



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2024 – 12:59 pm GMT

PDB ID : 8R6S  
EMDB ID : EMD-18935  
Title : Plastid-encoded RNA polymerase (Integrated model)  
Authors : Webster, M.W.; Pramanick, I.; Vergara-Cruces, A.  
Deposited on : 2023-11-22  
Resolution : 2.49 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

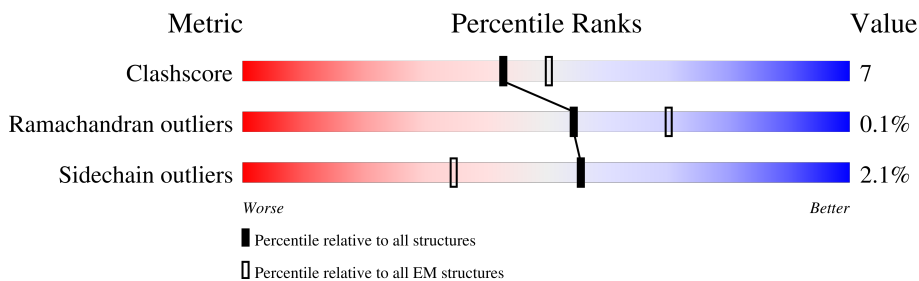
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.49 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.








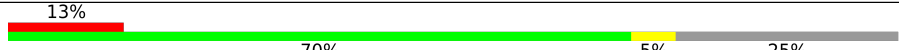
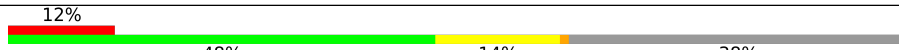
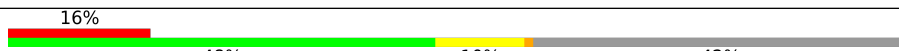


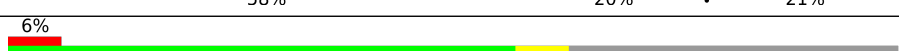


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	327	
1	B	327	
2	C	1072	
3	D	680	
4	E	1373	
5	F	911	
6	G	862	
7	H	675	

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Mol	Chain	Length	Quality of chain
8	I	263	
9	J	529	
10	K	460	
11	L	483	
12	M	334	
13	N	297	
14	O	185	
14	P	185	
15	Q	768	
16	R	162	
17	S	611	
18	T	140	
19	U	187	

## 2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 67366 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	301	Total	C	N	O	S	0	0
			2449	1571	422	446	10		
1	B	283	Total	C	N	O	S	0	0
			2292	1461	395	425	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	PHE	SER	conflict	UNP A0A6C0M610
B	67	PHE	SER	conflict	UNP A0A6C0M610

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	961	Total	C	N	O	S	0	0
			7685	4910	1340	1405	30		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	113	PHE	SER	conflict	UNP A0A6C0M5W1
C	657	VAL	ILE	conflict	UNP A0A6C0M5W1

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	571	Total	C	N	O	S	0	0
			4664	3006	815	817	26		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta''.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	1091	Total	C	N	O	S	0	0
			8758	5612	1554	1561	31		

- Molecule 5 is a protein called PAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	629	Total	C	N	O	S	0	0
			5052	3198	879	942	33		

- Molecule 6 is a protein called PAP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	748	Total	C	N	O	S	0	0
			5887	3723	994	1131	39		

- Molecule 7 is a protein called PAP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	549	Total	C	N	O	S	0	0
			4607	2937	799	854	17		

- Molecule 8 is a protein called PAP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	215	Total	C	N	O	S	0	0
			1771	1141	300	324	6		

- Molecule 9 is a protein called PAP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	234	Total	C	N	O	S	0	0
			1970	1247	350	363	10		

- Molecule 10 is a protein called PAP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	384	Total	C	N	O	S	0	0
			3103	1985	520	583	15		

- Molecule 11 is a protein called PAP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	416	3403	2183	580	620	20	0	0

- Molecule 12 is a protein called PAP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	215	1803	1142	312	341	8	0	0

- Molecule 13 is a protein called PAP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	224	1819	1168	309	338	4	0	0

- Molecule 14 is a protein called PAP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	114	923	588	148	178	9	0	0
14	P	108	865	550	139	167	9	0	0

- Molecule 15 is a protein called PAP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Q	539	4148	2584	706	833	25	0	0

- Molecule 16 is a protein called PAP12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	R	128	1069	672	193	201	3	0	0

- Molecule 17 is a protein called FLN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	386	3056	1941	516	578	21	0	0

- Molecule 18 is a protein called PTAC18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	104	Total	C	N	O	S	0	0
			881	572	148	157	4		

- Molecule 19 is a protein called PRIN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	109	Total	C	N	O	S	0	0
			877	561	144	169	3		

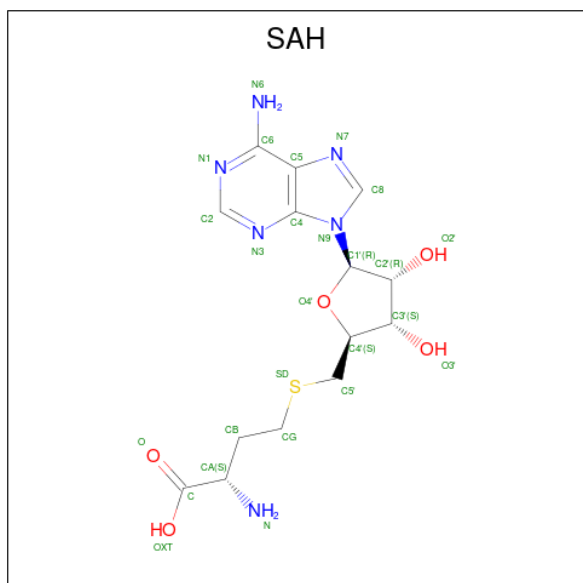
- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	E	1	Total	Zn	0
			1	1	

- Molecule 21 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
21	I	1	Total	Fe	0
			1	1	
21	N	1	Total	Fe	0
			1	1	

- Molecule 22 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
22	L	1	26	14	6	5	1	0

- Molecule 23 is water.

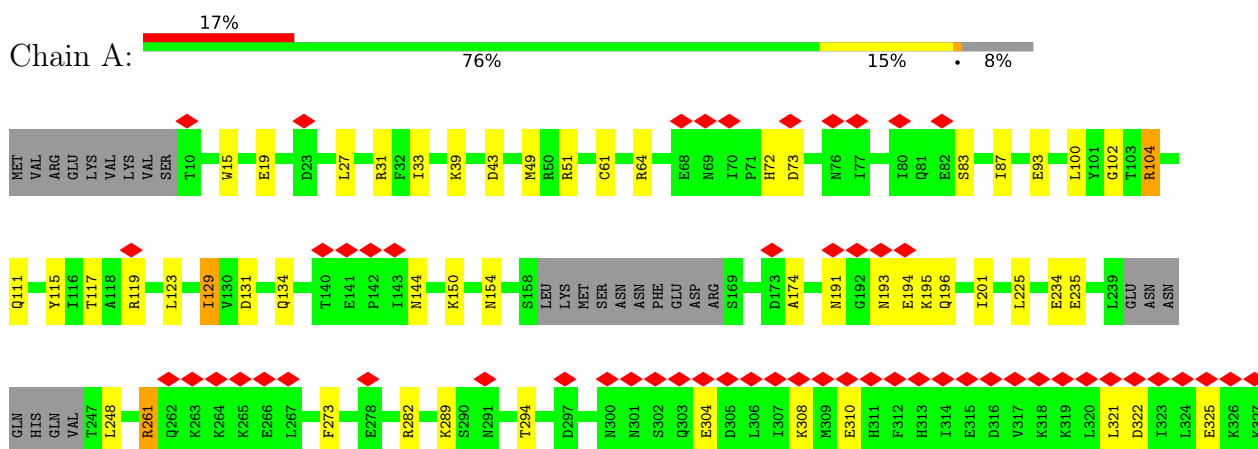
Mol	Chain	Residues	Atoms		AltConf
23	A	18	Total 18	O 18	0
23	B	13	Total 13	O 13	0
23	C	57	Total 57	O 57	0
23	D	21	Total 21	O 21	0
23	E	25	Total 25	O 25	0
23	F	1	Total 1	O 1	0
23	H	6	Total 6	O 6	0
23	I	4	Total 4	O 4	0
23	J	31	Total 31	O 31	0
23	K	15	Total 15	O 15	0
23	L	19	Total 19	O 19	0
23	M	13	Total 13	O 13	0
23	N	3	Total 3	O 3	0
23	O	2	Total 2	O 2	0
23	P	2	Total 2	O 2	0
23	R	2	Total 2	O 2	0
23	S	23	Total 23	O 23	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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

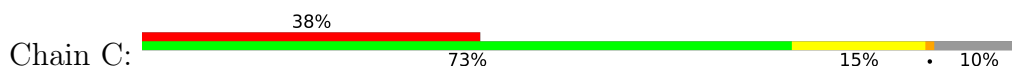
- Molecule 1: DNA-directed RNA polymerase subunit alpha

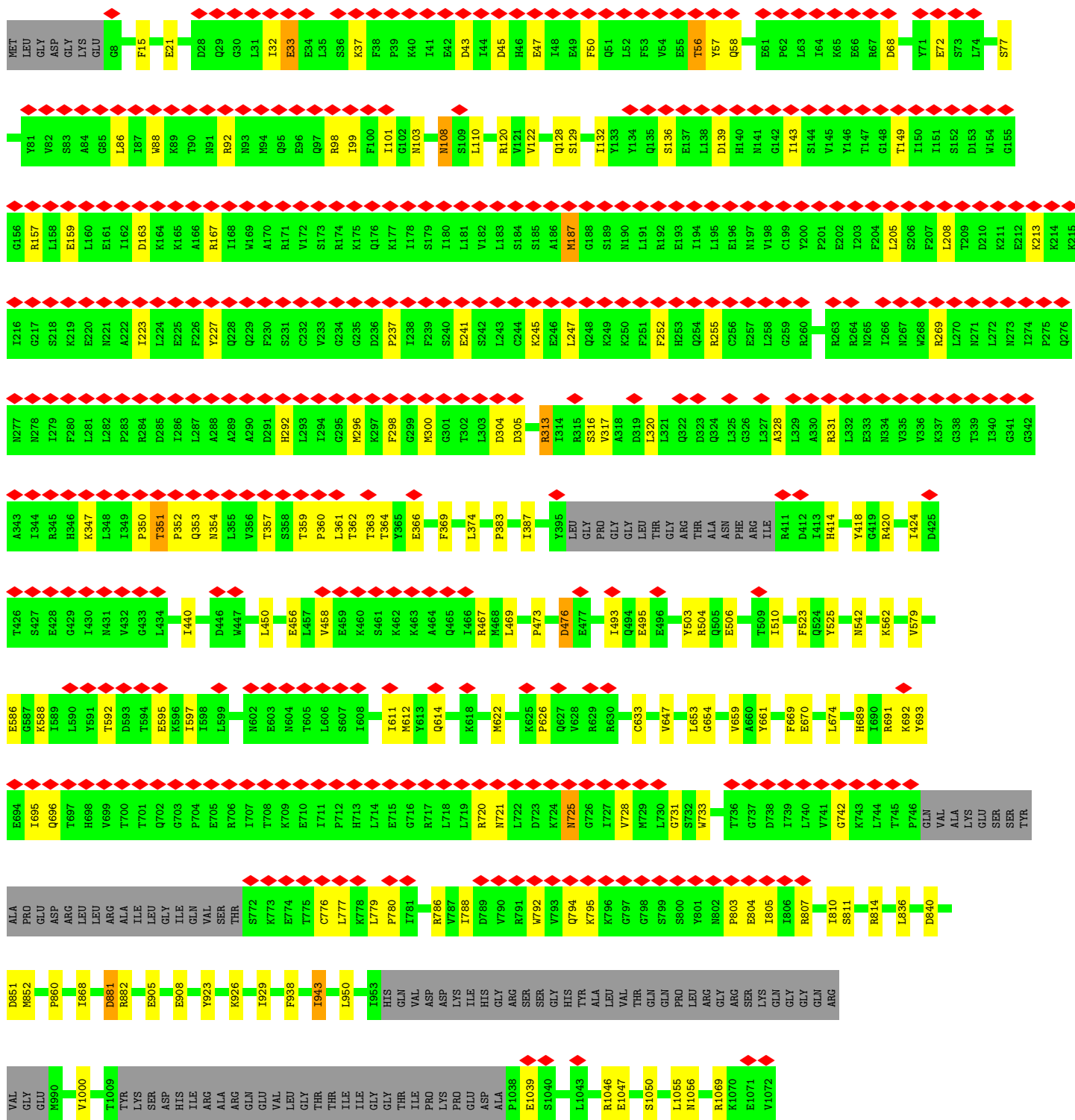


- Molecule 1: DNA-directed RNA polymerase subunit alpha

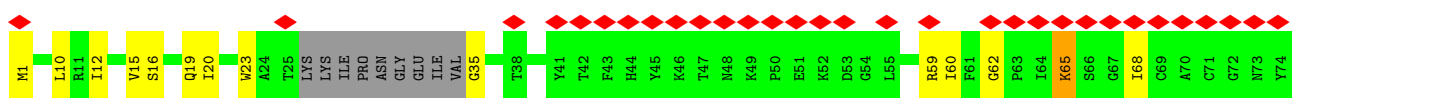


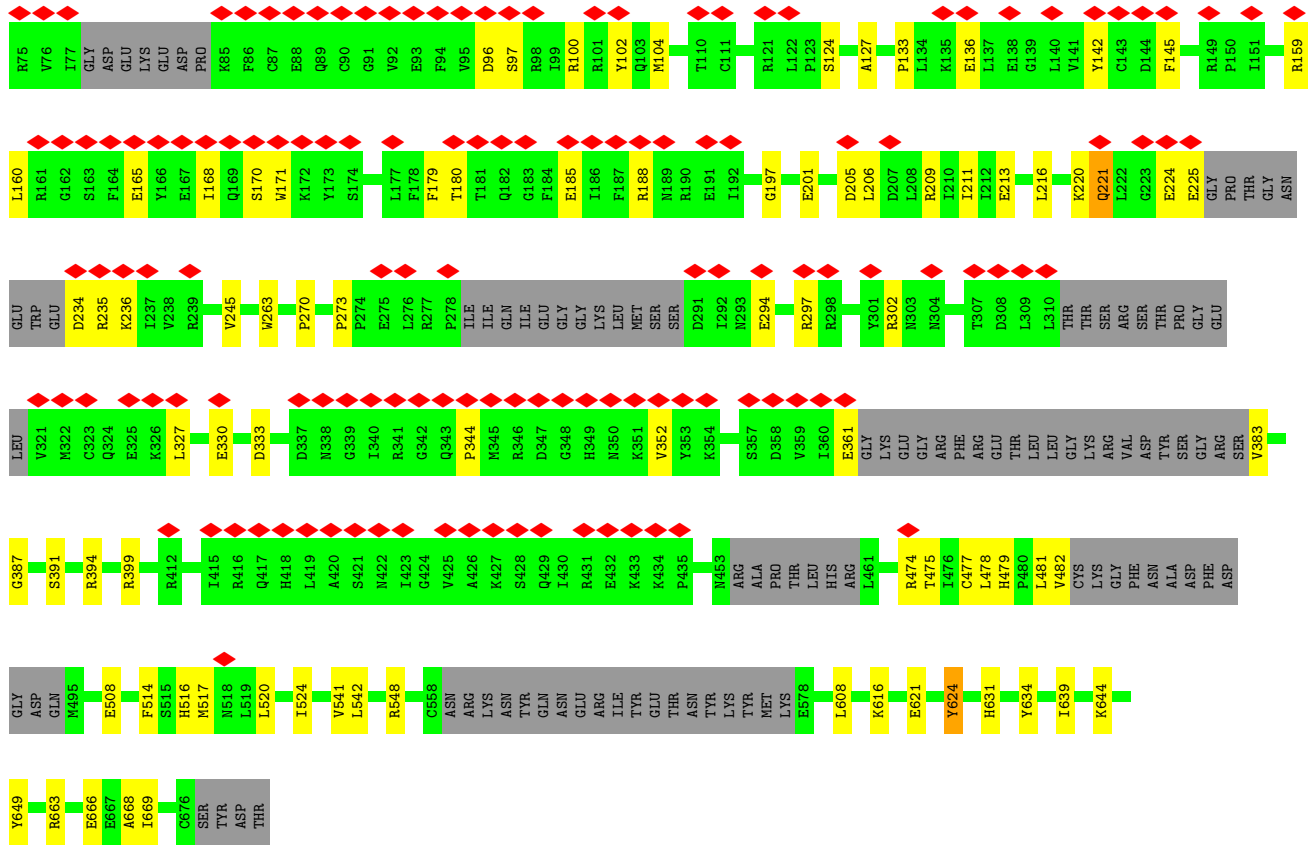
- Molecule 2: DNA-directed RNA polymerase subunit beta



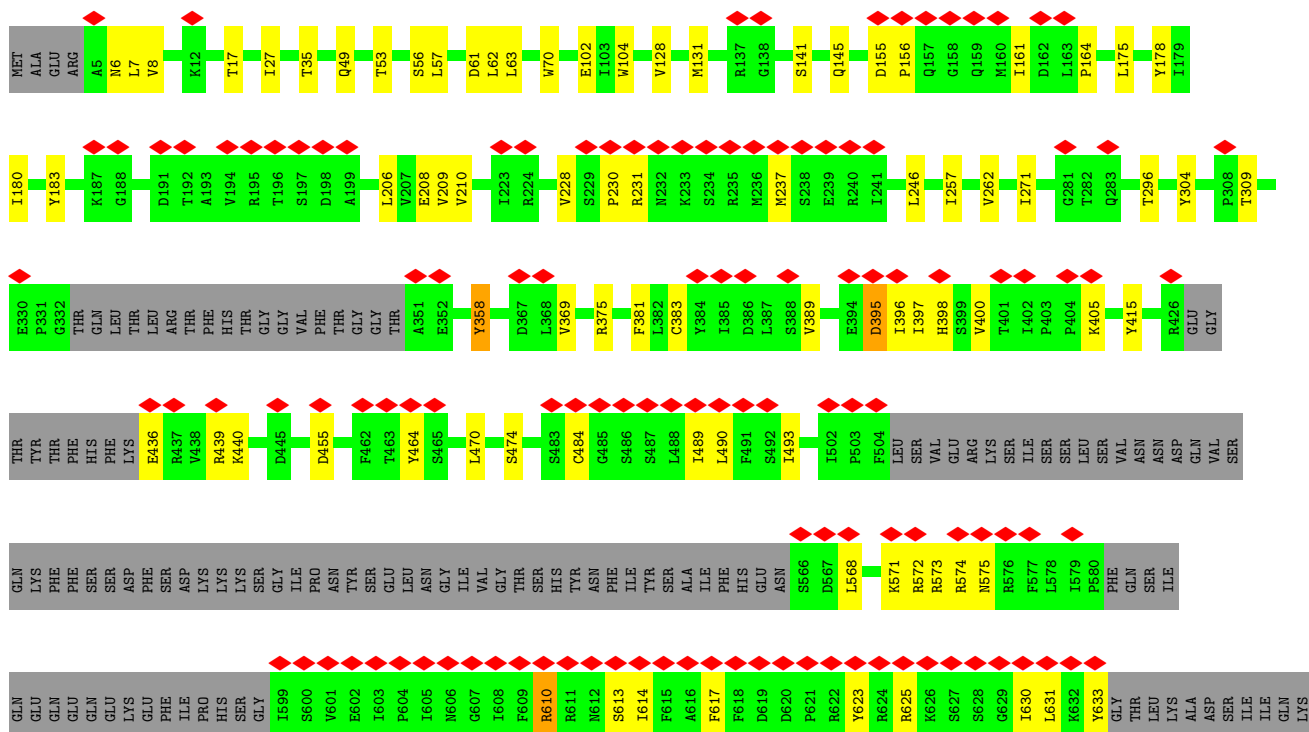


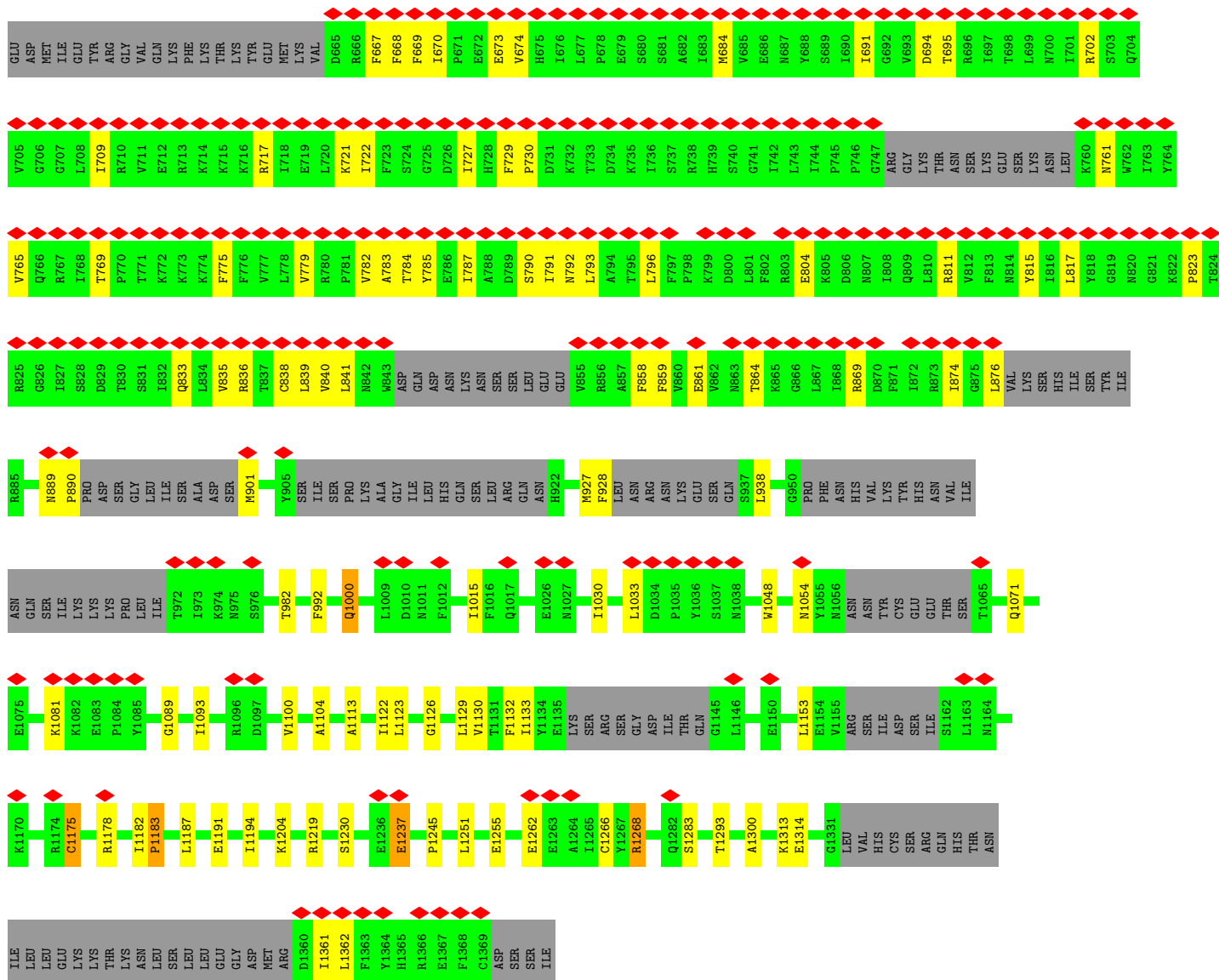
• Molecule 3: DNA-directed RNA polymerase subunit beta'



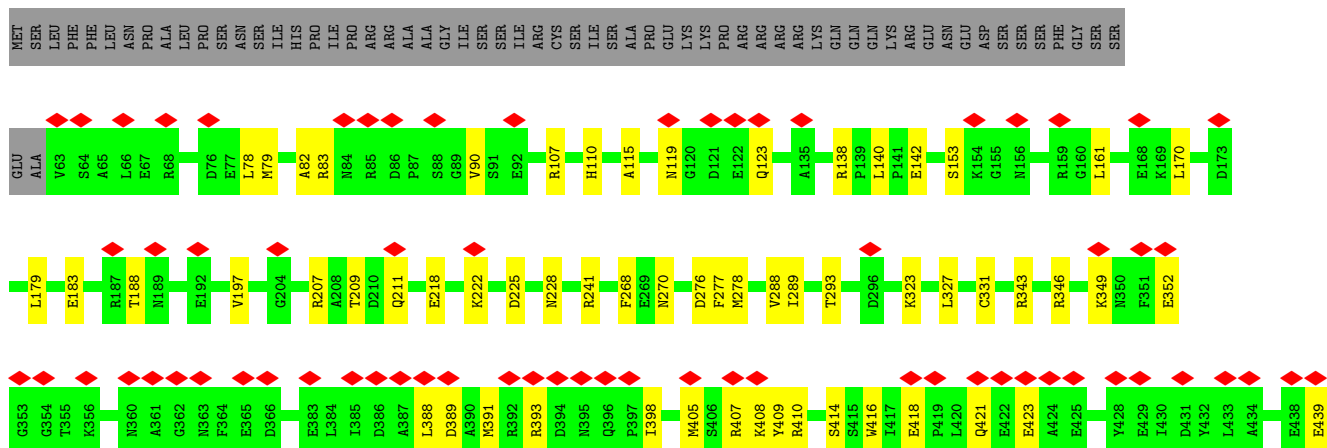


• Molecule 4: DNA-directed RNA polymerase subunit beta”

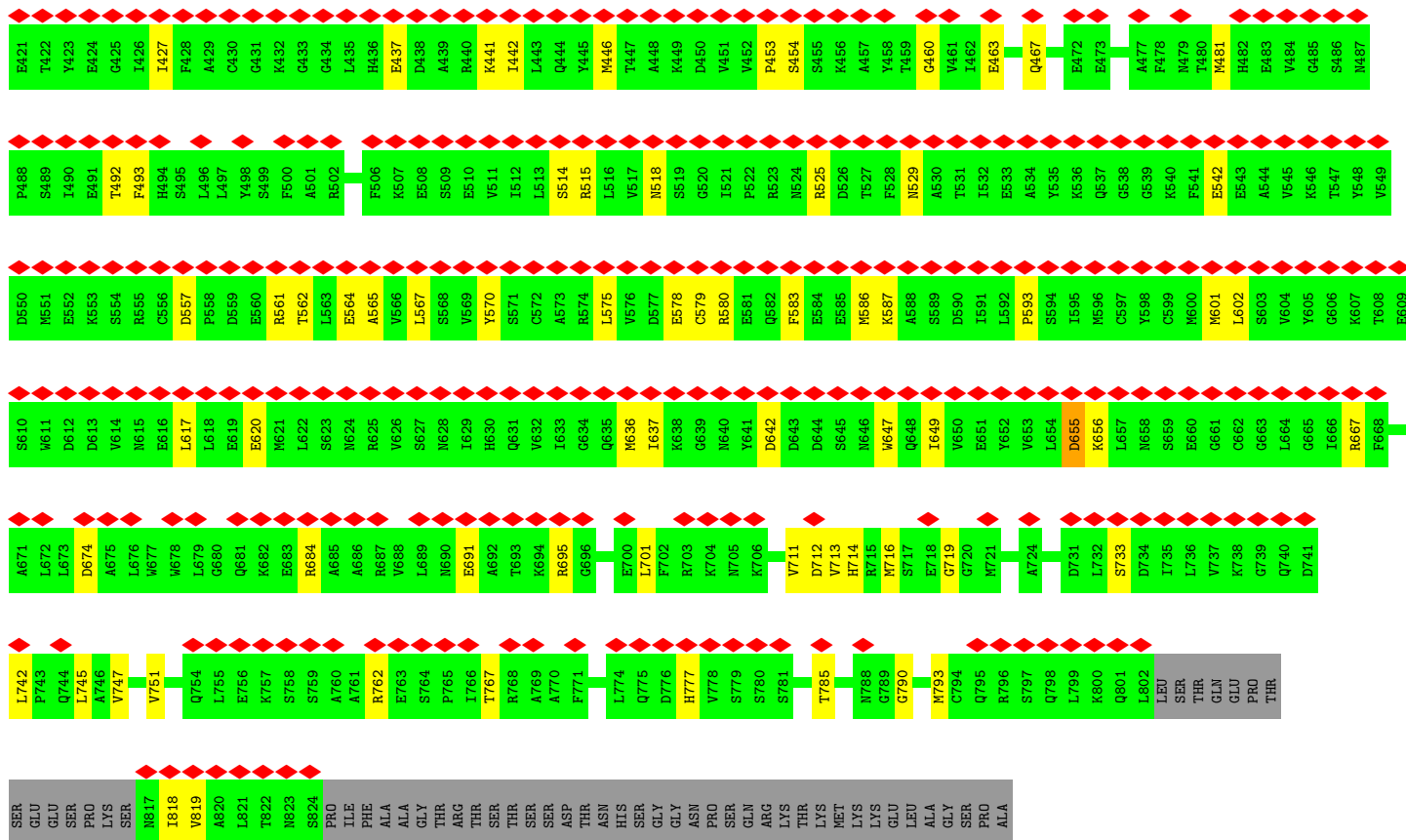




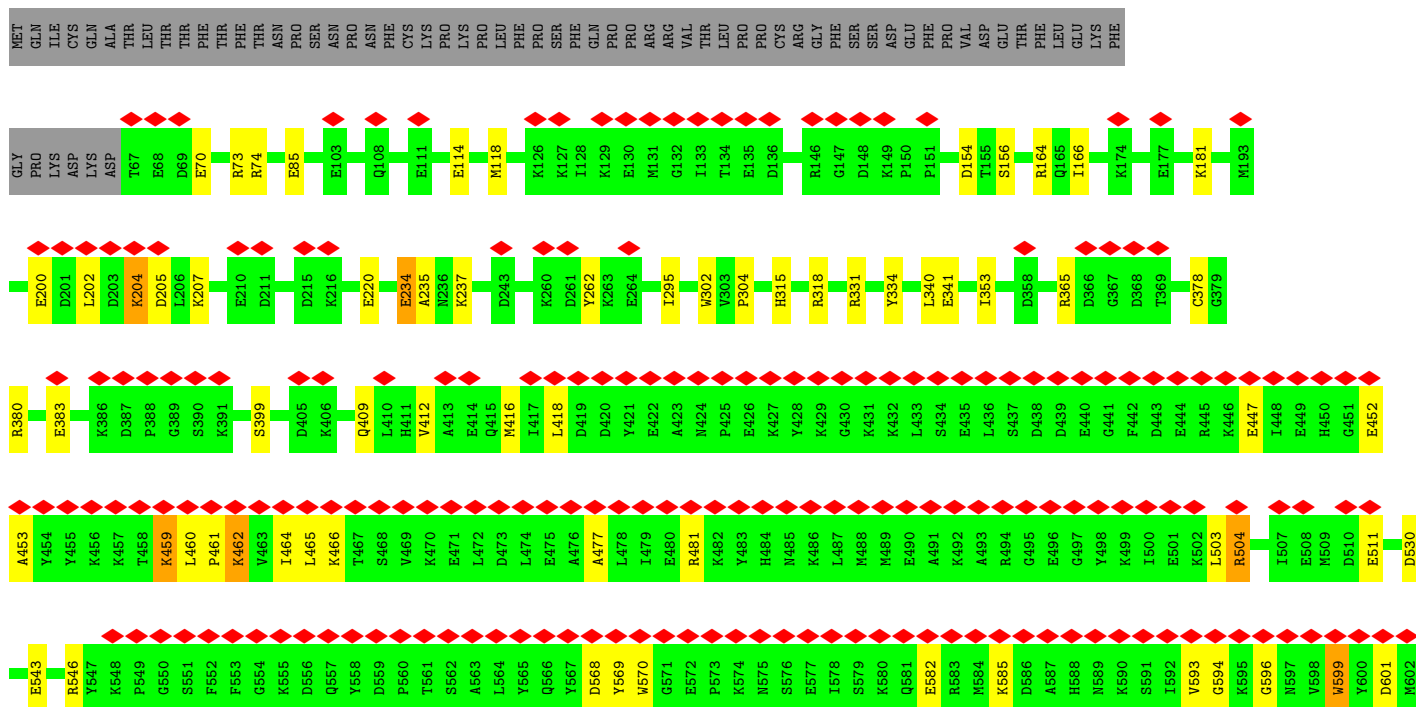
• Molecule 5: PAP1

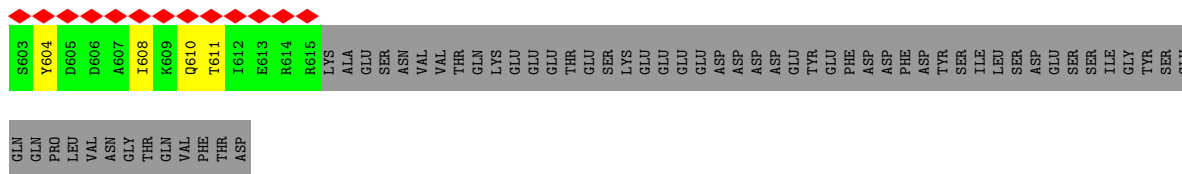




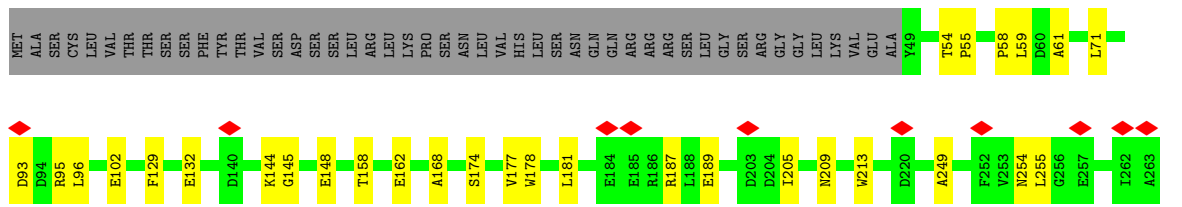


• Molecule 7: PAP3

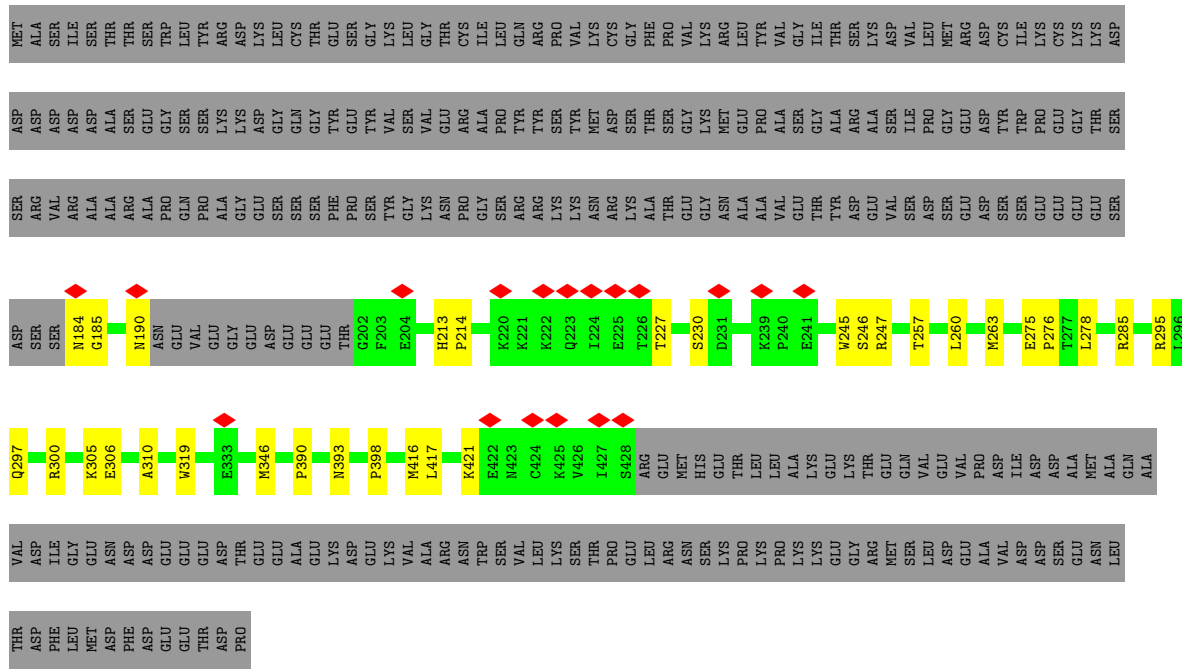
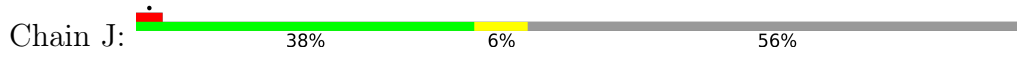




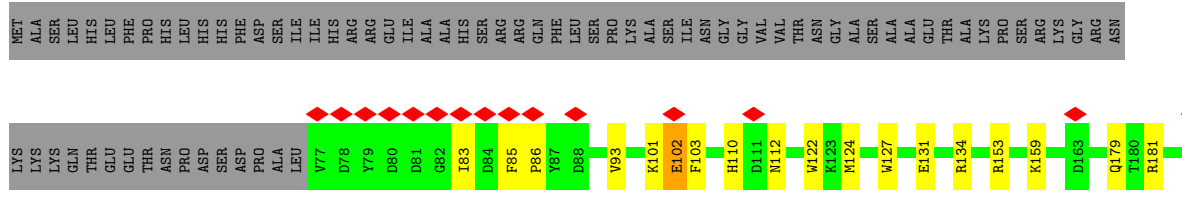
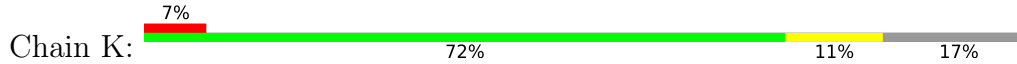
Molecule 8: PAP4

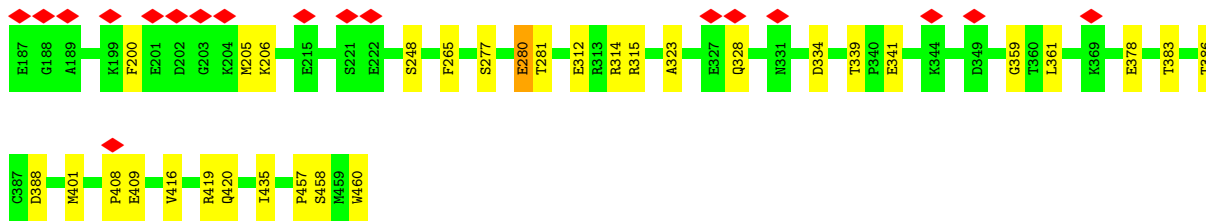


Molecule 9: PAP5

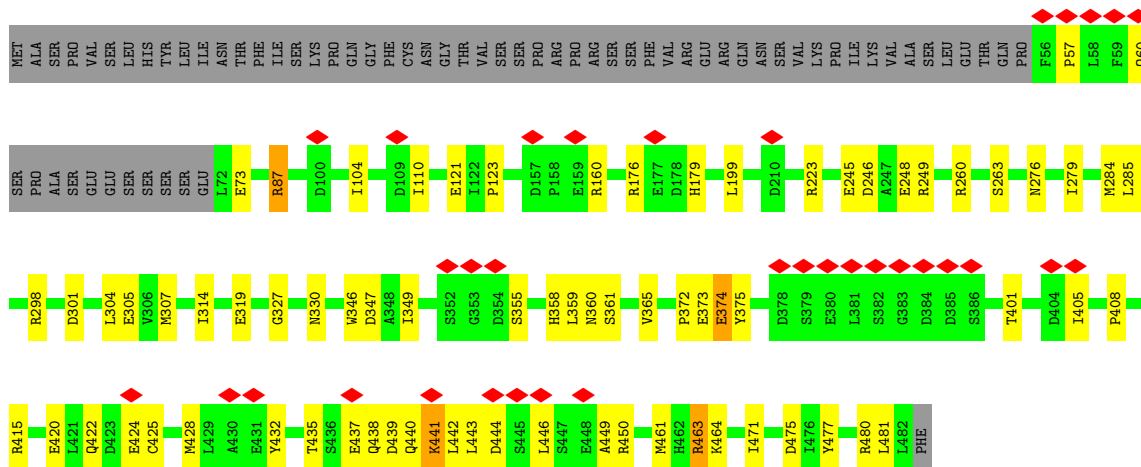


Molecule 10: PAP6

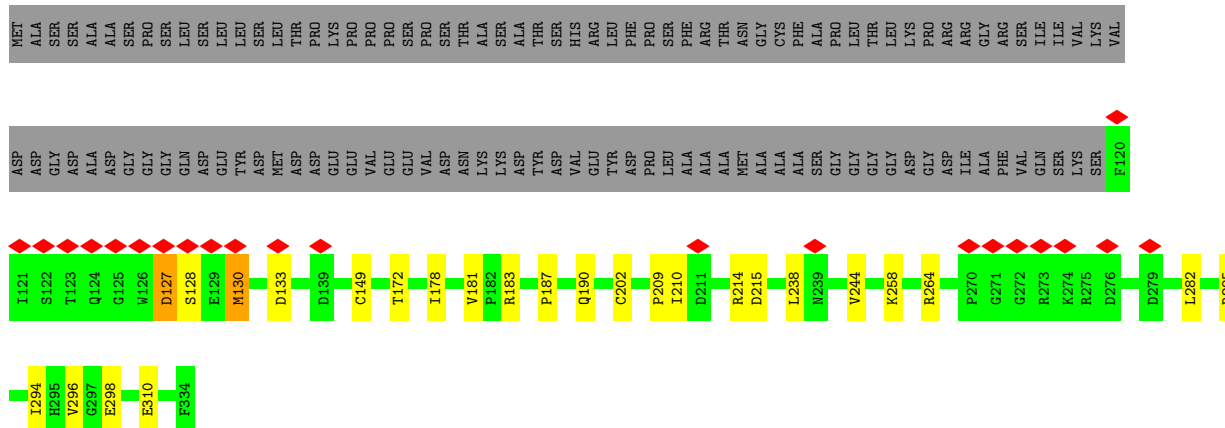




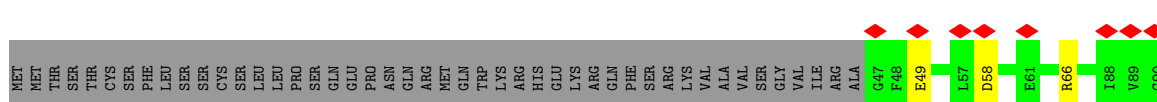
• Molecule 11: PAP7



• Molecule 12: PAP8

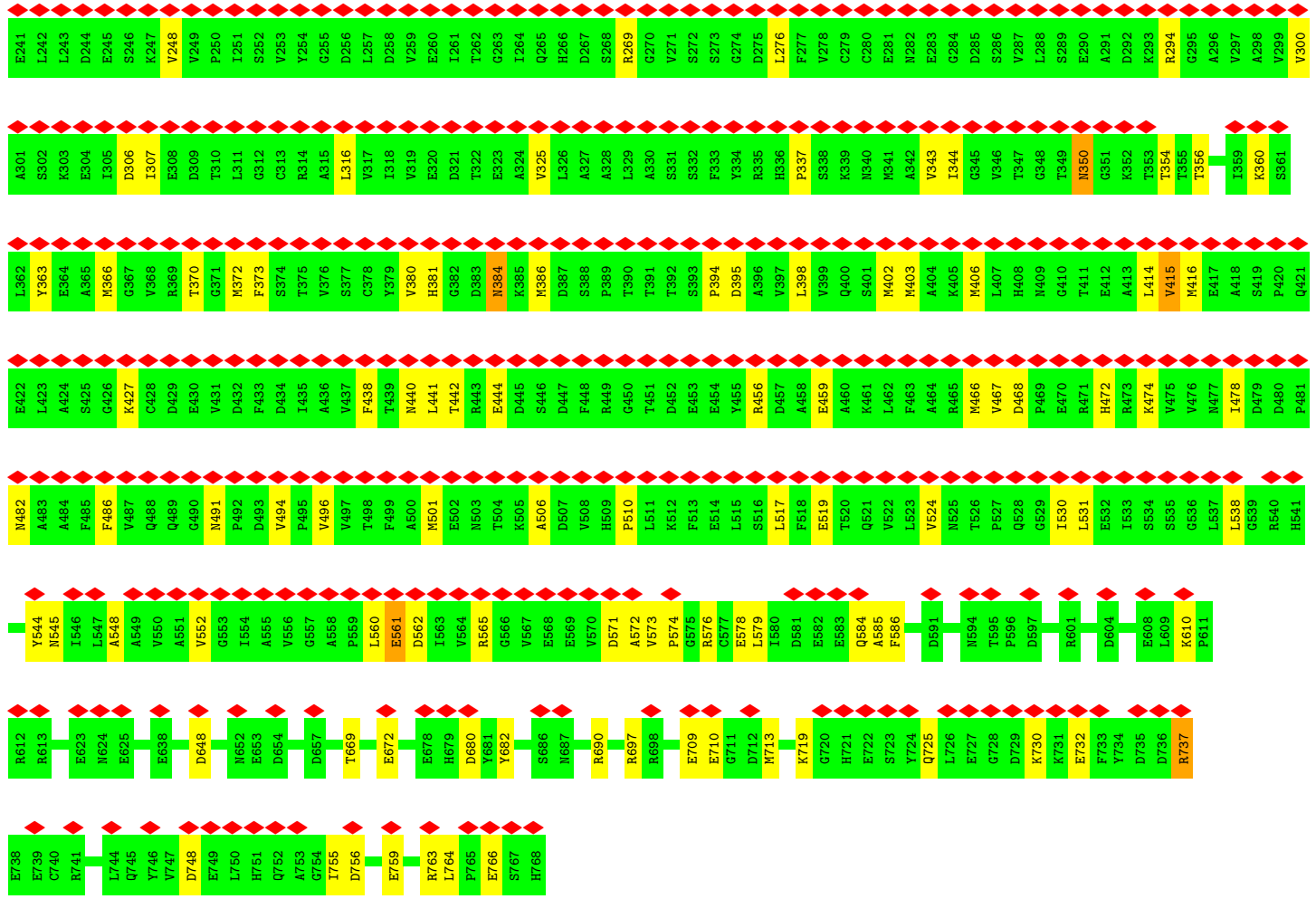


• Molecule 13: PAP9

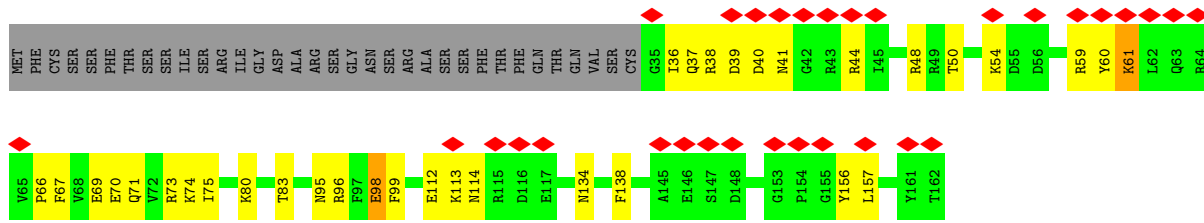




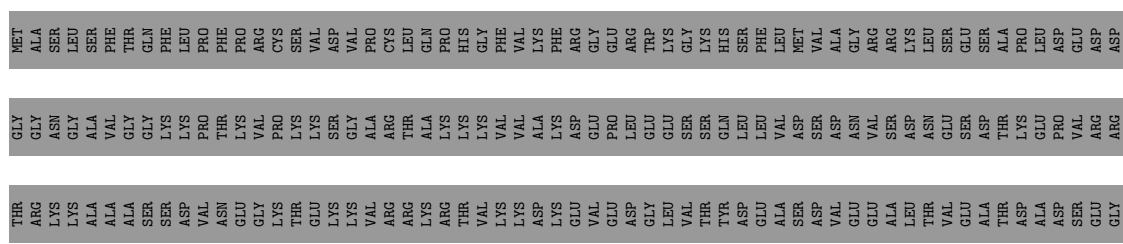


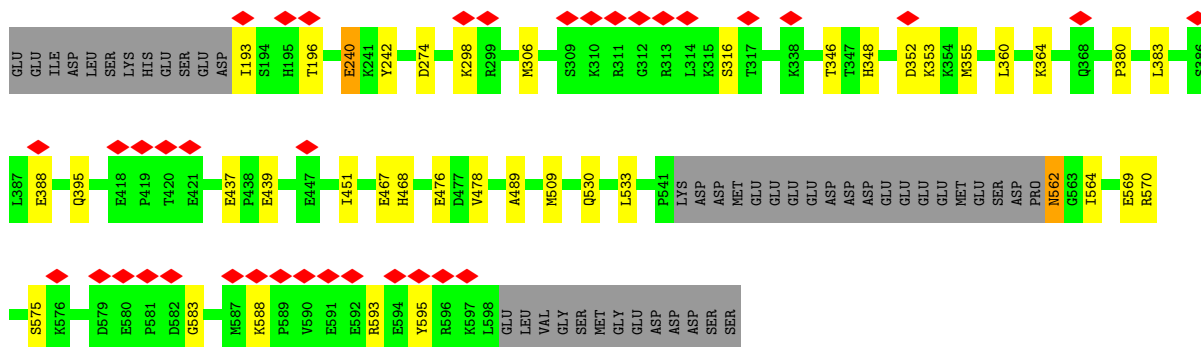


• Molecule 16: PAP12

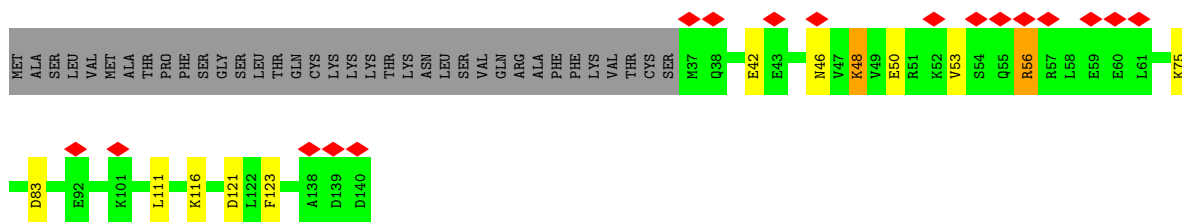


• Molecule 17: FLN2

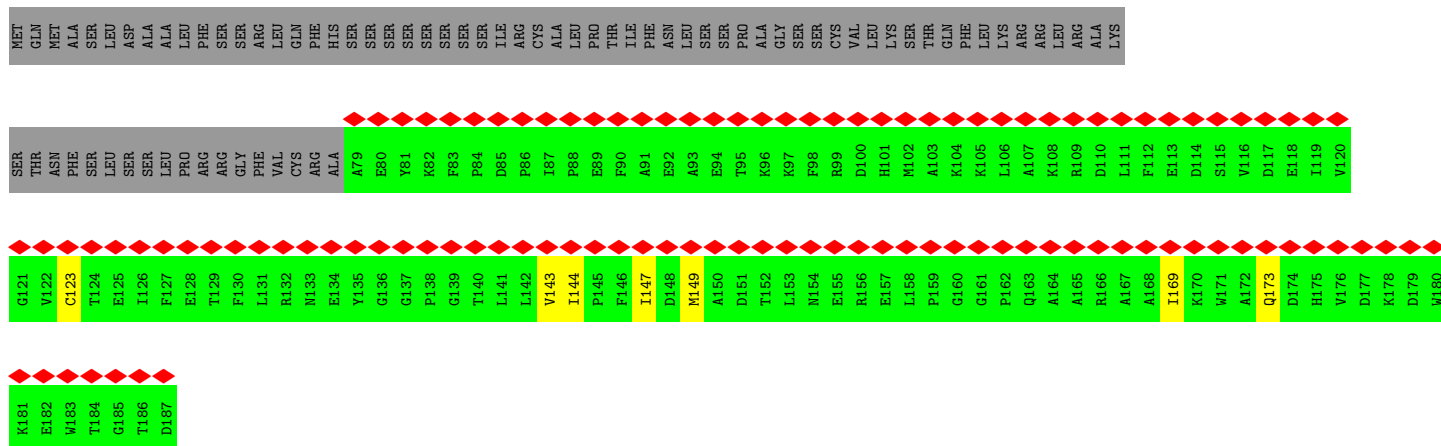




• Molecule 18: PTAC18



• Molecule 19: PRIN2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	613537	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	300.0, 300.0, 300.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	Depositor

## 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: SAH, ZN, FE

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	0.27	0/2498	0.50	0/3377
1	B	0.27	0/2336	0.52	0/3159
2	C	0.27	0/7842	0.50	0/10587
3	D	0.28	0/4765	0.50	0/6437
4	E	0.27	0/8932	0.52	1/12058 (0.0%)
5	F	0.27	0/5154	0.48	0/6964
6	G	0.25	0/5997	0.44	0/8096
7	H	0.27	0/4736	0.48	0/6386
8	I	0.28	0/1825	0.47	0/2481
9	J	0.27	0/2021	0.50	0/2724
10	K	0.27	0/3184	0.48	0/4320
11	L	0.29	0/3492	0.48	0/4727
12	M	0.31	0/1848	0.53	0/2502
13	N	0.27	0/1873	0.47	0/2549
14	O	0.27	0/939	0.50	0/1268
14	P	0.30	0/879	0.53	0/1187
15	Q	0.26	0/4218	0.49	0/5720
16	R	0.28	0/1089	0.52	0/1462
17	S	0.28	0/3123	0.49	0/4226
18	T	0.29	0/906	0.51	0/1225
19	U	0.24	0/900	0.40	0/1219
All	All	0.27	0/68557	0.49	1/92674 (0.0%)

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	B	0	1
5	F	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	890	PRO	CA-N-CD	-8.57	99.50	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	158	SER	Peptide
5	F	418	GLU	Peptide
5	F	825	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	2449	0	2490	32	0
1	B	2292	0	2311	41	0
2	C	7685	0	7774	125	0
3	D	4664	0	4741	76	0
4	E	8758	0	8895	176	0
5	F	5052	0	5003	77	0
6	G	5887	0	5803	116	0
7	H	4607	0	4464	65	0
8	I	1771	0	1696	19	0
9	J	1970	0	1923	23	0
10	K	3103	0	3026	47	0
11	L	3403	0	3347	59	0
12	M	1803	0	1756	18	0
13	N	1819	0	1746	8	0
14	O	923	0	917	30	0
14	P	865	0	867	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Q	4148	0	4046	86	0
16	R	1069	0	1058	31	0
17	S	3056	0	3042	26	0
18	T	881	0	860	8	0
19	U	877	0	840	32	0
20	E	1	0	0	0	0
21	I	1	0	0	0	0
21	N	1	0	0	0	0
22	L	26	0	19	1	0
23	A	18	0	0	0	0
23	B	13	0	0	0	0
23	C	57	0	0	1	0
23	D	21	0	0	0	0
23	E	25	0	0	0	0
23	F	1	0	0	0	0
23	H	6	0	0	0	0
23	I	4	0	0	0	0
23	J	31	0	0	0	0
23	K	15	0	0	0	0
23	L	19	0	0	1	0
23	M	13	0	0	1	0
23	N	3	0	0	0	0
23	O	2	0	0	0	0
23	P	2	0	0	0	0
23	R	2	0	0	0	0
23	S	23	0	0	0	0
All	All	67366	0	66624	953	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 7.

All (953) 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)
4:E:729:PHE:CD1	19:U:143:VAL:HB	1.35	1.58
4:E:729:PHE:CG	19:U:143:VAL:CG2	1.82	1.55
4:E:729:PHE:CE2	19:U:169:ILE:HD11	1.45	1.51
4:E:729:PHE:CG	19:U:143:VAL:HG21	1.40	1.45
4:E:729:PHE:CB	19:U:143:VAL:HG21	0.97	1.43
4:E:729:PHE:CD1	19:U:143:VAL:CB	2.12	1.31
4:E:729:PHE:CB	19:U:143:VAL:CG2	1.94	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:236:LYS:O	3:D:236:LYS:HD3	1.30	1.26
4:E:729:PHE:CD2	19:U:169:ILE:HD11	1.72	1.23
15:Q:468:ASP:H	15:Q:472:HIS:CD2	1.58	1.21
4:E:729:PHE:CG	19:U:143:VAL:HG23	1.75	1.08
6:G:212:TYR:HB3	6:G:236:MET:CE	1.82	1.08
4:E:670:ILE:HG22	4:E:782:VAL:HG22	1.23	1.08
4:E:729:PHE:CE2	19:U:169:ILE:CD1	2.36	1.08
4:E:729:PHE:HB2	19:U:143:VAL:HG21	1.22	1.08
3:D:663:ARG:NH1	3:D:666:GLU:OE1	1.89	1.05
4:E:1182:ILE:HG13	4:E:1183:PRO:HD2	1.38	1.04
4:E:729:PHE:CD1	19:U:143:VAL:CG2	2.38	1.03
4:E:729:PHE:HB3	19:U:143:VAL:HG21	1.06	1.03
4:E:729:PHE:CD2	19:U:169:ILE:CD1	2.43	1.02
4:E:729:PHE:CD2	19:U:143:VAL:HG23	1.96	1.00
4:E:729:PHE:HD1	19:U:143:VAL:HB	1.18	0.98
3:D:236:LYS:HD3	3:D:236:LYS:C	1.80	0.97
6:G:248:TYR:CD2	6:G:271:MET:SD	2.58	0.96
15:Q:468:ASP:N	15:Q:472:HIS:CD2	2.34	0.94
6:G:212:TYR:HB3	6:G:236:MET:HE1	1.48	0.94
15:Q:466:MET:HE1	15:Q:472:HIS:HB3	1.49	0.94
11:L:435:THR:OG1	11:L:437:GLU:OE2	1.86	0.94
6:G:212:TYR:CG	6:G:236:MET:CE	2.51	0.94
6:G:233:PHE:HA	6:G:236:MET:HG3	1.50	0.94
6:G:212:TYR:HB3	6:G:236:MET:HE3	1.51	0.92
4:E:729:PHE:HB3	19:U:143:VAL:CG2	1.81	0.91
6:G:745:LEU:HD11	6:G:793:MET:CE	2.01	0.90
6:G:212:TYR:CB	6:G:236:MET:CE	2.51	0.88
11:L:438:GLN:HA	11:L:441:LYS:HE3	1.54	0.88
6:G:745:LEU:HD11	6:G:793:MET:HE3	1.57	0.87
4:E:668:PHE:HB3	4:E:782:VAL:HG11	1.57	0.87
2:C:108:ASN:OD1	2:C:110:LEU:N	2.08	0.87
15:Q:730:LYS:HE3	15:Q:732:GLU:HG2	1.55	0.86
4:E:729:PHE:CE1	19:U:143:VAL:HB	2.10	0.85
10:K:93:VAL:HG11	10:K:401:MET:CE	2.06	0.85
1:B:309:MET:CE	1:B:312:PHE:HB2	2.07	0.84
2:C:32:ILE:HD11	2:C:57:TYR:CZ	2.12	0.84
5:F:827:PRO:HA	5:F:830:PHE:CD1	2.13	0.84
4:E:670:ILE:HG22	4:E:782:VAL:CG2	2.07	0.84
5:F:393:ARG:HG3	5:F:393:ARG:HH11	1.42	0.83
3:D:479:HIS:CE1	3:D:482:VAL:HG13	2.15	0.82
15:Q:468:ASP:HB3	15:Q:472:HIS:CE1	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:248:TYR:CG	6:G:271:MET:SD	2.74	0.81
4:E:729:PHE:CG	19:U:143:VAL:CB	2.50	0.80
10:K:205:MET:HE3	14:O:88:GLN:HE21	1.43	0.80
10:K:205:MET:CE	14:O:88:GLN:HA	2.13	0.79
4:E:57:LEU:HD11	4:E:128:VAL:HG22	1.64	0.79
4:E:1268:ARG:HE	4:E:1268:ARG:HA	1.46	0.79
6:G:248:TYR:CZ	6:G:271:MET:CE	2.65	0.79
1:B:309:MET:HE3	1:B:312:PHE:HB2	1.66	0.78
6:G:165:MET:HE2	6:G:171:ALA:HA	1.65	0.76
4:E:729:PHE:CD2	19:U:143:VAL:CG2	2.57	0.76
16:R:95:ASN:HB3	16:R:98:GLU:HG3	1.66	0.76
6:G:248:TYR:CE2	6:G:271:MET:SD	2.77	0.76
4:E:727:ILE:HB	19:U:173:GLN:NE2	2.01	0.75
15:Q:307:ILE:HD11	15:Q:316:LEU:HD22	1.68	0.75
4:E:861:GLU:HB3	7:H:464:ILE:HD12	1.68	0.74
6:G:226:TRP:HH2	6:G:251:LEU:HA	1.54	0.73
6:G:212:TYR:CB	6:G:236:MET:HE3	2.17	0.73
5:F:138:ARG:NH2	5:F:170:LEU:O	2.21	0.73
6:G:212:TYR:CB	6:G:236:MET:HE1	2.15	0.73
4:E:1268:ARG:HA	4:E:1268:ARG:NE	2.04	0.72
5:F:123:GLN:OE1	5:F:123:GLN:N	2.22	0.72
5:F:827:PRO:HA	5:F:830:PHE:CE1	2.23	0.72
7:H:234:GLU:C	7:H:234:GLU:OE2	2.27	0.72
15:Q:466:MET:CE	15:Q:472:HIS:HB3	2.19	0.72
4:E:1178:ARG:HA	5:F:492:ARG:HH22	1.54	0.71
4:E:782:VAL:HG12	4:E:783:ALA:N	2.04	0.71
4:E:811:ARG:NH2	7:H:601:ASP:OD2	2.24	0.71
6:G:248:TYR:CE2	6:G:271:MET:HE1	2.26	0.71
4:E:617:PHE:HA	4:E:838:CYS:HA	1.73	0.70
1:B:309:MET:SD	1:B:310:GLU:O	2.49	0.70
6:G:602:LEU:HD21	6:G:617:LEU:CD2	2.21	0.70
15:Q:478:ILE:HD11	15:Q:506:ALA:HB2	1.72	0.70
4:E:790:SER:HB3	7:H:610:GLN:HB3	1.73	0.70
6:G:271:MET:HA	6:G:271:MET:HE2	1.73	0.70
2:C:692:LYS:HD2	2:C:807:ARG:HD2	1.72	0.70
10:K:408:PRO:HD2	10:K:409:GLU:OE1	1.91	0.70
4:E:761:ASN:HA	4:E:784:THR:HG21	1.74	0.69
6:G:330:SER:HB3	6:G:333:GLU:HB2	1.75	0.69
10:K:205:MET:CE	14:O:88:GLN:HE21	2.05	0.69
6:G:248:TYR:CE2	6:G:271:MET:CE	2.76	0.69
4:E:729:PHE:HE2	19:U:169:ILE:HD11	1.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:141:GLU:HA	14:O:141:GLU:OE1	1.92	0.69
6:G:567:LEU:HD11	6:G:601:MET:HE1	1.74	0.69
5:F:393:ARG:HG3	5:F:393:ARG:NH1	2.03	0.69
10:K:419:ARG:NH2	10:K:458:SER:O	2.26	0.69
17:S:360:LEU:HD22	17:S:364:LYS:HE2	1.75	0.69
4:E:455:ASP:HB2	4:E:474:SER:HB2	1.73	0.68
4:E:727:ILE:HB	19:U:173:GLN:HE21	1.56	0.68
10:K:93:VAL:HG11	10:K:401:MET:HE3	1.74	0.68
2:C:851:ASP:OD2	23:C:1101:HOH:O	2.11	0.68
4:E:6:ASN:HD21	16:R:61:LYS:HE2	1.59	0.68
7:H:70:GLU:OE1	7:H:74:ARG:NH2	2.27	0.68
15:Q:530:ILE:HD12	15:Q:530:ILE:O	1.93	0.68
4:E:859:PHE:CE1	7:H:460:LEU:HB2	2.29	0.67
7:H:462:LYS:HE2	7:H:464:ILE:HD11	1.76	0.67
11:L:279:ILE:HD13	11:L:304:LEU:HD22	1.76	0.67
10:K:131:GLU:OE2	10:K:134:ARG:NH1	2.27	0.67
4:E:927:MET:HE2	4:E:938:LEU:HD12	1.77	0.67
11:L:286:ASN:ND2	11:L:319:GLU:OE2	2.27	0.67
4:E:206:LEU:HD21	4:E:1153:LEU:HD13	1.76	0.67
4:E:729:PHE:HB3	19:U:143:VAL:HG11	1.77	0.67
4:E:815:TYR:CZ	7:H:593:VAL:HB	2.30	0.67
2:C:328:ALA:HB2	2:C:364:THR:HG21	1.76	0.67
2:C:21:GLU:OE1	2:C:21:GLU:HA	1.95	0.66
4:E:610:ARG:HG2	7:H:585:LYS:HD3	1.78	0.66
5:F:824:ALA:HB1	5:F:826:MET:CE	2.26	0.66
2:C:595:GLU:HG2	2:C:612:MET:HE3	1.78	0.66
4:E:484:CYS:HB3	4:E:938:LEU:HD22	1.78	0.66
2:C:503:TYR:O	2:C:506:GLU:CD	2.35	0.66
4:E:440:LYS:HB3	4:E:1132:PHE:HB2	1.76	0.66
6:G:352:THR:O	6:G:356:LEU:HD22	1.96	0.66
9:J:185:GLY:O	12:M:264:ARG:NH1	2.29	0.65
6:G:212:TYR:CG	6:G:236:MET:HE2	2.32	0.65
5:F:826:MET:SD	5:F:826:MET:N	2.70	0.65
1:A:289:LYS:NZ	1:A:310:GLU:OE2	2.25	0.64
3:D:548:ARG:NH1	12:M:310:GLU:OE2	2.30	0.64
17:S:380:PRO:HD2	17:S:383:LEU:HD12	1.80	0.64
2:C:359:THR:O	2:C:363:THR:OG1	2.15	0.64
6:G:745:LEU:HD11	6:G:793:MET:HE1	1.80	0.64
2:C:316:SER:O	2:C:320:LEU:HD12	1.97	0.63
5:F:179:LEU:O	5:F:183:GLU:HG3	1.97	0.63
1:B:309:MET:HE3	1:B:312:PHE:CB	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:211:GLN:CD	5:F:211:GLN:H	2.02	0.63
4:E:228:VAL:HG21	4:E:246:LEU:HD21	1.81	0.63
5:F:811:ILE:HD13	5:F:842:TYR:HB3	1.79	0.63
2:C:696:GLN:HG2	2:C:805:ILE:HG12	1.81	0.63
6:G:602:LEU:CD2	6:G:617:LEU:HD22	2.28	0.63
15:Q:337:PRO:HG2	15:Q:403:MET:HG2	1.81	0.63
10:K:205:MET:HE1	14:O:88:GLN:HA	1.81	0.63
1:B:21:ARG:HH22	16:R:69:GLU:HG2	1.64	0.62
6:G:248:TYR:HA	6:G:251:LEU:HB2	1.79	0.62
15:Q:572:ALA:HB1	15:Q:578:GLU:HG3	1.81	0.62
4:E:791:ILE:HG23	4:E:793:LEU:HD13	1.82	0.62
5:F:410:ARG:HD3	5:F:816:VAL:HG21	1.80	0.62
19:U:123:CYS:HA	19:U:149:MET:CE	2.29	0.62
6:G:586:MET:HB3	6:G:593:PRO:HG3	1.81	0.62
6:G:224:LEU:O	6:G:258:ARG:NH2	2.32	0.62
8:I:187:ARG:NH1	8:I:189:GLU:OE2	2.31	0.62
9:J:297:GLN:OE1	9:J:300:ARG:NH1	2.32	0.62
4:E:1000:GLN:HG3	7:H:154:ASP:HB3	1.82	0.62
5:F:388:LEU:HD22	5:F:398:ILE:HD11	1.81	0.61
10:K:93:VAL:HG11	10:K:401:MET:HE1	1.79	0.61
15:Q:441:LEU:HD21	15:Q:459:GLU:CD	2.20	0.61
2:C:792:TRP:HE1	2:C:794:GLN:HE22	1.47	0.61
5:F:323:LYS:HE2	5:F:327:LEU:HD11	1.82	0.61
6:G:493:PHE:HE2	6:G:515:ARG:HD2	1.64	0.61
11:L:438:GLN:CA	11:L:441:LYS:HE3	2.29	0.61
15:Q:719:LYS:HE3	15:Q:725:GLN:NE2	2.14	0.61
2:C:721:ASN:HB3	2:C:728:VAL:HG23	1.80	0.61
2:C:418:TYR:HH	4:E:183:TYR:HH	1.49	0.61
6:G:82:SER:OG	6:G:116:ARG:NH1	2.34	0.61
2:C:163:ASP:OD1	2:C:167:ARG:N	2.34	0.61
3:D:297:ARG:HH11	3:D:297:ARG:HG3	1.64	0.61
4:E:729:PHE:HB3	19:U:143:VAL:CG1	2.31	0.61
1:B:113:PRO:HD3	1:B:142:PRO:HA	1.83	0.61
5:F:123:GLN:N	5:F:123:GLN:CD	2.54	0.61
15:Q:360:LYS:NZ	15:Q:370:THR:O	2.34	0.61
10:K:312:GLU:OE1	10:K:315:ARG:NH2	2.34	0.60
12:M:190:GLN:HA	12:M:190:GLN:NE2	2.15	0.60
18:T:48:LYS:HE3	18:T:48:LYS:O	2.01	0.60
15:Q:380:VAL:HG22	15:Q:384:ASN:HB2	1.83	0.60
4:E:982:THR:HB	7:H:166:ILE:HD12	1.82	0.60
11:L:437:GLU:OE1	11:L:438:GLN:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:437:GLU:O	11:L:441:LYS:HE3	2.01	0.60
15:Q:648:ASP:O	15:Q:725:GLN:OE1	2.19	0.60
2:C:1055:LEU:HD13	3:D:12:ILE:HG23	1.83	0.60
14:P:85:GLN:CD	14:P:85:GLN:H	2.05	0.60
2:C:493:ILE:CD1	2:C:495:GLU:HB2	2.32	0.60
15:Q:363:TYR:HA	15:Q:366:MET:HE2	1.83	0.60
3:D:221:GLN:OE1	3:D:221:GLN:C	2.39	0.59
8:I:102:GLU:CD	8:I:102:GLU:H	2.05	0.59
8:I:145:GLY:HA2	8:I:148:GLU:OE2	2.00	0.59
1:B:288:LYS:HE2	10:K:153:ARG:HD2	1.83	0.59
11:L:298:ARG:NH1	11:L:301:ASP:OD2	2.35	0.59
2:C:320:LEU:HD21	2:C:374:LEU:HD12	1.85	0.59
15:Q:468:ASP:CB	15:Q:472:HIS:NE2	2.64	0.59
10:K:205:MET:HE3	14:O:88:GLN:NE2	2.15	0.59
11:L:73:GLU:OE2	16:R:48:ARG:NH2	2.32	0.59
11:L:414:GLU:OE1	11:L:477:TYR:OH	2.19	0.59
5:F:824:ALA:HB1	5:F:826:MET:HE1	1.82	0.59
6:G:515:ARG:HA	6:G:518:ASN:HD21	1.67	0.59
7:H:452:GLU:HA	7:H:461:PRO:HA	1.83	0.59
13:N:58:ASP:OD2	13:N:66:ARG:HG3	2.01	0.59
10:K:323:ALA:HB1	10:K:328:GLN:HB3	1.84	0.59
11:L:199:LEU:O	11:L:450:ARG:NH2	2.35	0.59
14:O:172:ILE:HD12	14:O:176:MET:HE2	1.83	0.59
1:A:261:ARG:NH1	17:S:274:ASP:OD1	2.36	0.59
4:E:493:ILE:O	7:H:380:ARG:NH1	2.35	0.59
4:E:1194:ILE:HD13	4:E:1251:LEU:HD22	1.84	0.59
15:Q:561:GLU:C	15:Q:561:GLU:OE2	2.41	0.59
4:E:102:GLU:OE1	4:E:375:ARG:NH2	2.35	0.59
6:G:315:ILE:HD11	6:G:346:CYS:HB3	1.85	0.59
6:G:602:LEU:HD21	6:G:617:LEU:HD22	1.83	0.59
15:Q:584:GLN:NE2	15:Q:586:PHE:O	2.34	0.59
4:E:415:TYR:HB2	9:J:227:THR:HG21	1.85	0.59
15:Q:344:ILE:HB	15:Q:415:VAL:HG12	1.85	0.59
15:Q:474:LYS:HB2	15:Q:496:VAL:HG22	1.85	0.58
3:D:479:HIS:CE1	3:D:482:VAL:CG1	2.85	0.58
4:E:765:VAL:HG22	4:E:779:VAL:HG22	1.86	0.58
2:C:88:TRP:HE1	2:C:350:PRO:HD2	1.68	0.58
6:G:81:LEU:HD23	6:G:84:LEU:HD12	1.84	0.58
2:C:92:ARG:HH22	4:E:817:LEU:HB3	1.67	0.58
4:E:815:TYR:OH	7:H:596:GLY:N	2.31	0.58
4:E:631:LEU:HD12	4:E:669:PHE:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:212:TYR:CD1	6:G:236:MET:CE	2.86	0.58
6:G:564:GLU:OE2	6:G:667:ARG:NH1	2.37	0.58
15:Q:501:MET:HB2	15:Q:544:TYR:CZ	2.39	0.58
3:D:206:LEU:HD22	3:D:211:ILE:HD11	1.83	0.58
4:E:729:PHE:HB2	19:U:143:VAL:CG2	1.99	0.58
6:G:248:TYR:CZ	6:G:271:MET:HE1	2.39	0.58
11:L:121:GLU:OE2	11:L:298:ARG:NH2	2.34	0.58
1:B:191:ASN:OD1	1:B:191:ASN:O	2.22	0.57
10:K:200:PHE:HE1	10:K:205:MET:HE2	1.69	0.57
1:A:100:LEU:HD13	17:S:575:SER:HB3	1.86	0.57
1:B:85:HIS:O	1:B:89:MET:HG2	2.03	0.57
17:S:306:MET:CE	17:S:316:SER:HB3	2.34	0.57
15:Q:530:ILE:HD12	15:Q:530:ILE:C	2.24	0.57
4:E:574:ARG:NH1	4:E:804:GLU:OE1	2.37	0.57
5:F:209:THR:HB	5:F:211:GLN:OE1	2.03	0.57
7:H:331:ARG:NH1	7:H:341:GLU:OE1	2.27	0.57
15:Q:690:ARG:NH1	15:Q:759:GLU:OE1	2.33	0.57
3:D:608:LEU:HD22	16:R:60:TYR:HB3	1.86	0.57
16:R:70:GLU:O	16:R:74:LYS:HG3	2.05	0.57
5:F:107:ARG:HG2	5:F:140:LEU:HD11	1.86	0.57
3:D:16:SER:HB3	3:D:263:TRP:CZ2	2.40	0.57
16:R:59:ARG:H	16:R:59:ARG:HD3	1.70	0.57
7:H:73:ARG:HB2	7:H:73:ARG:NH1	2.20	0.57
14:O:91:VAL:O	14:O:95:ARG:NH1	2.37	0.57
3:D:35:GLY:HA2	3:D:60:ILE:HG23	1.87	0.57
8:I:54:THR:HG22	8:I:55:PRO:O	2.05	0.57
6:G:248:TYR:CZ	6:G:271:MET:HE3	2.38	0.56
10:K:383:THR:HG1	10:K:386:THR:HG1	1.47	0.56
15:Q:719:LYS:CE	15:Q:725:GLN:NE2	2.67	0.56
5:F:83:ARG:NH1	11:L:408:PRO:O	2.33	0.56
2:C:352:PRO:HG2	2:C:353:GLN:HE21	1.69	0.56
4:E:209:VAL:HG13	4:E:210:VAL:HG13	1.87	0.56
4:E:396:ILE:HG22	4:E:397:ILE:H	1.70	0.56
4:E:729:PHE:HB3	19:U:143:VAL:CB	2.34	0.56
15:Q:276:LEU:HD11	15:Q:300:VAL:HG23	1.88	0.56
15:Q:380:VAL:HG12	15:Q:386:MET:CE	2.34	0.56
15:Q:441:LEU:HD21	15:Q:459:GLU:OE1	2.05	0.56
18:T:56:ARG:HG3	18:T:56:ARG:HH11	1.70	0.56
3:D:142:TYR:OH	3:D:333:ASP:OD2	2.17	0.56
4:E:729:PHE:HE2	19:U:169:ILE:CD1	2.10	0.56
5:F:123:GLN:CD	5:F:123:GLN:H	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:819:ARG:O	5:F:823:ARG:HG3	2.06	0.56
11:L:432:TYR:OH	11:L:463:ARG:HD3	2.05	0.56
1:B:26:ARG:NH1	1:B:131:ASP:OD2	2.38	0.56
6:G:319:ASN:OD1	6:G:352:THR:OG1	2.22	0.56
15:Q:585:ALA:HB1	15:Q:710:GLU:HG3	1.87	0.56
3:D:12:ILE:HD11	4:E:1300:ALA:HB3	1.86	0.56
4:E:804:GLU:OE2	7:H:399:SER:N	2.37	0.56
11:L:327:GLY:HA2	11:L:346:TRP:CE2	2.41	0.56
4:E:572:ARG:NH1	4:E:573:ARG:O	2.38	0.56
15:Q:468:ASP:HB3	15:Q:472:HIS:NE2	2.20	0.56
4:E:27:ILE:HG13	4:E:35:THR:HG21	1.88	0.56
4:E:793:LEU:HD23	4:E:796:LEU:HD11	1.87	0.56
16:R:37:GLN:HE22	16:R:39:ASP:CG	2.09	0.56
11:L:359:LEU:HB2	11:L:401:THR:HB	1.87	0.55
4:E:396:ILE:HB	4:E:398:HIS:CE1	2.40	0.55
11:L:330:ASN:ND2	11:L:347:ASP:OD2	2.38	0.55
11:L:424:GLU:O	11:L:428:MET:HG3	2.07	0.55
7:H:452:GLU:HB3	7:H:459:LYS:HD3	1.87	0.55
15:Q:467:VAL:N	15:Q:472:HIS:HD2	2.05	0.55
1:B:70:ILE:HA	1:B:168:ARG:HH22	1.71	0.55
2:C:296:MET:HE3	2:C:300:MET:O	2.05	0.55
2:C:504:ARG:NH1	4:E:1126:GLY:O	2.39	0.55
2:C:208:LEU:HB3	2:C:213:LYS:HE3	1.88	0.55
5:F:107:ARG:NH2	5:F:142:GLU:OE2	2.39	0.55
6:G:212:TYR:CG	6:G:236:MET:HE3	2.35	0.55
15:Q:466:MET:SD	15:Q:472:HIS:HB3	2.46	0.55
15:Q:548:ALA:O	15:Q:552:VAL:HG23	2.07	0.55
16:R:112:GLU:OE1	16:R:112:GLU:HA	2.07	0.55
7:H:234:GLU:OE2	7:H:235:ALA:N	2.40	0.55
9:J:319:TRP:CG	9:J:346:MET:HG3	2.41	0.55
6:G:514:SER:O	6:G:518:ASN:ND2	2.39	0.55
2:C:504:ARG:O	2:C:506:GLU:OE1	2.24	0.55
10:K:205:MET:HE3	14:O:88:GLN:HA	1.86	0.55
4:E:436:GLU:N	4:E:436:GLU:OE2	2.40	0.55
8:I:59:LEU:HD22	8:I:71:LEU:HB3	1.88	0.55
14:O:172:ILE:HG21	14:O:176:MET:HE1	1.87	0.55
15:Q:360:LYS:HD2	15:Q:372:MET:HB2	1.88	0.54
17:S:388:GLU:OE1	17:S:388:GLU:HA	2.06	0.54
2:C:101:ILE:HG22	2:C:361:LEU:HD22	1.89	0.54
3:D:361:GLU:HG2	4:E:1293:THR:HB	1.88	0.54
5:F:827:PRO:HB2	5:F:861:GLU:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:437:GLU:CD	11:L:438:GLN:HG3	2.28	0.54
2:C:661:TYR:HB2	2:C:943:ILE:HG23	1.89	0.54
3:D:62:GLY:O	3:D:100:ARG:NH1	2.39	0.54
4:E:610:ARG:NH1	7:H:585:LYS:HB3	2.23	0.54
6:G:587:LYS:NZ	6:G:620:GLU:OE2	2.40	0.54
2:C:654:GLY:HA3	2:C:950:LEU:HD23	1.89	0.54
4:E:104:TRP:CD1	4:E:164:PRO:HG3	2.43	0.54
15:Q:468:ASP:CB	15:Q:472:HIS:CE1	2.90	0.54
3:D:624:TYR:HB3	12:M:282:LEU:HB3	1.90	0.54
1:A:73:ASP:N	1:A:73:ASP:OD1	2.41	0.53
5:F:408:LYS:NZ	5:F:421:GLN:O	2.31	0.53
6:G:420:MET:HE1	6:G:454:SER:H	1.73	0.53
10:K:206:LYS:HG2	14:O:145:ASP:HB3	1.89	0.53
14:P:160:ASP:OD2	14:P:162:SER:N	2.41	0.53
1:A:64:ARG:HG2	1:A:150:LYS:HB2	1.90	0.53
1:A:123:LEU:HD11	1:A:129:ILE:HD12	1.89	0.53
2:C:926:LYS:NZ	4:E:61:ASP:OD2	2.35	0.53
4:E:161:ILE:HD12	4:E:180:ILE:HG23	1.89	0.53
14:P:100:ILE:HD11	14:P:181:ILE:HD11	1.90	0.53
17:S:346:THR:HG23	17:S:348:HIS:H	1.73	0.53
3:D:168:ILE:HB	3:D:171:TRP:HB3	1.90	0.53
17:S:569:GLU:OE1	17:S:569:GLU:N	2.22	0.53
3:D:159:ARG:NH2	15:Q:680:ASP:OD1	2.42	0.53
7:H:295:ILE:HD11	7:H:340:LEU:HD13	1.91	0.53
15:Q:571:ASP:OD1	15:Q:571:ASP:N	2.38	0.53
2:C:1000:VAL:HG12	3:D:508:GLU:HB3	1.91	0.53
4:E:668:PHE:HB3	4:E:782:VAL:CG1	2.35	0.53
10:K:200:PHE:CE1	10:K:205:MET:HE2	2.44	0.53
6:G:481:MET:HE1	6:G:492:THR:HG21	1.90	0.53
4:E:833:GLN:NE2	4:E:835:VAL:O	2.41	0.52
4:E:861:GLU:CB	7:H:464:ILE:HD12	2.39	0.52
6:G:442:ILE:O	6:G:446:MET:HG3	2.09	0.52
5:F:225:ASP:OD2	5:F:228:ASN:ND2	2.35	0.52
6:G:247:THR:O	6:G:251:LEU:N	2.40	0.52
1:A:51:ARG:NH2	2:C:840:ASP:OD1	2.30	0.52
3:D:479:HIS:NE2	3:D:482:VAL:HG13	2.24	0.52
1:B:118:ALA:HB1	1:B:129:ILE:HD13	1.91	0.52
2:C:424:ILE:HD11	4:E:178:TYR:HE2	1.75	0.52
16:R:98:GLU:OE1	16:R:98:GLU:C	2.47	0.52
7:H:453:ALA:HB2	7:H:462:LYS:HD2	1.90	0.52
10:K:361:LEU:HD21	10:K:378:GLU:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:719:LYS:HE2	15:Q:725:GLN:HE22	1.73	0.52
1:B:124:PRO:HG2	1:B:127:VAL:HG21	1.91	0.52
5:F:832:LYS:O	5:F:836:THR:HG22	2.09	0.52
6:G:379:SER:OG	6:G:381:THR:OG1	2.26	0.52
12:M:210:ILE:HG23	12:M:215:ASP:HB2	1.92	0.52
3:D:216:LEU:HG	3:D:220:LYS:HZ2	1.73	0.52
4:E:389:VAL:HB	4:E:400:VAL:HG23	1.92	0.52
2:C:50:PHE:HD1	2:C:86:LEU:HD13	1.74	0.52
15:Q:467:VAL:H	15:Q:472:HIS:HD2	1.58	0.52
2:C:362:THR:O	2:C:366:GLU:HG2	2.10	0.52
2:C:868:ILE:HG23	2:C:943:ILE:HD13	1.92	0.52
14:O:141:GLU:OE1	14:O:144:ARG:NH2	2.43	0.52
1:A:225:LEU:HD22	1:B:45:ILE:HD11	1.92	0.52
4:E:928:PHE:HZ	4:E:1122:ILE:HD11	1.74	0.52
1:A:39:LYS:CD	1:B:159:LEU:HD21	2.40	0.51
11:L:358:HIS:CE1	11:L:360:ASN:HB2	2.45	0.51
15:Q:697:ARG:HD3	15:Q:725:GLN:NE2	2.25	0.51
16:R:60:TYR:HB2	16:R:61:LYS:NZ	2.25	0.51
11:L:437:GLU:OE2	11:L:438:GLN:HG3	2.11	0.51
2:C:32:ILE:HD13	2:C:32:ILE:N	2.25	0.51
3:D:15:VAL:HG13	3:D:19:GLN:HB3	1.93	0.51
6:G:427:ILE:HG22	6:G:460:GLY:HA3	1.93	0.51
7:H:409:GLN:HE21	7:H:465:LEU:HB3	1.75	0.51
11:L:439:ASP:HB3	11:L:461:MET:HE2	1.92	0.51
18:T:75:LYS:HG3	18:T:123:PHE:CE2	2.46	0.51
1:A:102:GLY:O	1:A:104:ARG:NE	2.41	0.51
2:C:316:SER:OG	2:C:317:VAL:N	2.44	0.51
6:G:318:TYR:HB3	6:G:341:MET:HE3	1.93	0.51
10:K:205:MET:CE	14:O:88:GLN:NE2	2.73	0.51
17:S:306:MET:HE2	17:S:316:SER:HB3	1.91	0.51
2:C:420:ARG:NH2	2:C:476:ASP:OD2	2.42	0.51
14:P:166:ILE:HD12	14:P:185:MET:HE1	1.92	0.51
2:C:157:ARG:O	2:C:255:ARG:NH1	2.43	0.51
3:D:297:ARG:HG3	3:D:297:ARG:NH1	2.26	0.51
5:F:410:ARG:HD2	5:F:414:SER:O	2.11	0.51
15:Q:269:ARG:O	15:Q:294:ARG:NH1	2.44	0.51
2:C:695:ILE:HB	2:C:777:LEU:HD22	1.92	0.51
10:K:134:ARG:HG2	10:K:359:GLY:HA3	1.93	0.51
9:J:263:MET:SD	9:J:295:ARG:NH2	2.84	0.51
17:S:583:GLY:O	17:S:588:LYS:NZ	2.44	0.51
18:T:83:ASP:OD1	18:T:116:LYS:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1047:GLU:O	2:C:1050:SER:OG	2.26	0.50
4:E:694:ASP:O	4:E:702:ARG:NH2	2.43	0.50
4:E:1093:ILE:HB	4:E:1100:VAL:HB	1.93	0.50
4:E:1237:GLU:OE1	4:E:1237:GLU:O	2.29	0.50
6:G:318:TYR:HB3	6:G:341:MET:CE	2.41	0.50
2:C:689:HIS:CD2	2:C:814:ARG:HD2	2.46	0.50
11:L:263:SER:OG	11:L:276:ASN:OD1	2.27	0.50
13:N:108:ARG:NH1	13:N:108:ARG:HG2	2.26	0.50
2:C:68:ASP:O	2:C:72:GLU:HG2	2.12	0.50
3:D:621:GLU:OE1	12:M:285:ARG:NE	2.37	0.50
4:E:613:SER:HA	7:H:585:LYS:HD2	1.93	0.50
5:F:512:ARG:HG3	5:F:594:VAL:HG13	1.94	0.50
12:M:285:ARG:NH2	23:M:401:HOH:O	2.45	0.50
1:A:83:SER:O	1:A:87:ILE:HG12	2.11	0.50
3:D:20:ILE:HD13	3:D:270:PRO:HD3	1.93	0.50
5:F:825:PRO:HB3	5:F:859:LEU:HD21	1.92	0.50
6:G:326:ALA:HA	6:G:359:LEU:HD13	1.93	0.50
10:K:277:SER:HB3	10:K:280:GLU:HG3	1.94	0.50
14:P:120:MET:SD	14:P:174:LEU:HD11	2.51	0.50
14:P:160:ASP:HB3	14:P:163:LYS:HD2	1.92	0.50
2:C:503:TYR:O	2:C:506:GLU:OE1	2.29	0.50
2:C:882:ARG:NH2	2:C:908:GLU:OE2	2.45	0.50
17:S:242:TYR:OH	17:S:476:GLU:OE2	2.24	0.50
6:G:114:ALA:HA	6:G:148:LEU:HD13	1.94	0.50
6:G:141:ILE:O	6:G:145:MET:HG2	2.10	0.50
6:G:212:TYR:CD1	6:G:236:MET:HE3	2.47	0.50
8:I:158:THR:O	8:I:162:GLU:HG2	2.12	0.50
3:D:302:ARG:HD3	3:D:327:LEU:HB3	1.93	0.50
4:E:439:ARG:HE	4:E:1133:ILE:HD11	1.76	0.50
2:C:120:ARG:HD2	2:C:369:PHE:HB3	1.94	0.50
10:K:388:ASP:HB2	10:K:435:ILE:HD13	1.94	0.50
1:B:209:LEU:HD11	1:B:213:GLU:CB	2.42	0.50
2:C:21:GLU:OE1	2:C:21:GLU:CA	2.60	0.50
4:E:859:PHE:CZ	7:H:460:LEU:HD13	2.47	0.50
4:E:575:ASN:HB3	4:E:876:LEU:HB3	1.93	0.49
6:G:602:LEU:HD21	6:G:617:LEU:HD23	1.94	0.49
15:Q:248:VAL:HG21	15:Q:325:VAL:HG13	1.93	0.49
2:C:205:LEU:HD23	2:C:208:LEU:HD12	1.94	0.49
4:E:62:LEU:HD23	4:E:128:VAL:HG21	1.92	0.49
5:F:391:MET:HE2	5:F:398:ILE:HD12	1.94	0.49
2:C:733:TRP:HB2	2:C:786:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1175:CYS:SG	5:F:745:PRO:HG2	2.52	0.49
4:E:1182:ILE:CG1	4:E:1183:PRO:HD2	2.25	0.49
6:G:331:ILE:HG23	6:G:360:PHE:HE1	1.77	0.49
15:Q:531:LEU:HD21	15:Q:560:LEU:HB3	1.93	0.49
4:E:787:ILE:HD12	7:H:599:TRP:CE3	2.47	0.49
6:G:751:VAL:HB	6:G:790:GLY:HA3	1.93	0.49
7:H:593:VAL:HG23	7:H:594:GLY:H	1.77	0.49
16:R:37:GLN:C	16:R:37:GLN:OE1	2.51	0.49
1:B:209:LEU:HD11	1:B:213:GLU:HB3	1.94	0.49
2:C:32:ILE:HD11	2:C:57:TYR:CE1	2.47	0.49
2:C:58:GLN:NE2	2:C:98:ARG:HH22	2.11	0.49
3:D:644:LYS:NZ	12:M:238:LEU:O	2.45	0.49
5:F:489:LYS:O	5:F:493:THR:HG22	2.13	0.49
6:G:570:TYR:HD1	6:G:575:LEU:HD12	1.77	0.49
14:P:160:ASP:OD2	14:P:160:ASP:C	2.51	0.49
1:A:193:ASN:ND2	1:A:194:GLU:OE1	2.46	0.49
4:E:304:TYR:O	4:E:1219:ARG:HD3	2.13	0.49
8:I:129:PHE:HD2	8:I:209:ASN:HB2	1.76	0.49
15:Q:468:ASP:N	15:Q:472:HIS:HD2	2.06	0.49
16:R:37:GLN:OE1	16:R:38:ARG:N	2.45	0.49
1:A:248:LEU:HD12	17:S:564:ILE:HD13	1.94	0.49
2:C:779:LEU:HD12	2:C:780:PRO:HD2	1.94	0.49
2:C:792:TRP:NE1	2:C:804:GLU:OE2	2.46	0.49
3:D:221:GLN:NE2	3:D:225:GLU:OE2	2.45	0.49
4:E:901:MET:SD	4:E:901:MET:N	2.85	0.49
5:F:218:GLU:HG2	5:F:222:LYS:HE2	1.95	0.49
3:D:669:ILE:HD12	4:E:7:LEU:HD11	1.94	0.49
14:O:128:ASN:OD1	14:O:128:ASN:N	2.43	0.49
3:D:15:VAL:HG21	3:D:23:TRP:CH2	2.48	0.49
7:H:205:ASP:OD2	7:H:207:LYS:NZ	2.45	0.49
2:C:223:ILE:HG12	7:H:570:TRP:HE1	1.78	0.48
15:Q:456:ARG:HG3	15:Q:482:ASN:HD21	1.77	0.48
15:Q:491:ASN:HB3	15:Q:494:VAL:HG23	1.95	0.48
17:S:467:GLU:HG2	17:S:468:HIS:CD2	2.48	0.48
6:G:244:ASP:OD1	6:G:244:ASP:N	2.46	0.48
1:B:309:MET:CE	1:B:312:PHE:CB	2.85	0.48
2:C:99:ILE:CD1	2:C:353:GLN:HA	2.43	0.48
2:C:669:PHE:CD2	2:C:670:GLU:HG3	2.49	0.48
4:E:630:ILE:HG22	4:E:823:PRO:HA	1.95	0.48
4:E:1054:ASN:OD1	4:E:1054:ASN:C	2.52	0.48
5:F:276:ASP:OD1	5:F:277:PHE:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:70:GLU:HG2	16:R:73:ARG:HH12	1.77	0.48
3:D:399:ARG:HH21	16:R:157:LEU:HD12	1.78	0.48
4:E:782:VAL:HG12	4:E:783:ALA:H	1.74	0.48
5:F:346:ARG:HA	5:F:349:LYS:HD3	1.95	0.48
13:N:108:ARG:HG2	13:N:108:ARG:HH11	1.77	0.48
16:R:98:GLU:OE1	16:R:99:PHE:N	2.46	0.48
17:S:489:ALA:HB2	17:S:533:LEU:HD22	1.95	0.48
6:G:655:ASP:OD1	6:G:695:ARG:NH2	2.45	0.48
2:C:45:ASP:HB2	2:C:47:GLU:HG3	1.95	0.48
2:C:860:PRO:HG2	4:E:131:MET:SD	2.53	0.48
3:D:542:LEU:HD13	4:E:49:GLN:HG3	1.94	0.48
6:G:647:TRP:NE1	6:G:691:GLU:OE2	2.43	0.48
6:G:762:ARG:NH2	6:G:785:THR:O	2.47	0.48
15:Q:356:THR:HG23	15:Q:415:VAL:HB	1.96	0.48
2:C:292:HIS:O	2:C:296:MET:N	2.41	0.48
5:F:293:THR:HG22	5:F:331:CYS:HB2	1.94	0.48
12:M:128:SER:HB2	12:M:183:ARG:HG2	1.95	0.48
2:C:149:THR:HG23	2:C:159:GLU:HG2	1.96	0.48
2:C:633:CYS:SG	14:O:124:GLU:HG2	2.53	0.48
3:D:302:ARG:NH1	3:D:330:GLU:OE1	2.46	0.48
4:E:674:VAL:HG22	4:E:721:LYS:HG2	1.96	0.48
4:E:815:TYR:HE2	4:E:817:LEU:HD23	1.78	0.48
4:E:1361:ILE:HG22	4:E:1362:LEU:H	1.78	0.48
5:F:414:SER:O	5:F:414:SER:OG	2.32	0.48
6:G:358:ASN:HD21	6:G:362:GLN:HE21	1.61	0.48
11:L:372:PRO:HA	11:L:375:TYR:CZ	2.49	0.48
3:D:19:GLN:HE21	3:D:23:TRP:HE1	1.62	0.48
6:G:248:TYR:CD1	6:G:271:MET:SD	3.07	0.48
8:I:144:LYS:O	8:I:148:GLU:OE2	2.30	0.48
17:S:395:GLN:O	17:S:395:GLN:NE2	2.47	0.48
2:C:92:ARG:NH2	4:E:817:LEU:O	2.46	0.48
6:G:583:PHE:HB2	6:G:601:MET:CE	2.43	0.48
1:B:288:LYS:NZ	10:K:179:GLN:HE21	2.12	0.47
2:C:56:THR:O	2:C:56:THR:OG1	2.30	0.47
2:C:493:ILE:HD12	2:C:495:GLU:N	2.28	0.47
2:C:586:GLU:OE2	14:O:74:ARG:NH2	2.31	0.47
3:D:209:ARG:O	3:D:213:GLU:HG2	2.14	0.47
4:E:358:TYR:CE1	4:E:398:HIS:CG	3.02	0.47
4:E:1237:GLU:OE1	4:E:1237:GLU:C	2.53	0.47
4:E:1262:GLU:OE1	5:F:343:ARG:NH1	2.47	0.47
5:F:115:ALA:O	5:F:119:ASN:ND2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:165:MET:SD	6:G:172:ARG:HG3	2.54	0.47
7:H:418:LEU:HD13	7:H:481:ARG:HB2	1.96	0.47
11:L:301:ASP:OD1	11:L:301:ASP:N	2.47	0.47
1:A:234:GLU:HG2	1:A:235:GLU:HG3	1.95	0.47
8:I:93:ASP:OD1	8:I:96:LEU:N	2.31	0.47
16:R:75:ILE:HG23	16:R:80:LYS:HB2	1.95	0.47
16:R:134:ASN:HA	16:R:138:PHE:O	2.14	0.47
17:S:451:ILE:HD11	17:S:509:MET:HG2	1.96	0.47
2:C:357:THR:O	2:C:360:PRO:HD2	2.15	0.47
6:G:529:ASN:ND2	6:G:562:THR:OG1	2.45	0.47
11:L:437:GLU:C	11:L:441:LYS:HE3	2.35	0.47
17:S:439:GLU:CD	17:S:439:GLU:H	2.18	0.47
1:A:322:ASP:HA	1:A:325:GLU:HB2	1.97	0.47
1:B:191:ASN:ND2	16:R:156:TYR:CZ	2.83	0.47
5:F:289:ILE:O	5:F:293:THR:HG23	2.14	0.47
6:G:583:PHE:HB2	6:G:601:MET:HE3	1.96	0.47
11:L:298:ARG:HD2	11:L:301:ASP:OD1	2.14	0.47
16:R:66:PRO:HG2	16:R:67:PHE:CE2	2.50	0.47
17:S:240:GLU:H	17:S:240:GLU:CD	2.16	0.47
15:Q:343:VAL:HG22	15:Q:414:LEU:HD21	1.97	0.47
1:A:321:LEU:O	1:A:325:GLU:N	2.40	0.47
1:B:131:ASP:HB3	1:B:134:GLN:HG3	1.97	0.47
6:G:315:ILE:N	6:G:315:ILE:HD13	2.29	0.47
11:L:438:GLN:HA	11:L:441:LYS:CE	2.37	0.47
15:Q:586:PHE:HB3	15:Q:709:GLU:O	2.15	0.47
2:C:562:LYS:HG3	2:C:647:VAL:HB	1.96	0.47
5:F:389:ASP:HB3	5:F:393:ARG:HH12	1.80	0.47
11:L:104:ILE:HD12	11:L:285:LEU:HG	1.97	0.47
11:L:246:ASP:OD1	11:L:249:ARG:N	2.45	0.47
14:P:79:VAL:HG13	14:P:131:ILE:HG22	1.96	0.47
1:A:195:LYS:HB2	1:B:159:LEU:HD13	1.97	0.47
4:E:610:ARG:HH11	7:H:585:LYS:HB3	1.78	0.47
6:G:248:TYR:CZ	6:G:271:MET:SD	3.08	0.47
11:L:446:LEU:HD22	11:L:449:ALA:HB2	1.96	0.47
15:Q:442:THR:OG1	15:Q:444:GLU:OE2	2.24	0.47
15:Q:467:VAL:H	15:Q:472:HIS:CD2	2.33	0.47
1:A:61:CYS:SG	1:A:174:ALA:HB1	2.55	0.47
2:C:296:MET:CE	2:C:296:MET:HA	2.45	0.47
4:E:155:ASP:HB2	4:E:156:PRO:HD2	1.96	0.47
13:N:267:GLN:HG2	13:N:270:GLN:HE21	1.80	0.47
15:Q:538:LEU:HD11	15:Q:579:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:353:LYS:HD2	17:S:353:LYS:HA	1.73	0.47
2:C:58:GLN:HE21	2:C:98:ARG:HH22	1.63	0.47
2:C:296:MET:HA	2:C:296:MET:HE2	1.98	0.47
3:D:344:PRO:HB2	3:D:352:VAL:HG13	1.97	0.47
7:H:334:TYR:CZ	7:H:365:ARG:HD3	2.51	0.47
11:L:361:SER:HB3	11:L:481:LEU:HD11	1.96	0.47
15:Q:350:ASN:HD22	15:Q:440:ASN:ND2	2.13	0.47
5:F:408:LYS:HB3	5:F:423:GLU:HG2	1.97	0.46
17:S:193:ILE:O	17:S:196:THR:OG1	2.28	0.46
2:C:458:VAL:H	2:C:467:ARG:HH12	1.62	0.46
3:D:387:GLY:HA3	3:D:477:CYS:SG	2.55	0.46
4:E:673:GLU:HB3	4:E:722:ILE:HB	1.97	0.46
4:E:792:ASN:HA	7:H:611:THR:HG21	1.97	0.46
6:G:266:MET:O	6:G:270:THR:OG1	2.31	0.46
6:G:561:ARG:O	6:G:565:ALA:N	2.45	0.46
9:J:257:THR:HG23	9:J:276:PRO:HG2	1.96	0.46
18:T:53:VAL:HG21	18:T:111:LEU:HB2	1.96	0.46
1:A:191:ASN:OD1	1:A:191:ASN:N	2.49	0.46
2:C:929:ILE:HG13	2:C:938:PHE:HD2	1.81	0.46
3:D:668:ALA:HA	16:R:71:GLN:OE1	2.14	0.46
19:U:123:CYS:HA	19:U:149:MET:SD	2.56	0.46
1:A:111:GLN:NE2	1:A:144:ASN:OD1	2.49	0.46
2:C:77:SER:OG	2:C:103:ASN:HB3	2.15	0.46
2:C:450:LEU:O	2:C:473:PRO:HD3	2.16	0.46
4:E:395:ASP:OD1	4:E:395:ASP:N	2.39	0.46
5:F:788:GLN:NE2	5:F:791:GLU:OE1	2.48	0.46
1:B:77:ILE:HG22	1:B:80:ILE:HG13	1.97	0.46
2:C:720:ARG:HB3	2:C:720:ARG:CZ	2.46	0.46
4:E:63:LEU:HD11	9:J:285:ARG:HD2	1.98	0.46
6:G:212:TYR:CD1	6:G:236:MET:HE2	2.49	0.46
11:L:437:GLU:O	11:L:441:LYS:CE	2.63	0.46
2:C:597:ILE:HD11	2:C:626:PRO:HB3	1.95	0.46
9:J:319:TRP:CD2	9:J:346:MET:HG3	2.50	0.46
10:K:409:GLU:OE1	10:K:409:GLU:N	2.46	0.46
3:D:185:GLU:OE2	3:D:188:ARG:NH2	2.35	0.46
5:F:826:MET:HG2	5:F:829:SER:OG	2.16	0.46
10:K:124:MET:HG2	10:K:127:TRP:CZ2	2.51	0.46
10:K:280:GLU:OE2	10:K:281:THR:N	2.48	0.46
15:Q:561:GLU:OE1	15:Q:562:ASP:OD1	2.34	0.46
6:G:383:PRO:HG2	6:G:388:TYR:OH	2.16	0.46
6:G:583:PHE:O	6:G:586:MET:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:216:LEU:HG	3:D:220:LYS:NZ	2.31	0.46
4:E:858:PHE:HB2	7:H:461:PRO:O	2.16	0.46
11:L:411:PRO:O	11:L:415:ARG:HG3	2.15	0.46
15:Q:468:ASP:H	15:Q:472:HIS:HD2	1.43	0.46
15:Q:510:PRO:HA	15:Q:524:VAL:HA	1.98	0.46
3:D:15:VAL:HG21	3:D:23:TRP:HH2	1.80	0.45
11:L:57:PRO:HA	11:L:60:GLN:HG2	1.97	0.45
14:O:175:GLN:NE2	14:O:179:ASP:OD1	2.49	0.45
2:C:674:LEU:HD11	2:C:836:LEU:HG	1.98	0.45
2:C:1046:ARG:NH2	3:D:102:TYR:HB3	2.32	0.45
4:E:383:CYS:O	4:E:405:LYS:N	2.49	0.45
4:E:729:PHE:CD2	19:U:169:ILE:HD13	2.44	0.45
7:H:164:ARG:HB2	7:H:166:ILE:HD11	1.98	0.45
3:D:160:LEU:HD21	15:Q:764:LEU:HD12	1.97	0.45
5:F:78:LEU:HG	5:F:90:VAL:HG13	1.97	0.45
9:J:246:SER:O	9:J:247:ARG:HB3	2.17	0.45
11:L:422:GLN:HG2	11:L:471:ILE:HG23	1.99	0.45
13:N:213:VAL:HG23	13:N:214:TRP:CD1	2.51	0.45
14:O:164:ASP:OD1	14:O:164:ASP:N	2.38	0.45
15:Q:730:LYS:HE3	15:Q:732:GLU:CG	2.38	0.45
2:C:132:ILE:HG23	2:C:269:ARG:HG2	1.98	0.45
6:G:525:ARG:HD3	6:G:557:ASP:O	2.15	0.45
12:M:172:THR:HG23	12:M:178:ILE:O	2.17	0.45
1:B:275:ASP:HB3	10:K:181:ARG:N	2.32	0.45
3:D:541:VAL:HG11	4:E:53:THR:HG21	1.99	0.45
7:H:459:LYS:HB3	7:H:459:LYS:HE3	1.79	0.45
10:K:85:PHE:CG	10:K:86:PRO:HD2	2.52	0.45
6:G:733:SER:HB3	6:G:818:ILE:HD11	1.99	0.45
7:H:543:GLU:OE1	7:H:546:ARG:NH2	2.46	0.45
2:C:510:ILE:HD12	2:C:510:ILE:O	2.17	0.45
2:C:788:ILE:HD13	2:C:811:SER:HB2	1.97	0.45
3:D:168:ILE:HG23	15:Q:766:GLU:HG3	1.98	0.45
6:G:777:HIS:CE1	6:G:819:VAL:HG13	2.51	0.45
2:C:139:ASP:OD1	2:C:143:ILE:N	2.44	0.45
2:C:612:MET:O	2:C:614:GLN:NE2	2.46	0.45
3:D:294:GLU:OE1	3:D:297:ARG:NH2	2.50	0.45
4:E:296:THR:HG21	4:E:1230:SER:HB2	1.98	0.45
4:E:769:THR:HG23	4:E:775:PHE:HB3	1.98	0.45
5:F:393:ARG:HH11	5:F:393:ARG:CG	2.20	0.45
7:H:200:GLU:O	7:H:204:LYS:NZ	2.35	0.45
9:J:190:ASN:OD1	9:J:190:ASN:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:284:MET:HA	22:L:8001:SAH:HB1	1.98	0.45
11:L:374:GLU:OE2	11:L:374:GLU:O	2.35	0.45
1:A:49:MET:HG2	1:A:201:ILE:HD13	1.99	0.45
6:G:463:GLU:O	6:G:467:GLN:HG2	2.16	0.45
14:O:172:ILE:HD12	14:O:176:MET:CE	2.47	0.45
1:B:155:ARG:HB2	1:B:158:SER:HB2	1.99	0.45
4:E:470:LEU:HD13	4:E:1113:ALA:HB3	1.98	0.45
4:E:793:LEU:HD23	4:E:796:LEU:CD1	2.47	0.45
5:F:398:ILE:HD13	5:F:805:LEU:HB3	1.99	0.45
5:F:597:LEU:O	5:F:600:ARG:HG3	2.17	0.45
6:G:575:LEU:HB3	6:G:578:GLU:HB2	1.98	0.45
7:H:418:LEU:HD11	7:H:477:ALA:HB1	1.99	0.45
10:K:205:MET:HB2	14:O:88:GLN:HE21	1.81	0.45
15:Q:380:VAL:HG12	15:Q:386:MET:HE1	1.98	0.45
15:Q:395:ASP:OD1	15:Q:398:LEU:N	2.40	0.45
1:B:145:LEU:HD21	1:B:147:ILE:HD11	1.99	0.44
1:B:209:LEU:CD1	1:B:213:GLU:CB	2.95	0.44
2:C:1056:ASN:OD1	2:C:1069:ARG:NH1	2.50	0.44
3:D:399:ARG:NH2	16:R:157:LEU:HD12	2.31	0.44
4:E:782:VAL:CG1	4:E:783:ALA:N	2.76	0.44
6:G:178:THR:HG23	6:G:211:THR:HA	1.99	0.44
6:G:713:VAL:HA	6:G:716:MET:HG3	1.99	0.44
10:K:102:GLU:HG2	14:O:171:LEU:HD12	1.99	0.44
16:R:113:LYS:HD2	16:R:114:ASN:OD1	2.17	0.44
1:A:93:GLU:OE1	1:A:134:GLN:NE2	2.50	0.44
1:A:304:GLU:O	1:A:308:LYS:HG2	2.17	0.44
1:B:280:PRO:HD2	1:B:283:ILE:HD12	1.98	0.44
7:H:353:ILE:O	8:I:254:ASN:ND2	2.40	0.44
14:P:122:ALA:HB2	14:P:131:ILE:HD12	1.99	0.44
14:P:174:LEU:HD12	17:S:562:ASN:N	2.32	0.44
1:A:72:HIS:HB3	2:C:731:GLY:HA2	1.99	0.44
2:C:241:GLU:HG2	2:C:245:LYS:HE3	1.99	0.44
4:E:861:GLU:HB3	7:H:464:ILE:CD1	2.42	0.44
5:F:352:GLU:H	5:F:352:GLU:CD	2.19	0.44
5:F:602:LYS:HG3	5:F:604:HIS:NE2	2.32	0.44
5:F:824:ALA:CB	5:F:826:MET:CE	2.95	0.44
8:I:178:TRP:CE3	8:I:209:ASN:OD1	2.70	0.44
12:M:127:ASP:CG	12:M:130:MET:HB2	2.38	0.44
1:A:194:GLU:HG2	1:A:196:GLN:HG3	1.99	0.44
2:C:33:GLU:OE1	2:C:37:LYS:NZ	2.46	0.44
3:D:65:LYS:HB3	3:D:68:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:815:TYR:CE1	7:H:593:VAL:HB	2.53	0.44
4:E:1314:GLU:OE1	4:E:1314:GLU:N	2.35	0.44
5:F:83:ARG:HG2	11:L:408:PRO:HD2	1.99	0.44
6:G:437:GLU:O	6:G:441:LYS:HG2	2.18	0.44
6:G:637:ILE:O	6:G:684:ARG:NH1	2.51	0.44
8:I:174:SER:HB3	8:I:213:TRP:CD2	2.53	0.44
11:L:442:LEU:O	11:L:446:LEU:HG	2.18	0.44
1:B:123:LEU:HD11	1:B:129:ILE:HG13	2.00	0.44
2:C:99:ILE:HD13	2:C:353:GLN:HA	2.00	0.44
4:E:625:ARG:HD3	4:E:785:TYR:OH	2.17	0.44
5:F:824:ALA:HB1	5:F:826:MET:HE3	1.97	0.44
7:H:302:TRP:CZ2	7:H:304:PRO:HB3	2.52	0.44
10:K:277:SER:HB3	10:K:280:GLU:CG	2.47	0.44
11:L:248:GLU:CD	11:L:248:GLU:H	2.21	0.44
1:B:209:LEU:HD12	1:B:210:THR:N	2.33	0.44
3:D:124:SER:HB3	3:D:127:ALA:HB3	1.98	0.44
4:E:691:ILE:HD12	4:E:695:THR:HB	1.99	0.44
4:E:1015:ILE:HG23	7:H:156:SER:HB3	2.00	0.44
6:G:71:SER:HB3	6:G:74:VAL:HG23	1.99	0.44
6:G:86:PRO:O	6:G:124:ARG:NH1	2.51	0.44
7:H:530:ASP:OD2	18:T:116:LYS:NZ	2.49	0.44
11:L:176:ARG:HB2	11:L:179:HIS:HB2	1.99	0.44
13:N:175:TRP:CE2	13:N:211:PRO:HD3	2.53	0.44
15:Q:610:LYS:HA	15:Q:610:LYS:HD3	1.58	0.44
1:A:273:PHE:HA	1:A:294:THR:HA	2.00	0.44
4:E:568:LEU:HD13	7:H:503:LEU:HG	2.00	0.44
5:F:815:ALA:O	5:F:819:ARG:N	2.43	0.44
9:J:275:GLU:OE2	9:J:275:GLU:HA	2.17	0.44
11:L:365:VAL:HG13	11:L:480:ARG:HD2	1.99	0.44
15:Q:478:ILE:HD11	15:Q:506:ALA:CB	2.44	0.44
16:R:39:ASP:O	16:R:41:ASN:N	2.49	0.44
2:C:359:THR:OG1	2:C:360:PRO:HD3	2.17	0.44
3:D:96:ASP:OD1	3:D:97:SER:N	2.51	0.44
4:E:1089:GLY:HA2	4:E:1104:ALA:HB3	1.98	0.44
5:F:409:TYR:OH	5:F:439:GLU:OE2	2.29	0.44
6:G:248:TYR:HD1	6:G:267:VAL:HG13	1.81	0.44
6:G:414:GLU:HB2	6:G:416:ILE:HD12	2.00	0.44
11:L:373:GLU:CD	11:L:373:GLU:H	2.22	0.44
14:P:95:ARG:HA	14:P:95:ARG:HD2	1.78	0.44
2:C:882:ARG:NH1	2:C:905:GLU:OE1	2.49	0.44
4:E:208:GLU:OE1	4:E:1313:LYS:NZ	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1251:LEU:O	4:E:1255:GLU:HG3	2.18	0.44
5:F:153:SER:HA	5:F:188:THR:HG21	2.00	0.44
8:I:58:PRO:HG2	8:I:61:ALA:HB2	2.00	0.44
9:J:260:LEU:HD23	9:J:260:LEU:HA	1.89	0.44
9:J:421:LYS:HE2	14:O:72:PHE:CE1	2.53	0.44
2:C:43:ASP:OD1	2:C:43:ASP:N	2.49	0.43
4:E:257:ILE:HD12	4:E:262:VAL:HG11	1.98	0.43
1:B:209:LEU:CD1	1:B:213:GLU:HB2	2.48	0.43
4:E:571:LYS:HD2	4:E:571:LYS:HA	1.85	0.43
4:E:730:PRO:HG3	4:E:775:PHE:CE2	2.52	0.43
6:G:561:ARG:HH21	6:G:667:ARG:HD3	1.82	0.43
8:I:174:SER:HB3	8:I:213:TRP:CE2	2.53	0.43
9:J:245:TRP:CH2	9:J:247:ARG:HB2	2.53	0.43
12:M:127:ASP:O	12:M:181:VAL:HB	2.18	0.43
15:Q:354:THR:HB	15:Q:545:ASN:HD22	1.84	0.43
15:Q:373:PHE:HB2	15:Q:416:MET:HB3	2.00	0.43
1:B:309:MET:SD	1:B:309:MET:C	2.96	0.43
2:C:592:THR:HG22	2:C:597:ILE:HG23	2.01	0.43
4:E:864:THR:O	4:E:864:THR:HG23	2.18	0.43
5:F:161:LEU:HD21	5:F:197:VAL:HG13	2.01	0.43
6:G:260:LEU:HB3	6:G:263:GLU:HB2	1.99	0.43
12:M:149:CYS:HB3	12:M:258:LYS:HE2	2.00	0.43
17:S:437:GLU:HB3	17:S:439:GLU:OE2	2.18	0.43
2:C:298:PHE:HB3	4:E:464:TYR:CE1	2.53	0.43
3:D:474:ARG:NH1	3:D:475:THR:HG22	2.33	0.43
11:L:443:LEU:O	16:R:38:ARG:NH2	2.51	0.43
13:N:253:THR:O	13:N:257:ARG:HG3	2.18	0.43
1:B:86:GLU:HG3	3:D:649:TYR:CE2	2.53	0.43
3:D:213:GLU:OE2	3:D:213:GLU:CA	2.66	0.43
4:E:231:ARG:NE	4:E:231:ARG:HA	2.33	0.43
5:F:823:ARG:C	5:F:825:PRO:HD2	2.39	0.43
5:F:829:SER:HA	5:F:832:LYS:HE3	2.00	0.43
18:T:50:GLU:O	18:T:53:VAL:HG22	2.19	0.43
1:B:209:LEU:HD12	1:B:213:GLU:HB2	2.00	0.43
2:C:247:LEU:HB3	7:H:570:TRP:CZ3	2.52	0.43
5:F:407:ARG:HD2	15:Q:669:THR:HG21	2.01	0.43
5:F:469:ASN:N	5:F:469:ASN:OD1	2.47	0.43
9:J:390:PRO:HG2	9:J:393:ASN:ND2	2.34	0.43
1:A:195:LYS:HD2	1:B:159:LEU:HD22	2.01	0.43
2:C:328:ALA:HA	2:C:331:ARG:HD2	2.01	0.43
4:E:841:LEU:HD11	4:E:874:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:852:ILE:HD12	5:F:868:ILE:HD13	2.00	0.43
9:J:184:ASN:ND2	12:M:187:PRO:HG2	2.32	0.43
9:J:305:LYS:HB2	9:J:305:LYS:HE2	1.83	0.43
11:L:260:ARG:NH1	23:L:8101:HOH:O	2.38	0.43
1:A:19:GLU:OE1	1:A:31:ARG:NH1	2.42	0.43
1:B:173:ASP:OD1	1:B:173:ASP:N	2.50	0.43
2:C:88:TRP:NE1	2:C:350:PRO:HD2	2.32	0.43
2:C:742:GLY:HA2	2:C:776:CYS:SG	2.58	0.43
3:D:245:VAL:HG21	4:E:1245:PRO:HG2	2.00	0.43
5:F:82:ALA:HA	5:F:115:ALA:HB2	2.00	0.43
3:D:634:TYR:CE1	3:D:639:ILE:HD12	2.54	0.43
4:E:1237:GLU:OE2	4:E:1266:CYS:SG	2.71	0.43
5:F:389:ASP:O	5:F:393:ARG:NH1	2.52	0.43
7:H:315:HIS:O	7:H:318:ARG:NH2	2.52	0.43
10:K:200:PHE:CE1	14:O:88:GLN:NE2	2.87	0.43
11:L:355:SER:OG	11:L:420:GLU:OE1	2.31	0.43
13:N:191:PRO:HB2	13:N:192:LEU:HD13	2.01	0.43
15:Q:755:ILE:HG23	15:Q:764:LEU:HD23	2.01	0.43
15:Q:756:ASP:HB3	15:Q:763:ARG:HB2	2.01	0.43
2:C:58:GLN:NE2	2:C:98:ARG:HH12	2.16	0.42
2:C:88:TRP:O	2:C:92:ARG:N	2.52	0.42
2:C:122:VAL:CG1	2:C:320:LEU:HD13	2.49	0.42
6:G:385:ALA:HA	6:G:388:TYR:CD2	2.53	0.42
6:G:742:LEU:HD12	6:G:742:LEU:HA	1.92	0.42
11:L:87:ARG:HD2	12:M:214:ARG:HD3	2.00	0.42
2:C:420:ARG:NH1	2:C:476:ASP:OD2	2.48	0.42
5:F:407:ARG:NH1	15:Q:672:GLU:OE2	2.52	0.42
10:K:159:LYS:HD3	10:K:186:ASP:HB2	2.01	0.42
15:Q:719:LYS:CE	15:Q:725:GLN:HE22	2.31	0.42
2:C:129:SER:HA	2:C:313:ARG:HD3	2.01	0.42
3:D:179:PHE:O	3:D:180:THR:OG1	2.31	0.42
3:D:616:LYS:HG2	12:M:202:CYS:SG	2.59	0.42
7:H:447:GLU:HA	7:H:466:LYS:HB3	2.01	0.42
3:D:478:LEU:HD13	3:D:482:VAL:HG23	2.01	0.42
4:E:709:ILE:HD13	4:E:722:ILE:HG12	2.01	0.42
5:F:405:MET:HG2	5:F:409:TYR:HA	2.02	0.42
2:C:383:PRO:HG3	2:C:579:VAL:HG21	2.01	0.42
2:C:653:LEU:CB	2:C:950:LEU:HD22	2.50	0.42
2:C:1055:LEU:HD11	3:D:10:LEU:HD13	2.00	0.42
3:D:236:LYS:C	3:D:236:LYS:CD	2.58	0.42
3:D:383:VAL:HG22	3:D:474:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:610:ARG:NH2	7:H:582:GLU:OE1	2.53	0.42
4:E:1081:LYS:HE2	4:E:1081:LYS:HB3	1.49	0.42
6:G:367:ASP:N	6:G:367:ASP:OD1	2.52	0.42
6:G:245:ILE:HD12	6:G:245:ILE:HA	1.92	0.42
6:G:248:TYR:CD1	6:G:267:VAL:HG13	2.54	0.42
10:K:457:PRO:HA	10:K:460:TRP:CE2	2.55	0.42
16:R:113:LYS:HB3	16:R:113:LYS:HE3	1.76	0.42
4:E:796:LEU:HD12	7:H:604:TYR:CE2	2.55	0.42
6:G:165:MET:HE2	6:G:171:ALA:CA	2.41	0.42
9:J:213:HIS:ND1	9:J:214:PRO:O	2.47	0.42
14:O:149:ARG:NH2	14:O:169:GLU:OE1	2.53	0.42
19:U:144:ILE:HD13	19:U:147:ILE:HD12	2.02	0.42
2:C:525:TYR:CE2	4:E:175:LEU:HD21	2.55	0.42
3:D:524:ILE:HD12	3:D:524:ILE:HA	1.89	0.42
4:E:859:PHE:HB2	7:H:462:LYS:HB2	2.01	0.42
5:F:110:HIS:CE1	5:F:142:GLU:HG3	2.54	0.42
6:G:280:LEU:HD13	6:G:316:THR:HB	2.02	0.42
7:H:237:LYS:HD2	7:H:262:TYR:OH	2.20	0.42
9:J:306:GLU:HB3	9:J:310:ALA:HB3	2.02	0.42
11:L:441:LYS:HB3	11:L:441:LYS:HE2	1.75	0.42
2:C:456:GLU:HB2	2:C:469:LEU:HD22	2.00	0.42
3:D:234:ASP:N	3:D:234:ASP:OD1	2.53	0.42
3:D:479:HIS:CD2	3:D:481:LEU:H	2.37	0.42
3:D:516:HIS:CE1	16:R:83:THR:HG23	2.55	0.42
4:E:1129:LEU:HG	4:E:1130:VAL:HG23	2.02	0.42
5:F:414:SER:OG	5:F:813:ASP:OD1	2.36	0.42
7:H:114:GLU:O	7:H:118:MET:HG2	2.20	0.42
7:H:604:TYR:O	7:H:608:ILE:HG12	2.20	0.42
10:K:122:TRP:CE2	14:O:106:THR:HG22	2.55	0.42
16:R:38:ARG:HG2	16:R:44:ARG:HG2	2.01	0.42
2:C:351:THR:HG23	2:C:354:ASN:H	1.83	0.42
2:C:493:ILE:HD12	2:C:495:GLU:H	1.85	0.42
3:D:197:GLY:O	3:D:201:GLU:HG2	2.20	0.42
4:E:141:SER:O	4:E:145:GLN:HG2	2.20	0.42
4:E:623:TYR:CD2	4:E:835:VAL:HB	2.54	0.42
6:G:712:ASP:OD1	6:G:714:HIS:ND1	2.41	0.42
6:G:762:ARG:HA	6:G:767:THR:HG21	2.01	0.42
8:I:205:ILE:HG21	8:I:249:ALA:HB2	2.02	0.42
10:K:101:LYS:HE2	10:K:101:LYS:HB2	1.61	0.42
15:Q:370:THR:O	15:Q:381:HIS:HA	2.20	0.42
15:Q:394:PRO:O	15:Q:427:LYS:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:36:ILE:HD11	16:R:38:ARG:NH2	2.35	0.42
2:C:15:PHE:HB2	2:C:387:ILE:HD11	2.02	0.41
2:C:440:ILE:HD12	2:C:523:PHE:HB3	2.02	0.41
6:G:271:MET:CE	6:G:271:MET:HA	2.45	0.41
11:L:440:GLN:NE2	11:L:444:ASP:OD2	2.51	0.41
15:Q:441:LEU:HD11	15:Q:486:PHE:HE2	1.85	0.41
1:B:119:ARG:CZ	1:B:132:ASN:HD22	2.34	0.41
3:D:391:SER:HB2	3:D:394:ARG:HG3	2.01	0.41
10:K:200:PHE:HD1	14:O:88:GLN:HE22	1.67	0.41
10:K:339:THR:OG1	10:K:341:GLU:HG2	2.20	0.41
15:Q:748:ASP:OD1	15:Q:748:ASP:N	2.52	0.41
1:A:117:THR:OG1	1:A:119:ARG:HG2	2.20	0.41
2:C:588:LYS:HE2	14:O:123:VAL:O	2.20	0.41
3:D:520:LEU:O	4:E:309:THR:HG22	2.20	0.41
4:E:1182:ILE:HD12	4:E:1182:ILE:HA	1.94	0.41
6:G:162:PHE:CG	6:G:180:LEU:HD22	2.56	0.41
1:A:195:LYS:HB2	1:B:159:LEU:HD22	2.01	0.41
2:C:305:ASP:OD2	2:C:414:HIS:NE2	2.46	0.41
6:G:181:ILE:HG22	6:G:193:SER:HA	2.02	0.41
6:G:233:PHE:CD1	6:G:247:THR:HG21	2.56	0.41
7:H:568:ASP:OD1	7:H:568:ASP:N	2.51	0.41
8:I:178:TRP:CZ3	8:I:209:ASN:OD1	2.73	0.41
11:L:435:THR:OG1	11:L:437:GLU:CD	2.57	0.41
17:S:352:ASP:HB3	17:S:355:MET:HB2	2.03	0.41
1:A:131:ASP:HB3	1:A:134:GLN:HG3	2.02	0.41
1:B:158:SER:C	1:B:159:LEU:HG	2.40	0.41
4:E:358:TYR:CD1	4:E:398:HIS:CD2	3.08	0.41
4:E:633:TYR:HB3	4:E:667:PHE:HB2	2.03	0.41
6:G:254:ALA:HA	6:G:257:ILE:HD12	2.02	0.41
8:I:168:ALA:HA	8:I:177:VAL:HG21	2.01	0.41
11:L:110:ILE:HB	11:L:314:ILE:HB	2.01	0.41
15:Q:343:VAL:HG13	15:Q:414:LEU:HD11	2.03	0.41
15:Q:441:LEU:HD11	15:Q:486:PHE:CE2	2.55	0.41
2:C:725:ASN:OD1	2:C:725:ASN:N	2.54	0.41
3:D:170:SER:HB2	15:Q:755:ILE:HD11	2.01	0.41
4:E:369:VAL:HB	4:E:381:PHE:HB3	2.03	0.41
4:E:1187:LEU:O	4:E:1191:GLU:HG2	2.21	0.41
7:H:412:VAL:HG12	7:H:416:MET:HE2	2.01	0.41
7:H:585:LYS:HB3	7:H:585:LYS:HE2	1.87	0.41
10:K:314:ARG:NH2	10:K:334:ASP:OD2	2.53	0.41
15:Q:517:LEU:HD22	15:Q:713:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:659:VAL:HG22	2:C:852:MET:HB2	2.02	0.41
4:E:70:TRP:CZ2	9:J:278:LEU:HD12	2.55	0.41
4:E:230:PRO:HA	4:E:237:MET:HE1	2.01	0.41
4:E:271:ILE:HG21	12:M:209:PRO:HB2	2.03	0.41
4:E:1030:ILE:HD13	7:H:202:LEU:HD23	2.02	0.41
6:G:446:MET:HE1	6:G:453:PRO:HB3	2.03	0.41
6:G:579:CYS:O	6:G:601:MET:HE3	2.20	0.41
9:J:417:LEU:HG	9:J:421:LYS:HD2	2.03	0.41
12:M:294:ILE:HD12	12:M:298:GLU:HB2	2.03	0.41
14:P:147:GLN:HG3	17:S:316:SER:HB2	2.01	0.41
15:Q:384:ASN:OD1	15:Q:384:ASN:N	2.53	0.41
15:Q:561:GLU:C	15:Q:561:GLU:CD	2.79	0.41
15:Q:574:PRO:HB3	15:Q:737:ARG:HH12	1.86	0.41
18:T:46:ASN:CG	18:T:46:ASN:O	2.58	0.41
4:E:1033:LEU:HD22	4:E:1048:TRP:CG	2.56	0.41
6:G:701:LEU:O	6:G:711:VAL:HA	2.21	0.41
11:L:87:ARG:HD3	11:L:123:PRO:HG3	2.03	0.41
11:L:160:ARG:NE	11:L:223:ARG:HD3	2.35	0.41
14:O:98:PRO:HB3	14:O:185:MET:HB3	2.03	0.41
16:R:95:ASN:HB3	16:R:98:GLU:CG	2.44	0.41
2:C:611:ILE:HG23	2:C:614:GLN:HG2	2.03	0.41
2:C:693:TYR:CE1	2:C:810:ILE:HD12	2.56	0.41
2:C:881:ASP:OD1	9:J:398:PRO:HG2	2.20	0.41
2:C:1039:GLU:OE1	3:D:102:TYR:OH	2.39	0.41
3:D:145:PHE:CE2	3:D:165:GLU:HG2	2.56	0.41
4:E:490:LEU:HD12	7:H:383:GLU:OE1	2.20	0.41
4:E:610:ARG:NH1	7:H:585:LYS:HE2	2.35	0.41
5:F:268:PHE:HB2	5:F:288:VAL:HG21	2.03	0.41
6:G:226:TRP:CZ3	6:G:254:ALA:HB3	2.56	0.41
7:H:504:ARG:NH2	7:H:511:GLU:OE2	2.54	0.41
10:K:416:VAL:O	10:K:420:GLN:HG2	2.21	0.41
11:L:432:TYR:CG	11:L:464:LYS:HE2	2.55	0.41
14:P:97:VAL:HG11	14:P:127:SER:O	2.21	0.41
15:Q:466:MET:HE1	15:Q:472:HIS:CB	2.33	0.41
15:Q:576:ARG:HA	15:Q:576:ARG:HD3	1.95	0.41
15:Q:682:TYR:O	15:Q:690:ARG:NH2	2.53	0.41
17:S:478:VAL:HG21	17:S:530:GLN:HG2	2.03	0.41
2:C:187:MET:CE	2:C:252:PHE:CZ	3.04	0.41
4:E:889:ASN:HD22	4:E:889:ASN:HA	1.70	0.41
5:F:608:THR:HG22	5:F:612:LYS:HD2	2.02	0.41
6:G:570:TYR:CD1	6:G:575:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:795:LYS:HB2	2:C:803:PRO:HG2	2.02	0.40
4:E:614:ILE:HG12	4:E:840:VAL:HG22	2.03	0.40
4:E:1071:GLN:HG2	7:H:85:GLU:HB2	2.03	0.40
10:K:110:HIS:CE1	10:K:112:ASN:HB3	2.56	0.40
16:R:66:PRO:HG2	16:R:67:PHE:CD2	2.55	0.40
4:E:815:TYR:CE2	4:E:817:LEU:HD23	2.55	0.40
5:F:277:PHE:CD1	5:F:278:MET:HG3	2.56	0.40
6:G:216:ILE:HD13	6:G:247:THR:HG23	2.02	0.40
6:G:656:LYS:HE2	6:G:656:LYS:HB3	1.90	0.40
10:K:383:THR:OG1	10:K:386:THR:OG1	2.29	0.40
11:L:305:GLU:HB3	11:L:307:MET:SD	2.62	0.40
11:L:327:GLY:HA2	11:L:346:TRP:CD2	2.56	0.40
11:L:425:CYS:HA	11:L:428:MET:HE2	2.03	0.40
14:O:113:LEU:O	14:O:117:GLU:HG2	2.21	0.40
1:B:309:MET:SD	1:B:312:PHE:HB2	2.60	0.40
2:C:227:TYR:HD2	2:C:237:PRO:HG3	1.87	0.40
2:C:595:GLU:HA	2:C:612:MET:HE3	2.02	0.40
3:D:474:ARG:HH11	3:D:475:THR:HG22	1.85	0.40
4:E:793:LEU:HD21	4:E:839:LEU:HD11	2.02	0.40
6:G:279:ASP:O	6:G:282:THR:OG1	2.38	0.40
6:G:674:ASP:HA	6:G:719:GLY:HA3	2.04	0.40
9:J:190:ASN:OD1	9:J:190:ASN:C	2.59	0.40
17:S:593:ARG:NH1	17:S:595:TYR:OH	2.55	0.40
1:A:15:TRP:HA	1:A:33:ILE:O	2.22	0.40
2:C:328:ALA:CB	2:C:364:THR:HG21	2.48	0.40
2:C:347:LYS:HB2	4:E:717:ARG:HH22	1.87	0.40
3:D:104:MET:SD	3:D:273:PRO:HD3	2.61	0.40
4:E:358:TYR:CE1	4:E:398:HIS:CD2	3.10	0.40
4:E:992:PHE:HE1	8:I:132:GLU:HG3	1.86	0.40
5:F:410:ARG:NH1	5:F:816:VAL:HG11	2.37	0.40
5:F:443:THR:O	5:F:443:THR:OG1	2.35	0.40
5:F:890:ALA:O	5:F:894:ASN:ND2	2.54	0.40
6:G:196:LEU:O	6:G:200:MET:HG3	2.21	0.40
8:I:181:LEU:HD11	8:I:255:LEU:HD21	2.03	0.40
10:K:103:PHE:CE1	14:O:169:GLU:HB3	2.57	0.40
11:L:349:ILE:HD13	11:L:349:ILE:HA	1.96	0.40
15:Q:573:VAL:HA	15:Q:574:PRO:HD3	1.99	0.40
1:B:282:ARG:HD2	10:K:83:ILE:HG21	2.02	0.40
3:D:133:PRO:HG2	3:D:136:GLU:HG2	2.03	0.40
5:F:352:GLU:CD	5:F:352:GLU:N	2.75	0.40
5:F:797:VAL:O	5:F:801:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:165:MET:CE	6:G:171:ALA:HA	2.44	0.40
7:H:409:GLN:NE2	7:H:465:LEU:HB3	2.37	0.40
10:K:85:PHE:CD1	10:K:86:PRO:HD2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/327 (90%)	284 (96%)	11 (4%)	0	100	100
1	B	279/327 (85%)	268 (96%)	11 (4%)	0	100	100
2	C	951/1072 (89%)	932 (98%)	19 (2%)	0	100	100
3	D	551/680 (81%)	533 (97%)	18 (3%)	0	100	100
4	E	1057/1373 (77%)	1019 (96%)	36 (3%)	2 (0%)	47	68
5	F	621/911 (68%)	601 (97%)	19 (3%)	1 (0%)	47	68
6	G	744/862 (86%)	725 (97%)	19 (3%)	0	100	100
7	H	547/675 (81%)	533 (97%)	14 (3%)	0	100	100
8	I	213/263 (81%)	205 (96%)	8 (4%)	0	100	100
9	J	230/529 (44%)	222 (96%)	8 (4%)	0	100	100
10	K	382/460 (83%)	369 (97%)	13 (3%)	0	100	100
11	L	412/483 (85%)	403 (98%)	8 (2%)	1 (0%)	47	68
12	M	213/334 (64%)	210 (99%)	3 (1%)	0	100	100
13	N	222/297 (75%)	216 (97%)	6 (3%)	0	100	100
14	O	112/185 (60%)	110 (98%)	2 (2%)	0	100	100
14	P	106/185 (57%)	103 (97%)	3 (3%)	0	100	100
15	Q	537/768 (70%)	527 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	R	126/162 (78%)	119 (94%)	6 (5%)	1 (1%)	19	35
17	S	382/611 (62%)	365 (96%)	17 (4%)	0	100	100
18	T	102/140 (73%)	98 (96%)	4 (4%)	0	100	100
19	U	107/187 (57%)	104 (97%)	3 (3%)	0	100	100
All	All	8189/10831 (76%)	7946 (97%)	238 (3%)	5 (0%)	54	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	1183	PRO
5	F	825	PRO
11	L	405	ILE
16	R	40	ASP
4	E	489	ILE

### 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 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	275/301 (91%)	267 (97%)	8 (3%)	42	69
1	B	258/301 (86%)	249 (96%)	9 (4%)	36	62
2	C	843/931 (90%)	826 (98%)	17 (2%)	55	79
3	D	514/608 (84%)	503 (98%)	11 (2%)	53	78
4	E	969/1230 (79%)	953 (98%)	16 (2%)	60	82
5	F	538/782 (69%)	522 (97%)	16 (3%)	41	68
6	G	642/740 (87%)	628 (98%)	14 (2%)	52	77
7	H	488/609 (80%)	478 (98%)	10 (2%)	55	79
8	I	187/230 (81%)	186 (100%)	1 (0%)	88	96
9	J	212/469 (45%)	210 (99%)	2 (1%)	78	92
10	K	338/401 (84%)	334 (99%)	4 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	369/431 (86%)	363 (98%)	6 (2%)	62	84
12	M	205/299 (69%)	200 (98%)	5 (2%)	49	74
13	N	192/259 (74%)	188 (98%)	4 (2%)	53	78
14	O	103/169 (61%)	100 (97%)	3 (3%)	42	69
14	P	97/169 (57%)	94 (97%)	3 (3%)	40	67
15	Q	458/661 (69%)	447 (98%)	11 (2%)	49	74
16	R	114/144 (79%)	109 (96%)	5 (4%)	28	52
17	S	336/532 (63%)	332 (99%)	4 (1%)	71	88
18	T	93/126 (74%)	89 (96%)	4 (4%)	29	53
19	U	91/160 (57%)	91 (100%)	0	100	100
All	All	7322/9552 (77%)	7169 (98%)	153 (2%)	56	78

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	43	ASP
1	A	104	ARG
1	A	115	TYR
1	A	129	ILE
1	A	154	ASN
1	A	261	ARG
1	A	282	ARG
1	B	43	ASP
1	B	66	LYS
1	B	100	LEU
1	B	109	CYS
1	B	158	SER
1	B	162	SER
1	B	165	PHE
1	B	167	ASP
1	B	309	MET
2	C	33	GLU
2	C	56	THR
2	C	108	ASN
2	C	128	GLN
2	C	136	SER
2	C	187	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	304	ASP
2	C	313	ARG
2	C	351	THR
2	C	476	ASP
2	C	542	ASN
2	C	622	MET
2	C	691	ARG
2	C	725	ASN
2	C	881	ASP
2	C	923	TYR
2	C	943	ILE
3	D	1	MET
3	D	59	ARG
3	D	65	LYS
3	D	205	ASP
3	D	221	GLN
3	D	224	GLU
3	D	235	ARG
3	D	514	PHE
3	D	517	MET
3	D	624	TYR
3	D	631	HIS
4	E	8	VAL
4	E	17	THR
4	E	56	SER
4	E	358	TYR
4	E	395	ASP
4	E	610	ARG
4	E	684	MET
4	E	836	ARG
4	E	869	ARG
4	E	1000	GLN
4	E	1123	LEU
4	E	1175	CYS
4	E	1204	LYS
4	E	1237	GLU
4	E	1268	ARG
4	E	1283	SER
5	F	79	MET
5	F	207	ARG
5	F	241	ARG
5	F	270	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	F	416	TRP
5	F	443	THR
5	F	452	ARG
5	F	492	ARG
5	F	511	MET
5	F	602	LYS
5	F	818	LEU
5	F	826	MET
5	F	835	GLN
5	F	848	LEU
5	F	863	ASP
5	F	871	ASP
6	G	113	PHE
6	G	165	MET
6	G	212	TYR
6	G	325	TYR
6	G	367	ASP
6	G	376	MET
6	G	393	ASP
6	G	542	GLU
6	G	580	ARG
6	G	636	MET
6	G	642	ASP
6	G	649	ILE
6	G	655	ASP
6	G	747	VAL
7	H	181	LYS
7	H	204	LYS
7	H	220	GLU
7	H	234	GLU
7	H	378	CYS
7	H	459	LYS
7	H	462	LYS
7	H	504	ARG
7	H	569	TYR
7	H	599	TRP
8	I	95	ARG
9	J	230	SER
9	J	416	MET
10	K	102	GLU
10	K	248	SER
10	K	265	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	K	280	GLU
11	L	87	ARG
11	L	245	GLU
11	L	374	GLU
11	L	441	LYS
11	L	463	ARG
11	L	475	ASP
12	M	127	ASP
12	M	130	MET
12	M	133	ASP
12	M	244	VAL
12	M	296	VAL
13	N	49	GLU
13	N	156	ASP
13	N	214	TRP
13	N	252	GLU
14	O	85	GLN
14	O	127	SER
14	O	128	ASN
14	P	85	GLN
14	P	144	ARG
14	P	176	MET
15	Q	306	ASP
15	Q	350	ASN
15	Q	384	ASN
15	Q	402	MET
15	Q	406	MET
15	Q	415	VAL
15	Q	438	PHE
15	Q	519	GLU
15	Q	561	GLU
15	Q	565	ARG
15	Q	737	ARG
16	R	50	THR
16	R	54	LYS
16	R	61	LYS
16	R	96	ARG
16	R	98	GLU
17	S	240	GLU
17	S	298	LYS
17	S	562	ASN
17	S	570	ARG

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Mol	Chain	Res	Type
18	T	42	GLU
18	T	48	LYS
18	T	56	ARG
18	T	121	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	105	ASN
1	A	111	GLN
1	A	196	GLN
1	A	301	ASN
1	A	303	GLN
1	B	132	ASN
1	B	191	ASN
1	B	196	GLN
1	B	311	HIS
2	C	58	GLN
2	C	135	GLN
2	C	278	ASN
2	C	353	GLN
2	C	542	ASN
2	C	623	HIS
2	C	794	GLN
3	D	324	GLN
3	D	479	HIS
4	E	6	ASN
4	E	370	HIS
4	E	398	HIS
4	E	739	HIS
4	E	863	ASN
4	E	889	ASN
4	E	1027	ASN
4	E	1038	ASN
4	E	1212	GLN
4	E	1282	GLN
4	E	1291	GLN
5	F	495	GLN
5	F	894	ASN
6	G	358	ASN
6	G	518	ASN

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Mol	Chain	Res	Type
6	G	754	GLN
6	G	777	HIS
7	H	308	ASN
7	H	588	HIS
8	I	111	ASN
8	I	159	ASN
9	J	184	ASN
9	J	329	GLN
10	K	110	HIS
10	K	179	GLN
10	K	255	GLN
10	K	331	ASN
11	L	132	GLN
11	L	438	GLN
12	M	190	GLN
14	O	88	GLN
14	O	183	ASN
15	Q	350	ASN
15	Q	472	HIS
15	Q	725	GLN
15	Q	751	HIS
19	U	173	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	SAH	L	8001	11	24,28,28	1.19	3 (12%)	25,40,40	1.68	5 (20%)

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
22	SAH	L	8001	11	-	6/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	8001	SAH	C2-N3	3.72	1.38	1.32
22	L	8001	SAH	C2-N1	2.23	1.38	1.33
22	L	8001	SAH	OXT-C	-2.20	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	8001	SAH	N3-C2-N1	-5.27	120.44	128.68
22	L	8001	SAH	C5'-SD-CG	-3.44	91.96	102.27
22	L	8001	SAH	C3'-C2'-C1'	3.05	105.56	100.98
22	L	8001	SAH	OXT-C-O	-2.65	118.08	124.09
22	L	8001	SAH	OXT-C-CA	2.10	120.55	113.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	L	8001	SAH	N-CA-CB-CG
22	L	8001	SAH	C-CA-CB-CG
22	L	8001	SAH	C3'-C4'-C5'-SD
22	L	8001	SAH	O-C-CA-CB
22	L	8001	SAH	OXT-C-CA-CB

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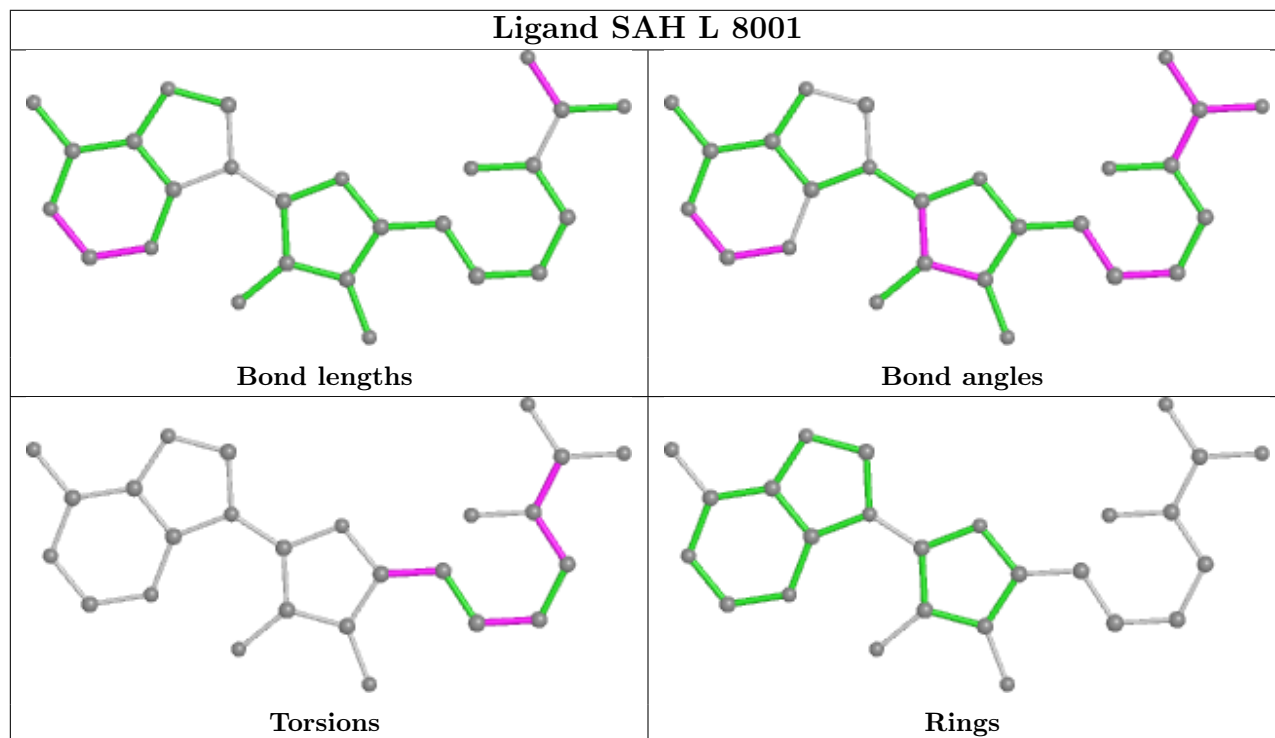
Mol	Chain	Res	Type	Atoms
22	L	8001	SAH	CB-CG-SD-C5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	L	8001	SAH	1	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.

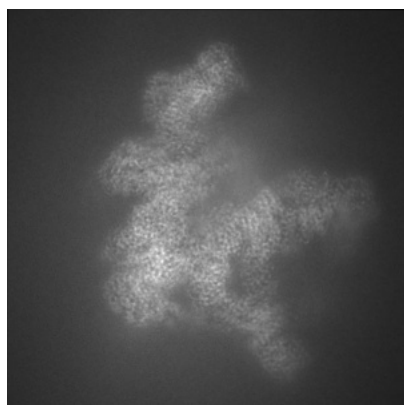
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18935. These allow visual inspection of the internal detail of the map and identification of artifacts.

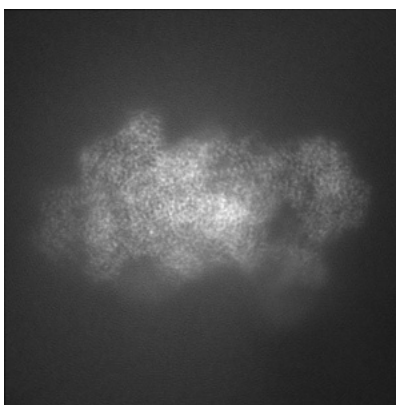
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

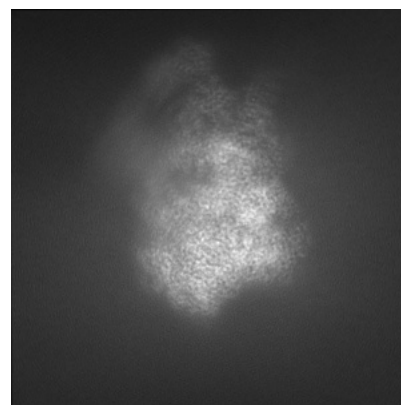
#### 6.1.1 Primary map



X



Y

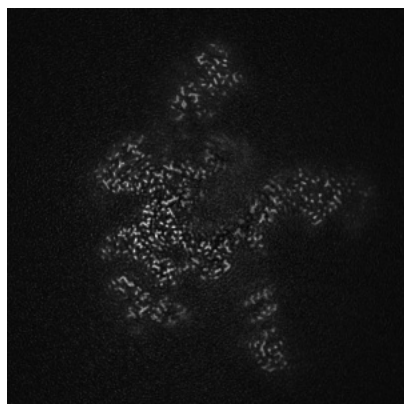


Z

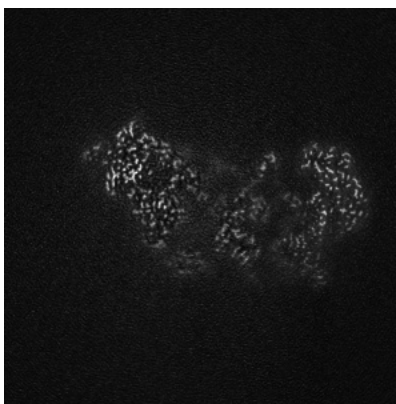
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

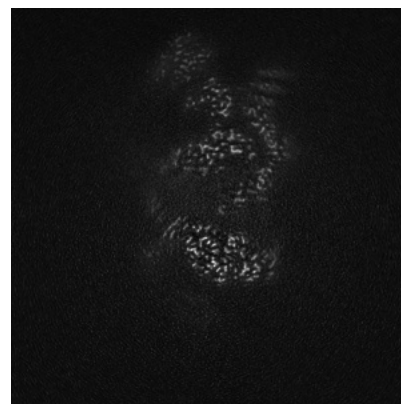
#### 6.2.1 Primary map



X Index: 300



Y Index: 300

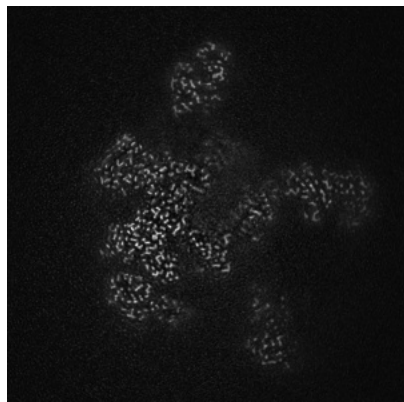


Z Index: 300

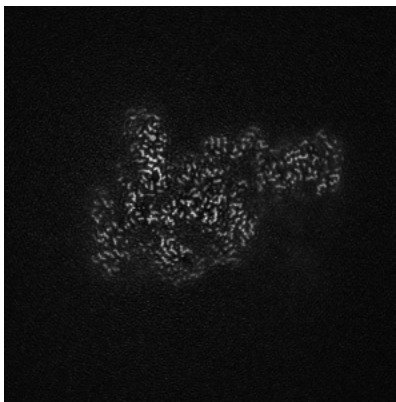
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

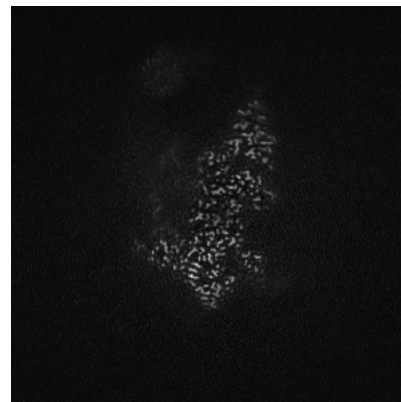
### 6.3.1 Primary map



X Index: 289



Y Index: 232

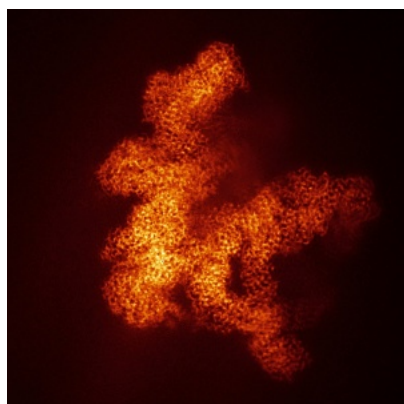


Z Index: 253

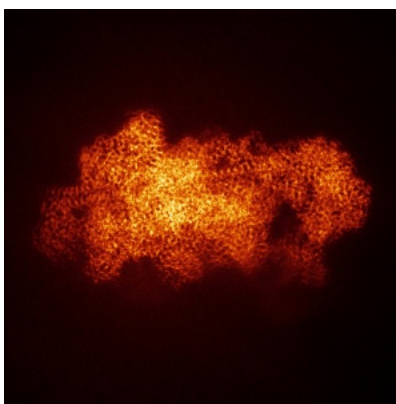
The images above show the largest variance slices of the map in three orthogonal directions.

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

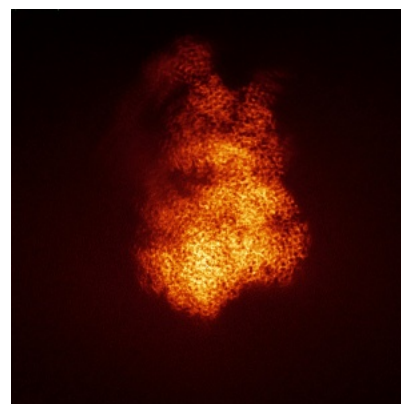
### 6.4.1 Primary map



X



Y

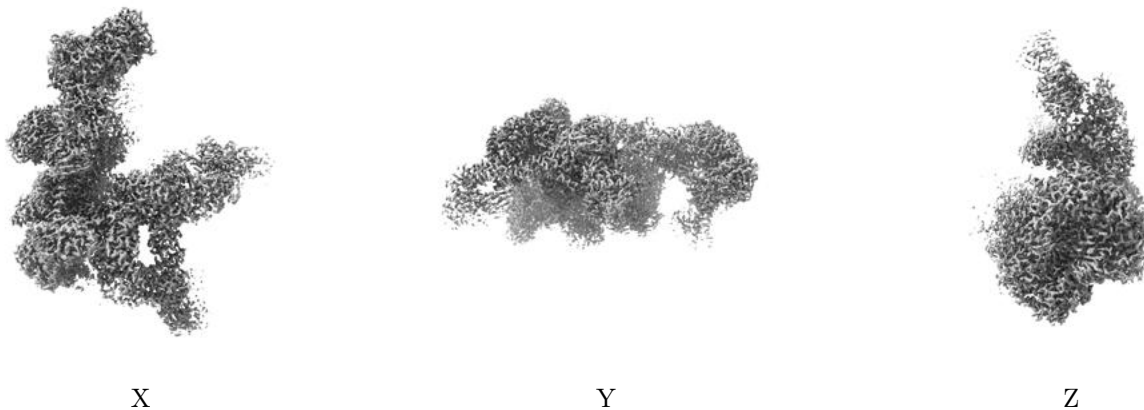


Z

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

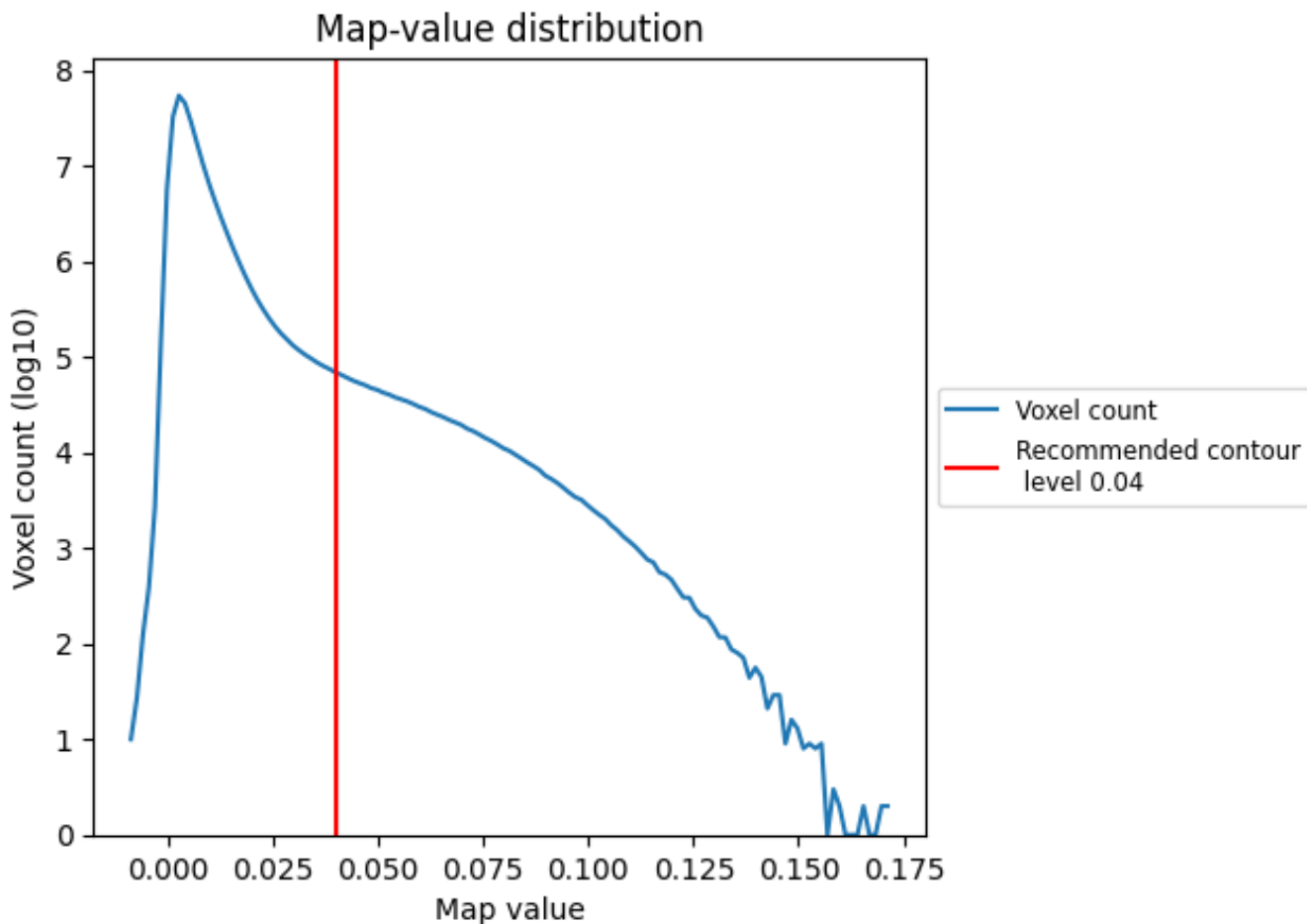
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

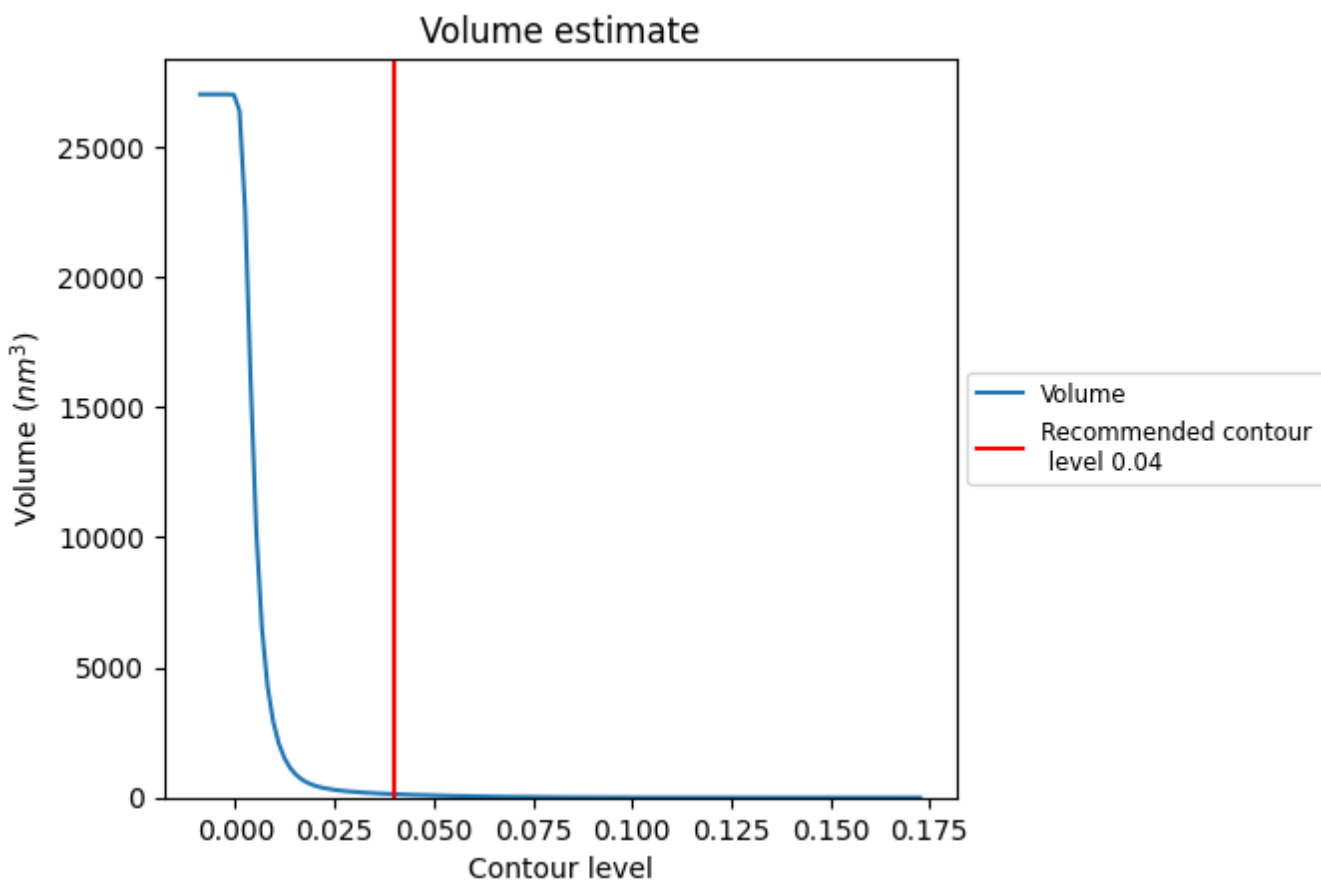
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

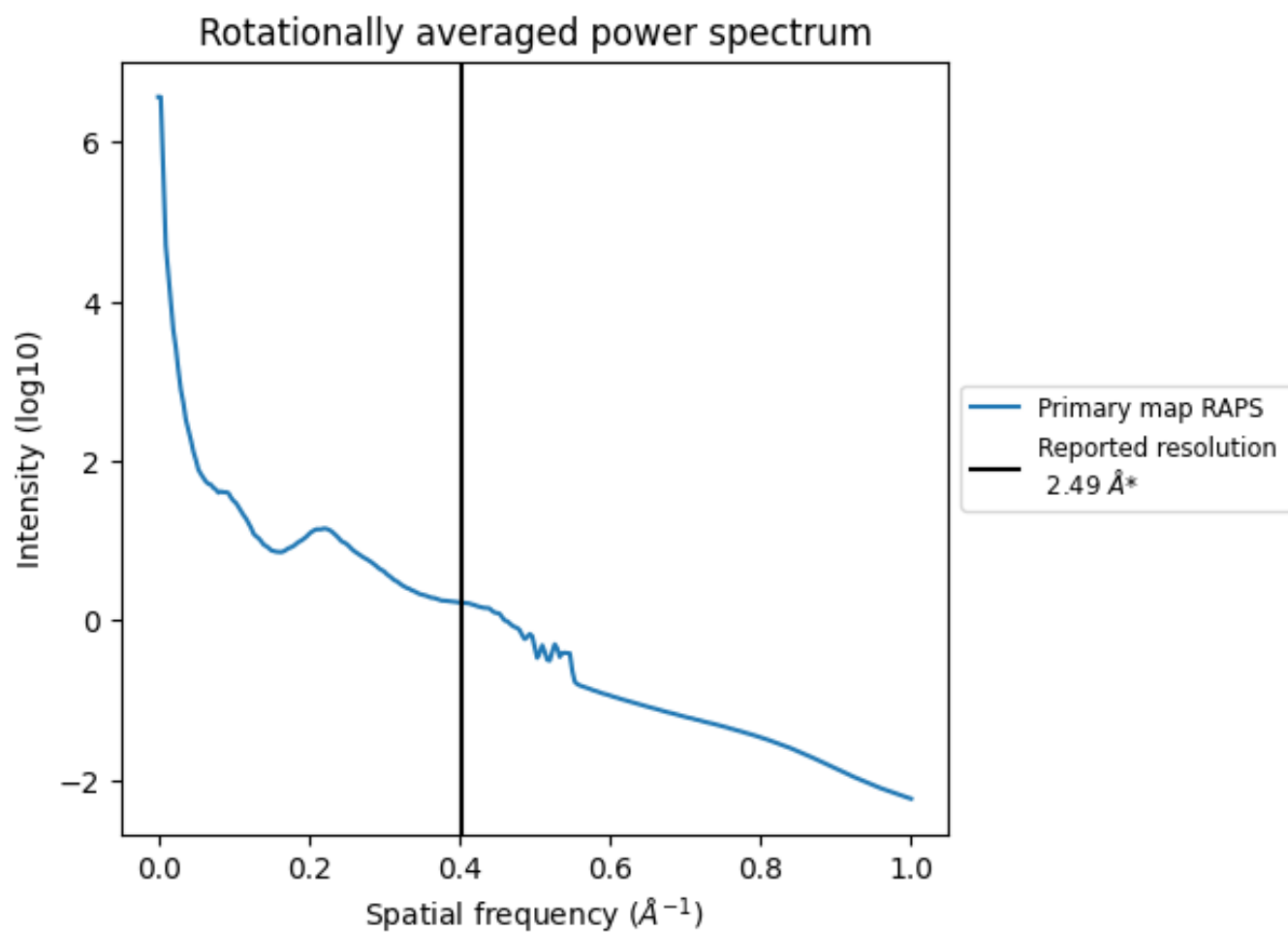
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is  $132 \text{ nm}^3$ ; this corresponds to an approximate mass of 119 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 0.402 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

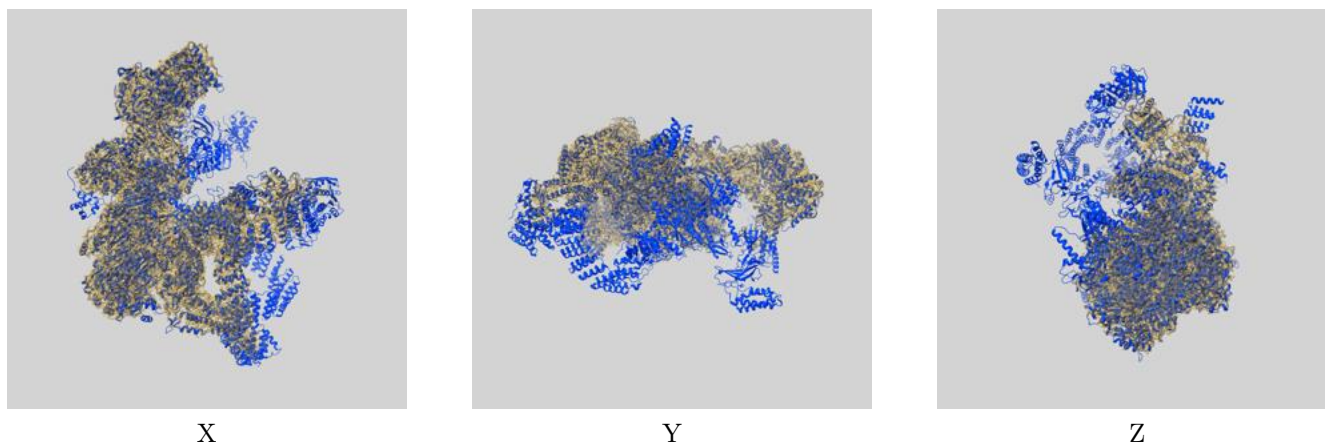
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

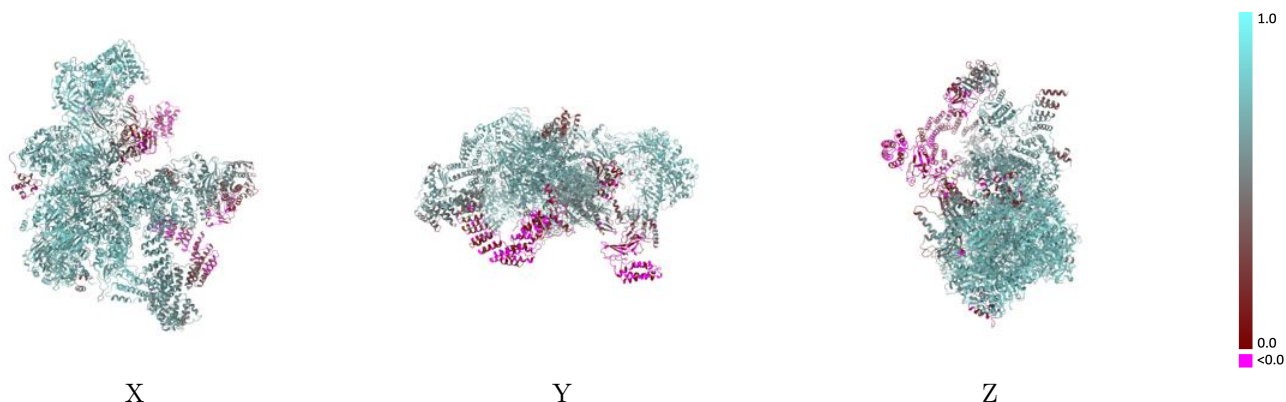
This section contains information regarding the fit between EMDB map EMD-18935 and PDB model 8R6S. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)



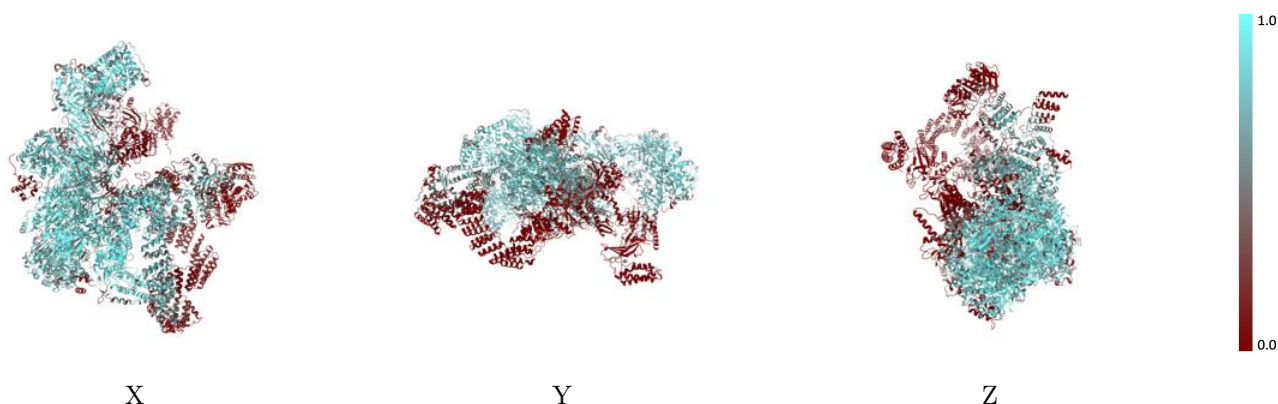
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



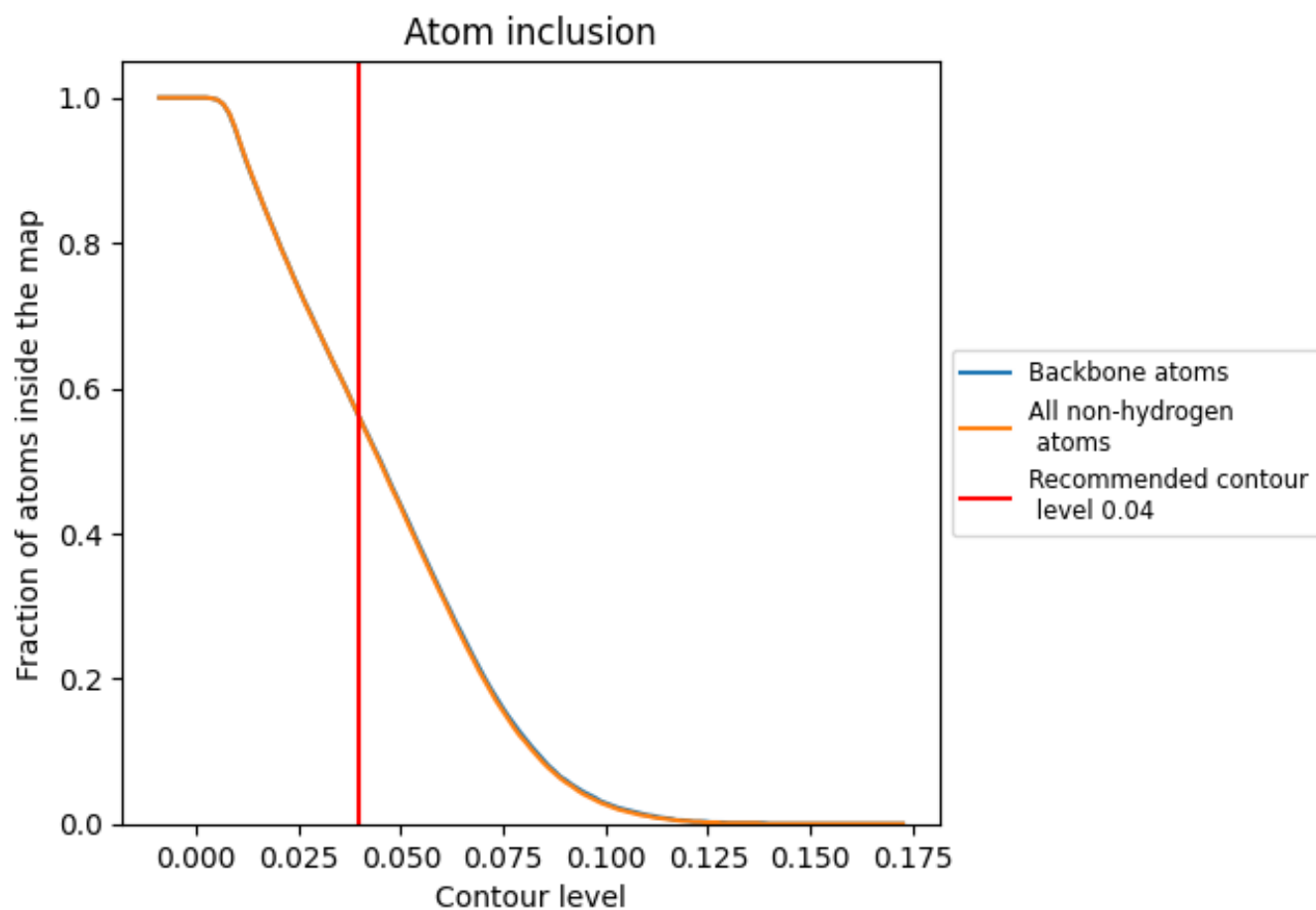
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 56% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5590	 0.6030
A	 0.7100	 0.6970
B	 0.5840	 0.5800
C	 0.5160	 0.5900
D	 0.6150	 0.6510
E	 0.5840	 0.6060
F	 0.5610	 0.6250
G	 0.1060	 0.3550
H	 0.5420	 0.6210
I	 0.8260	 0.7430
J	 0.8240	 0.7410
K	 0.7920	 0.7240
L	 0.8130	 0.7120
M	 0.7980	 0.7110
N	 0.7080	 0.6890
O	 0.6940	 0.7100
P	 0.6350	 0.6800
Q	 0.2160	 0.4070
R	 0.6550	 0.6650
S	 0.7870	 0.7250
T	 0.7270	 0.7140
U	 0.0000	 -0.0200

