



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:12 PM UTC

PDB ID : 8AS8 / pdb_00008as8
EMDB ID : EMD-15609
Title : E. coli Wadjet JetABC monomer
Authors : Roisne-Hamelin, F.; Beckert, B.; Li, Y.; Myasnikov, A.; Gruber, S.
Deposited on : 2022-08-18
Resolution : 3.00 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

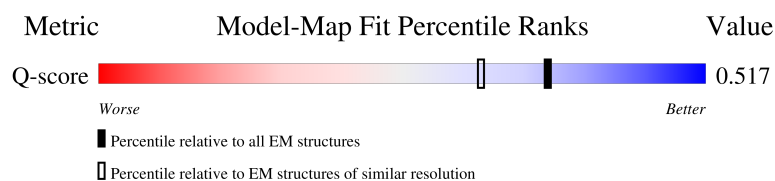
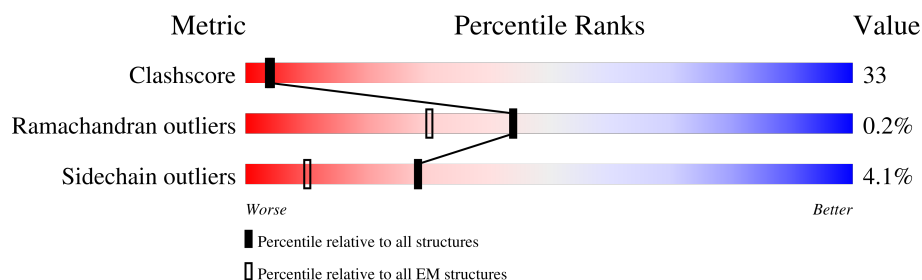
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	A	1096	
1	B	1096	
2	C	250	
2	D	250	

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Mol	Chain	Length	Quality of chain
3	E	554	 A horizontal bar chart showing the quality of chain E. The bar is divided into three segments: green (49%), yellow (39%), and grey (10%). The green segment is the largest, followed by yellow, and then grey. The percentages are labeled below the segments.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16724 atoms, of which 24 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 JetC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	597	Total	C	N	O	S	0	0
			4735	2955	869	899	12		
1	B	597	Total	C	N	O	S	0	0
			4735	2955	869	899	12		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	LEU	GLN	conflict	UNP A0A4T5T6V2
A	298	SER	ASN	conflict	UNP A0A4T5T6V2
A	386	SER	ILE	conflict	UNP A0A4T5T6V2
A	398	GLU	ALA	conflict	UNP A0A4T5T6V2
A	400	ARG	LEU	conflict	UNP A0A4T5T6V2
A	576	HIS	ARG	conflict	UNP A0A4T5T6V2
A	625	ALA	THR	conflict	UNP A0A4T5T6V2
A	705	ILE	VAL	conflict	UNP A0A4T5T6V2
A	729	LEU	SER	conflict	UNP A0A4T5T6V2
A	823	PRO	THR	conflict	UNP A0A4T5T6V2
A	889	ASP	TYR	conflict	UNP A0A4T5T6V2
A	933	VAL	ILE	conflict	UNP A0A4T5T6V2
A	1096	GLY	-	insertion	UNP A0A4T5T6V2
B	283	LEU	GLN	conflict	UNP A0A4T5T6V2
B	298	SER	ASN	conflict	UNP A0A4T5T6V2
B	386	SER	ILE	conflict	UNP A0A4T5T6V2
B	398	GLU	ALA	conflict	UNP A0A4T5T6V2
B	400	ARG	LEU	conflict	UNP A0A4T5T6V2
B	576	HIS	ARG	conflict	UNP A0A4T5T6V2
B	625	ALA	THR	conflict	UNP A0A4T5T6V2
B	705	ILE	VAL	conflict	UNP A0A4T5T6V2
B	729	LEU	SER	conflict	UNP A0A4T5T6V2
B	823	PRO	THR	conflict	UNP A0A4T5T6V2
B	889	ASP	TYR	conflict	UNP A0A4T5T6V2
B	933	VAL	ILE	conflict	UNP A0A4T5T6V2
B	1096	GLY	-	insertion	UNP A0A4T5T6V2

- Molecule 2 is a protein called JetB.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	195	Total	C	N	O	0	0
			1566	991	280	295		
2	D	195	Total	C	N	O	0	0
			1566	991	280	295		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	THR	conflict	UNP A0A4C9B499
C	7	LYS	ARG	conflict	UNP A0A4C9B499
C	35	ASP	GLU	conflict	UNP A0A4C9B499
C	46	GLN	LYS	conflict	UNP A0A4C9B499
C	240	PRO	ARG	conflict	UNP A0A4C9B499
C	250	GLY	-	insertion	UNP A0A4C9B499
D	2	ALA	THR	conflict	UNP A0A4C9B499
D	7	LYS	ARG	conflict	UNP A0A4C9B499
D	35	ASP	GLU	conflict	UNP A0A4C9B499
D	46	GLN	LYS	conflict	UNP A0A4C9B499
D	240	PRO	ARG	conflict	UNP A0A4C9B499
D	250	GLY	-	insertion	UNP A0A4C9B499

- Molecule 3 is a protein called JetA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	498	Total	C	N	O	S	0	0
			4044	2512	752	772	8		

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-54	MET	-	initiating methionine	UNP A0A4V3QHV5
E	-53	ALA	-	expression tag	UNP A0A4V3QHV5
E	-52	HIS	-	expression tag	UNP A0A4V3QHV5
E	-51	HIS	-	expression tag	UNP A0A4V3QHV5
E	-50	HIS	-	expression tag	UNP A0A4V3QHV5
E	-49	HIS	-	expression tag	UNP A0A4V3QHV5
E	-48	HIS	-	expression tag	UNP A0A4V3QHV5
E	-47	HIS	-	expression tag	UNP A0A4V3QHV5
E	-46	HIS	-	expression tag	UNP A0A4V3QHV5
E	-45	HIS	-	expression tag	UNP A0A4V3QHV5
E	-44	HIS	-	expression tag	UNP A0A4V3QHV5

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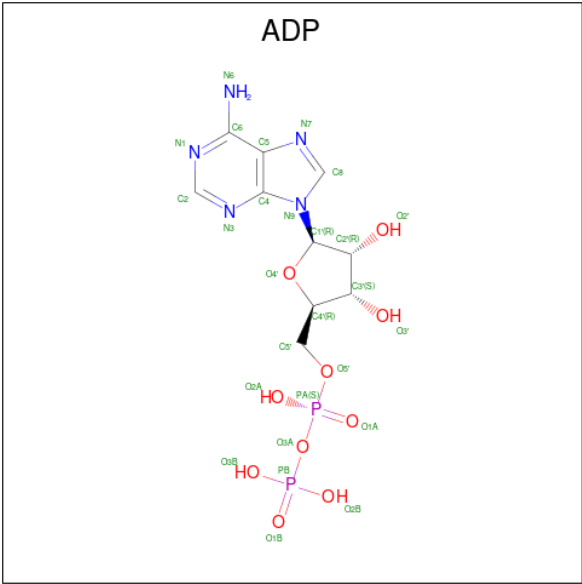
Chain	Residue	Modelled	Actual	Comment	Reference
E	-43	HIS	-	expression tag	UNP A0A4V3QHV5
E	-42	GLY	-	expression tag	UNP A0A4V3QHV5
E	-41	GLY	-	expression tag	UNP A0A4V3QHV5
E	-40	SER	-	expression tag	UNP A0A4V3QHV5
E	-39	SER	-	expression tag	UNP A0A4V3QHV5
E	-38	ALA	-	expression tag	UNP A0A4V3QHV5
E	-37	TRP	-	expression tag	UNP A0A4V3QHV5
E	-36	SER	-	expression tag	UNP A0A4V3QHV5
E	-35	HIS	-	expression tag	UNP A0A4V3QHV5
E	-34	PRO	-	expression tag	UNP A0A4V3QHV5
E	-33	GLN	-	expression tag	UNP A0A4V3QHV5
E	-32	PHE	-	expression tag	UNP A0A4V3QHV5
E	-31	GLU	-	expression tag	UNP A0A4V3QHV5
E	-30	LYS	-	expression tag	UNP A0A4V3QHV5
E	-29	GLY	-	expression tag	UNP A0A4V3QHV5
E	-28	GLY	-	expression tag	UNP A0A4V3QHV5
E	-27	GLY	-	expression tag	UNP A0A4V3QHV5
E	-26	SER	-	expression tag	UNP A0A4V3QHV5
E	-25	GLY	-	expression tag	UNP A0A4V3QHV5
E	-24	GLY	-	expression tag	UNP A0A4V3QHV5
E	-23	GLY	-	expression tag	UNP A0A4V3QHV5
E	-22	SER	-	expression tag	UNP A0A4V3QHV5
E	-21	GLY	-	expression tag	UNP A0A4V3QHV5
E	-20	GLY	-	expression tag	UNP A0A4V3QHV5
E	-19	GLY	-	expression tag	UNP A0A4V3QHV5
E	-18	SER	-	expression tag	UNP A0A4V3QHV5
E	-17	TRP	-	expression tag	UNP A0A4V3QHV5
E	-16	SER	-	expression tag	UNP A0A4V3QHV5
E	-15	HIS	-	expression tag	UNP A0A4V3QHV5
E	-14	PRO	-	expression tag	UNP A0A4V3QHV5
E	-13	GLN	-	expression tag	UNP A0A4V3QHV5
E	-12	PHE	-	expression tag	UNP A0A4V3QHV5
E	-11	GLU	-	expression tag	UNP A0A4V3QHV5
E	-10	LYS	-	expression tag	UNP A0A4V3QHV5
E	-9	LEU	-	expression tag	UNP A0A4V3QHV5
E	-8	GLU	-	expression tag	UNP A0A4V3QHV5
E	-7	VAL	-	expression tag	UNP A0A4V3QHV5
E	-6	LEU	-	expression tag	UNP A0A4V3QHV5
E	-5	PHE	-	expression tag	UNP A0A4V3QHV5
E	-4	GLN	-	expression tag	UNP A0A4V3QHV5
E	-3	GLY	-	expression tag	UNP A0A4V3QHV5
E	-2	PRO	-	expression tag	UNP A0A4V3QHV5

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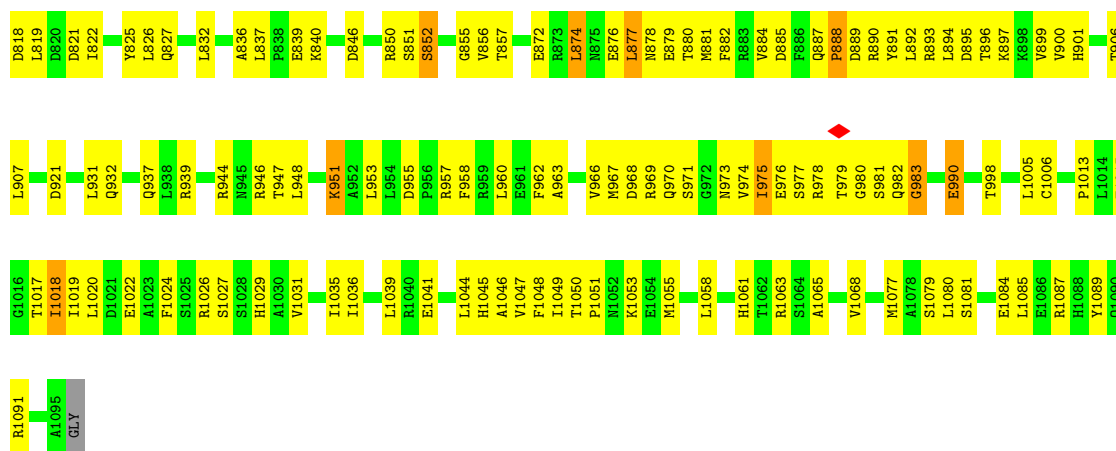
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ALA	-	expression tag	UNP A0A4V3QHV5
E	0	ALA	-	expression tag	UNP A0A4V3QHV5
E	187	ASP	GLU	conflict	UNP A0A4V3QHV5
E	435	GLU	ALA	conflict	UNP A0A4V3QHV5
E	499	GLY	-	insertion	UNP A0A4V3QHV5

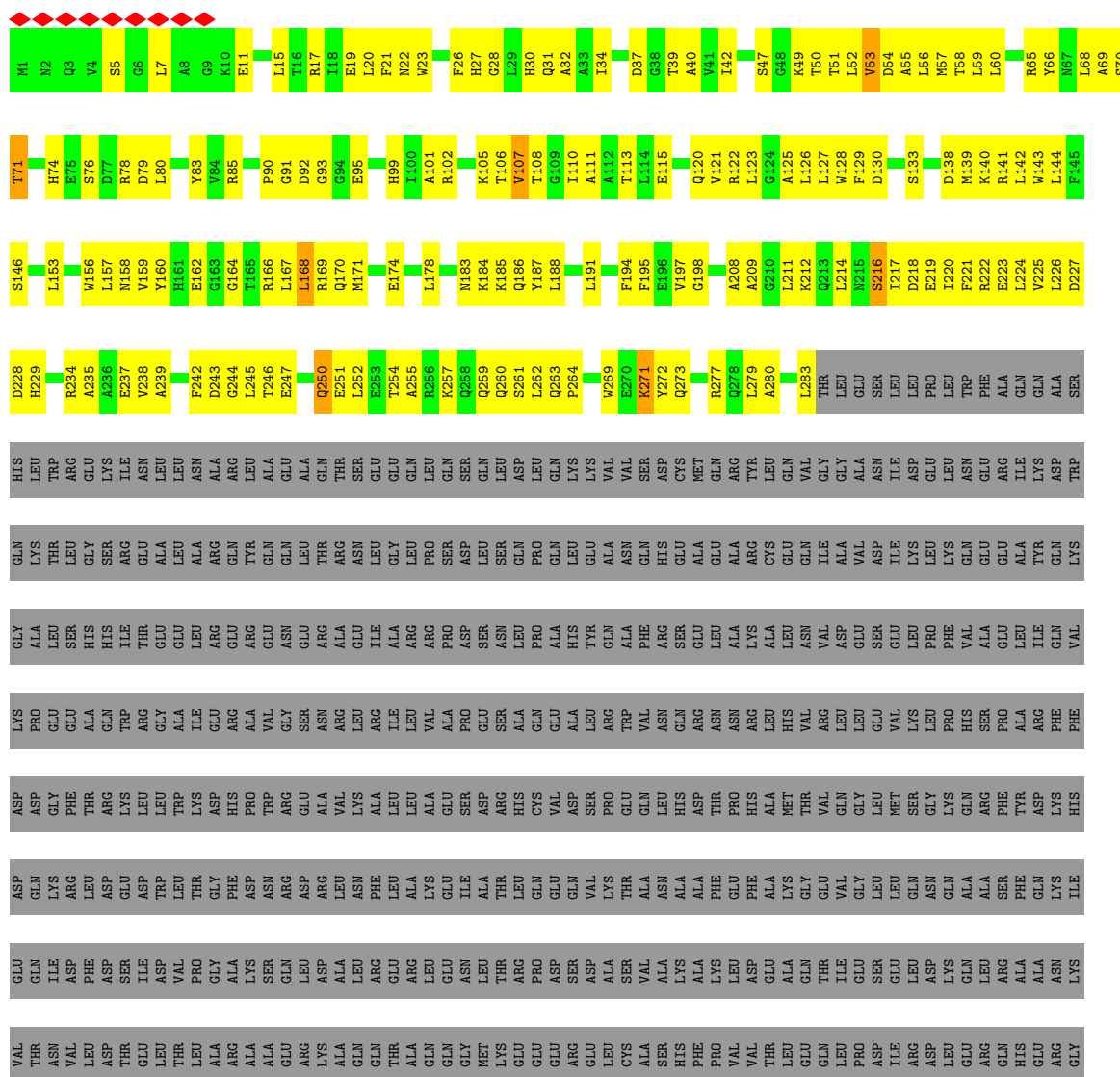
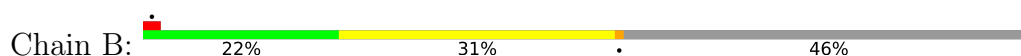
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

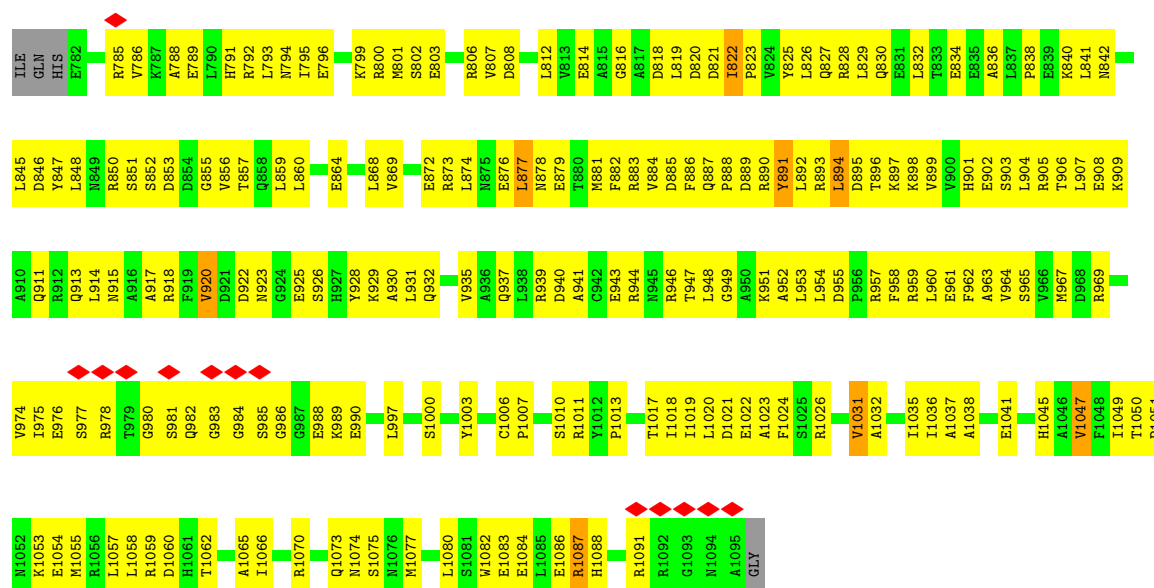


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
4	A	1	39	10	12	5	10	2	0
4	B	1	39	10	12	5	10	2	0



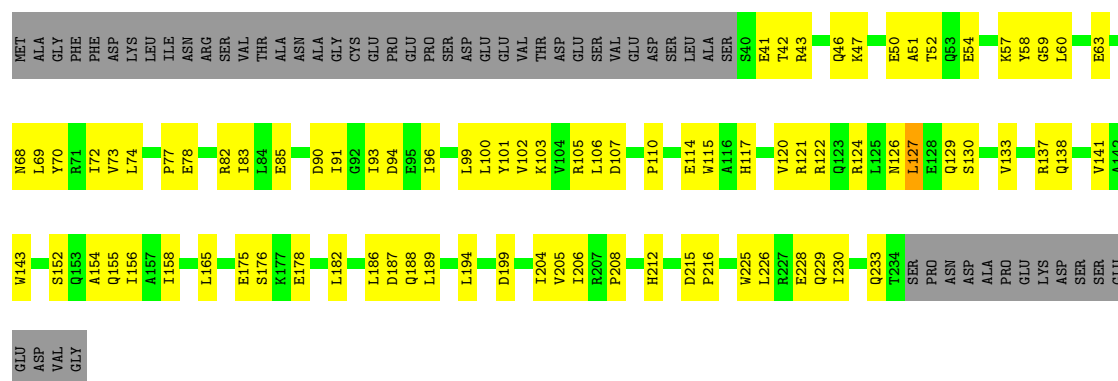
• Molecule 1: JetC





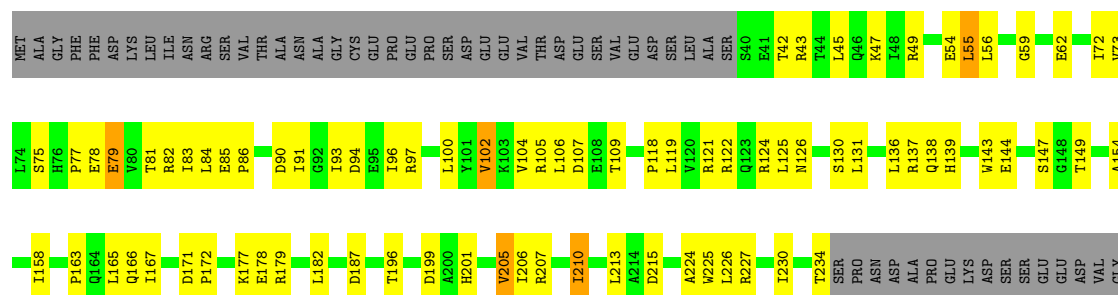
• Molecule 2: JetB

Chain C: 44% 33% 22%



• Molecule 2: JetB

Chain D: 46% 30% 22%



• Molecule 3: JetA

Chain E: 49% 39% 10%

L437	P438	P439	A440	H441	D442	L443	E444	T445	W449	M452	A453	R454	E455	V460	I461	D462	S463	Q464	R465	L470	S471	R476	R477	W478	R479	F480	N481	T484	T485	G486	L487	E488	S489	Q490	A491	L492	M493	E498	GLY												
P355	L356	P357	A358	V363	P367	A368	I369	E370	R371	L372	R373	F374	E375	E376	E380	A381	E382	L387	A391	A392	D399	D400	F401	W402	L408	D409	R410	E411	V412	L413	I414	Q415	T416	T417	L418	Q419	L420	L421	A422	K423	E424	N425	R426	F427	V428	A431	E432	L433	A434	E435	L436
R266	E265	L267	R268	V269	L270	L271	S275	A276	S277	D278	A279	R282	R285	L288	R289	W290	L291	V292	K293	R294	L295	E298	S299	Q300	Q304	A305	R306	A307	R308	S309	E310	V313	R314	M317	K318	T319	H330	L331	L332	N333	E334	N337	K341	L342	Q352	E353	V354				
H179	Q180	A181	V182	E183	D187	R196	F199	W206	D210	L213	R214	I217	E220	H223	R224	G225	D226	I227	V228	E229	R230	N233	D234	Q235	D236	A237	L238	L239	N240	T241	P242	E243	G244	R245	V246	F247	Q251	Q252	Q253	L254	R255	Q256	S257	S258	L260	K261					
E96	R97	D98	F102	E108	F113	V114	L117	T125	A126	S127	R128	L129	S130	T131	V132	E135	I136	E137	N138	L139	E140	T141	R142	L143	M146	P147	A148	S149	R150	V151	A152	T153	L154	R155	R156	R157	I158	S159	E160	R163	E164	L165	Q166	E169	I173	E174	E177	T178			
L24	L25	A26	T27	R28	R29	A30	P31	L32	V33	L34	S35	C36	SER	L40	S44	H45	D46	G47	I48	P49	L50	I54	L57	S58	L61	I62	V65	S66	Q67	E68	Q69	I72	P77	F78	L79	Q80	A81	S82	R83	E84	L85	R86	W88	I89	K90	R91	R92	L93	I94	V95	
MET	ALA	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	GLY	SER	SER	ALA	TRP	SER	HIS	PRO	PHE	GLN	GLY	GLY	GLY	SER	GLY	GLY	SER	TRP	SER	HIS	HIS	PRO	GLN	PHE	GLU	LYS	LEU	GLU	VAL	LEU	PHE	GLN	PRO	ALA	ALA	M1	E2	E3	I94	Q7

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124689	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.00183	Depositor
Map size (Å)	464.63998, 464.63998, 464.63998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1616, 1.1616, 1.1616	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/4817	0.40	1/6502 (0.0%)
1	B	0.21	0/4817	0.37	1/6502 (0.0%)
2	C	0.17	0/1592	0.29	0/2164
2	D	0.14	0/1592	0.24	0/2164
3	E	0.13	0/4110	0.28	0/5560
All	All	0.20	0/16928	0.34	2/22892 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	888	PRO	CA-N-CD	-6.43	102.99	112.00
1	B	95	GLU	CB-CA-C	-5.01	110.41	117.23

There are no chirality outliers.

There are no planarity outliers.

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	A	4735	0	4689	287	0
1	B	4735	0	4689	429	0
2	C	1566	0	1605	85	0
2	D	1566	0	1605	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	4044	0	4007	274	0
4	A	27	12	12	0	0
4	B	27	12	12	0	0
All	All	16700	24	16619	1087	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 33.

All (1087) 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)
3:E:414:ILE:HD13	3:E:452:MET:HE1	1.22	1.12
1:B:42:ILE:HD12	1:B:1055:MET:HE1	1.30	1.06
1:B:982:GLN:HA	1:B:988:GLU:HB2	1.28	1.06
2:D:59:GLY:HA3	3:E:367:PRO:HG2	1.38	1.04
1:A:801:MET:HG2	1:A:825:TYR:HE2	1.27	0.99
1:B:262:LEU:HB3	1:B:829:LEU:HD23	1.45	0.98
1:B:32:ALA:HB1	1:B:1066:ILE:HD13	1.48	0.96
1:B:279:LEU:HD12	1:B:786:VAL:HG12	1.49	0.95
1:A:887:GLN:HB3	1:A:888:PRO:HD3	1.48	0.94
3:E:261:LYS:H	3:E:261:LYS:HE2	1.30	0.94
1:A:268:SER:HB3	1:A:797:LEU:HD22	1.51	0.92
2:C:68:ASN:O	2:C:72:ILE:HD12	1.68	0.91
1:B:19:GLU:HB2	1:B:111:ALA:HB3	1.52	0.91
2:C:78:GLU:N	2:C:78:GLU:OE2	2.04	0.90
3:E:414:ILE:CD1	3:E:452:MET:HE1	2.01	0.90
1:A:801:MET:HG2	1:A:825:TYR:CE2	2.07	0.89
1:A:1039:LEU:HD21	1:A:1046:ALA:HB2	1.52	0.88
2:D:47:LYS:HB3	2:D:72:ILE:HD13	1.56	0.88
3:E:417:THR:O	3:E:421:LEU:HD12	1.74	0.87
1:B:47:SER:HA	1:B:1070:ARG:HB2	1.57	0.86
3:E:177:GLU:HB2	3:E:180:GLN:HB2	1.56	0.86
1:B:223:GLU:N	1:B:223:GLU:OE1	2.08	0.85
2:C:91:ILE:HD11	2:C:100:LEU:HB3	1.58	0.85
2:C:107:ASP:OD1	2:D:43:ARG:NH1	2.07	0.85
1:B:982:GLN:HG2	1:B:984:GLY:H	1.41	0.85
2:D:126:ASN:O	2:D:130:SER:OG	1.95	0.84
1:A:797:LEU:HD12	1:A:822:ILE:HD11	1.59	0.84
1:B:280:ALA:HA	1:B:283:LEU:HB3	1.60	0.83
1:A:237:GLU:N	1:A:237:GLU:OE1	2.11	0.83
2:C:99:LEU:HD13	2:C:208:PRO:HB2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD11	1:A:1077:MET:HE1	1.61	0.83
1:B:887:GLN:HB3	1:B:888:PRO:HD2	1.61	0.82
3:E:92:ARG:HG3	3:E:92:ARG:HH11	1.42	0.82
3:E:137:GLU:O	3:E:141:THR:HG23	1.78	0.82
3:E:233:ASN:HD21	3:E:235:GLN:HB2	1.44	0.82
3:E:24:LEU:HB2	3:E:93:LEU:HD11	1.61	0.81
1:B:982:GLN:HG3	1:B:986:GLY:H	1.46	0.81
1:A:971:SER:OG	1:A:973:ASN:OD1	1.98	0.81
1:A:20:LEU:HD11	1:A:52:LEU:HD12	1.63	0.80
1:B:953:LEU:HB3	1:B:954:LEU:HD22	1.64	0.80
1:B:1058:LEU:O	1:B:1062:THR:OG1	1.99	0.80
2:C:230:ILE:HD12	3:E:341:LYS:HB2	1.64	0.80
1:B:785:ARG:NH1	1:B:785:ARG:O	2.15	0.80
1:A:17:ARG:NH2	1:A:31:GLN:OE1	2.14	0.80
1:B:250:GLN:O	1:B:254:THR:HG23	1.82	0.80
3:E:44:SER:OG	3:E:46:ASP:OD1	2.00	0.80
1:B:168:LEU:O	1:B:171:MET:HG2	1.82	0.80
1:B:827:GLN:O	1:B:830:GLN:HG3	1.82	0.79
1:B:1032:ALA:HA	1:B:1035:ILE:HD12	1.63	0.79
1:B:911:GLN:O	1:B:915:ASN:ND2	2.16	0.79
2:D:55:LEU:HD22	2:D:102:VAL:HG13	1.62	0.79
1:B:1026:ARG:H	1:B:1026:ARG:HD3	1.48	0.79
3:E:58:SER:O	3:E:62:ILE:HG13	1.83	0.79
1:A:162:GLU:HG2	1:A:167:LEU:HD22	1.65	0.78
1:B:224:LEU:HD23	1:B:997:LEU:HD11	1.65	0.78
1:A:887:GLN:HB2	1:A:890:ARG:HG3	1.66	0.78
1:B:216:SER:OG	1:B:218:ASP:OD2	2.02	0.78
1:A:52:LEU:CD1	1:A:1077:MET:HE1	2.14	0.78
1:B:792:ARG:HB2	1:B:792:ARG:NH1	1.98	0.78
1:B:876:GLU:O	1:B:879:GLU:HG3	1.84	0.78
1:B:925:GLU:N	1:B:925:GLU:OE1	2.17	0.77
1:B:897:LYS:HG3	1:B:898:LYS:H	1.49	0.77
1:A:946:ARG:HD2	1:B:946:ARG:HH12	1.48	0.77
1:A:154:GLU:OE2	2:D:126:ASN:ND2	2.17	0.77
1:A:797:LEU:O	1:A:801:MET:HE3	1.85	0.77
2:D:55:LEU:CD2	2:D:102:VAL:HG13	2.15	0.77
3:E:367:PRO:O	3:E:371:ARG:NH1	2.18	0.77
1:B:1054:GLU:HG2	1:B:1057:LEU:CD2	2.15	0.76
1:B:164:GLY:O	1:B:168:LEU:HD22	1.85	0.76
3:E:87:GLU:OE2	3:E:91:ARG:NH1	2.18	0.76
1:A:268:SER:HB3	1:A:797:LEU:CD2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:LEU:O	1:B:881:MET:HG3	1.85	0.76
2:D:225:TRP:HZ2	3:E:382:GLU:HG2	1.48	0.76
2:D:93:ILE:HD12	2:D:100:LEU:HD22	1.67	0.76
3:E:419:GLN:HG3	3:E:423:LYS:HE2	1.66	0.76
3:E:87:GLU:HA	3:E:90:LYS:NZ	2.00	0.76
1:B:893:ARG:NH1	1:B:967:MET:HE3	2.01	0.76
3:E:490:GLN:HA	3:E:493:MET:HE2	1.67	0.76
3:E:408:LEU:HB2	3:E:441:HIS:HD2	1.52	0.75
3:E:258:SER:HB2	3:E:259:GLU:OE1	1.86	0.75
1:A:15:LEU:HB3	1:A:1017:THR:HG21	1.69	0.75
1:B:102:ARG:HB3	1:B:106:THR:HG21	1.67	0.75
2:D:56:LEU:HD11	2:D:84:LEU:HD21	1.69	0.75
1:A:888:PRO:HD2	1:A:889:ASP:H	1.50	0.75
1:A:832:LEU:HD23	1:A:836:ALA:HB3	1.69	0.75
1:B:238:VAL:CG2	1:B:856:VAL:HG22	2.18	0.74
1:B:902:GLU:OE1	1:B:905:ARG:NH1	2.20	0.74
2:C:215:ASP:HB2	2:C:216:PRO:HD2	1.70	0.74
1:B:262:LEU:CB	1:B:829:LEU:HD23	2.16	0.74
1:B:1031:VAL:O	1:B:1035:ILE:HD12	1.86	0.74
1:B:983:GLY:H	1:B:988:GLU:H	1.36	0.74
1:A:884:VAL:HG22	1:A:1041:GLU:HG2	1.70	0.73
1:B:1059:ARG:NH1	3:E:442:ASP:OD2	2.21	0.73
1:B:1087:ARG:HG3	3:E:477:ARG:HE	1.53	0.73
1:B:869:VAL:O	1:B:872:GLU:HG3	1.87	0.73
1:A:808:ASP:OD2	1:A:812:LEU:HB2	1.88	0.73
1:B:816:GLY:O	1:B:825:TYR:OH	2.04	0.73
1:A:814:GLU:OE1	1:A:814:GLU:N	2.21	0.73
2:C:137:ARG:HG3	3:E:332:LEU:HD11	1.71	0.72
1:B:53:VAL:HG22	1:B:1019:ILE:HG21	1.71	0.72
1:A:877:LEU:O	1:A:880:THR:HG22	1.88	0.72
1:B:948:LEU:HD12	1:B:949:GLY:N	2.03	0.72
3:E:128:ARG:O	3:E:132:VAL:HG23	1.89	0.72
1:A:1024:PHE:CE1	1:A:1035:ILE:HG21	2.24	0.72
1:B:1088:HIS:NE2	1:B:1091:ARG:HB2	2.03	0.72
1:A:892:LEU:HD23	1:A:893:ARG:N	2.05	0.71
3:E:84:GLU:HA	3:E:84:GLU:OE2	1.88	0.71
2:C:158:ILE:HD11	2:C:204:ILE:HG23	1.71	0.71
3:E:34:LEU:HD13	3:E:114:VAL:HG21	1.73	0.71
3:E:431:ALA:O	3:E:435:GLU:HG3	1.90	0.71
1:A:966:VAL:CG1	1:A:976:GLU:HB3	2.20	0.71
2:C:93:ILE:HG12	2:C:100:LEU:HD23	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:GLU:OE2	1:A:1024:PHE:HA	1.90	0.71
1:B:22:ASN:O	1:B:108:THR:OG1	2.07	0.71
2:D:93:ILE:HD12	2:D:100:LEU:CD2	2.20	0.71
3:E:449:TRP:O	3:E:452:MET:HB2	1.91	0.71
1:A:272:TYR:HD1	1:A:793:LEU:HB3	1.55	0.71
1:A:796:GLU:O	1:A:800:ARG:HG2	1.90	0.71
1:B:69:ALA:HB1	1:B:1022:GLU:HG3	1.71	0.71
1:B:244:GLY:O	1:B:247:GLU:HG3	1.90	0.70
1:B:247:GLU:O	1:B:250:GLN:HG3	1.91	0.70
3:E:432:GLU:O	3:E:436:LEU:HG	1.90	0.70
1:B:860:LEU:HD21	1:B:907:LEU:HD11	1.73	0.70
1:B:211:LEU:HD13	1:B:212:LYS:O	1.91	0.70
1:B:896:THR:OG1	1:B:960:LEU:HD12	1.91	0.70
1:A:192:ARG:HG3	1:A:197:VAL:O	1.92	0.70
1:A:887:GLN:HB2	1:A:890:ARG:CG	2.22	0.70
1:B:263:GLN:OE1	1:B:829:LEU:HD21	1.92	0.70
3:E:261:LYS:H	3:E:261:LYS:CE	2.03	0.70
1:B:964:VAL:H	1:B:978:ARG:HH12	1.40	0.70
1:A:162:GLU:HG2	1:A:167:LEU:CD2	2.21	0.69
1:B:71:THR:HG23	1:B:74:HIS:H	1.56	0.69
1:B:159:VAL:HG11	1:B:171:MET:SD	2.33	0.69
1:B:107:VAL:HG11	1:B:160:TYR:CE1	2.26	0.69
2:C:143:TRP:CD2	2:C:154:ALA:HB2	2.28	0.69
1:A:119:LYS:HE2	1:A:119:LYS:HA	1.75	0.69
1:B:257:LYS:NZ	1:B:260:GLN:OE1	2.25	0.69
1:B:261:SER:O	1:B:264:PRO:HD2	1.92	0.69
1:B:251:GLU:C	1:B:840:LYS:HZ1	2.01	0.68
1:B:893:ARG:HG2	1:B:893:ARG:HH11	1.57	0.68
1:B:34:ILE:HG23	1:B:39:THR:HG21	1.75	0.68
1:B:105:LYS:HE3	1:B:130:ASP:HA	1.74	0.68
2:D:59:GLY:CA	3:E:367:PRO:HG2	2.18	0.68
1:B:5:SER:OG	1:B:37:ASP:OD2	2.04	0.68
3:E:137:GLU:HA	3:E:137:GLU:OE1	1.92	0.68
3:E:128:ARG:HB2	3:E:187:ASP:OD1	1.92	0.68
1:A:217:ILE:HD12	1:A:217:ILE:H	1.58	0.68
2:C:63:GLU:HG3	2:C:70:TYR:CD1	2.28	0.68
3:E:461:ILE:HD11	3:E:484:THR:HB	1.75	0.68
1:A:64:PRO:HA	1:A:206:ASN:ND2	2.09	0.68
1:B:105:LYS:CE	1:B:130:ASP:HA	2.24	0.68
2:D:137:ARG:HD3	2:D:210:ILE:HG22	1.75	0.68
1:A:225:VAL:O	1:A:226:LEU:HD12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:SER:HB2	1:B:178:LEU:HD23	1.76	0.68
1:B:252:LEU:HA	1:B:840:LYS:CE	2.23	0.67
1:A:84:VAL:HG13	1:A:108:THR:CG2	2.25	0.67
1:A:900:VAL:HG12	1:A:900:VAL:O	1.94	0.67
3:E:470:LEU:HD13	3:E:471:SER:N	2.09	0.67
1:B:953:LEU:HB3	1:B:954:LEU:CD2	2.24	0.67
1:B:218:ASP:HB3	1:B:222:ARG:HH21	1.59	0.67
1:A:243:ASP:OD1	1:A:939:ARG:NH2	2.17	0.67
1:B:915:ASN:HA	1:B:918:ARG:CD	2.24	0.67
2:C:127:LEU:HD21	2:C:225:TRP:CH2	2.28	0.67
3:E:487:LEU:HG	3:E:492:LEU:HD11	1.76	0.67
1:A:20:LEU:HD11	1:A:52:LEU:CD1	2.25	0.66
1:B:252:LEU:HA	1:B:840:LYS:HE2	1.77	0.66
1:B:234:ARG:HA	1:B:237:GLU:OE1	1.95	0.66
1:A:946:ARG:CD	1:B:946:ARG:HH12	2.08	0.66
1:B:917:ALA:O	1:B:920:VAL:HG23	1.96	0.66
1:A:128:TRP:CE2	1:A:140:LYS:HB2	2.31	0.66
1:A:832:LEU:HA	1:A:836:ALA:HB3	1.78	0.66
1:B:252:LEU:HA	1:B:840:LYS:NZ	2.10	0.66
3:E:95:VAL:HG23	3:E:102:PHE:HB2	1.76	0.66
3:E:380:GLU:N	3:E:380:GLU:OE1	2.28	0.66
3:E:409:ASP:OD2	3:E:412:VAL:HB	1.96	0.66
3:E:455:GLU:OE2	3:E:455:GLU:HA	1.95	0.66
1:A:948:LEU:HD12	1:A:948:LEU:O	1.96	0.66
3:E:206:TRP:CZ3	3:E:306:ARG:HB2	2.31	0.66
1:B:59:LEU:O	1:B:187:TYR:OH	2.12	0.66
3:E:290:TRP:O	3:E:294:ARG:HG2	1.95	0.66
3:E:310:GLU:OE1	3:E:314:ARG:NH2	2.24	0.66
1:B:878:ASN:HD21	1:B:893:ARG:HB2	1.62	0.65
3:E:226:ASP:OD1	3:E:230:ARG:NH2	2.29	0.65
3:E:267:LEU:HD11	3:E:288:LEU:HD11	1.78	0.65
1:A:53:VAL:O	1:A:57:MET:HG2	1.95	0.65
2:D:107:ASP:O	2:D:109:THR:HG22	1.97	0.65
1:A:81:ILE:HD12	1:A:129:PHE:HZ	1.62	0.65
1:A:893:ARG:HG2	1:A:894:LEU:H	1.60	0.65
1:A:946:ARG:HD2	1:B:946:ARG:NH1	2.10	0.65
1:B:129:PHE:CZ	1:B:139:MET:HG3	2.32	0.65
3:E:151:VAL:HG13	3:E:155:ARG:HE	1.61	0.65
1:B:982:GLN:HA	1:B:988:GLU:CB	2.16	0.65
2:D:77:PRO:O	2:D:81:THR:HG22	1.97	0.65
1:B:273:GLN:O	1:B:277:ARG:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:461:ILE:CG1	3:E:484:THR:HB	2.27	0.65
2:C:127:LEU:HD21	2:C:225:TRP:HH2	1.62	0.65
3:E:241:THR:HA	3:E:245:ARG:NH1	2.12	0.65
1:A:1027:SER:HB2	1:A:1031:VAL:CG2	2.27	0.65
2:C:74:LEU:O	2:C:77:PRO:HD3	1.97	0.65
1:A:812:LEU:HG	1:A:825:TYR:CE1	2.32	0.65
1:B:128:TRP:CD1	1:B:160:TYR:HH	2.15	0.64
1:B:195:PHE:O	1:B:197:VAL:HG23	1.97	0.64
2:C:114:GLU:OE2	3:E:358:ALA:N	2.21	0.64
1:B:982:GLN:HG3	1:B:986:GLY:N	2.11	0.64
2:C:52:THR:HG21	2:C:83:ILE:HG21	1.79	0.64
3:E:135:GLU:OE2	3:E:135:GLU:HA	1.96	0.64
1:A:1036:ILE:HG21	1:A:1061:HIS:HB3	1.80	0.64
1:B:914:LEU:HD23	1:B:918:ARG:HE	1.61	0.64
1:A:818:ASP:OD1	1:A:819:LEU:N	2.30	0.64
1:A:1026:ARG:HH21	1:B:70:SER:HA	1.61	0.64
1:B:246:THR:HG23	1:B:928:TYR:OH	1.97	0.64
1:B:1020:LEU:CD1	1:B:1023:ALA:HA	2.28	0.64
2:C:68:ASN:OD1	2:C:72:ILE:HD11	1.98	0.64
1:A:966:VAL:O	1:A:975:ILE:HG13	1.98	0.64
1:B:1020:LEU:HD12	1:B:1023:ALA:HA	1.79	0.64
1:A:64:PRO:HA	1:A:206:ASN:HD21	1.62	0.64
1:A:784:GLU:CD	1:A:784:GLU:H	2.05	0.64
3:E:241:THR:HG23	3:E:245:ARG:HH12	1.61	0.64
1:A:21:PHE:HA	1:A:28:GLY:O	1.97	0.64
1:A:128:TRP:CG	1:A:160:TYR:HH	2.15	0.64
3:E:461:ILE:HD12	3:E:464:GLN:HB2	1.79	0.64
1:A:227:ASP:OD1	1:A:227:ASP:N	2.31	0.63
1:A:832:LEU:HD23	1:A:836:ALA:CB	2.29	0.63
3:E:490:GLN:HG2	3:E:493:MET:HE2	1.81	0.63
2:D:131:LEU:HD13	2:D:226:LEU:HD12	1.79	0.63
3:E:318:LYS:O	3:E:319:THR:OG1	2.12	0.63
1:A:247:GLU:O	1:A:251:GLU:HG3	1.99	0.63
2:D:166:GLN:NE2	2:D:171:ASP:HB2	2.14	0.63
1:A:119:LYS:HE2	1:A:119:LYS:CA	2.29	0.63
1:B:129:PHE:CE2	1:B:139:MET:HG3	2.34	0.63
1:B:975:ILE:HG22	1:B:976:GLU:OE1	1.99	0.63
2:C:99:LEU:CD1	2:C:208:PRO:HB2	2.26	0.63
3:E:454:ARG:HH21	3:E:460:VAL:H	1.44	0.63
1:B:92:ASP:OD1	1:B:93:GLY:N	2.25	0.63
2:D:47:LYS:HE3	2:D:72:ILE:CD1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:158:ILE:HD11	2:C:204:ILE:CG2	2.28	0.63
1:A:135:SER:HB3	1:A:138:ASP:OD1	1.99	0.62
3:E:165:LEU:O	3:E:165:LEU:HD12	1.98	0.62
3:E:226:ASP:O	3:E:227:ILE:HD13	2.00	0.62
2:C:106:LEU:O	2:C:106:LEU:HD12	1.98	0.62
1:A:946:ARG:HD2	1:B:946:ARG:HH22	1.65	0.62
1:B:269:TRP:CE3	1:B:822:ILE:HG21	2.33	0.62
1:B:814:GLU:N	1:B:814:GLU:OE1	2.30	0.62
2:C:143:TRP:HZ2	2:C:152:SER:HB3	1.64	0.62
3:E:92:ARG:HG3	3:E:92:ARG:NH1	2.10	0.62
1:B:42:ILE:HG22	1:B:1050:THR:CG2	2.29	0.62
1:B:965:SER:HB3	1:B:974:VAL:HG21	1.81	0.62
3:E:125:THR:OG1	3:E:127:SER:O	2.17	0.62
1:A:192:ARG:HB2	1:A:192:ARG:CZ	2.30	0.62
1:B:975:ILE:HG22	1:B:976:GLU:CD	2.25	0.62
3:E:155:ARG:HD3	3:E:155:ARG:N	2.14	0.62
1:B:42:ILE:HG22	1:B:1050:THR:HG23	1.81	0.62
3:E:173:ILE:O	3:E:173:ILE:HG13	2.00	0.62
1:B:57:MET:HE3	1:B:57:MET:HA	1.80	0.61
2:D:225:TRP:CZ2	3:E:382:GLU:HG2	2.33	0.61
3:E:257:SER:HA	3:E:261:LYS:NZ	2.15	0.61
1:B:225:VAL:HG12	1:B:226:LEU:H	1.65	0.61
1:A:217:ILE:O	1:A:220:ILE:HG12	2.00	0.61
3:E:236:ASP:OD2	3:E:306:ARG:NH1	2.33	0.61
3:E:62:ILE:O	3:E:65:VAL:HG13	2.01	0.61
3:E:77:PRO:HA	3:E:80:GLN:OE1	2.00	0.61
1:B:242:PHE:CG	1:B:935:VAL:HG21	2.35	0.61
1:B:1084:GLU:CD	3:E:476:ARG:HD2	2.26	0.61
3:E:166:GLN:HA	3:E:169:GLU:OE1	2.01	0.61
3:E:45:HIS:ND1	3:E:298:GLU:OE2	2.33	0.61
3:E:32:LEU:H	3:E:32:LEU:HD22	1.66	0.61
1:A:91:GLY:HA2	1:B:982:GLN:HE22	1.64	0.61
1:B:133:SER:HB3	1:B:138:ASP:OD2	2.01	0.61
1:B:1032:ALA:HA	1:B:1035:ILE:CD1	2.31	0.61
1:B:15:LEU:HG	1:B:34:ILE:HD12	1.84	0.60
1:B:158:ASN:O	1:B:162:GLU:HG3	2.00	0.60
1:B:845:LEU:HD12	1:B:846:ASP:N	2.16	0.60
2:D:54:GLU:OE2	2:D:54:GLU:HA	2.01	0.60
1:A:907:LEU:HD22	1:A:953:LEU:HD11	1.83	0.60
1:B:183:ASN:HB2	1:B:185:LYS:NZ	2.17	0.60
1:B:982:GLN:HG2	1:B:984:GLY:N	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:46:GLN:NE2	2:C:47:LYS:HG3	2.15	0.60
3:E:67:GLN:HB3	3:E:69:GLN:OE1	2.00	0.60
3:E:465:ARG:NH2	3:E:481:ASN:O	2.31	0.60
1:B:227:ASP:N	1:B:227:ASP:OD1	2.33	0.60
1:B:808:ASP:OD2	1:B:812:LEU:HD12	2.00	0.60
1:A:5:SER:HB3	1:A:37:ASP:OD1	2.00	0.60
1:A:887:GLN:CB	1:A:888:PRO:HD3	2.27	0.60
1:B:899:VAL:HG12	1:B:959:ARG:O	2.02	0.60
2:C:138:GLN:O	2:C:141:VAL:HG12	2.02	0.60
2:D:136:LEU:HD22	2:D:206:ILE:CD1	2.31	0.60
1:B:217:ILE:HA	1:B:220:ILE:HD13	1.82	0.60
1:B:219:GLU:N	1:B:219:GLU:OE1	2.34	0.60
3:E:24:LEU:O	3:E:27:THR:HG22	2.01	0.60
3:E:28:ARG:HH12	3:E:69:GLN:HA	1.66	0.60
1:A:877:LEU:HD12	1:A:880:THR:CG2	2.32	0.60
2:C:82:ARG:HH11	2:C:82:ARG:HB2	1.66	0.60
3:E:50:LEU:O	3:E:54:ILE:HG12	2.02	0.60
1:B:878:ASN:ND2	1:B:894:LEU:H	1.99	0.60
1:B:1036:ILE:CD1	1:B:1057:LEU:HD13	2.32	0.60
1:A:211:LEU:HD12	1:A:211:LEU:O	2.01	0.60
1:A:1089:TYR:HB2	3:E:402:TRP:CZ3	2.36	0.60
1:B:242:PHE:O	1:B:246:THR:OG1	2.19	0.60
3:E:151:VAL:HG13	3:E:155:ARG:HH21	1.66	0.60
1:B:1054:GLU:HG2	1:B:1057:LEU:HD23	1.83	0.60
3:E:87:GLU:HA	3:E:90:LYS:HZ1	1.64	0.59
1:A:1024:PHE:CE2	1:A:1036:ILE:HD11	2.37	0.59
1:A:57:MET:HE2	1:A:206:ASN:HA	1.83	0.59
1:A:794:ASN:O	1:A:798:THR:HG22	2.02	0.59
1:B:806:ARG:HG3	1:B:806:ARG:HH11	1.67	0.59
1:B:183:ASN:HB2	1:B:185:LYS:CE	2.32	0.59
1:B:32:ALA:HB1	1:B:1066:ILE:CD1	2.29	0.59
1:B:1084:GLU:HB2	3:E:478:TRP:CZ3	2.37	0.59
1:B:788:ALA:O	1:B:791:HIS:HB3	2.02	0.59
1:A:1035:ILE:HG22	1:A:1036:ILE:HD13	1.84	0.59
1:B:967:MET:HA	1:B:974:VAL:HA	1.84	0.59
3:E:233:ASN:OD1	3:E:235:GLN:N	2.33	0.59
1:B:34:ILE:HG23	1:B:39:THR:CG2	2.32	0.59
1:B:251:GLU:HG2	1:B:840:LYS:HZ1	1.67	0.59
3:E:267:LEU:O	3:E:271:LEU:HD23	2.02	0.59
1:B:56:LEU:CD2	1:B:1019:ILE:HG13	2.33	0.59
1:B:224:LEU:CD2	1:B:997:LEU:HD11	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:H	1:A:206:ASN:HD21	1.49	0.58
2:D:121:ARG:O	3:E:371:ARG:HD2	2.03	0.58
1:A:84:VAL:HG13	1:A:108:THR:HG22	1.83	0.58
1:A:170:GLN:O	1:A:174:GLU:HG3	2.03	0.58
2:C:59:GLY:O	2:C:102:VAL:HG23	2.04	0.58
2:D:172:PRO:CG	2:D:178:GLU:HG3	2.33	0.58
3:E:179:HIS:CE1	3:E:180:GLN:HG3	2.38	0.58
2:C:189:LEU:HD22	2:C:194:LEU:HD12	1.85	0.58
1:A:960:LEU:H	1:A:960:LEU:HD23	1.67	0.58
1:B:234:ARG:HH21	1:B:859:LEU:HA	1.67	0.58
1:A:65:ARG:HB3	1:A:68:LEU:HD13	1.84	0.58
1:A:272:TYR:HA	1:A:793:LEU:HD23	1.85	0.58
1:B:789:GLU:HA	1:B:789:GLU:OE1	2.02	0.58
3:E:461:ILE:CD1	3:E:464:GLN:HB2	2.34	0.58
1:A:851:SER:O	1:A:852:SER:HB3	2.04	0.58
1:A:1053:LYS:NZ	1:B:1054:GLU:OE2	2.31	0.58
3:E:417:THR:HG21	3:E:449:TRP:HE1	1.69	0.58
3:E:432:GLU:N	3:E:432:GLU:OE1	2.37	0.58
1:B:915:ASN:O	1:B:918:ARG:HD2	2.04	0.58
1:B:1019:ILE:HG23	1:B:1047:VAL:CG2	2.34	0.58
3:E:54:ILE:HD12	3:E:82:SER:HA	1.86	0.58
3:E:400:ASP:N	3:E:400:ASP:OD1	2.37	0.58
1:A:121:VAL:HG21	1:A:194:PHE:CZ	2.39	0.57
1:A:242:PHE:CE1	1:A:931:LEU:HD23	2.39	0.57
1:B:20:LEU:HD11	1:B:52:LEU:CD1	2.34	0.57
1:B:242:PHE:CE1	1:B:931:LEU:HB3	2.40	0.57
1:B:251:GLU:O	1:B:840:LYS:NZ	2.35	0.57
1:A:1036:ILE:HG21	1:A:1061:HIS:CB	2.34	0.57
2:C:156:ILE:HG12	2:C:206:ILE:HD11	1.86	0.57
3:E:408:LEU:HB2	3:E:441:HIS:CD2	2.37	0.57
2:C:85:GLU:OE2	2:D:43:ARG:HA	2.03	0.57
3:E:239:LEU:HD12	3:E:239:LEU:H	1.68	0.57
1:A:884:VAL:CG2	1:A:1041:GLU:HG2	2.34	0.57
1:B:58:THR:OG1	1:B:66:TYR:OH	2.21	0.57
1:B:183:ASN:OD1	1:B:186:GLN:HG2	2.04	0.57
1:B:1051:PRO:HG2	1:B:1053:LYS:HD3	1.86	0.57
3:E:265:GLU:HA	3:E:268:ARG:HD3	1.86	0.57
1:B:897:LYS:HG3	1:B:898:LYS:N	2.18	0.57
3:E:3:GLU:O	3:E:7:GLN:HG3	2.03	0.57
3:E:275:SER:HA	3:E:278:ASP:OD2	2.05	0.57
1:A:836:ALA:O	1:A:840:LYS:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:TRP:CD2	1:B:822:ILE:HG21	2.40	0.57
1:B:891:TYR:OH	1:B:967:MET:SD	2.52	0.57
2:D:125:LEU:HD12	3:E:374:PHE:HD1	1.68	0.57
1:A:1029:HIS:CE1	3:E:410:ARG:HD2	2.39	0.57
1:B:115:GLU:OE2	1:B:115:GLU:HA	2.03	0.57
1:B:914:LEU:CD2	1:B:918:ARG:HH21	2.18	0.57
3:E:259:GLU:OE1	3:E:259:GLU:N	2.38	0.57
1:A:978:ARG:HA	1:B:90:PRO:HG3	1.87	0.57
1:B:234:ARG:O	1:B:237:GLU:HG2	2.05	0.57
1:B:915:ASN:HA	1:B:918:ARG:NE	2.20	0.57
1:A:118:GLY:C	1:A:119:LYS:HE2	2.30	0.57
1:B:1084:GLU:OE1	3:E:476:ARG:HD2	2.05	0.57
1:B:121:VAL:HG21	1:B:194:PHE:CZ	2.39	0.56
2:C:130:SER:OG	3:E:354:VAL:HG21	2.05	0.56
3:E:182:VAL:HG13	3:E:279:ALA:HA	1.86	0.56
3:E:310:GLU:O	3:E:313:VAL:HG12	2.05	0.56
3:E:408:LEU:HD11	3:E:445:THR:HG22	1.86	0.56
1:A:51:THR:HG23	1:A:83:TYR:HE1	1.70	0.56
1:A:192:ARG:HB2	1:A:192:ARG:NH1	2.20	0.56
1:B:47:SER:HA	1:B:1070:ARG:CB	2.33	0.56
1:B:242:PHE:CZ	1:B:932:GLN:HA	2.40	0.56
3:E:196:ARG:HG3	3:E:196:ARG:HH11	1.70	0.56
3:E:217:ILE:HG23	3:E:227:ILE:HD11	1.86	0.56
3:E:419:GLN:HG3	3:E:423:LYS:CE	2.34	0.56
3:E:461:ILE:CD1	3:E:484:THR:HB	2.35	0.56
1:A:967:MET:HE2	1:A:974:VAL:HG23	1.88	0.56
1:B:53:VAL:O	1:B:57:MET:HG2	2.06	0.56
1:B:974:VAL:HG21	1:B:977:SER:HA	1.85	0.56
2:C:43:ARG:NE	2:D:85:GLU:OE2	2.38	0.56
2:C:93:ILE:HG12	2:C:100:LEU:CD2	2.36	0.56
1:A:128:TRP:CD1	1:A:160:TYR:HH	2.22	0.56
1:A:1050:THR:HG21	1:A:1058:LEU:CD2	2.36	0.56
1:B:944:ARG:HG2	1:B:944:ARG:HH11	1.70	0.56
1:B:235:ALA:O	1:B:238:VAL:HG12	2.06	0.56
1:B:905:ARG:O	1:B:908:GLU:HG3	2.05	0.56
1:A:1055:MET:HE1	3:E:401:PHE:CD1	2.41	0.56
3:E:227:ILE:HD12	3:E:317:MET:HG3	1.88	0.56
1:B:143:TRP:C	1:B:144:LEU:HD12	2.30	0.56
1:A:784:GLU:OE1	1:A:784:GLU:N	2.32	0.55
1:A:885:ASP:HB3	1:A:887:GLN:O	2.06	0.55
1:B:1054:GLU:HG2	1:B:1057:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:151:VAL:O	3:E:155:ARG:HG2	2.06	0.55
1:A:26:PHE:HB3	1:A:30:HIS:CD2	2.41	0.55
1:A:899:VAL:HG12	1:A:901:HIS:H	1.71	0.55
1:B:159:VAL:HG21	1:B:171:MET:CE	2.36	0.55
1:A:57:MET:CE	1:A:206:ASN:HA	2.36	0.55
1:A:887:GLN:HB3	1:A:888:PRO:CD	2.30	0.55
1:B:901:HIS:ND1	1:B:903:SER:OG	2.39	0.55
3:E:233:ASN:OD1	3:E:234:ASP:N	2.40	0.55
1:A:782:GLU:N	1:A:784:GLU:OE1	2.39	0.55
1:A:807:VAL:HG12	1:A:807:VAL:O	2.06	0.55
1:B:234:ARG:HB3	1:B:859:LEU:HD12	1.88	0.55
1:A:215:ASN:HB2	1:A:219:GLU:OE1	2.07	0.55
1:A:797:LEU:CD1	1:A:822:ILE:HD11	2.34	0.55
1:B:20:LEU:HD11	1:B:52:LEU:HD12	1.88	0.55
2:C:124:ARG:HD3	3:E:353:GLU:OE1	2.05	0.55
1:A:176:ILE:HD12	2:C:187:ASP:OD2	2.07	0.55
1:A:1018:ILE:HD11	1:A:1039:LEU:HD11	1.89	0.55
1:B:1032:ALA:CA	1:B:1035:ILE:HD12	2.36	0.55
1:B:887:GLN:OE1	1:B:888:PRO:HD2	2.07	0.55
1:B:899:VAL:HG13	1:B:904:LEU:HD11	1.88	0.55
3:E:24:LEU:HD22	3:E:93:LEU:HD13	1.89	0.55
1:B:794:ASN:ND2	1:B:819:LEU:HD11	2.21	0.55
1:A:51:THR:HG23	1:A:83:TYR:CE1	2.41	0.55
1:A:846:ASP:OD2	1:A:850:ARG:NH2	2.40	0.54
1:B:17:ARG:NH1	1:B:31:GLN:OE1	2.40	0.54
1:B:27:HIS:HD2	1:B:1074:ASN:HB3	1.72	0.54
1:B:40:ALA:O	1:B:1065:ALA:HA	2.07	0.54
1:B:917:ALA:HA	1:B:920:VAL:CG2	2.38	0.54
1:B:953:LEU:C	1:B:954:LEU:HD22	2.32	0.54
2:D:158:ILE:HG23	2:D:182:LEU:HD12	1.89	0.54
1:A:122:ARG:NH1	1:A:151:GLN:O	2.38	0.54
1:B:40:ALA:HB1	1:B:1058:LEU:HD13	1.90	0.54
1:B:872:GLU:O	1:B:876:GLU:HG2	2.07	0.54
2:C:230:ILE:CD1	3:E:341:LYS:HB2	2.34	0.54
3:E:282:ARG:HB3	3:E:282:ARG:NH1	2.22	0.54
1:B:806:ARG:HG3	1:B:806:ARG:NH1	2.21	0.54
2:C:126:ASN:HA	3:E:352:GLN:O	2.07	0.54
3:E:449:TRP:HA	3:E:452:MET:HG2	1.88	0.54
1:B:263:GLN:HB2	1:B:264:PRO:HD3	1.89	0.54
1:B:1070:ARG:HA	1:B:1075:SER:HA	1.89	0.54
1:B:1020:LEU:HD12	1:B:1020:LEU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:107:ASP:OD2	2:D:43:ARG:HD3	2.08	0.54
3:E:29:ARG:HG2	3:E:32:LEU:HD23	1.90	0.54
1:B:214:LEU:CD2	1:B:990:GLU:HG3	2.38	0.54
1:B:874:LEU:HD22	1:B:894:LEU:HG	1.90	0.54
1:A:852:SER:O	1:A:857:THR:HB	2.08	0.54
1:A:84:VAL:HG13	1:A:108:THR:HG21	1.90	0.54
1:A:92:ASP:HB2	1:B:980:GLY:O	2.08	0.54
1:A:42:ILE:HG22	1:A:1050:THR:OG1	2.07	0.54
1:A:946:ARG:HD2	1:B:946:ARG:NH2	2.22	0.54
1:A:974:VAL:HG11	1:A:977:SER:HB3	1.90	0.54
1:B:153:LEU:HD13	1:B:157:LEU:HD23	1.89	0.54
1:B:101:ALA:HB2	1:B:1073:GLN:NE2	2.24	0.53
1:B:183:ASN:HB2	1:B:185:LYS:HE2	1.89	0.53
1:A:813:VAL:HG12	1:A:814:GLU:OE1	2.08	0.53
1:A:893:ARG:NH1	1:A:967:MET:HE1	2.23	0.53
1:B:56:LEU:HD23	1:B:1019:ILE:HG13	1.90	0.53
1:B:123:LEU:HD23	1:B:187:TYR:HE1	1.73	0.53
1:B:940:ASP:OD2	1:B:941:ALA:N	2.41	0.53
2:D:55:LEU:O	2:D:59:GLY:N	2.40	0.53
1:B:878:ASN:ND2	1:B:893:ARG:HB2	2.23	0.53
1:B:899:VAL:HG13	1:B:904:LEU:CD1	2.38	0.53
2:C:228:GLU:OE2	2:C:229:GLN:NE2	2.41	0.53
3:E:163:ARG:HH11	3:E:163:ARG:HB3	1.74	0.53
1:B:252:LEU:HD12	1:B:252:LEU:O	2.08	0.53
2:C:117:HIS:HB3	2:C:120:VAL:HG23	1.90	0.53
3:E:462:ASP:O	3:E:465:ARG:HD2	2.08	0.53
1:B:126:LEU:C	1:B:127:LEU:HD22	2.33	0.53
1:B:1070:ARG:HG3	1:B:1075:SER:HB2	1.90	0.53
2:D:125:LEU:HD12	3:E:374:PHE:CD1	2.44	0.53
1:A:40:ALA:O	1:A:1065:ALA:HA	2.07	0.53
1:A:272:TYR:CA	1:A:793:LEU:HD23	2.39	0.53
1:B:185:LYS:HE2	1:B:185:LYS:H	1.73	0.53
2:C:57:LYS:HD2	2:D:118:PRO:O	2.08	0.53
2:D:96:ILE:HG21	2:D:149:THR:HG22	1.90	0.53
1:A:907:LEU:HD22	1:A:953:LEU:CD1	2.38	0.53
1:B:250:GLN:OE1	1:B:251:GLU:N	2.42	0.53
1:B:906:THR:HA	1:B:909:LYS:NZ	2.24	0.53
1:A:818:ASP:HB3	1:A:821:ASP:OD1	2.08	0.53
1:A:1019:ILE:HD13	1:A:1047:VAL:HB	1.90	0.53
2:D:124:ARG:HA	3:E:373:ARG:O	2.09	0.53
1:B:217:ILE:HD12	1:B:962:PHE:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:ILE:O	2:D:86:PRO:HD2	2.09	0.53
3:E:182:VAL:HG13	3:E:279:ALA:CB	2.38	0.53
3:E:265:GLU:OE1	3:E:268:ARG:HD3	2.09	0.53
1:A:41:VAL:HB	1:A:1049:ILE:HD13	1.90	0.53
1:A:1050:THR:HG21	1:A:1058:LEU:HD23	1.91	0.52
1:B:159:VAL:HG21	1:B:171:MET:HE1	1.90	0.52
3:E:153:THR:HG23	3:E:156:ARG:NH2	2.25	0.52
1:B:937:GLN:HA	1:B:940:ASP:OD1	2.09	0.52
1:A:815:ALA:HB1	1:A:821:ASP:HB3	1.91	0.52
1:A:893:ARG:HG2	1:A:894:LEU:N	2.23	0.52
3:E:128:ARG:HA	3:E:131:THR:HB	1.91	0.52
1:B:128:TRP:CE2	1:B:140:LYS:HB2	2.43	0.52
1:B:792:ARG:HB2	1:B:792:ARG:HH11	1.72	0.52
2:C:91:ILE:HD11	2:C:100:LEU:CD2	2.40	0.52
1:A:797:LEU:C	1:A:801:MET:HE3	2.34	0.52
1:B:851:SER:O	1:B:852:SER:HB2	2.09	0.52
1:A:827:GLN:OE1	1:A:827:GLN:C	2.53	0.52
1:A:882:PHE:O	1:A:969:ARG:NH2	2.43	0.52
1:A:85:ARG:NH2	1:A:133:SER:O	2.39	0.52
1:B:23:TRP:NE1	1:B:55:ALA:HB2	2.25	0.52
1:B:170:GLN:HG3	1:B:174:GLU:CD	2.35	0.52
2:D:122:ARG:NH2	3:E:373:ARG:HD3	2.25	0.52
3:E:28:ARG:NH1	3:E:69:GLN:O	2.43	0.52
1:A:81:ILE:CD1	1:A:129:PHE:HZ	2.23	0.52
1:B:1037:ALA:O	1:B:1041:GLU:HG3	2.09	0.52
1:B:829:LEU:C	1:B:829:LEU:HD13	2.35	0.52
1:B:946:ARG:HD2	1:B:946:ARG:C	2.35	0.52
2:D:187:ASP:OD1	2:D:187:ASP:C	2.54	0.52
3:E:282:ARG:CB	3:E:282:ARG:HH11	2.23	0.51
1:A:785:ARG:HE	1:A:786:VAL:HG23	1.74	0.51
1:A:982:GLN:O	1:A:983:GLY:C	2.51	0.51
1:A:1017:THR:HG23	1:A:1045:HIS:ND1	2.25	0.51
1:B:887:GLN:HB3	1:B:888:PRO:CD	2.37	0.51
1:A:17:ARG:HG3	1:A:17:ARG:HH11	1.74	0.51
1:A:1018:ILE:HG21	1:A:1044:LEU:HD13	1.91	0.51
2:C:68:ASN:C	2:C:72:ILE:HD12	2.33	0.51
2:C:77:PRO:HG2	2:C:78:GLU:OE2	2.11	0.51
2:D:90:ASP:OD2	2:D:91:ILE:N	2.44	0.51
3:E:44:SER:HB3	3:E:48:ILE:HD11	1.92	0.51
3:E:490:GLN:HG2	3:E:493:MET:CE	2.40	0.51
1:B:21:PHE:HA	1:B:28:GLY:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:799:LYS:O	1:B:802:SER:OG	2.19	0.51
2:D:172:PRO:HD2	2:D:178:GLU:HG3	1.92	0.51
3:E:54:ILE:CD1	3:E:82:SER:HA	2.41	0.51
1:A:57:MET:HE2	1:A:206:ASN:CG	2.35	0.51
2:C:129:GLN:NE2	2:C:188:GLN:OE1	2.32	0.51
2:D:137:ARG:HD3	2:D:210:ILE:CG2	2.41	0.51
1:A:92:ASP:H	1:B:981:SER:CB	2.24	0.51
1:A:203:THR:HG22	1:A:207:ARG:NH1	2.26	0.51
1:A:967:MET:HE2	1:A:974:VAL:CG2	2.40	0.51
1:B:806:ARG:HD2	1:B:806:ARG:O	2.10	0.51
1:B:1086:GLU:O	1:B:1087:ARG:C	2.54	0.51
3:E:266:ARG:O	3:E:270:ILE:HG13	2.10	0.51
1:A:998:THR:HG21	1:A:1039:LEU:HA	1.93	0.51
1:B:893:ARG:NH1	1:B:893:ARG:HG2	2.26	0.51
3:E:424:GLU:HB3	3:E:426:ARG:HG2	1.91	0.51
1:A:142:LEU:HD11	1:A:180:THR:HB	1.93	0.51
1:B:822:ILE:N	1:B:823:PRO:HD2	2.26	0.51
1:B:960:LEU:HD23	1:B:960:LEU:H	1.75	0.51
2:C:117:HIS:HB3	2:C:120:VAL:CG2	2.41	0.51
3:E:126:ALA:O	3:E:129:LEU:HB3	2.11	0.51
1:A:53:VAL:HG22	1:A:1019:ILE:HG21	1.92	0.50
1:B:909:LYS:O	1:B:913:GLN:HG2	2.11	0.50
3:E:433:LEU:O	3:E:433:LEU:HD12	2.09	0.50
1:B:238:VAL:HG21	1:B:856:VAL:HG22	1.92	0.50
1:B:1055:MET:HG3	3:E:444:GLU:HG3	1.93	0.50
2:D:144:GLU:HG2	2:D:149:THR:HA	1.92	0.50
3:E:174:GLU:HA	3:E:174:GLU:OE2	2.11	0.50
1:A:37:ASP:HB2	1:A:1063:ARG:CG	2.41	0.50
1:B:816:GLY:N	1:B:821:ASP:OD2	2.26	0.50
1:B:878:ASN:OD1	1:B:893:ARG:HB2	2.11	0.50
1:B:917:ALA:C	1:B:920:VAL:HG23	2.36	0.50
1:B:1038:ALA:HA	1:B:1041:GLU:HG3	1.93	0.50
2:C:51:ALA:HB1	2:C:73:VAL:HG23	1.93	0.50
2:C:69:LEU:HA	2:C:72:ILE:CD1	2.41	0.50
3:E:178:THR:O	3:E:182:VAL:HG23	2.12	0.50
1:B:257:LYS:HE3	1:B:257:LYS:HA	1.94	0.50
1:B:1087:ARG:HG3	3:E:477:ARG:HH21	1.77	0.50
1:A:874:LEU:HD11	1:A:962:PHE:CE1	2.46	0.50
1:B:113:THR:HG23	1:B:120:GLN:HG3	1.93	0.50
1:A:782:GLU:N	1:A:782:GLU:OE1	2.44	0.50
1:A:1022:GLU:HG3	1:A:1051:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1073:GLN:HG3	1:B:1073:GLN:O	2.10	0.50
2:C:94:ASP:HB2	2:C:212:HIS:CE1	2.47	0.50
1:A:65:ARG:CB	1:A:68:LEU:HD13	2.41	0.50
1:A:216:SER:O	1:A:220:ILE:HG23	2.11	0.50
3:E:420:LEU:HD12	3:E:437:LEU:HG	1.94	0.50
1:A:15:LEU:CB	1:A:1017:THR:HG21	2.41	0.50
1:B:228:ASP:OD1	1:B:229:HIS:N	2.43	0.50
1:B:1080:LEU:HD23	1:B:1080:LEU:C	2.37	0.50
2:C:143:TRP:CZ2	2:C:152:SER:HB3	2.46	0.50
3:E:27:THR:HG22	3:E:30:ALA:HB2	1.94	0.50
3:E:437:LEU:O	3:E:439:PRO:HD3	2.12	0.50
1:A:1087:ARG:O	1:A:1091:ARG:HG3	2.12	0.50
1:B:792:ARG:HB2	1:B:792:ARG:CZ	2.42	0.50
2:D:172:PRO:CD	2:D:178:GLU:HG3	2.41	0.50
3:E:376:GLU:OE1	3:E:376:GLU:N	2.34	0.50
1:B:66:TYR:OH	1:B:80:LEU:HD13	2.12	0.49
1:B:217:ILE:HD11	1:B:962:PHE:C	2.36	0.49
1:B:883:ARG:HD3	1:B:1011:ARG:CZ	2.41	0.49
1:B:1017:THR:HA	1:B:1045:HIS:O	2.12	0.49
1:A:1020:LEU:HD12	1:A:1048:PHE:CD1	2.46	0.49
1:B:211:LEU:HD21	1:B:224:LEU:HD22	1.94	0.49
1:B:1036:ILE:HD11	1:B:1057:LEU:CD1	2.42	0.49
1:B:30:HIS:HB3	1:B:1077:MET:HE2	1.94	0.49
3:E:257:SER:HA	3:E:261:LYS:HZ1	1.74	0.49
3:E:367:PRO:O	3:E:371:ARG:HD3	2.12	0.49
1:B:801:MET:CE	1:B:822:ILE:HG12	2.42	0.49
1:B:951:LYS:O	1:B:955:ASP:HB3	2.12	0.49
3:E:294:ARG:HB3	3:E:294:ARG:CZ	2.43	0.49
1:B:1024:PHE:HB2	1:B:1054:GLU:OE1	2.11	0.49
1:B:1026:ARG:HD3	1:B:1026:ARG:N	2.24	0.49
2:C:91:ILE:HD12	2:C:101:TYR:O	2.13	0.49
2:C:226:LEU:HD11	3:E:342:LEU:HD11	1.94	0.49
1:B:1059:ARG:HB2	3:E:443:LEU:HD22	1.95	0.49
3:E:88:TRP:CE3	3:E:93:LEU:HD12	2.47	0.49
1:A:1005:LEU:HD22	1:A:1015:PHE:HB3	1.95	0.49
1:B:115:GLU:OE2	1:B:120:GLN:HB2	2.13	0.49
1:B:20:LEU:HD23	1:B:110:ILE:HG22	1.95	0.49
1:B:1088:HIS:CE1	1:B:1091:ARG:HB2	2.48	0.49
2:C:50:GLU:O	2:C:54:GLU:HG2	2.13	0.49
1:A:92:ASP:HB2	1:B:981:SER:HB2	1.94	0.49
1:A:119:LYS:HE2	1:A:119:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LYS:HE2	1:B:130:ASP:HA	1.94	0.49
3:E:213:LEU:HD23	3:E:313:VAL:HG21	1.95	0.49
3:E:233:ASN:OD1	3:E:235:GLN:HG2	2.13	0.49
3:E:294:ARG:HG2	3:E:294:ARG:HH11	1.78	0.49
1:A:878:ASN:ND2	1:A:893:ARG:HG2	2.28	0.48
1:B:15:LEU:CD2	1:B:34:ILE:HD12	2.43	0.48
1:B:208:ALA:HA	1:B:211:LEU:HB2	1.94	0.48
1:B:855:GLY:O	1:B:857:THR:N	2.46	0.48
1:B:955:ASP:OD2	1:B:958:PHE:HD2	1.96	0.48
3:E:61:LEU:O	3:E:72:ILE:HD13	2.13	0.48
1:B:228:ASP:HA	1:B:957:ARG:CZ	2.42	0.48
1:B:868:LEU:C	1:B:868:LEU:HD13	2.38	0.48
1:B:891:TYR:HD2	1:B:969:ARG:HD3	1.76	0.48
1:B:892:LEU:HD13	1:B:964:VAL:CG1	2.43	0.48
2:C:90:ASP:HB2	2:C:105:ARG:HB2	1.94	0.48
1:A:946:ARG:CG	1:B:946:ARG:HH22	2.26	0.48
1:A:1020:LEU:HD12	1:A:1048:PHE:CE1	2.48	0.48
2:C:82:ARG:HB2	2:C:82:ARG:NH1	2.27	0.48
2:D:105:ARG:O	2:D:105:ARG:HG2	2.11	0.48
3:E:61:LEU:HD13	3:E:72:ILE:CD1	2.44	0.48
1:B:796:GLU:OE1	1:B:800:ARG:NH2	2.46	0.48
1:B:878:ASN:ND2	1:B:894:LEU:HD23	2.28	0.48
2:C:41:GLU:OE2	2:C:42:THR:HG22	2.12	0.48
2:C:73:VAL:HG11	2:C:100:LEU:HD13	1.94	0.48
3:E:160:GLU:OE1	3:E:163:ARG:NH1	2.46	0.48
1:A:888:PRO:HD2	1:A:889:ASP:N	2.18	0.48
1:A:970:GLN:OE1	1:A:971:SER:N	2.45	0.48
1:B:1036:ILE:HD11	1:B:1057:LEU:HD13	1.93	0.48
1:B:122:ARG:HG2	1:B:156:TRP:HH2	1.79	0.48
1:B:834:GLU:O	1:B:838:PRO:HG2	2.13	0.48
1:B:989:LYS:C	1:B:989:LYS:CD	2.86	0.48
2:C:158:ILE:HD12	2:C:186:LEU:HD11	1.96	0.48
2:D:93:ILE:CD1	2:D:100:LEU:HD22	2.41	0.48
3:E:128:ARG:O	3:E:128:ARG:HG2	2.14	0.48
3:E:490:GLN:O	3:E:493:MET:HG2	2.13	0.48
1:B:887:GLN:O	1:B:888:PRO:C	2.57	0.48
1:B:887:GLN:CB	1:B:888:PRO:HD2	2.36	0.48
3:E:151:VAL:CG1	3:E:155:ARG:HE	2.25	0.48
1:B:39:THR:HG22	1:B:1047:VAL:HG12	1.95	0.48
1:B:886:PHE:CG	1:B:892:LEU:HD23	2.49	0.48
1:B:1059:ARG:HG2	1:B:1059:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:96:ILE:HG23	3:E:319:THR:HB	1.96	0.48
2:D:78:GLU:HA	2:D:81:THR:CG2	2.43	0.48
3:E:419:GLN:CG	3:E:423:LYS:HE2	2.41	0.48
1:B:872:GLU:OE1	1:B:873:ARG:HG2	2.14	0.48
1:B:884:VAL:HG22	1:B:885:ASP:H	1.79	0.48
3:E:454:ARG:NH2	3:E:460:VAL:H	2.10	0.48
1:A:855:GLY:O	1:A:857:THR:N	2.47	0.48
3:E:98:ASP:CG	3:E:98:ASP:O	2.57	0.48
3:E:127:SER:O	3:E:128:ARG:HB3	2.14	0.48
3:E:210:ASP:O	3:E:214:ARG:HG3	2.12	0.48
1:A:228:ASP:HA	1:A:957:ARG:CZ	2.44	0.47
1:A:967:MET:HA	1:A:975:ILE:HG23	1.94	0.47
2:D:55:LEU:HD21	2:D:102:VAL:HG13	1.94	0.47
3:E:29:ARG:CG	3:E:32:LEU:HD23	2.43	0.47
3:E:310:GLU:C	3:E:310:GLU:OE2	2.57	0.47
1:A:808:ASP:CG	1:A:812:LEU:HB2	2.38	0.47
1:A:955:ASP:HB3	1:A:958:PHE:HB2	1.95	0.47
1:B:881:MET:HE1	1:B:892:LEU:HD11	1.96	0.47
1:B:906:THR:HA	1:B:909:LYS:HZ2	1.77	0.47
1:B:976:GLU:HB3	1:B:978:ARG:O	2.15	0.47
2:C:96:ILE:HD13	2:C:96:ILE:N	2.29	0.47
2:D:55:LEU:HD22	2:D:102:VAL:CG1	2.37	0.47
1:A:272:TYR:CE1	1:A:790:LEU:HD13	2.49	0.47
1:B:197:VAL:HG12	1:B:198:GLY:N	2.29	0.47
1:B:269:TRP:CD1	1:B:826:LEU:HD11	2.50	0.47
1:B:983:GLY:N	1:B:988:GLU:H	2.08	0.47
2:C:73:VAL:CG1	2:C:100:LEU:HD13	2.44	0.47
3:E:89:ILE:HD13	3:E:96:GLU:HB2	1.96	0.47
1:A:846:ASP:CG	1:A:850:ARG:HH21	2.21	0.47
1:B:144:LEU:HD12	1:B:144:LEU:N	2.29	0.47
1:B:183:ASN:HD21	1:B:186:GLN:HG2	1.79	0.47
2:D:158:ILE:HG23	2:D:182:LEU:CD1	2.44	0.47
1:A:60:LEU:HD21	1:A:1015:PHE:CZ	2.50	0.47
1:A:62:ALA:HB2	1:A:188:LEU:CD1	2.45	0.47
1:A:192:ARG:HH11	1:A:192:ARG:CG	2.28	0.47
1:A:269:TRP:CD1	1:A:826:LEU:HD21	2.49	0.47
1:A:792:ARG:CZ	1:A:792:ARG:HB3	2.43	0.47
1:B:139:MET:HE3	1:B:141:ARG:HH22	1.79	0.47
3:E:36:CYS:O	3:E:40:LEU:HG	2.14	0.47
1:A:282:TRP:CD1	1:A:783:ILE:HD11	2.50	0.47
1:B:897:LYS:HB3	1:B:961:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:VAL:CG1	1:B:904:LEU:HD11	2.44	0.47
3:E:95:VAL:CG2	3:E:102:PHE:HB2	2.43	0.47
3:E:426:ARG:O	3:E:428:VAL:HG23	2.13	0.47
1:A:37:ASP:HB2	1:A:1063:ARG:HG3	1.97	0.47
1:A:192:ARG:HG3	1:A:192:ARG:HH11	1.79	0.47
1:A:242:PHE:CD1	1:A:931:LEU:HD23	2.49	0.47
1:A:805:LYS:NZ	1:A:813:VAL:HA	2.29	0.47
1:B:39:THR:HG23	1:B:1047:VAL:HB	1.96	0.47
1:B:79:ASP:OD2	1:B:79:ASP:C	2.57	0.47
1:B:168:LEU:HA	1:B:171:MET:SD	2.55	0.47
1:B:943:GLU:CB	1:B:944:ARG:HH12	2.27	0.47
2:C:54:GLU:HG3	2:C:69:LEU:HD13	1.96	0.47
2:D:94:ASP:OD2	2:D:97:ARG:HB2	2.15	0.47
1:A:57:MET:HE2	1:A:206:ASN:OD1	2.13	0.47
1:A:274:LYS:HZ1	1:A:275:GLN:HG2	1.80	0.47
1:A:881:MET:HE1	1:A:894:LEU:CD1	2.44	0.47
1:B:221:PHE:HB3	1:B:226:LEU:HD22	1.95	0.47
2:D:163:PRO:O	2:D:167:ILE:HG12	2.15	0.47
3:E:199:PHE:HE1	3:E:247:PHE:HE1	1.61	0.47
1:A:1036:ILE:HD13	1:A:1036:ILE:N	2.28	0.47
1:B:221:PHE:O	1:B:226:LEU:HB2	2.15	0.47
1:B:226:LEU:O	1:B:957:ARG:HD3	2.15	0.47
1:B:257:LYS:HA	1:B:257:LYS:CE	2.44	0.47
1:B:794:ASN:C	1:B:794:ASN:HD22	2.23	0.47
1:B:890:ARG:HH21	1:B:975:ILE:HG12	1.80	0.47
2:D:73:VAL:HG11	2:D:100:LEU:HD13	1.97	0.47
3:E:28:ARG:HH12	3:E:69:GLN:CA	2.28	0.47
3:E:114:VAL:O	3:E:117:LEU:HB2	2.15	0.47
3:E:182:VAL:HG13	3:E:279:ALA:CA	2.44	0.47
3:E:423:LYS:HD3	3:E:423:LYS:N	2.29	0.47
1:A:92:ASP:C	1:B:981:SER:HB2	2.40	0.47
1:A:224:LEU:HD12	1:A:224:LEU:HA	1.81	0.47
1:A:238:VAL:CG1	1:A:856:VAL:HG22	2.45	0.47
1:A:968:ASP:OD2	1:A:970:GLN:NE2	2.48	0.47
1:B:997:LEU:HD12	1:B:997:LEU:HA	1.76	0.47
2:D:109:THR:HG23	2:D:109:THR:O	2.15	0.47
3:E:91:ARG:O	3:E:92:ARG:HB2	2.14	0.47
1:A:225:VAL:HG23	1:A:226:LEU:HG	1.97	0.46
1:A:1029:HIS:ND1	3:E:410:ARG:HD2	2.30	0.46
1:B:255:ALA:CB	1:B:840:LYS:HZ3	2.28	0.46
3:E:24:LEU:CB	3:E:93:LEU:HD11	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:THR:OG1	1:B:122:ARG:NH2	2.48	0.46
1:B:1084:GLU:OE2	3:E:476:ARG:HD2	2.16	0.46
3:E:210:ASP:OD2	3:E:210:ASP:C	2.59	0.46
3:E:288:LEU:HD12	3:E:288:LEU:O	2.14	0.46
3:E:408:LEU:CD1	3:E:445:THR:HG22	2.44	0.46
1:A:61:CYS:O	1:A:184:LYS:NZ	2.45	0.46
1:A:963:ALA:HB1	1:A:979:THR:HA	1.96	0.46
1:B:26:PHE:CE1	1:B:1077:MET:HG3	2.50	0.46
1:B:1007:PRO:HD2	1:B:1010:SER:HB3	1.97	0.46
1:B:246:THR:HG23	1:B:928:TYR:HH	1.80	0.46
1:B:895:ASP:OD2	1:B:963:ALA:HB3	2.16	0.46
1:B:1084:GLU:HB2	3:E:478:TRP:CE3	2.50	0.46
3:E:108:GLU:HA	3:E:108:GLU:OE1	2.15	0.46
1:A:791:HIS:CE1	1:B:791:HIS:ND1	2.84	0.46
1:B:914:LEU:HD23	1:B:914:LEU:C	2.41	0.46
1:B:963:ALA:HB1	1:B:978:ARG:NH1	2.30	0.46
2:D:62:GLU:OE1	2:D:207:ARG:NH2	2.46	0.46
3:E:233:ASN:CG	3:E:235:GLN:H	2.21	0.46
1:A:793:LEU:O	1:A:797:LEU:HD23	2.14	0.46
1:A:979:THR:O	1:A:979:THR:HG23	2.16	0.46
1:B:127:LEU:HD22	1:B:127:LEU:N	2.31	0.46
1:B:905:ARG:HA	1:B:908:GLU:HG3	1.98	0.46
3:E:58:SER:HB3	3:E:78:PHE:HA	1.97	0.46
3:E:87:GLU:HA	3:E:90:LYS:HZ2	1.80	0.46
1:A:946:ARG:CD	1:B:946:ARG:HH22	2.28	0.46
1:B:1031:VAL:C	1:B:1035:ILE:HD12	2.40	0.46
3:E:24:LEU:HD22	3:E:93:LEU:CD1	2.45	0.46
3:E:147:PRO:O	3:E:151:VAL:HG23	2.16	0.46
3:E:236:ASP:HB3	3:E:239:LEU:HG	1.97	0.46
1:A:272:TYR:HA	1:A:793:LEU:CD2	2.46	0.46
1:B:122:ARG:HG2	1:B:156:TRP:CH2	2.51	0.46
1:B:166:ARG:HG2	1:B:169:ARG:HH22	1.81	0.46
1:B:983:GLY:H	1:B:988:GLU:N	2.08	0.46
1:B:1055:MET:HB2	3:E:444:GLU:OE2	2.16	0.46
3:E:28:ARG:NH2	3:E:69:GLN:HB3	2.30	0.46
1:A:257:LYS:HB3	1:A:807:VAL:HG11	1.98	0.46
1:A:803:GLU:OE1	1:A:803:GLU:O	2.34	0.46
1:A:963:ALA:CB	1:A:979:THR:HA	2.45	0.46
1:A:980:GLY:O	1:A:981:SER:C	2.59	0.46
1:B:159:VAL:HG13	1:B:167:LEU:HG	1.98	0.46
2:C:101:TYR:HE2	2:C:103:LYS:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:277:SER:HA	3:E:285:ARG:NH1	2.31	0.46
1:A:15:LEU:HG	1:A:34:ILE:HD12	1.98	0.46
1:A:242:PHE:CZ	1:A:932:GLN:HA	2.51	0.46
1:A:884:VAL:HG22	1:A:1041:GLU:CG	2.43	0.46
1:B:17:ARG:NH1	1:B:31:GLN:HB3	2.31	0.46
1:B:917:ALA:HA	1:B:920:VAL:HG23	1.97	0.46
3:E:265:GLU:CD	3:E:268:ARG:HD3	2.41	0.46
3:E:391:ALA:O	3:E:392:ALA:HB3	2.16	0.46
1:A:968:ASP:HB3	1:A:971:SER:O	2.17	0.45
1:B:907:LEU:HD13	1:B:907:LEU:C	2.41	0.45
1:A:80:LEU:O	1:A:84:VAL:HG23	2.16	0.45
1:A:84:VAL:HG22	1:A:108:THR:HG21	1.96	0.45
1:B:846:ASP:OD2	1:B:850:ARG:NH2	2.49	0.45
3:E:223:HIS:O	3:E:227:ILE:HG12	2.16	0.45
3:E:470:LEU:HD13	3:E:470:LEU:C	2.41	0.45
1:A:269:TRP:CD2	1:A:822:ILE:HG21	2.51	0.45
1:A:887:GLN:CB	1:A:890:ARG:HG3	2.41	0.45
3:E:210:ASP:HA	3:E:238:LEU:HD21	1.97	0.45
1:B:183:ASN:ND2	1:B:186:GLN:HG2	2.32	0.45
1:B:252:LEU:HD21	1:B:841:LEU:HD13	1.97	0.45
1:A:27:HIS:O	3:E:387:LEU:HD11	2.16	0.45
1:B:91:GLY:HA3	1:B:99:HIS:CG	2.52	0.45
1:B:142:LEU:HD13	1:B:142:LEU:C	2.41	0.45
1:B:243:ASP:OD2	1:B:939:ARG:NH2	2.46	0.45
1:B:252:LEU:HA	1:B:840:LYS:HZ3	1.81	0.45
3:E:61:LEU:CD1	3:E:72:ILE:HG12	2.46	0.45
3:E:98:ASP:O	3:E:98:ASP:OD1	2.34	0.45
3:E:217:ILE:CG2	3:E:227:ILE:HD11	2.46	0.45
1:B:54:ASP:OD1	1:B:66:TYR:HB3	2.16	0.45
1:B:166:ARG:HA	1:B:169:ARG:NH2	2.31	0.45
3:E:282:ARG:NH1	3:E:282:ARG:CB	2.80	0.45
2:D:136:LEU:HD22	2:D:206:ILE:HD11	1.98	0.45
1:A:17:ARG:HG3	1:A:17:ARG:NH1	2.31	0.45
1:B:59:LEU:HD23	1:B:59:LEU:HA	1.75	0.45
1:B:183:ASN:HD22	1:B:185:LYS:HE2	1.81	0.45
2:D:47:LYS:HB3	2:D:47:LYS:HE3	1.59	0.45
1:A:233:ASP:OD1	1:A:234:ARG:N	2.49	0.45
1:A:981:SER:O	1:A:982:GLN:C	2.59	0.45
1:B:211:LEU:HD13	1:B:212:LYS:N	2.32	0.45
2:D:224:ALA:HA	2:D:227:ARG:HG2	1.99	0.45
3:E:182:VAL:HG13	3:E:279:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:229:GLU:O	3:E:229:GLU:HG2	2.16	0.45
1:A:47:SER:HB2	1:A:1068:VAL:HG12	1.99	0.44
1:A:67:ASN:O	1:A:71:THR:HG23	2.17	0.44
1:A:812:LEU:HG	1:A:825:TYR:CD1	2.52	0.44
1:B:211:LEU:HD13	1:B:211:LEU:C	2.42	0.44
1:A:123:LEU:HD22	1:A:191:LEU:HD21	1.98	0.44
1:A:982:GLN:CD	1:A:982:GLN:H	2.25	0.44
1:B:940:ASP:OD2	1:B:940:ASP:C	2.60	0.44
1:B:1036:ILE:CD1	1:B:1057:LEU:CD1	2.95	0.44
2:D:165:LEU:CD1	2:D:182:LEU:HD23	2.47	0.44
1:A:887:GLN:CB	1:A:888:PRO:CD	2.95	0.44
1:B:56:LEU:HG	1:B:60:LEU:HD23	1.98	0.44
3:E:28:ARG:HH22	3:E:69:GLN:HA	1.82	0.44
3:E:143:LEU:HD23	3:E:143:LEU:O	2.17	0.44
3:E:267:LEU:CD1	3:E:288:LEU:HD11	2.44	0.44
3:E:424:GLU:OE1	3:E:426:ARG:HD3	2.17	0.44
3:E:461:ILE:HG13	3:E:461:ILE:O	2.16	0.44
1:A:228:ASP:OD1	1:A:230:SER:N	2.33	0.44
1:A:906:THR:CG2	1:A:937:GLN:HE22	2.30	0.44
1:B:51:THR:HG23	1:B:83:TYR:CE1	2.52	0.44
1:B:818:ASP:OD1	1:B:820:ASP:N	2.30	0.44
2:C:96:ILE:CG2	3:E:319:THR:HB	2.47	0.44
1:A:105:LYS:O	1:A:105:LYS:HG3	2.18	0.44
1:B:926:SER:HA	1:B:929:LYS:HG2	1.98	0.44
1:B:943:GLU:HB2	1:B:944:ARG:HH12	1.82	0.44
2:C:127:LEU:HD22	3:E:354:VAL:HG12	2.00	0.44
2:D:143:TRP:CE2	2:D:154:ALA:HA	2.53	0.44
2:D:179:ARG:HB2	2:D:179:ARG:NH1	2.32	0.44
2:D:225:TRP:CE3	2:D:226:LEU:HD23	2.53	0.44
3:E:177:GLU:HB2	3:E:180:GLN:CB	2.39	0.44
1:B:952:ALA:O	1:B:959:ARG:HG2	2.17	0.44
1:B:1087:ARG:HG3	3:E:477:ARG:NE	2.27	0.44
3:E:233:ASN:ND2	3:E:235:GLN:HB2	2.23	0.44
3:E:260:LEU:HD12	3:E:292:VAL:HG13	1.98	0.44
1:A:944:ARG:HB3	1:A:947:THR:CG2	2.48	0.44
1:B:252:LEU:CA	1:B:840:LYS:HE2	2.46	0.44
1:B:915:ASN:O	1:B:918:ARG:CD	2.65	0.44
1:B:929:LYS:HG3	1:B:930:ALA:N	2.32	0.44
2:C:127:LEU:HD22	3:E:354:VAL:CG1	2.47	0.44
3:E:25:LEU:HD21	3:E:113:PHE:CD2	2.53	0.44
1:A:946:ARG:HD2	1:B:946:ARG:CZ	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:836:ALA:O	1:B:840:LYS:HB3	2.18	0.44
2:D:45:LEU:O	2:D:49:ARG:HG3	2.18	0.44
1:A:15:LEU:N	1:A:1017:THR:OG1	2.44	0.44
1:A:61:CYS:SG	1:A:62:ALA:N	2.91	0.44
1:A:99:HIS:CG	1:A:99:HIS:O	2.71	0.44
1:A:221:PHE:O	1:A:226:LEU:HD11	2.18	0.44
1:A:1081:SER:N	1:A:1084:GLU:OE1	2.41	0.44
1:B:15:LEU:CG	1:B:34:ILE:HD12	2.47	0.44
1:B:120:GLN:OE1	1:B:122:ARG:NH1	2.49	0.44
2:C:69:LEU:HA	2:C:72:ILE:HD13	2.00	0.44
1:B:803:GLU:O	1:B:807:VAL:HG22	2.18	0.43
1:B:891:TYR:CD2	1:B:969:ARG:HD3	2.53	0.43
2:C:43:ARG:HD2	2:C:43:ARG:HA	1.76	0.43
3:E:163:ARG:HH11	3:E:163:ARG:CB	2.31	0.43
1:B:272:TYR:HA	1:B:793:LEU:CD1	2.48	0.43
2:C:199:ASP:OD2	2:C:199:ASP:C	2.60	0.43
1:A:12:SER:C	1:A:116:ARG:HD3	2.43	0.43
1:A:216:SER:HB2	1:A:982:GLN:HG3	1.99	0.43
1:A:970:GLN:H	1:A:970:GLN:HG3	1.64	0.43
1:B:1006:CYS:HA	1:B:1013:PRO:HA	2.00	0.43
3:E:220:GLU:OE1	3:E:223:HIS:HA	2.18	0.43
3:E:241:THR:N	3:E:242:PRO:HD2	2.34	0.43
3:E:295:LEU:HD23	3:E:295:LEU:HA	1.86	0.43
3:E:465:ARG:HE	3:E:465:ARG:HB3	1.57	0.43
1:B:259:GLN:O	1:B:263:GLN:HG2	2.18	0.43
1:B:1019:ILE:HG23	1:B:1047:VAL:HG22	1.99	0.43
2:D:230:ILE:O	2:D:234:THR:HG22	2.17	0.43
3:E:29:ARG:HE	3:E:29:ARG:HB2	1.63	0.43
3:E:236:ASP:O	3:E:237:ALA:HB3	2.18	0.43
1:A:123:LEU:HD13	1:A:191:LEU:HD11	1.99	0.43
1:B:255:ALA:HB3	1:B:840:LYS:HZ3	1.83	0.43
1:B:272:TYR:CD1	1:B:272:TYR:C	2.96	0.43
1:B:802:SER:OG	1:B:803:GLU:OE2	2.36	0.43
1:B:1003:TYR:C	1:B:1003:TYR:CD1	2.97	0.43
1:B:252:LEU:HD13	1:B:840:LYS:HG3	2.01	0.43
1:B:893:ARG:NH1	1:B:965:SER:HB2	2.33	0.43
2:D:78:GLU:HA	2:D:81:THR:HG22	2.00	0.43
2:D:119:LEU:HD22	3:E:363:VAL:O	2.19	0.43
2:D:166:GLN:HE22	2:D:171:ASP:HB2	1.82	0.43
3:E:1:MET:SD	3:E:1:MET:N	2.73	0.43
3:E:440:ALA:O	3:E:441:HIS:ND1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ALA:CB	1:B:1022:GLU:HG3	2.45	0.43
1:B:184:LYS:HG2	1:B:188:LEU:CD1	2.48	0.43
2:D:79:GLU:HG3	2:D:82:ARG:HH21	1.83	0.43
3:E:261:LYS:N	3:E:261:LYS:CD	2.81	0.43
3:E:57:LEU:O	3:E:61:LEU:HD23	2.19	0.43
3:E:177:GLU:CB	3:E:180:GLN:HB2	2.38	0.43
3:E:242:PRO:O	3:E:243:GLU:C	2.62	0.43
3:E:265:GLU:HA	3:E:268:ARG:CD	2.49	0.43
3:E:412:VAL:O	3:E:415:GLN:HG2	2.19	0.43
3:E:442:ASP:HB3	3:E:480:PHE:CZ	2.53	0.43
1:A:1079:SER:O	2:D:177:LYS:HE3	2.19	0.43
1:B:159:VAL:HG11	1:B:171:MET:CE	2.49	0.43
1:B:796:GLU:O	1:B:800:ARG:HG2	2.19	0.43
2:C:94:ASP:HB2	2:C:212:HIS:NE2	2.34	0.43
2:C:115:TRP:CG	2:C:124:ARG:HG2	2.53	0.43
1:A:95:GLU:CD	1:A:98:SER:H	2.27	0.43
1:B:228:ASP:HA	1:B:957:ARG:HD3	2.00	0.43
1:B:1083:GLU:C	1:B:1083:GLU:OE1	2.62	0.43
2:D:104:VAL:CG1	2:D:106:LEU:HG	2.49	0.43
3:E:255:ARG:HB2	3:E:255:ARG:HH11	1.84	0.43
1:B:123:LEU:HD23	1:B:187:TYR:CE1	2.53	0.42
1:B:896:THR:HG1	1:B:960:LEU:HD12	1.84	0.42
1:A:966:VAL:HG13	1:A:975:ILE:HG13	2.01	0.42
1:B:209:ALA:HA	1:B:1019:ILE:O	2.18	0.42
1:B:269:TRP:O	1:B:273:GLN:HG2	2.19	0.42
1:B:271:LYS:NZ	1:B:271:LYS:HB3	2.34	0.42
1:B:940:ASP:O	1:B:944:ARG:HG2	2.19	0.42
1:B:1058:LEU:HD23	1:B:1058:LEU:HA	1.89	0.42
2:C:106:LEU:CB	2:C:110:PRO:HG2	2.50	0.42
3:E:238:LEU:HD23	3:E:238:LEU:HA	1.86	0.42
3:E:265:GLU:O	3:E:268:ARG:HG2	2.19	0.42
1:A:906:THR:HG22	1:A:937:GLN:HE22	1.83	0.42
1:B:110:ILE:HG13	1:B:125:ALA:HB3	2.01	0.42
1:B:220:ILE:O	1:B:224:LEU:HB3	2.20	0.42
1:B:901:HIS:CE1	1:B:903:SER:OG	2.72	0.42
2:C:165:LEU:HD12	2:C:182:LEU:HD13	2.02	0.42
3:E:443:LEU:HD23	3:E:444:GLU:H	1.84	0.42
1:B:225:VAL:HG12	1:B:226:LEU:N	2.34	0.42
1:B:825:TYR:CD1	1:B:825:TYR:N	2.88	0.42
2:C:57:LYS:HE3	2:C:58:TYR:CZ	2.54	0.42
2:C:156:ILE:CD1	2:C:206:ILE:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:226:LEU:CD1	3:E:342:LEU:HD11	2.49	0.42
2:D:136:LEU:HD22	2:D:206:ILE:HD12	2.00	0.42
3:E:417:THR:HG21	3:E:449:TRP:NE1	2.32	0.42
3:E:437:LEU:HA	3:E:437:LEU:HD23	1.79	0.42
3:E:465:ARG:HB3	3:E:481:ASN:OD1	2.19	0.42
1:A:30:HIS:CE1	3:E:387:LEU:HD22	2.54	0.42
1:A:121:VAL:HG21	1:A:194:PHE:CE2	2.54	0.42
1:A:1085:LEU:HD12	1:A:1085:LEU:HA	1.82	0.42
1:B:242:PHE:HZ	1:B:932:GLN:HG3	1.84	0.42
1:B:915:ASN:C	1:B:918:ARG:HD2	2.44	0.42
3:E:24:LEU:O	3:E:30:ALA:HB2	2.19	0.42
3:E:151:VAL:HG13	3:E:155:ARG:NE	2.32	0.42
3:E:368:ALA:O	3:E:370:GLU:N	2.52	0.42
1:B:828:ARG:CZ	1:B:832:LEU:HG	2.49	0.42
1:B:851:SER:C	1:B:853:ASP:H	2.26	0.42
2:D:182:LEU:HD22	2:D:182:LEU:O	2.18	0.42
1:A:948:LEU:HD12	1:A:948:LEU:C	2.44	0.42
1:A:1024:PHE:HE1	1:A:1035:ILE:HG21	1.78	0.42
1:B:66:TYR:HH	1:B:80:LEU:HD13	1.84	0.42
2:D:47:LYS:HB3	2:D:72:ILE:CD1	2.38	0.42
3:E:443:LEU:HD23	3:E:444:GLU:N	2.34	0.42
1:A:23:TRP:NE1	1:A:55:ALA:HB2	2.35	0.42
1:A:41:VAL:HB	1:A:1049:ILE:CD1	2.49	0.42
1:A:837:LEU:HD23	1:A:837:LEU:HA	1.85	0.42
1:A:851:SER:O	1:A:852:SER:CB	2.68	0.42
1:B:65:ARG:HB2	1:B:68:LEU:HD22	2.02	0.42
1:B:806:ARG:HD2	1:B:806:ARG:C	2.44	0.42
1:B:889:ASP:O	1:B:889:ASP:CG	2.63	0.42
2:C:85:GLU:OE2	2:D:43:ARG:NE	2.27	0.42
2:C:133:VAL:HG22	2:C:194:LEU:HD13	2.01	0.42
2:C:143:TRP:CE3	2:C:154:ALA:HB2	2.54	0.42
3:E:490:GLN:HA	3:E:493:MET:CE	2.44	0.42
1:A:874:LEU:HD11	1:A:962:PHE:HE1	1.85	0.42
1:A:1039:LEU:CD2	1:A:1046:ALA:HB2	2.36	0.42
1:B:157:LEU:HD13	1:B:157:LEU:HA	1.89	0.42
1:B:159:VAL:HG12	1:B:168:LEU:HD13	2.01	0.42
1:B:242:PHE:CE2	1:B:932:GLN:HA	2.54	0.42
3:E:254:LEU:HD22	3:E:260:LEU:HD11	2.01	0.42
3:E:330:HIS:CE1	3:E:334:GLU:OE1	2.73	0.42
3:E:461:ILE:HD12	3:E:464:GLN:CD	2.44	0.42
1:A:274:LYS:HE3	1:A:274:LYS:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:GLU:HG2	1:A:783:ILE:H	1.85	0.42
1:A:805:LYS:HE3	1:A:805:LYS:HB3	1.93	0.42
1:B:142:LEU:HD12	1:B:144:LEU:HD11	2.02	0.42
2:D:47:LYS:HE3	2:D:72:ILE:HD11	2.01	0.42
2:D:106:LEU:HD23	2:D:106:LEU:HA	1.79	0.42
2:D:213:LEU:O	2:D:215:ASP:N	2.53	0.42
1:A:15:LEU:HD12	1:A:113:THR:O	2.20	0.41
1:A:238:VAL:HG11	1:A:856:VAL:HG22	2.02	0.41
1:A:275:GLN:HB3	1:A:790:LEU:CD2	2.49	0.41
1:A:839:GLU:O	1:A:840:LYS:C	2.63	0.41
1:A:897:LYS:O	1:A:960:LEU:HB2	2.20	0.41
1:A:901:HIS:CD2	1:A:948:LEU:HG	2.55	0.41
1:A:1080:LEU:HD23	2:D:177:LYS:HD2	2.01	0.41
1:B:226:LEU:O	1:B:227:ASP:C	2.63	0.41
1:B:860:LEU:CD2	1:B:907:LEU:HD11	2.46	0.41
2:C:155:GLN:HG2	2:C:205:VAL:HG22	2.02	0.41
1:A:62:ALA:HA	1:A:188:LEU:HD11	2.02	0.41
1:A:65:ARG:H	1:A:206:ASN:ND2	2.15	0.41
1:B:242:PHE:CD2	1:B:935:VAL:HG11	2.55	0.41
1:B:914:LEU:HD23	1:B:914:LEU:O	2.20	0.41
1:B:922:ASP:O	1:B:923:ASN:HB2	2.19	0.41
3:E:265:GLU:HA	3:E:268:ARG:CG	2.50	0.41
1:A:129:PHE:CZ	1:A:139:MET:HB2	2.55	0.41
1:B:85:ARG:HD2	1:B:102:ARG:O	2.20	0.41
1:B:170:GLN:HG3	1:B:174:GLU:OE1	2.20	0.41
1:B:183:ASN:CG	1:B:186:GLN:HG2	2.45	0.41
2:C:91:ILE:HD11	2:C:100:LEU:HD22	2.01	0.41
2:D:93:ILE:N	2:D:93:ILE:HD13	2.35	0.41
3:E:87:GLU:O	3:E:91:ARG:HB2	2.19	0.41
3:E:97:ARG:NH2	3:E:102:PHE:CZ	2.89	0.41
3:E:139:LEU:O	3:E:143:LEU:HB2	2.20	0.41
1:A:921:ASP:OD2	1:A:921:ASP:C	2.63	0.41
1:B:7:LEU:HG	1:B:11:GLU:CG	2.51	0.41
1:B:1082:TRP:HB3	3:E:480:PHE:CD2	2.55	0.41
2:D:165:LEU:HD12	2:D:182:LEU:HD23	2.02	0.41
3:E:421:LEU:HB3	3:E:489:SER:HB2	2.03	0.41
1:B:23:TRP:HE3	1:B:108:THR:HG21	1.86	0.41
1:B:128:TRP:CG	1:B:160:TYR:HH	2.39	0.41
1:B:234:ARG:HA	1:B:237:GLU:CD	2.44	0.41
1:B:897:LYS:CG	1:B:898:LYS:H	2.26	0.41
2:D:199:ASP:OD1	2:D:201:HIS:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PHE:HD1	1:A:225:VAL:CG2	2.33	0.41
1:A:272:TYR:CE2	1:A:819:LEU:HD21	2.56	0.41
1:B:891:TYR:CZ	1:B:967:MET:HB2	2.56	0.41
1:B:960:LEU:HD23	1:B:960:LEU:N	2.36	0.41
3:E:46:ASP:OD1	3:E:46:ASP:N	2.37	0.41
1:A:271:LYS:HB2	1:A:271:LYS:HE2	1.56	0.41
1:A:895:ASP:OD2	1:A:895:ASP:C	2.64	0.41
1:B:26:PHE:HE1	1:B:1077:MET:HG3	1.84	0.41
1:B:122:ARG:CZ	1:B:122:ARG:HB2	2.51	0.41
1:B:905:ARG:O	1:B:909:LYS:NZ	2.54	0.41
2:C:155:GLN:CG	2:C:205:VAL:HG22	2.50	0.41
2:D:84:LEU:HD12	2:D:91:ILE:HG23	2.03	0.41
3:E:127:SER:OG	3:E:183:GLU:HG2	2.20	0.41
3:E:417:THR:CG2	3:E:449:TRP:HE1	2.33	0.41
1:A:12:SER:HB3	1:A:1013:PRO:O	2.20	0.41
1:A:45:THR:OG1	1:B:985:SER:HB2	2.20	0.41
1:A:946:ARG:HA	1:A:951:LYS:HD3	2.03	0.41
1:A:966:VAL:HG12	1:A:976:GLU:HB3	2.00	0.41
1:B:218:ASP:HB3	1:B:222:ARG:HE	1.86	0.41
1:B:245:LEU:HD11	1:B:848:LEU:HA	2.02	0.41
1:B:864:GLU:OE2	1:B:864:GLU:HA	2.20	0.41
1:B:951:LYS:O	1:B:955:ASP:N	2.50	0.41
2:D:196:THR:CG2	2:D:205:VAL:HG13	2.50	0.41
2:D:206:ILE:HG22	2:D:210:ILE:HG13	2.03	0.41
3:E:155:ARG:HA	3:E:158:ILE:HD12	2.02	0.41
3:E:163:ARG:NH1	3:E:163:ARG:CB	2.84	0.41
3:E:261:LYS:H	3:E:261:LYS:CD	2.34	0.41
3:E:308:ARG:HG2	3:E:309:SER:N	2.35	0.41
3:E:413:LEU:HD12	3:E:417:THR:HG23	2.03	0.41
3:E:461:ILE:HG12	3:E:484:THR:O	2.21	0.41
1:A:118:GLY:O	1:A:119:LYS:HE2	2.20	0.41
1:A:795:ILE:CD1	1:B:795:ILE:HD13	2.51	0.41
1:A:797:LEU:HD12	1:A:801:MET:CE	2.51	0.41
1:A:1006:CYS:HA	1:A:1013:PRO:HA	2.03	0.41
1:B:191:LEU:HD22	1:B:195:PHE:HD2	1.86	0.41
3:E:146:ASN:ND2	3:E:149:ASN:OD1	2.54	0.41
3:E:251:GLN:OE1	3:E:299:SER:HB3	2.21	0.41
3:E:300:GLN:HG3	3:E:304:GLN:OE1	2.21	0.41
1:A:147:ASP:OD2	1:A:147:ASP:C	2.63	0.40
1:A:782:GLU:HG2	1:A:783:ILE:N	2.36	0.40
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:874:LEU:HD11	1:B:962:PHE:CD1	2.56	0.40
1:B:905:ARG:HA	1:B:908:GLU:CG	2.51	0.40
1:B:915:ASN:HA	1:B:918:ARG:HD2	2.03	0.40
1:B:946:ARG:HD2	1:B:947:THR:N	2.35	0.40
1:B:1060:ASP:OD1	1:B:1060:ASP:N	2.54	0.40
2:C:121:ARG:O	2:C:122:ARG:HB2	2.21	0.40
1:A:951:LYS:HE3	1:A:958:PHE:CZ	2.56	0.40
1:B:128:TRP:CD2	1:B:140:LYS:HB2	2.56	0.40
1:B:239:ALA:HB1	1:B:939:ARG:NE	2.36	0.40
1:B:1019:ILE:CD1	1:B:1047:VAL:HG22	2.51	0.40
2:C:69:LEU:HA	2:C:72:ILE:HD12	2.03	0.40
2:C:70:TYR:CE1	2:C:74:LEU:HD12	2.56	0.40
2:C:175:GLU:O	2:C:178:GLU:HG2	2.20	0.40
2:D:166:GLN:O	2:D:166:GLN:HG3	2.20	0.40
1:A:92:ASP:CA	1:B:981:SER:HB2	2.52	0.40
1:A:874:LEU:HD12	1:A:896:THR:HG22	2.03	0.40
1:B:53:VAL:HG22	1:B:1019:ILE:CG2	2.46	0.40
1:B:818:ASP:OD1	1:B:819:LEU:N	2.54	0.40
1:B:953:LEU:HD12	1:B:953:LEU:HA	1.90	0.40
2:D:138:GLN:HG3	2:D:139:HIS:N	2.36	0.40
3:E:85:LEU:HD23	3:E:85:LEU:HA	1.82	0.40
1:A:234:ARG:HD3	3:E:66:SER:HB2	2.04	0.40
1:A:1058:LEU:N	1:A:1058:LEU:HD22	2.36	0.40
1:B:842:ASN:O	1:B:845:LEU:HG	2.21	0.40
2:D:182:LEU:C	2:D:182:LEU:HD13	2.47	0.40
3:E:117:LEU:HD23	3:E:117:LEU:HA	1.90	0.40
1:A:274:LYS:HZ1	1:A:275:GLN:CA	2.34	0.40
1:A:892:LEU:HD23	1:A:893:ARG:O	2.22	0.40
1:B:878:ASN:CG	1:B:893:ARG:HB2	2.46	0.40
1:B:882:PHE:HD2	1:B:891:TYR:CE1	2.40	0.40
2:D:230:ILE:HD13	2:D:230:ILE:HA	1.83	0.40
3:E:354:VAL:HG23	3:E:356:LEU:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	593/1096 (54%)	550 (93%)	40 (7%)	3 (0%)	24	60
1	B	593/1096 (54%)	557 (94%)	34 (6%)	2 (0%)	36	70
2	C	193/250 (77%)	178 (92%)	15 (8%)	0	100	100
2	D	193/250 (77%)	183 (95%)	10 (5%)	0	100	100
3	E	496/554 (90%)	470 (95%)	26 (5%)	0	100	100
All	All	2068/3246 (64%)	1938 (94%)	125 (6%)	5 (0%)	44	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	852	SER
1	B	891	TYR
1	B	1087	ARG
1	A	983	GLY
1	A	90	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	A	501/929 (54%)	480 (96%)	21 (4%)	26	61
1	B	501/929 (54%)	479 (96%)	22 (4%)	25	60
2	C	171/218 (78%)	167 (98%)	4 (2%)	44	74
2	D	171/218 (78%)	163 (95%)	8 (5%)	23	58
3	E	435/474 (92%)	417 (96%)	18 (4%)	27	61
All	All	1779/2768 (64%)	1706 (96%)	73 (4%)	28	61

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	79	ASP
1	A	87	VAL
1	A	88	SER
1	A	108	THR
1	A	121	VAL
1	A	191	LEU
1	A	196	GLU
1	A	237	GLU
1	A	790	LEU
1	A	796	GLU
1	A	872	GLU
1	A	874	LEU
1	A	876	GLU
1	A	877	LEU
1	A	879	GLU
1	A	891	TYR
1	A	951	LYS
1	A	975	ILE
1	A	990	GLU
1	A	1018	ILE
1	B	49	LYS
1	B	50	THR
1	B	53	VAL
1	B	71	THR
1	B	76	SER
1	B	78	ARG
1	B	107	VAL
1	B	168	LEU
1	B	216	SER
1	B	250	GLN
1	B	271	LYS
1	B	822	ILE
1	B	847	TYR
1	B	877	LEU
1	B	894	LEU
1	B	920	VAL
1	B	1000	SER
1	B	1018	ILE
1	B	1021	ASP
1	B	1031	VAL
1	B	1047	VAL
1	B	1049	ILE

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Mol	Chain	Res	Type
2	C	60	LEU
2	C	127	LEU
2	C	176	SER
2	C	233	GLN
2	D	42	THR
2	D	55	LEU
2	D	75	SER
2	D	79	GLU
2	D	102	VAL
2	D	147	SER
2	D	205	VAL
2	D	210	ILE
3	E	25	LEU
3	E	27	THR
3	E	143	LEU
3	E	166	GLN
3	E	173	ILE
3	E	227	ILE
3	E	253	GLN
3	E	258	SER
3	E	267	LEU
3	E	271	LEU
3	E	277	SER
3	E	291	LEU
3	E	317	MET
3	E	337	ASN
3	E	399	ASP
3	E	425	ASN
3	E	484	THR
3	E	485	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	206	ASN
1	A	937	GLN
1	A	982	GLN
1	A	1069	HIS
1	A	1076	ASN
1	B	27	HIS
1	B	278	GLN

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Mol	Chain	Res	Type
1	B	794	ASN
1	B	830	GLN
1	B	911	GLN
1	B	913	GLN
1	B	982	GLN
1	B	1029	HIS
1	B	1073	GLN
2	C	218	ASN
2	C	220	GLN
3	E	18	GLN
3	E	179	HIS
3	E	180	GLN
3	E	184	HIS
3	E	325	HIS

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
4	ADP	A	1101	-	28,29,29	0.46	0	43,45,45	0.48	0
4	ADP	B	1101	-	28,29,29	0.46	0	43,45,45	0.46	0

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
4	ADP	A	1101	-	-	8/16/32/32	0/3/3/3
4	ADP	B	1101	-	-	5/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

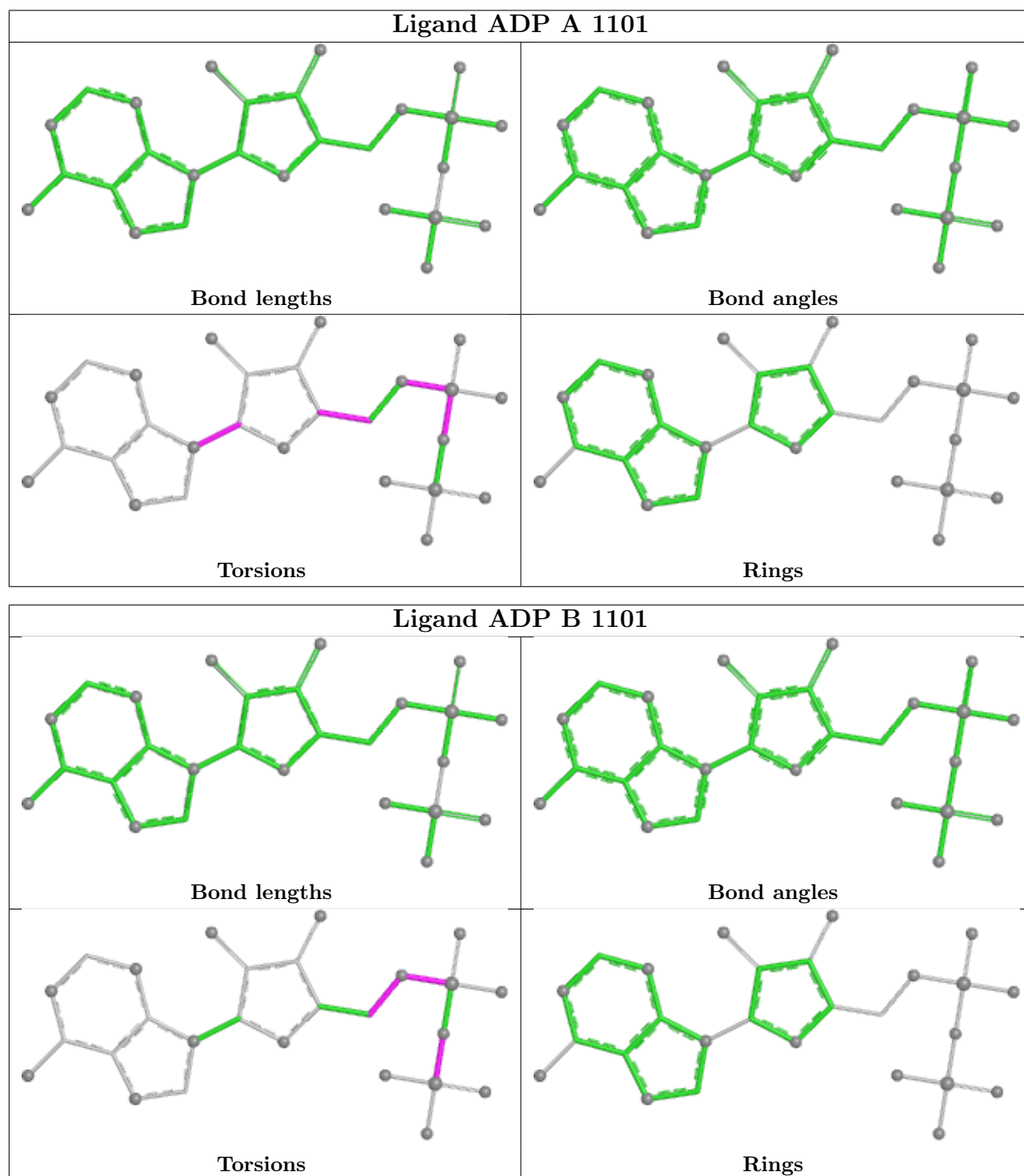
Mol	Chain	Res	Type	Atoms
4	A	1101	ADP	C5'-O5'-PA-O1A
4	A	1101	ADP	C5'-O5'-PA-O3A
4	B	1101	ADP	PA-O3A-PB-O3B
4	B	1101	ADP	C5'-O5'-PA-O3A
4	B	1101	ADP	C4'-C5'-O5'-PA
4	A	1101	ADP	C3'-C4'-C5'-O5'
4	A	1101	ADP	O4'-C4'-C5'-O5'
4	A	1101	ADP	C5'-O5'-PA-O2A
4	B	1101	ADP	C5'-O5'-PA-O1A
4	B	1101	ADP	PA-O3A-PB-O1B
4	A	1101	ADP	PB-O3A-PA-O1A
4	A	1101	ADP	PB-O3A-PA-O2A
4	A	1101	ADP	C2'-C1'-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

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.

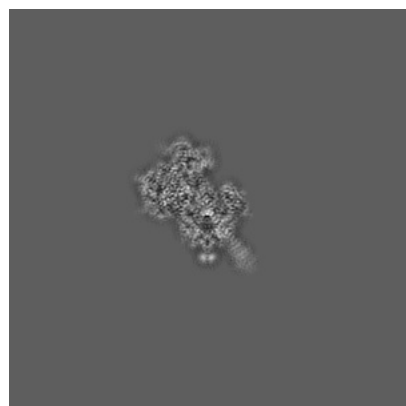
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15609. 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](#)

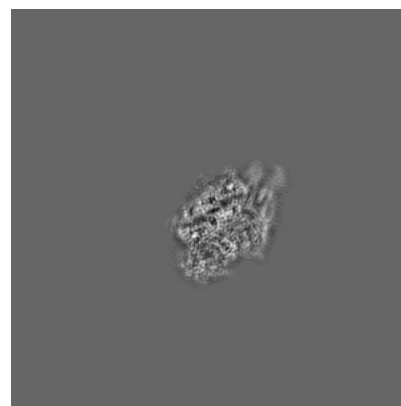
6.1.1 Primary map



X

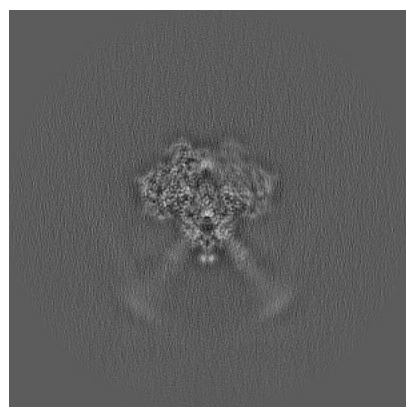


Y

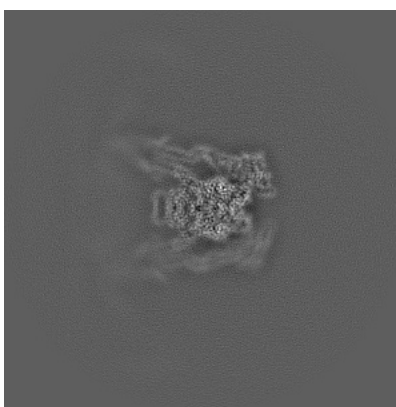


Z

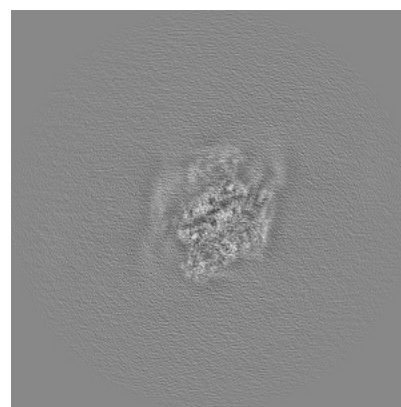
6.1.2 Raw map



X



Y



Z

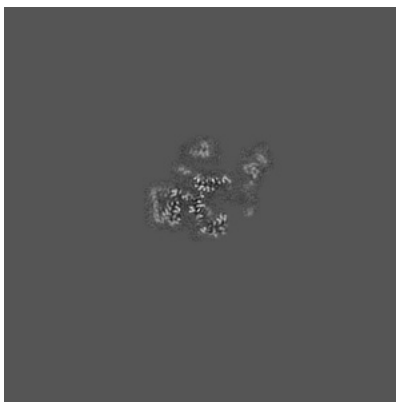
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

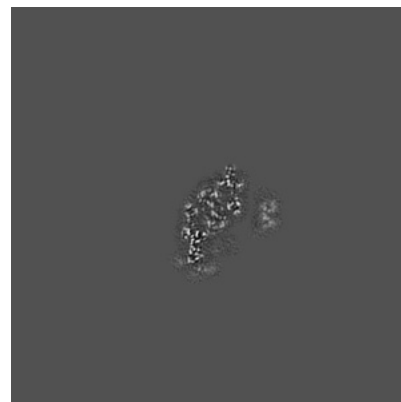
6.2.1 Primary map



X Index: 200

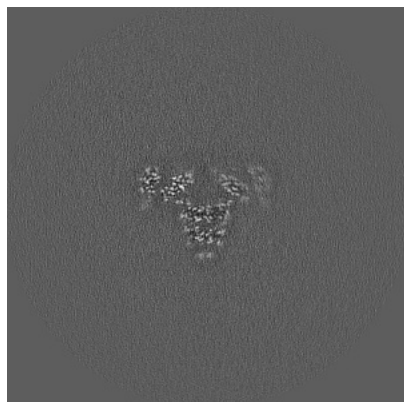


Y Index: 200

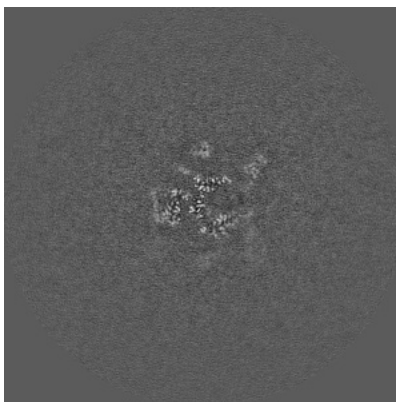


Z Index: 200

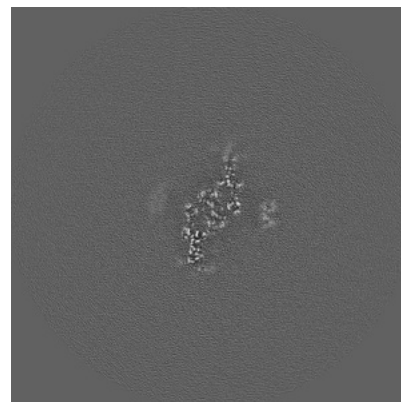
6.2.2 Raw map



X Index: 200



Y Index: 200

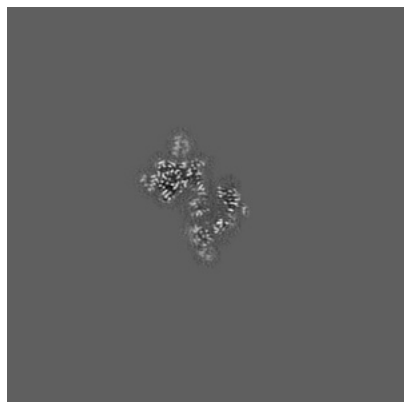


Z Index: 200

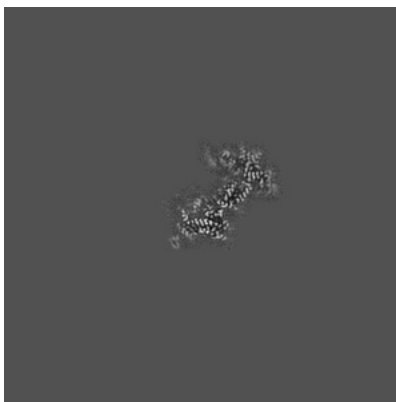
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

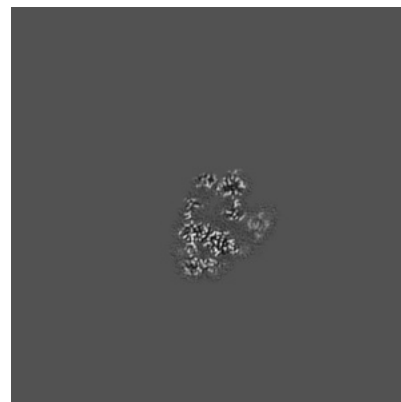
6.3.1 Primary map



X Index: 214

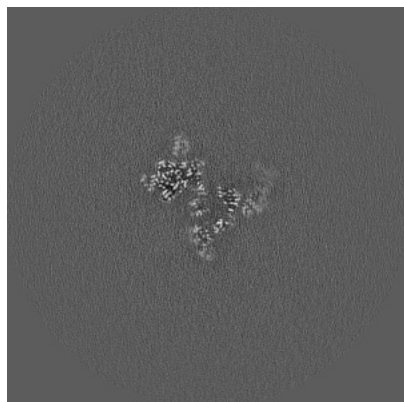


Y Index: 175

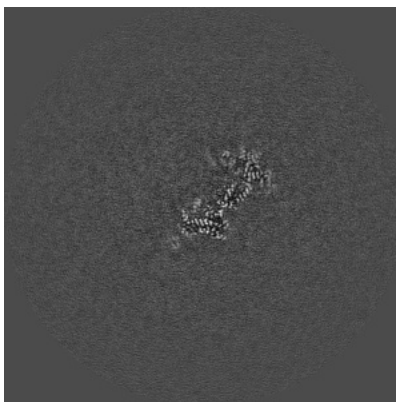


Z Index: 215

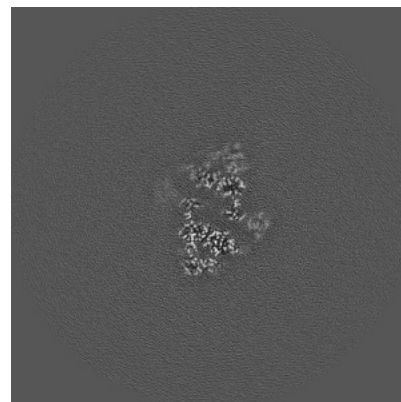
6.3.2 Raw map



X Index: 214



Y Index: 175

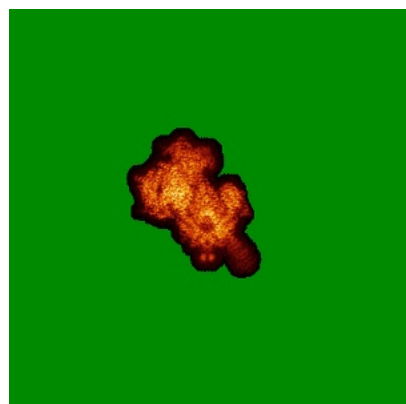


Z Index: 215

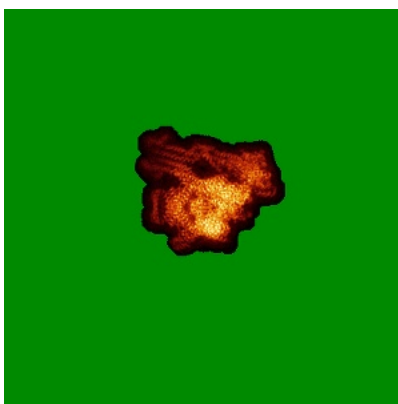
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

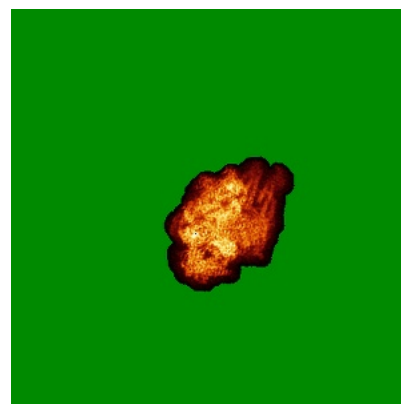
6.4.1 Primary map



X

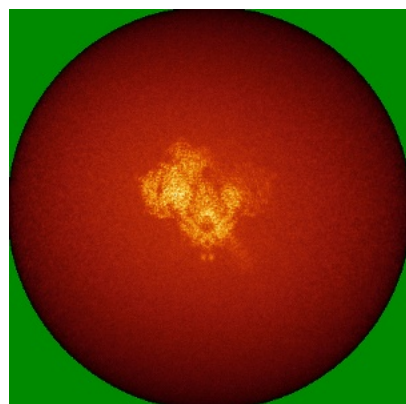


Y

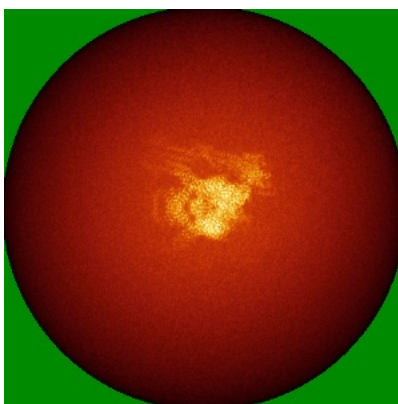


Z

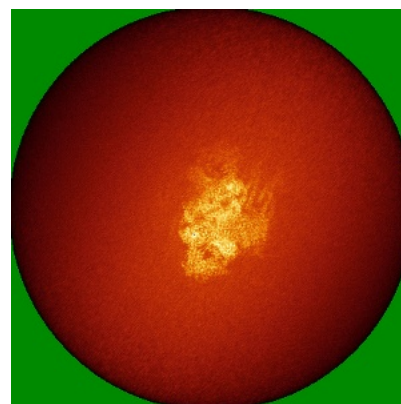
6.4.2 Raw map



X



Y

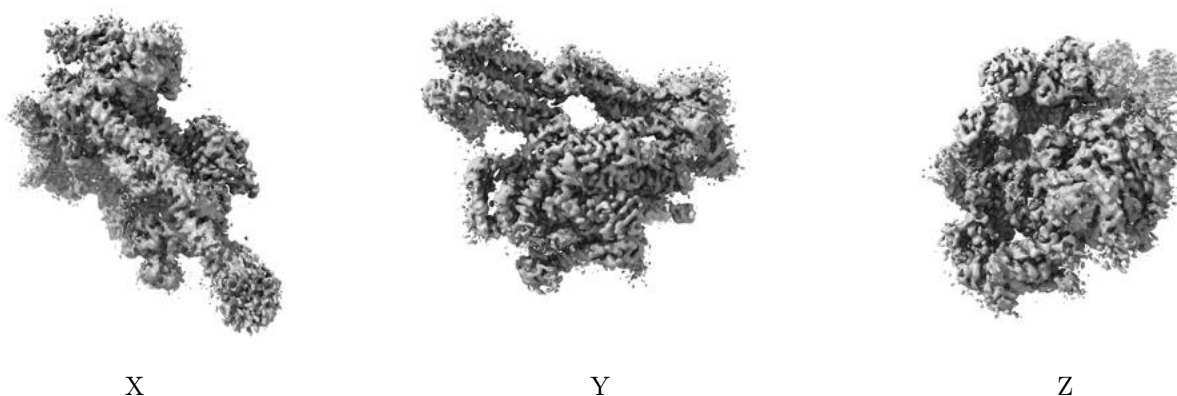


Z

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.

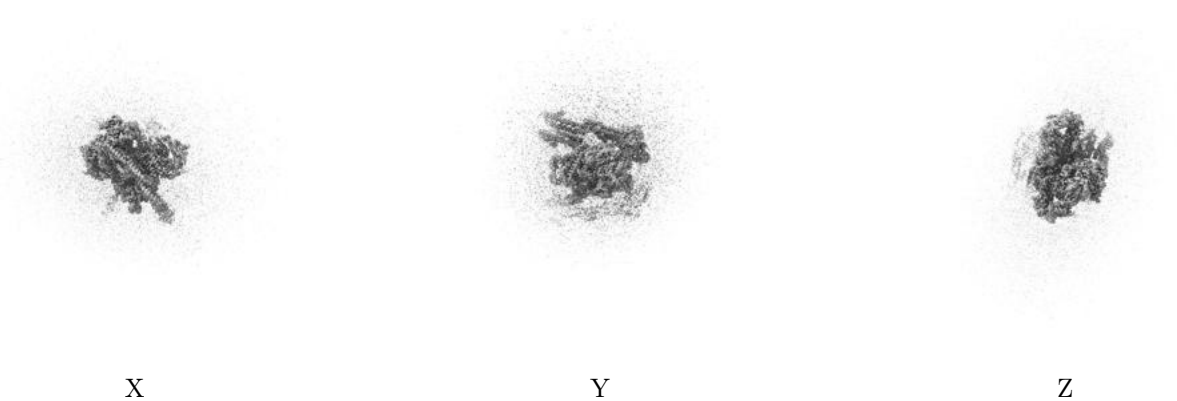
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00183. 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.

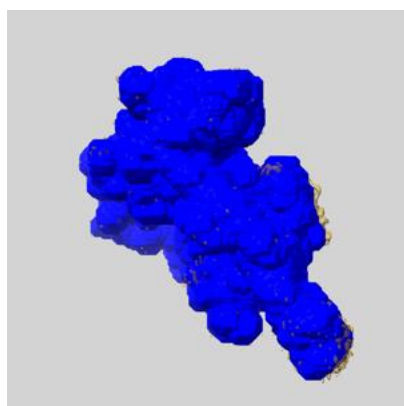
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

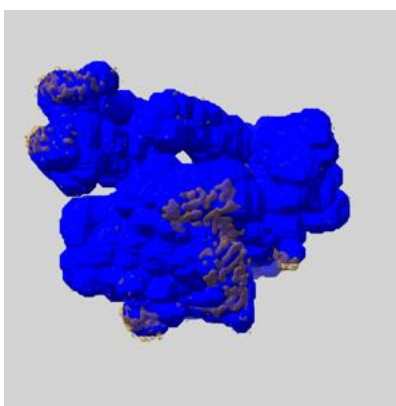
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

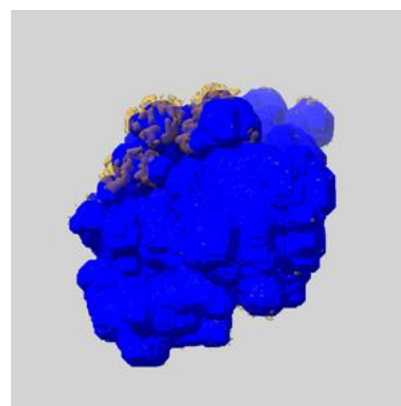
6.6.1 emd_15609_msk_1.map [i](#)



X



Y

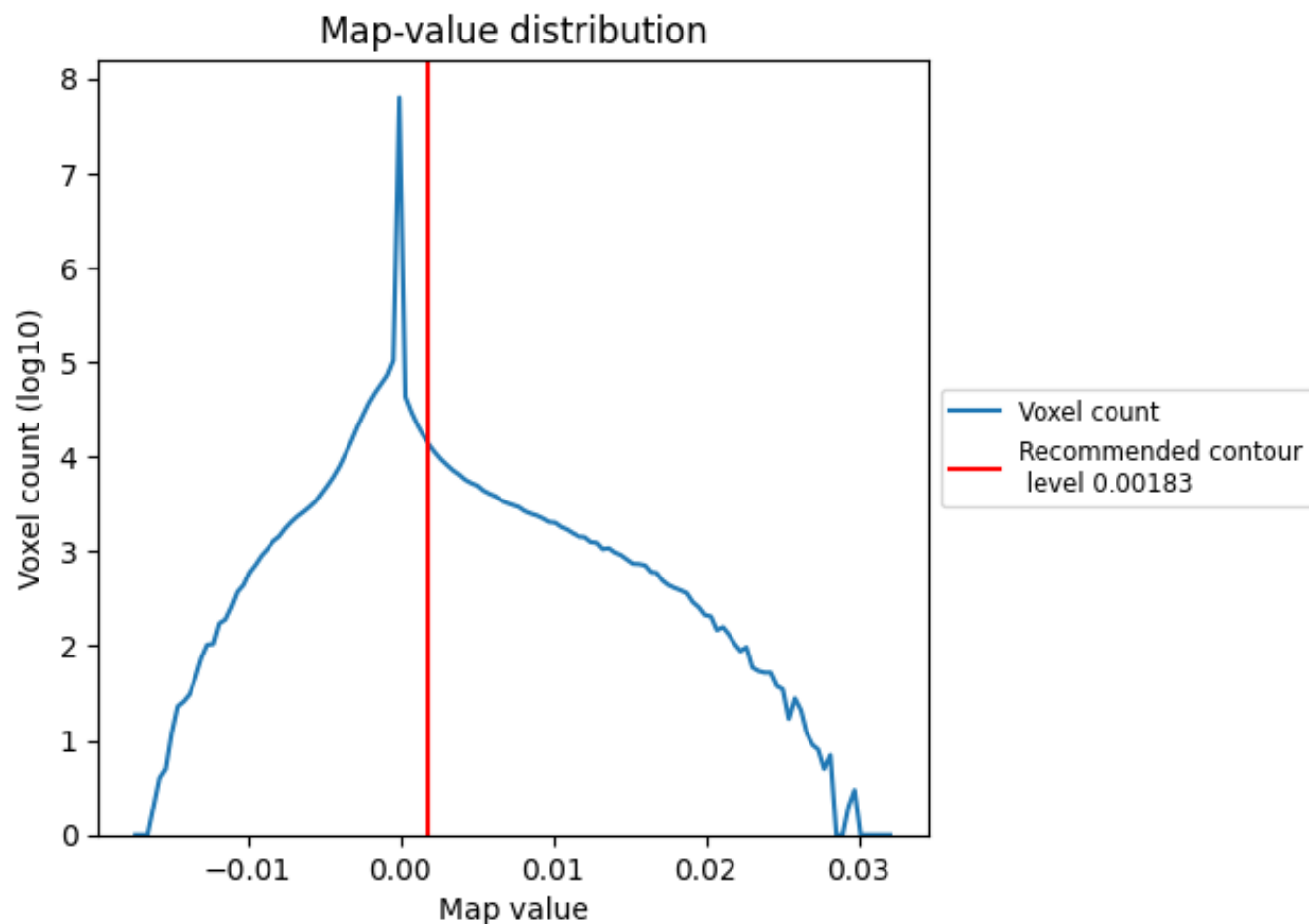


Z

7 Map analysis [i](#)

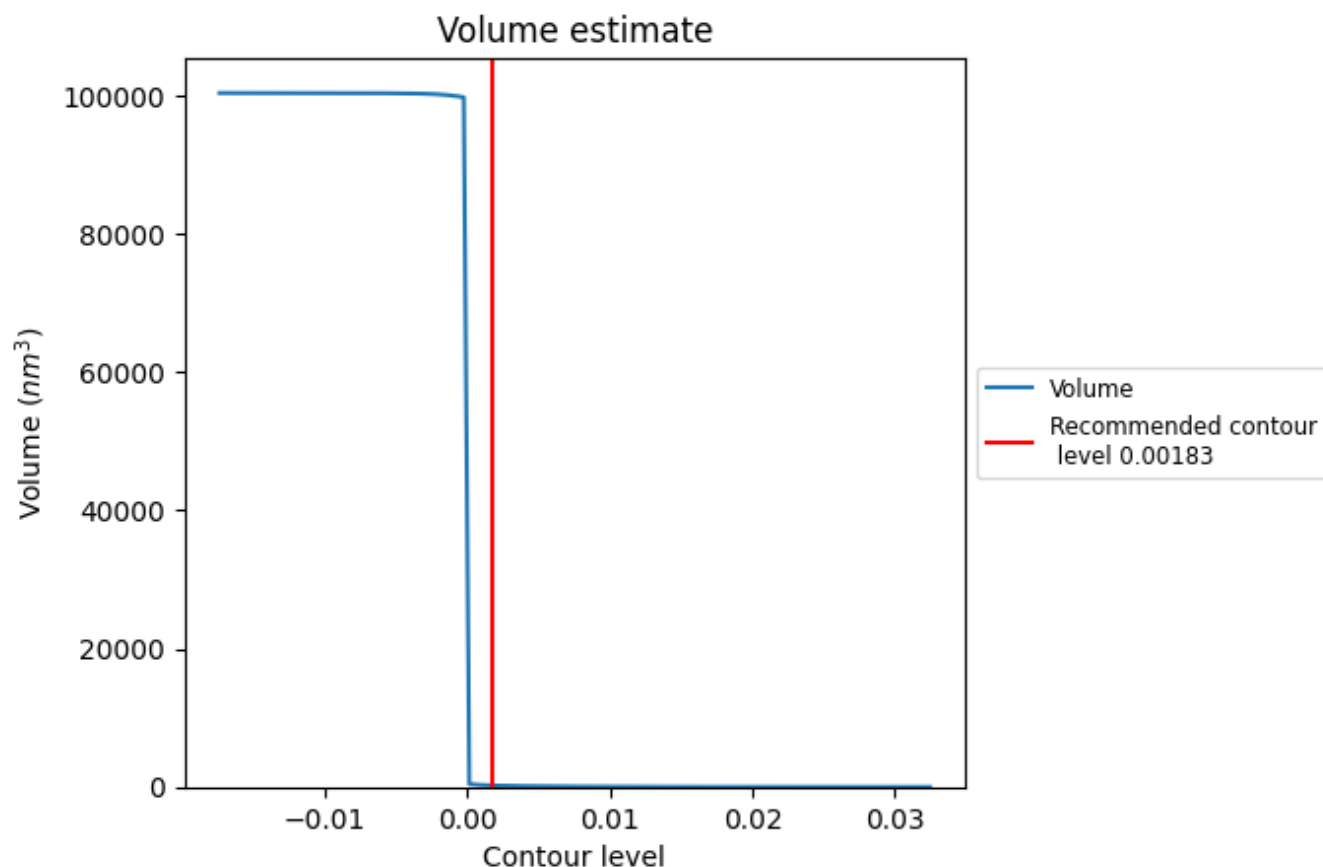
This section contains the results of statistical analysis of the map.

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.

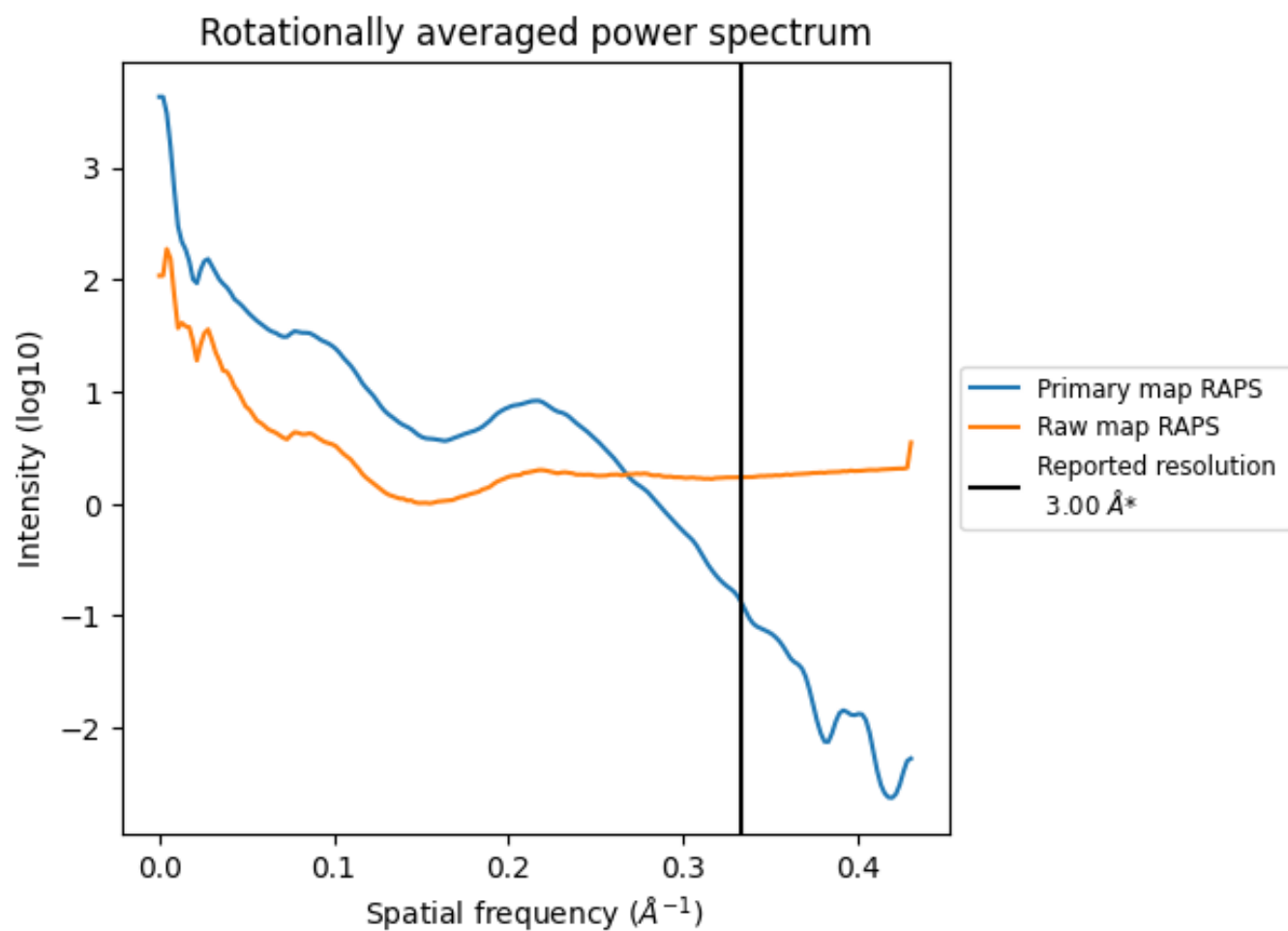
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm³; this corresponds to an approximate mass of 192 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 [i](#)

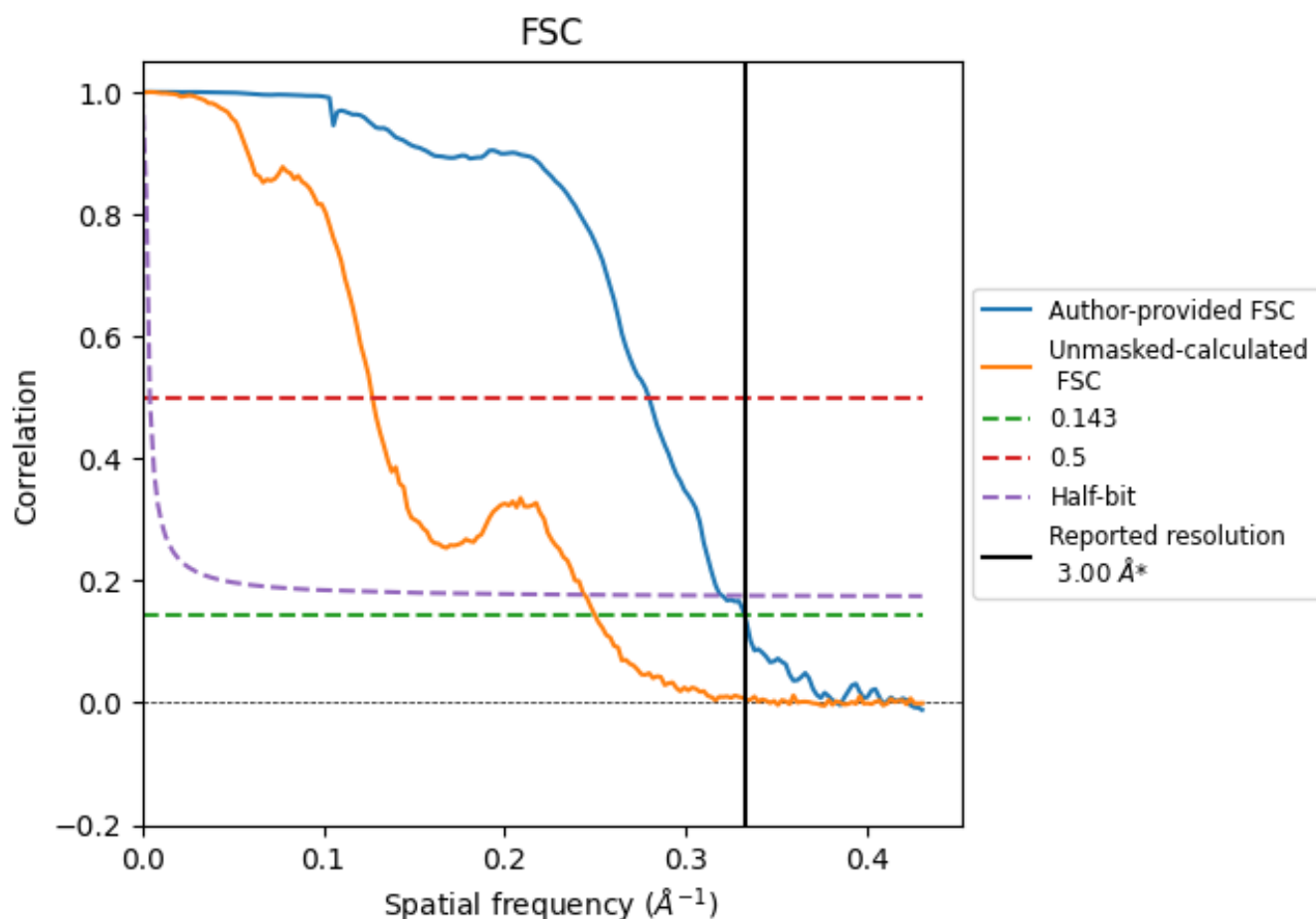


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.01	3.58	3.13
Unmasked-calculated*	4.00	7.87	4.10

*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 4.00 differs from the reported value 3.0 by more than 10 %

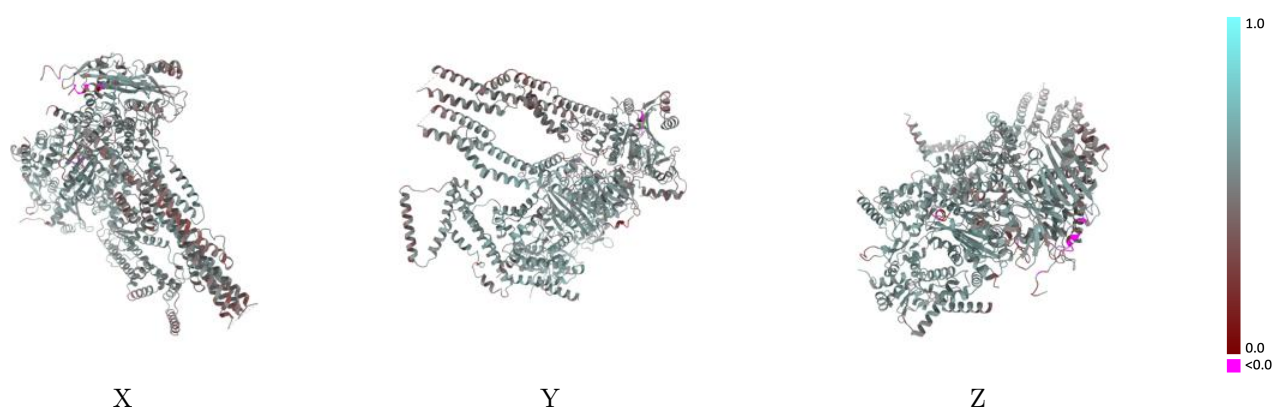
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15609 and PDB model 8AS8. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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



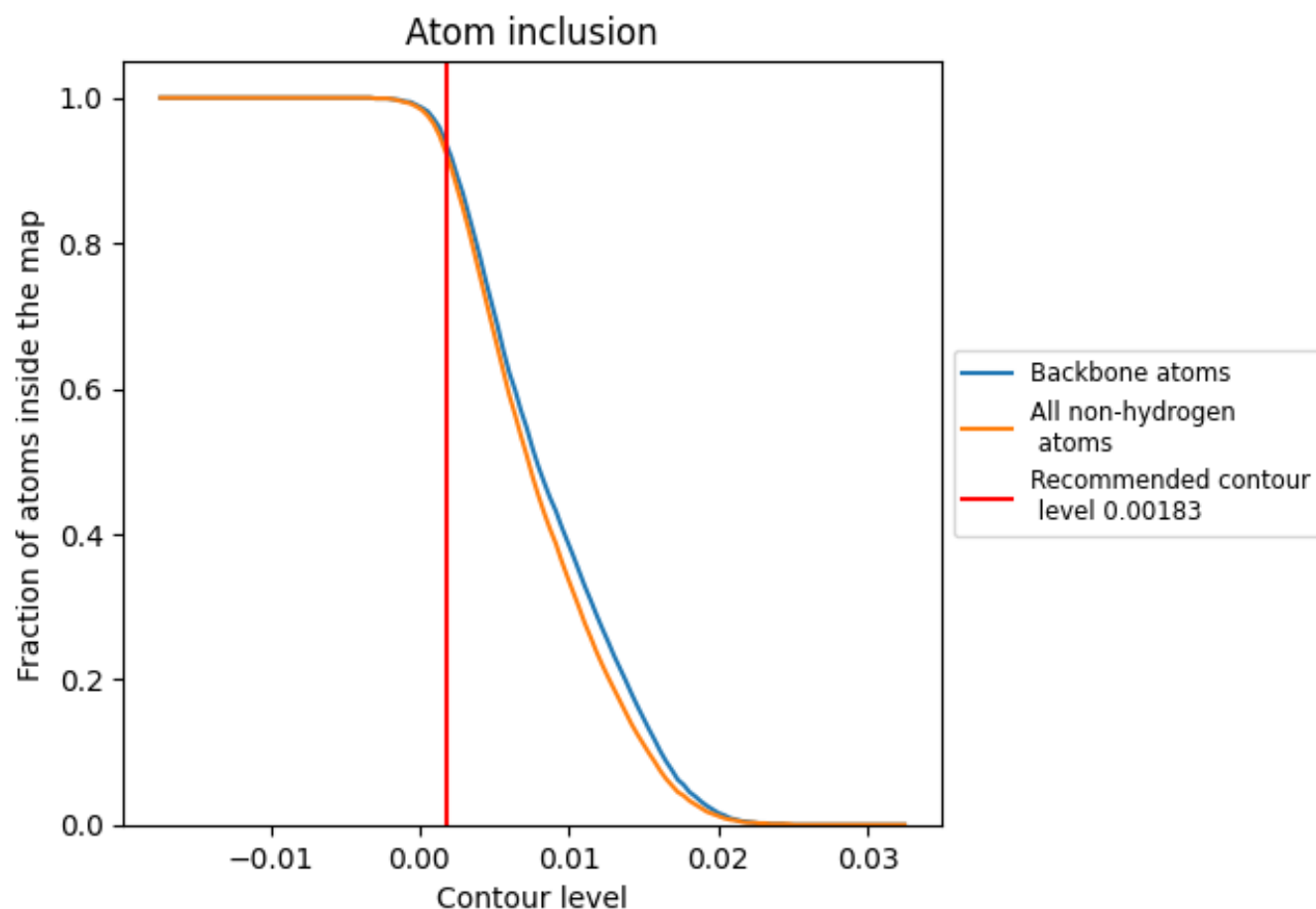
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00183).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.00183) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9210	0.5170
A	0.9220	0.5380
B	0.8940	0.4700
C	0.9500	0.5650
D	0.9600	0.5450
E	0.9320	0.5190

