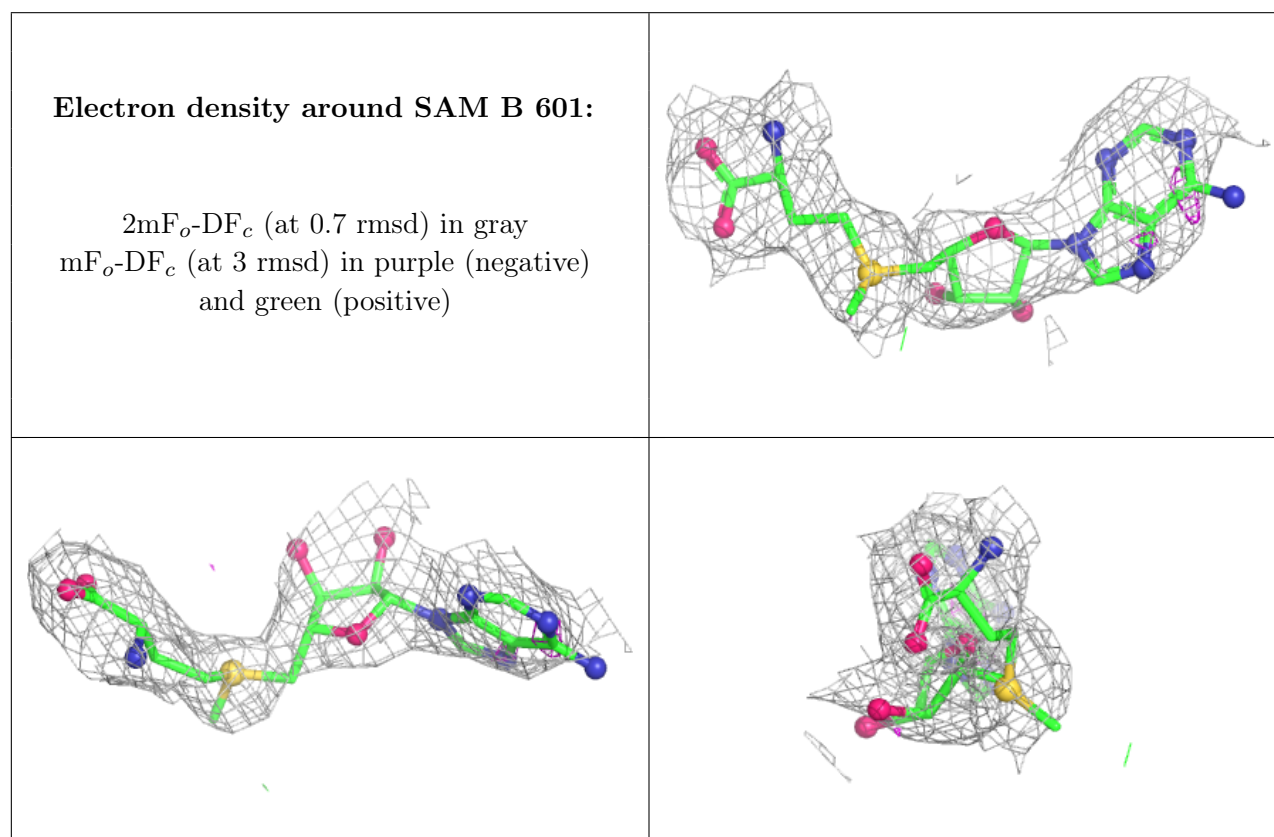
There are no oligosaccharides in this entry.

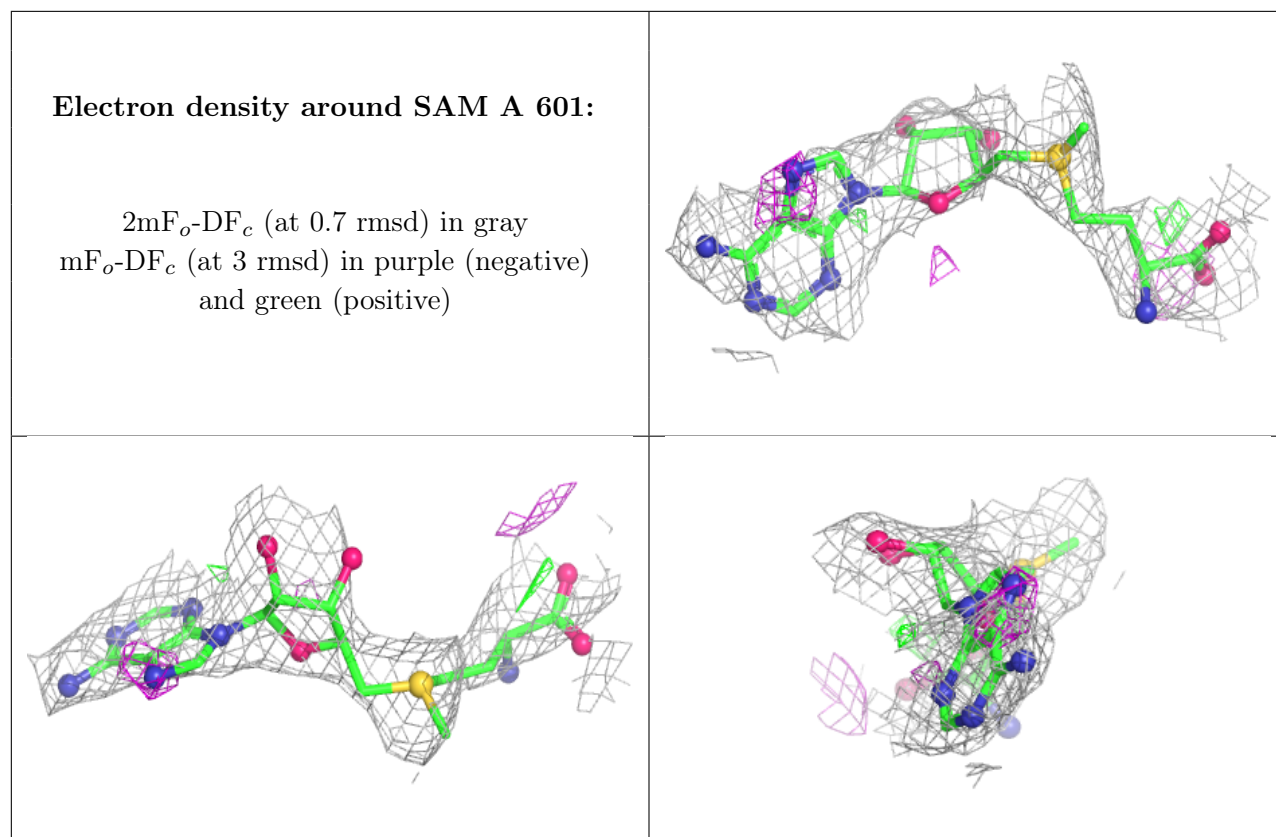
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SAM	B	601	27/27	0.97	0.10	93,137,149,189	0
5	SAM	A	601	27/27	0.98	0.10	106,142,155,271	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.