Full wwPDB EM Validation Report ⓘ

Mar 5, 2024 – 01:34 pm GMT

PDB ID	:	8R5O
EMDB ID	:	EMD-18935
Title	:	Plastid-encoded RNA polymerase
Authors	:	Webster, M.W.; Pramanick, I.; Vergara-Cruces, A.
Deposited on	:	2023-11-17
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*
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:

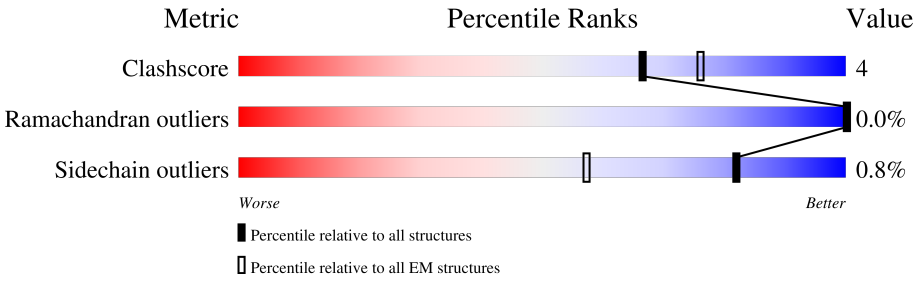
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 >=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 <=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	18% 79% 13% • 8%
1	B	327	8% 59% 7% 34%
2	C	1072	9% 52% 8% 40%
3	D	680	21% 69% 11% 20%
4	E	1373	13% 57% 9% 34%
5	F	911	13% 52% 7% 41%
6	G	862	36% 38% 6% 55%
7	H	675	16% 59% 6% 35%

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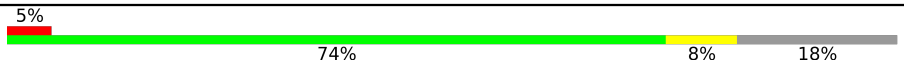
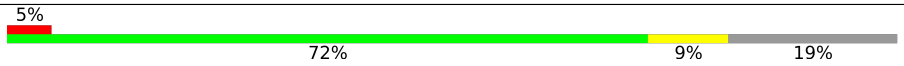
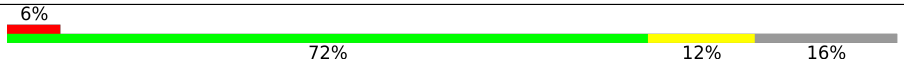
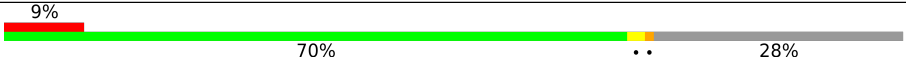
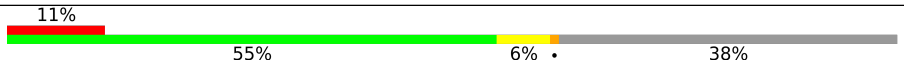
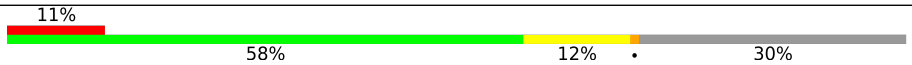
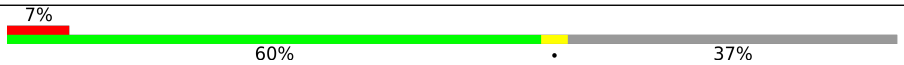
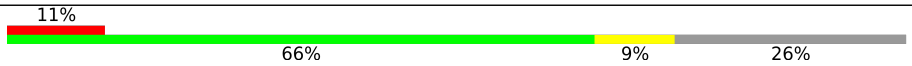
Mol	Chain	Length	Quality of chain
8	I	263	
9	J	529	
10	K	460	
11	L	483	
12	M	334	
13	N	297	
14	O	185	
14	P	185	
15	Q	768	
16	R	162	
17	S	611	
18	T	140	

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 54473 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
1	A	301	Total	C	N	O	S	0	0
			2449	1571	422	446	10		
1	B	216	Total	C	N	O	S	0	0
			1722	1091	302	321	8		

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
2	C	647	Total	C	N	O	S	0	0
			5170	3304	897	948	21		

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
3	D	545	Total	C	N	O	S	0	0
			4468	2884	782	780	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	912	Total	C	N	O	S	0	0
			7308	4683	1294	1305	26		

- Molecule 5 is a protein called PAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	537	Total	C	N	O	S	0	0
			4338	2750	760	801	27		

- Molecule 6 is a protein called PAP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	385	Total	C	N	O	S	0	0
			3040	1918	518	583	21		

- Molecule 7 is a protein called PAP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	440	Total	C	N	O	S	0	0
			3701	2369	643	676	13		

- 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	374	Total	C	N	O	S	0	0
			3022	1933	510	564	15		

- Molecule 11 is a protein called PAP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	408	Total	C	N	O	S	0	0
			3348	2153	572	603	20		

- Molecule 12 is a protein called PAP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	204	Total	C	N	O	S	0	0
			1714	1085	299	323	7		

- Molecule 13 is a protein called PAP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	215	Total	C	N	O	S	0	0
			1759	1132	300	323	4		

- Molecule 14 is a protein called PAP10.

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

- Molecule 15 is a protein called PAP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	220	Total	C	N	O	S	0	0
			1740	1082	307	341	10		

- Molecule 16 is a protein called PAP12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	114	Total	C	N	O	S	0	0
			944	596	167	178	3		

- Molecule 17 is a protein called FLN2.

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

- 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		

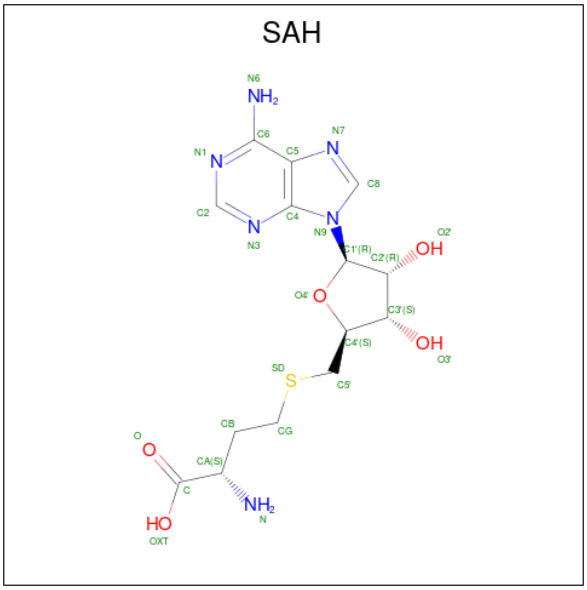
- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 20 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 21 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is water.

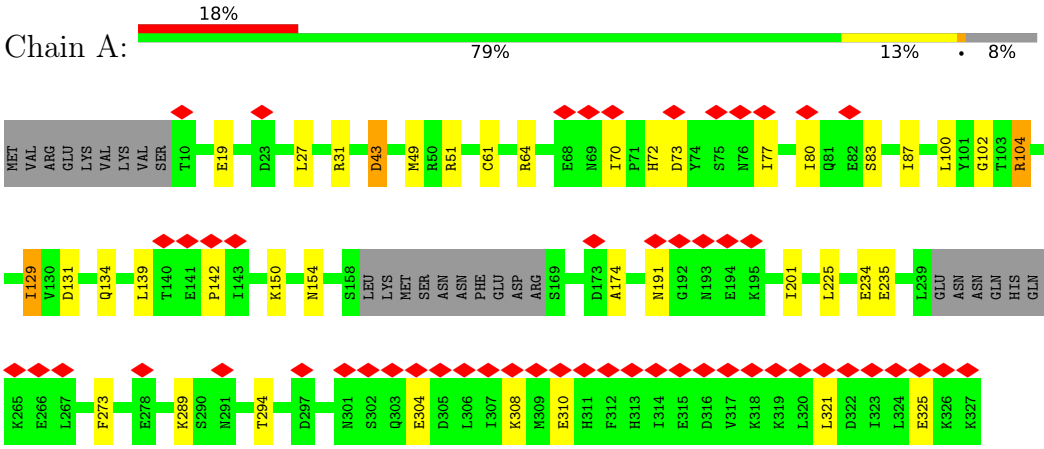
Mol	Chain	Residues	Atoms	AltConf
22	A	18	Total O 18 18	0
22	B	12	Total O 12 12	0
22	C	57	Total O 57 57	0
22	D	19	Total O 19 19	0
22	E	25	Total O 25 25	0
22	F	2	Total O 2 2	0
22	H	6	Total O 6 6	0
22	I	4	Total O 4 4	0
22	J	31	Total O 31 31	0
22	K	16	Total O 16 16	0
22	L	19	Total O 19 19	0
22	M	14	Total O 14 14	0
22	N	3	Total O 3 3	0
22	O	2	Total O 2 2	0
22	P	2	Total O 2 2	0
22	R	2	Total O 2 2	0
22	S	23	Total O 23 23	0

3 Residue-property plots (i)

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.

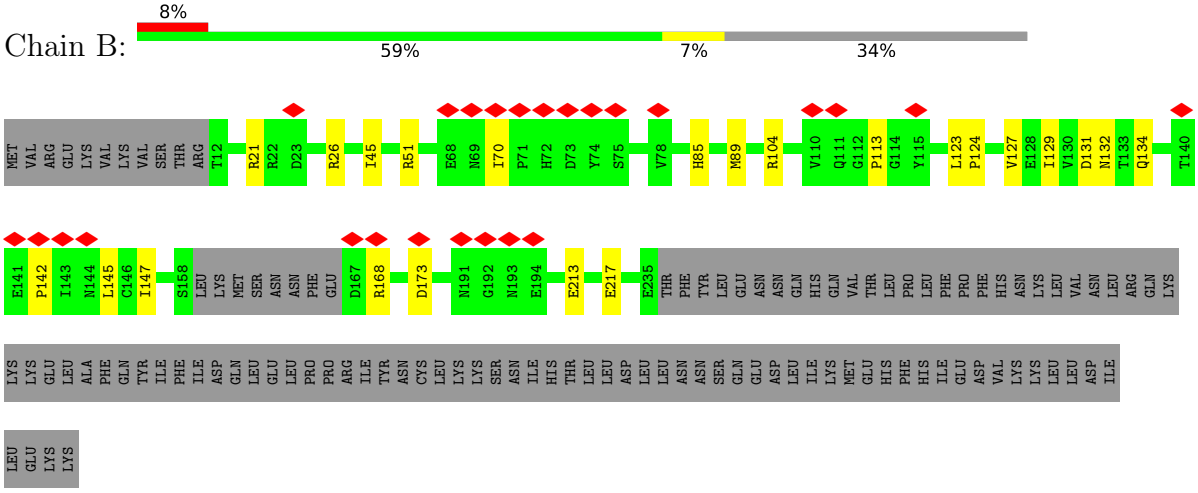
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



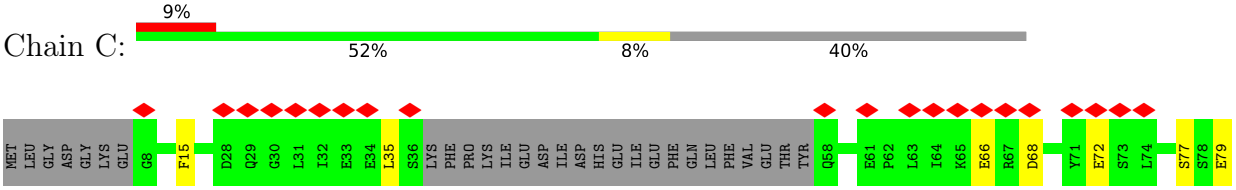
• Molecule 1: DNA-directed RNA polymerase subunit alpha

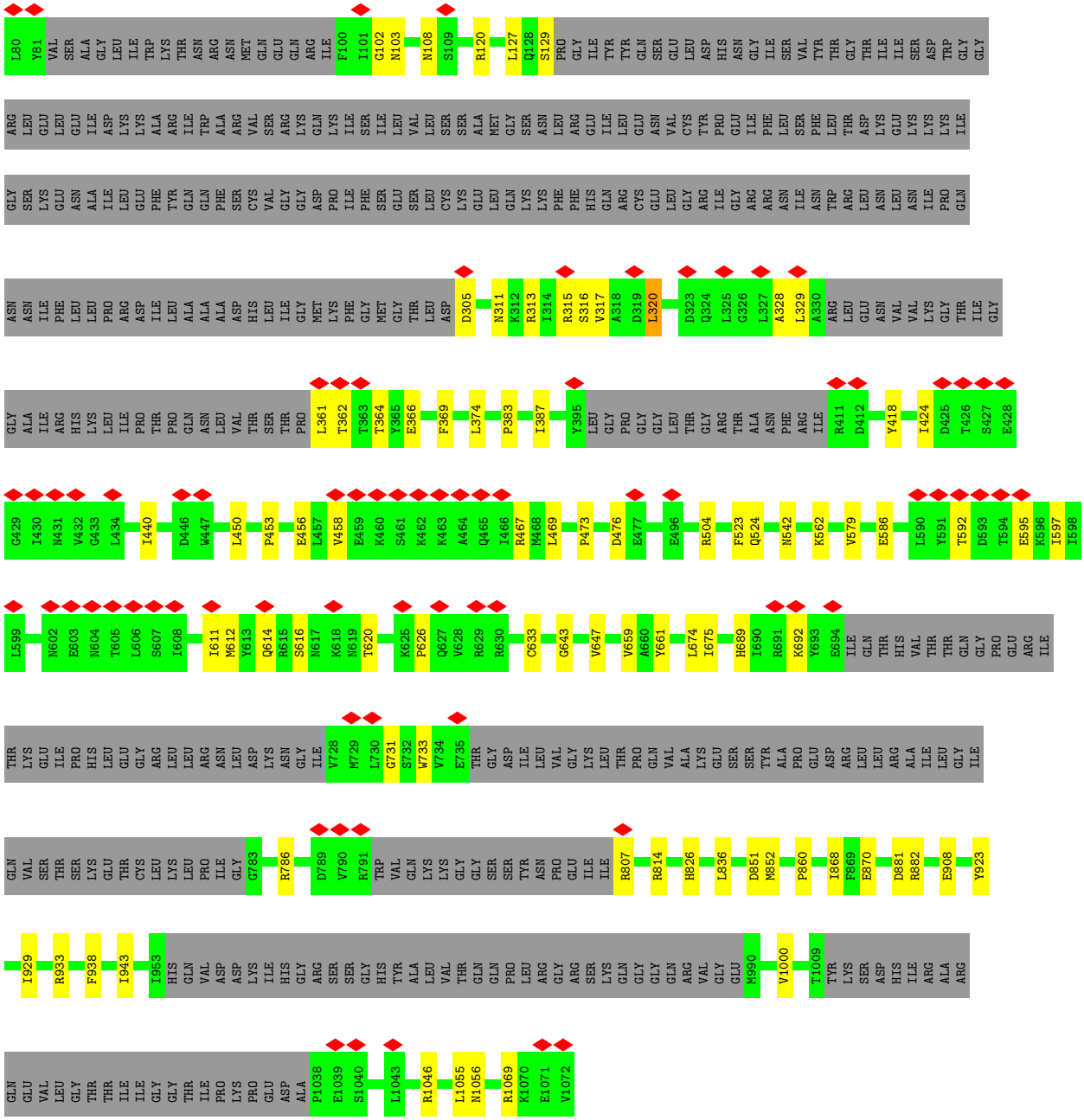
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

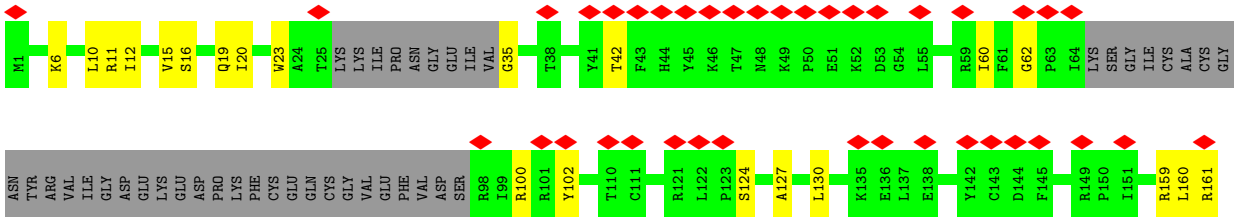
Chain C:

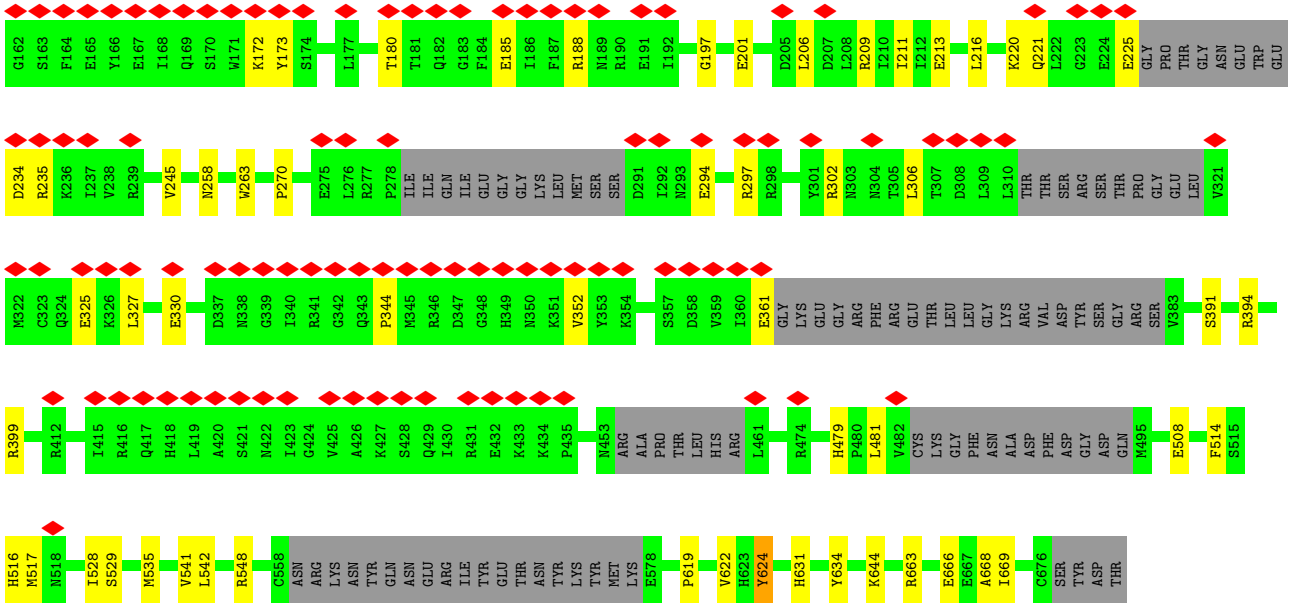




• Molecule 3: DNA-directed RNA polymerase subunit beta'

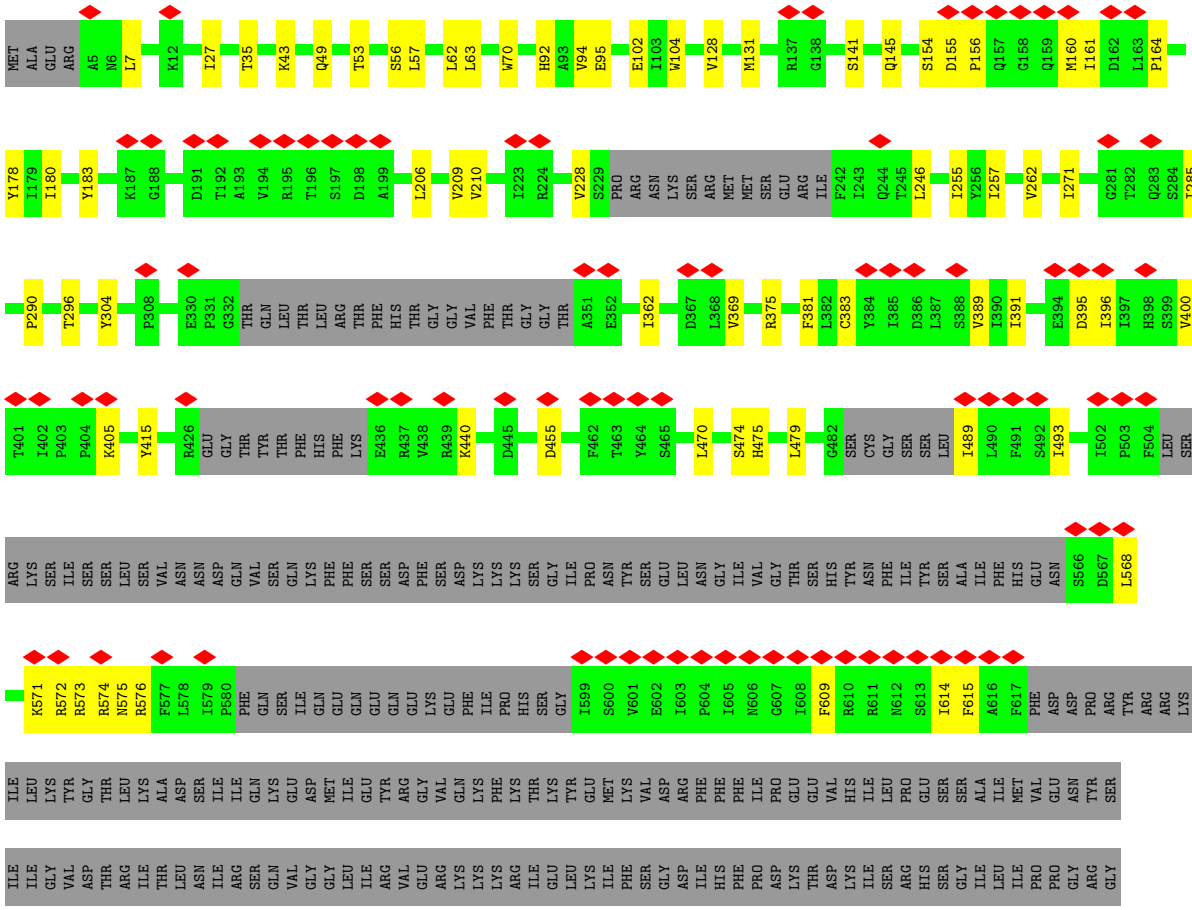
Chain D:

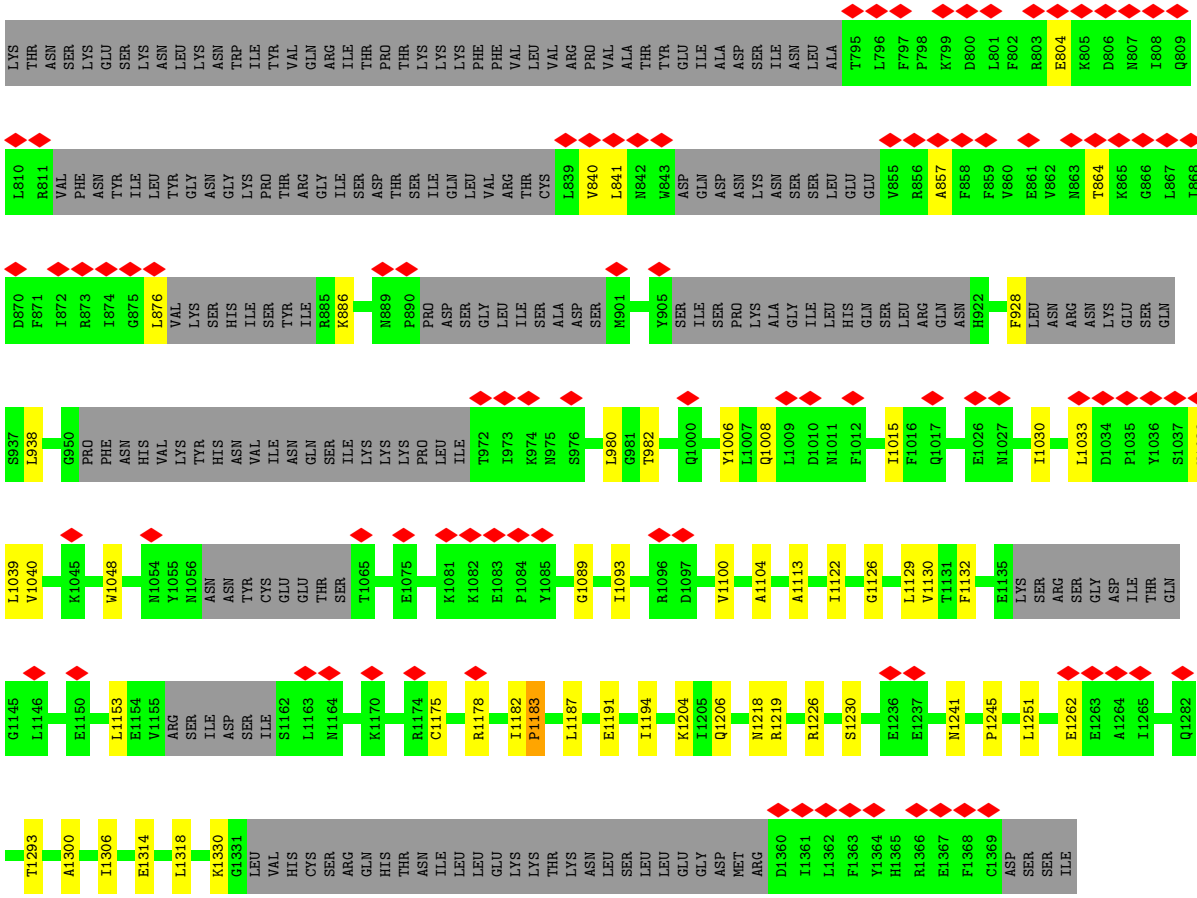




• Molecule 4: DNA-directed RNA polymerase subunit beta"

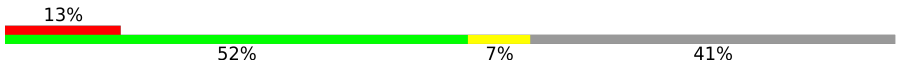
Chain E:

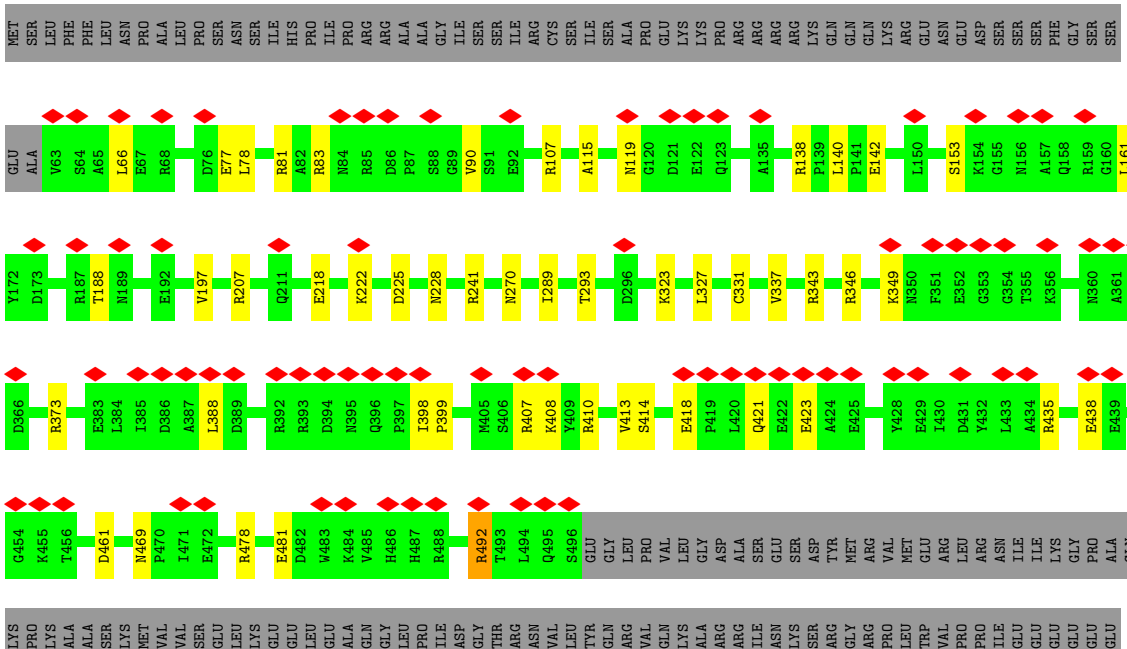


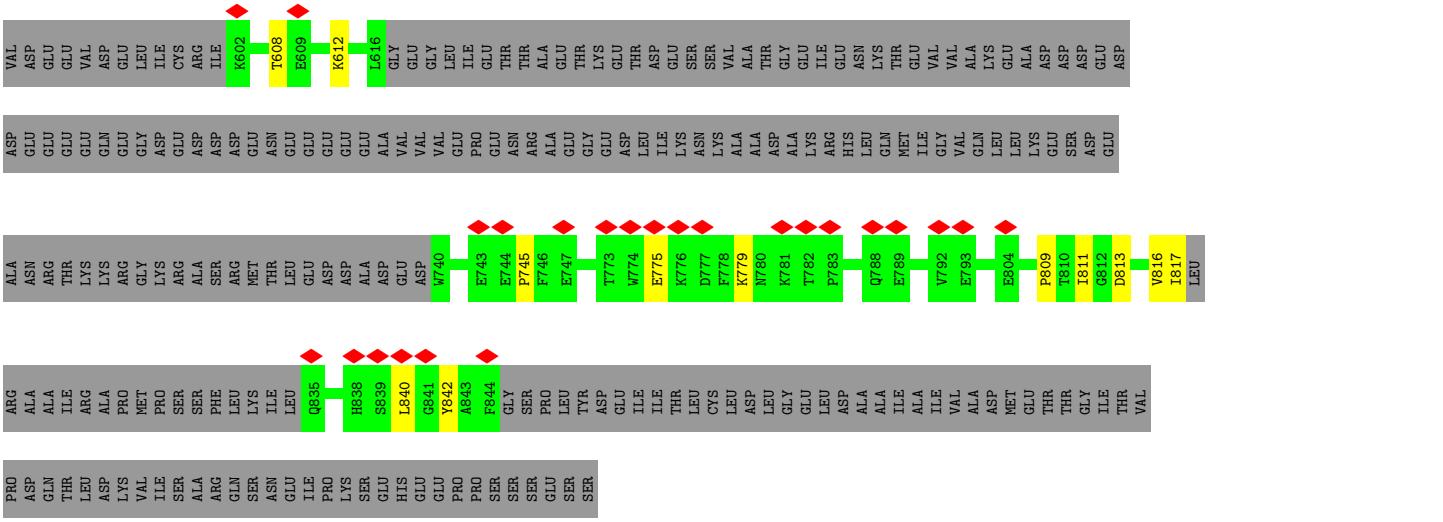


• Molecule 5: PAP1

Chain F:

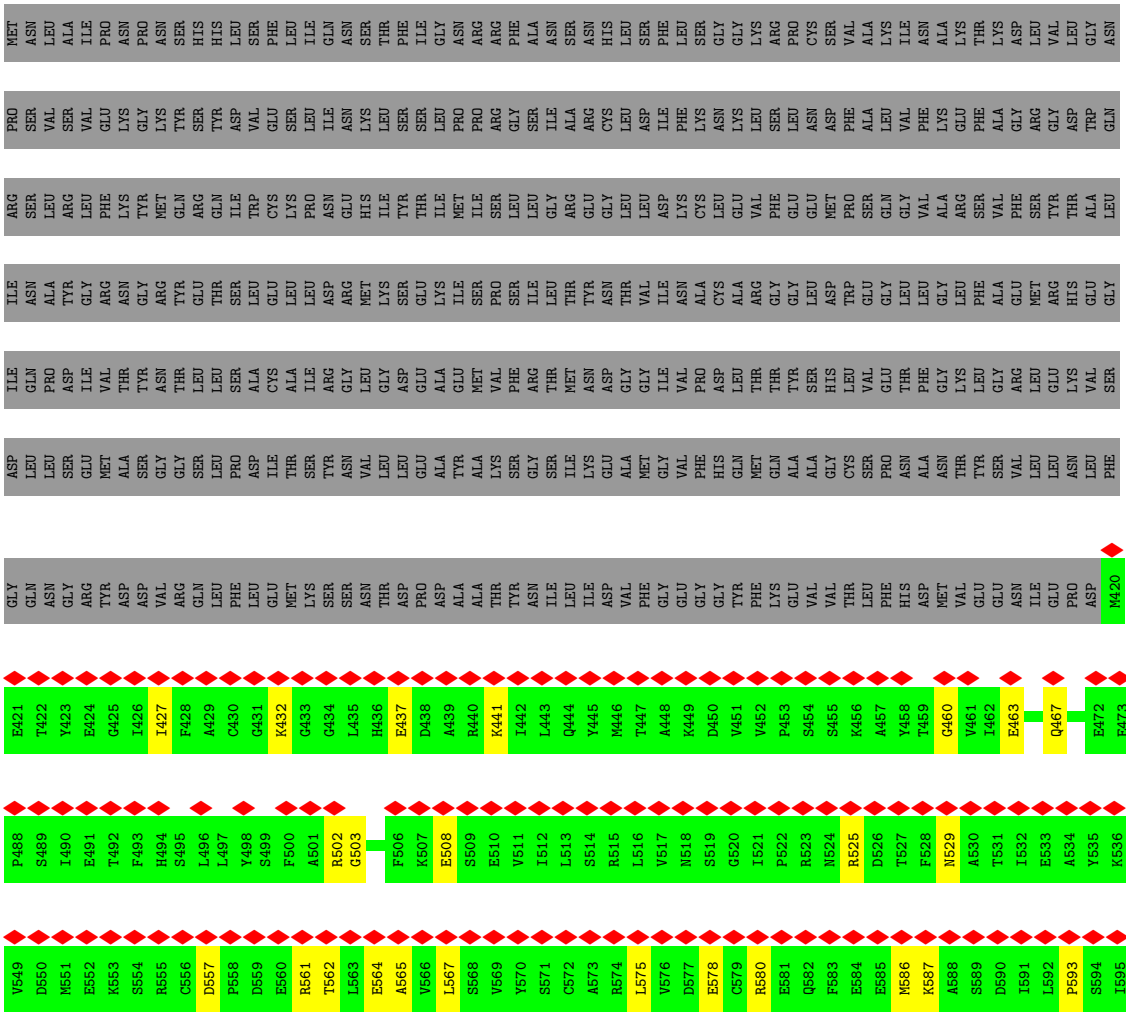


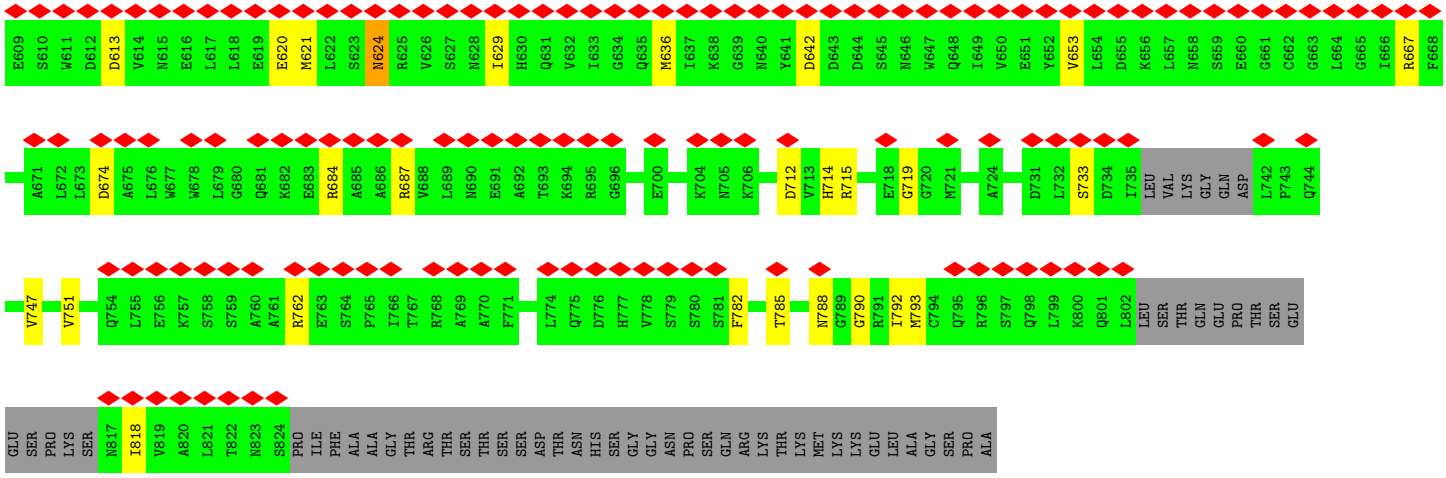




- Molecule 6: PAP2

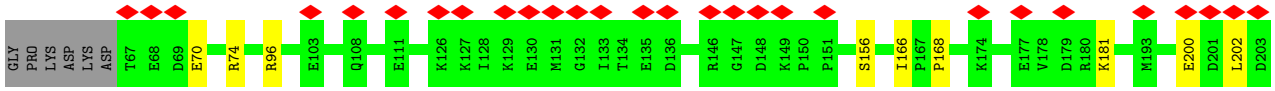
Chain G:

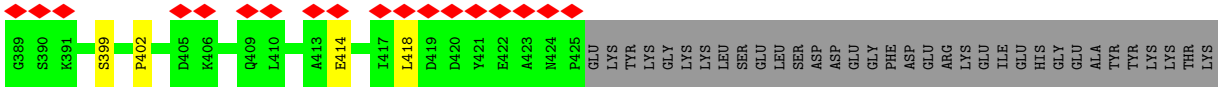


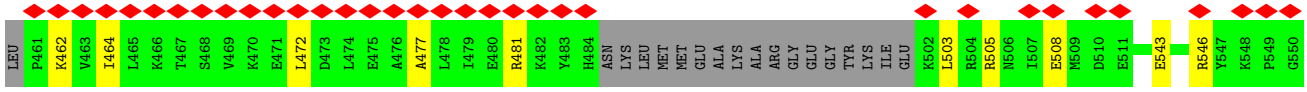


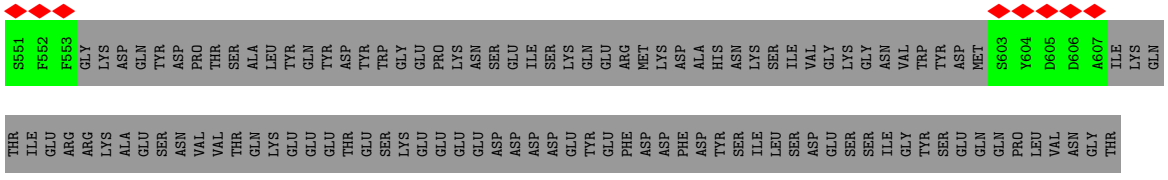
• Molecule 7: PAP3

Chain H:



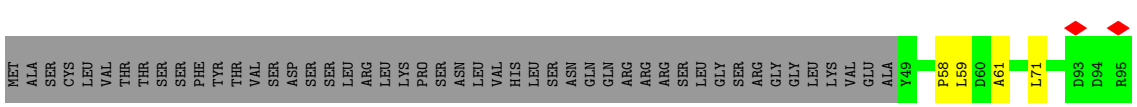


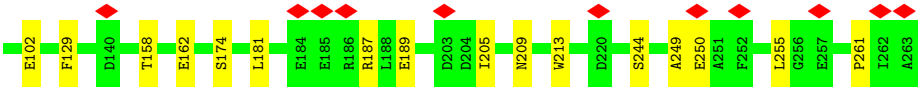




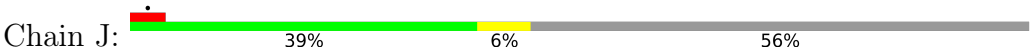
• Molecule 8: PAP4

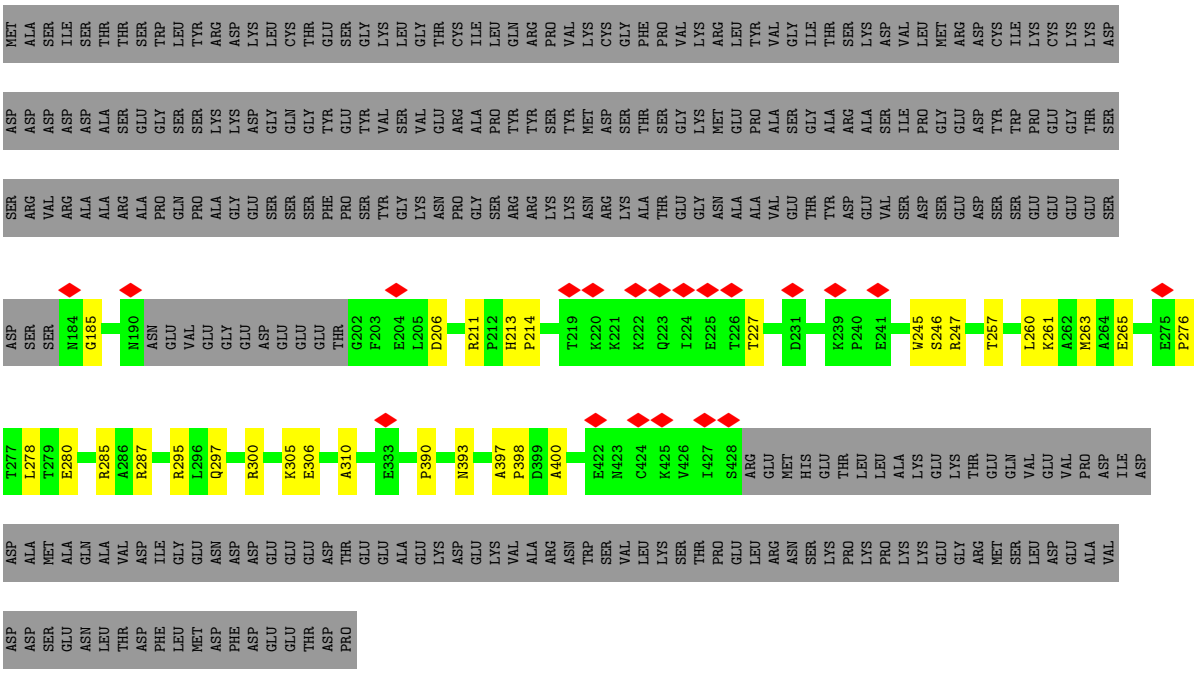
Chain I:



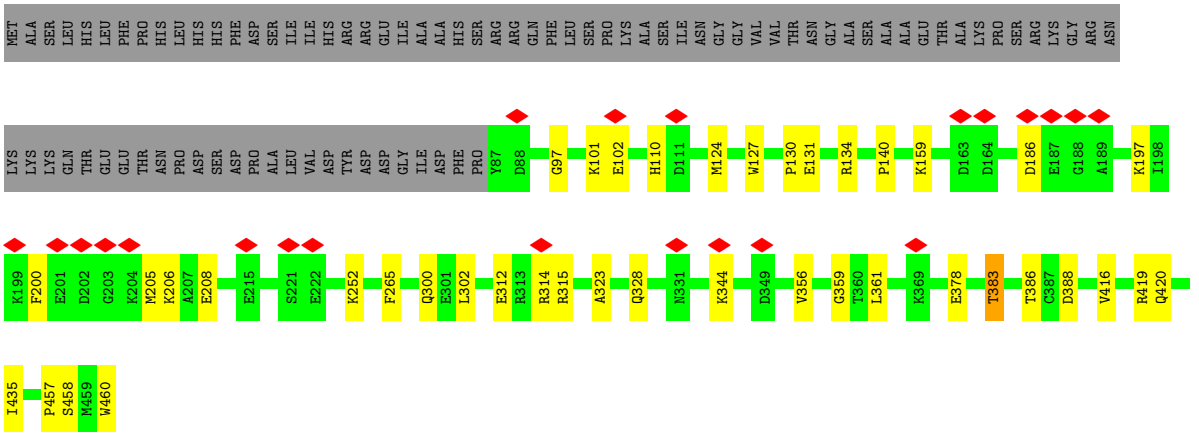


• Molecule 9: PAP5

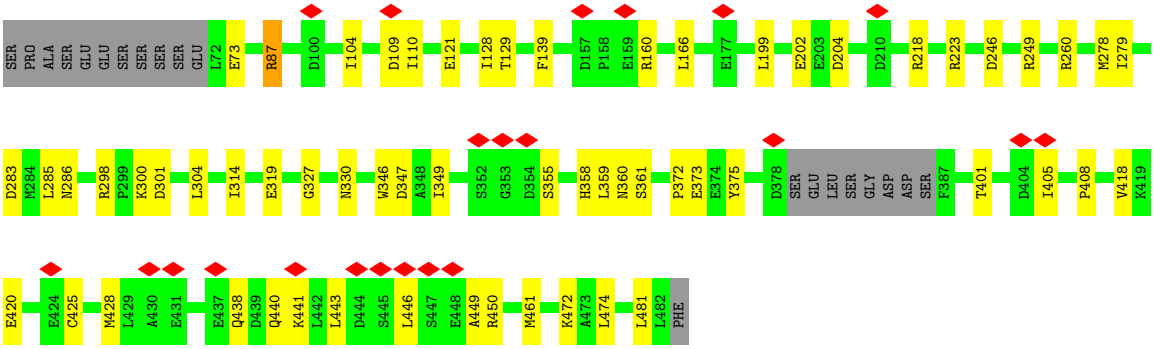




• Molecule 10: PAP6

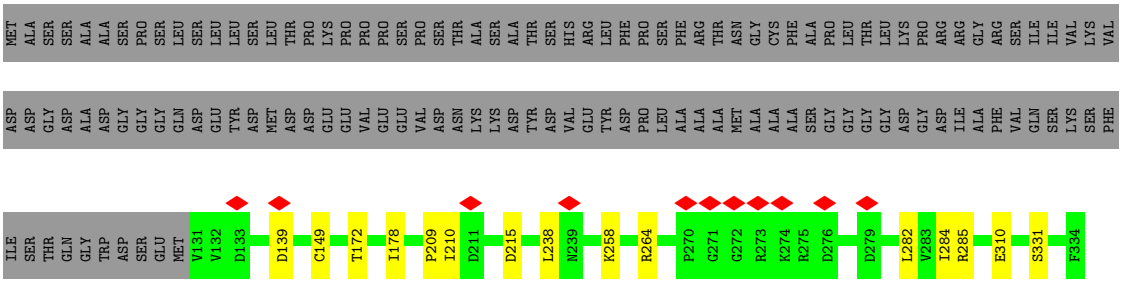


• Molecule 11: PAP7



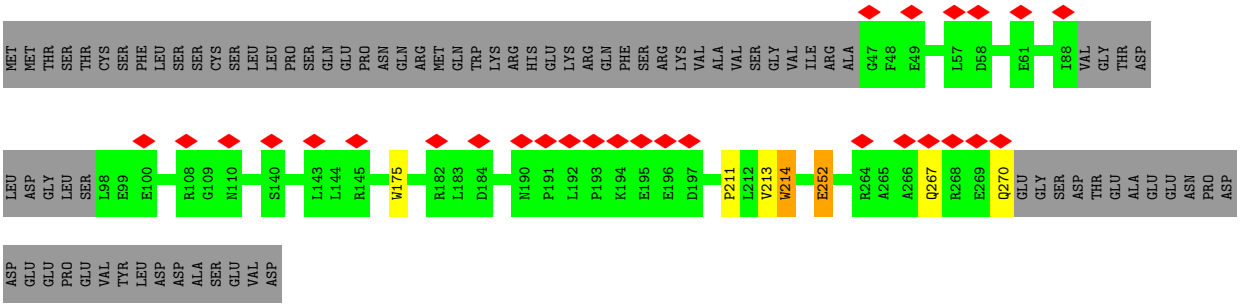
• Molecule 12: PAP8

Chain M:



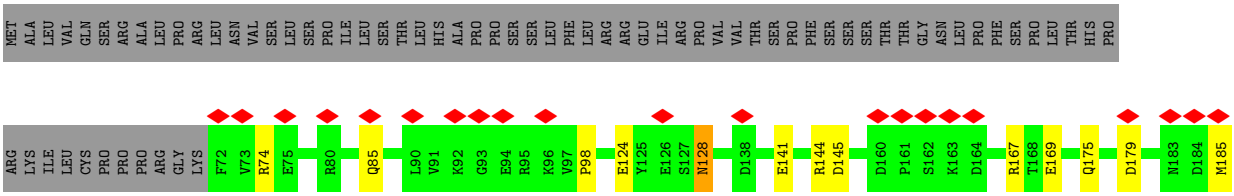
• Molecule 13: PAP9

Chain N:



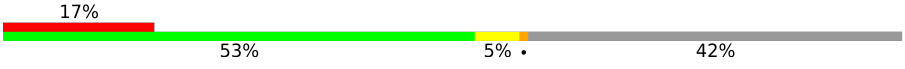
• Molecule 14: PAP10

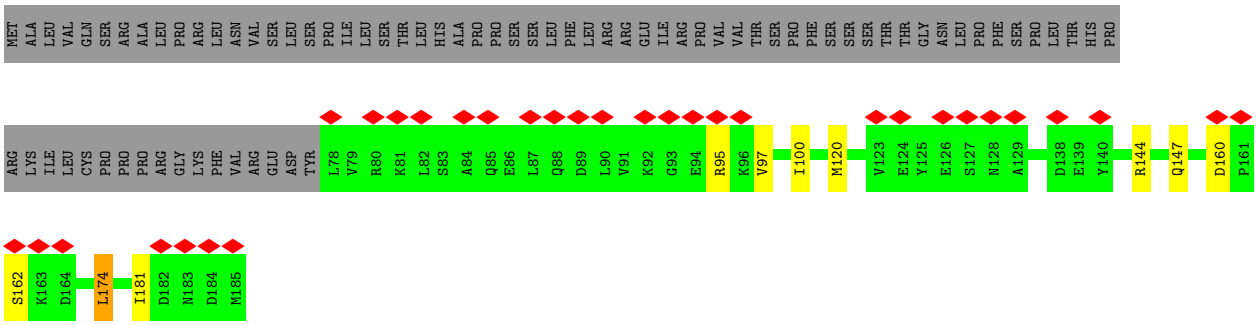
Chain O:



• Molecule 14: PAP10

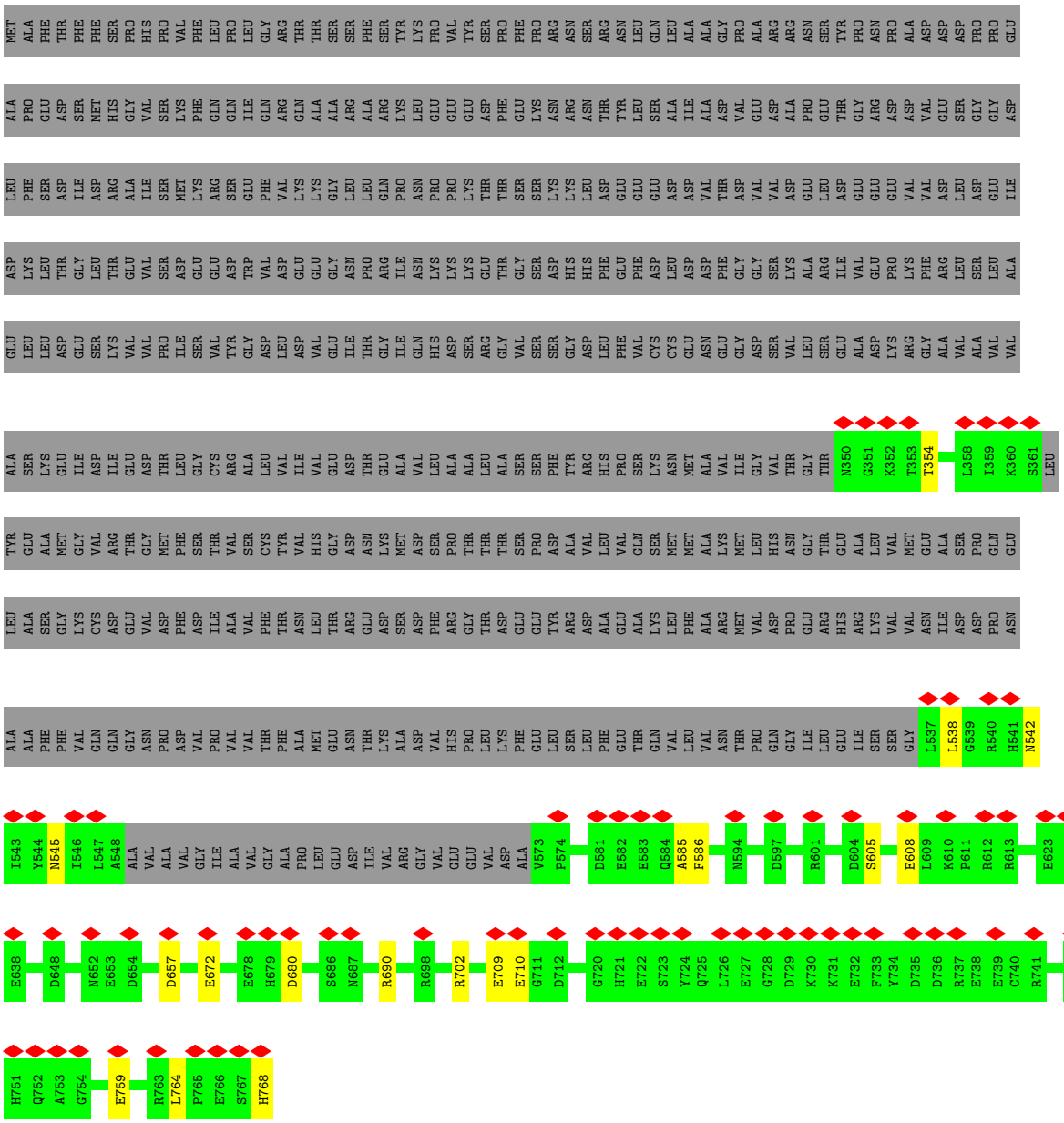
Chain P:





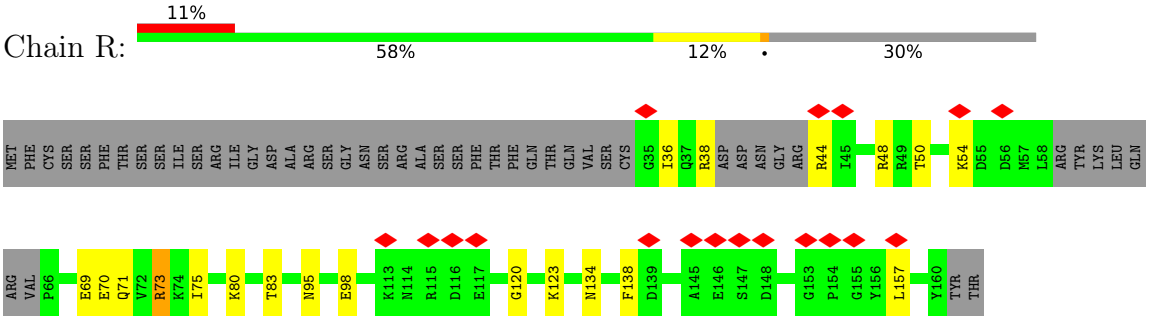
• Molecule 15: PAP11

Chain Q:



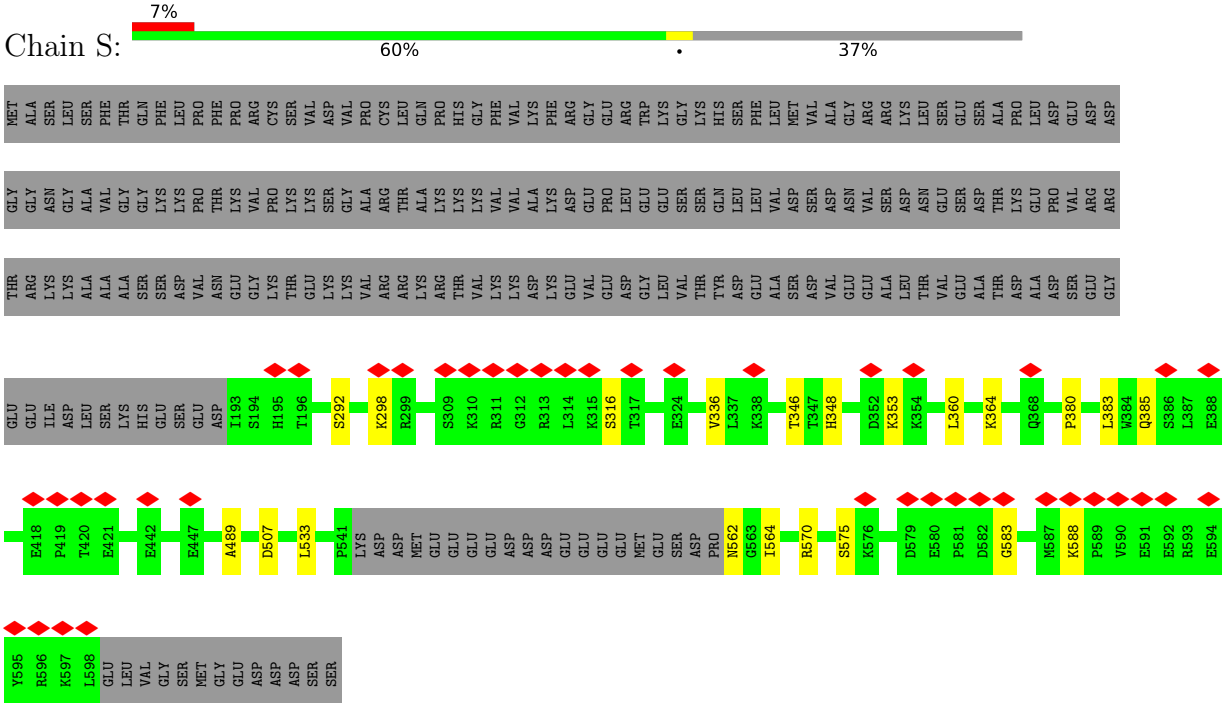
• Molecule 16: PAP12

Chain R:



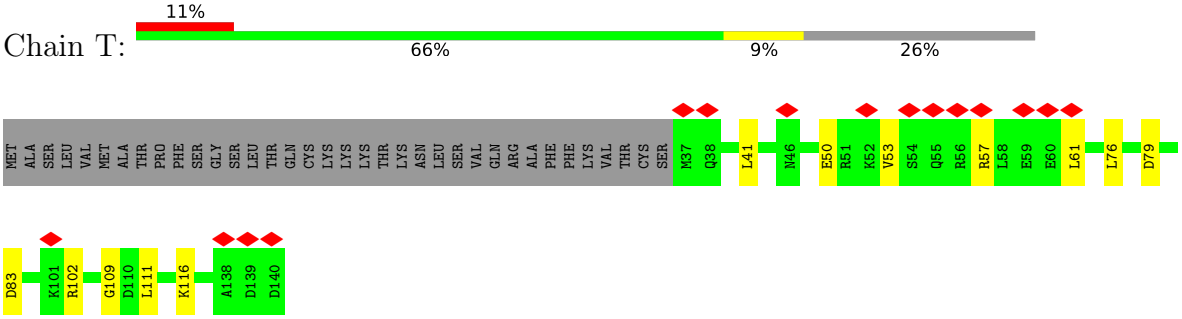
• Molecule 17: FLN2

Chain S:



• Molecule 18: PTAC18

Chain T:



4 Experimental information (i)

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 ($e^-/Å^2$)	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, FE, ZN

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	0.24	0/2498	0.47	0/3377
1	B	0.25	0/1755	0.50	0/2378
2	C	0.25	0/5271	0.48	0/7108
3	D	0.24	0/4566	0.48	0/6171
4	E	0.25	0/7449	0.49	0/10057
5	F	0.24	0/4433	0.46	0/5986
6	G	0.24	0/3095	0.44	0/4175
7	H	0.24	0/3809	0.47	0/5147
8	I	0.25	0/1825	0.46	0/2481
9	J	0.24	0/2021	0.47	0/2724
10	K	0.25	0/3100	0.47	0/4204
11	L	0.25	0/3436	0.46	0/4650
12	M	0.26	0/1756	0.51	0/2378
13	N	0.24	0/1812	0.44	0/2464
14	O	0.24	0/939	0.47	0/1268
14	P	0.24	0/879	0.47	0/1187
15	Q	0.24	0/1771	0.48	0/2392
16	R	0.25	0/960	0.48	0/1285
17	S	0.25	0/3123	0.47	0/4226
18	T	0.25	0/906	0.48	0/1225
All	All	0.24	0/55404	0.47	0/74883

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
5	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	418	GLU	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	26	0
1	B	1722	0	1726	14	0
2	C	5170	0	5183	55	0
3	D	4468	0	4552	55	0
4	E	7308	0	7386	86	0
5	F	4338	0	4265	41	0
6	G	3040	0	2986	29	0
7	H	3701	0	3579	26	0
8	I	1771	0	1696	15	0
9	J	1970	0	1923	19	0
10	K	3022	0	2962	23	0
11	L	3348	0	3302	37	0
12	M	1714	0	1679	11	0
13	N	1759	0	1688	4	0
14	O	923	0	917	8	0
14	P	865	0	867	6	0
15	Q	1740	0	1685	12	0
16	R	944	0	935	13	0
17	S	3056	0	3042	12	0
18	T	881	0	860	8	0
19	E	1	0	0	0	0
20	I	1	0	0	0	0
20	N	1	0	0	0	0
21	L	26	0	19	0	0
22	A	18	0	0	0	0
22	B	12	0	0	0	0
22	C	57	0	0	1	0
22	D	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	E	25	0	0	0	0
22	F	2	0	0	0	0
22	H	6	0	0	0	0
22	I	4	0	0	0	0
22	J	31	0	0	0	0
22	K	16	0	0	0	0
22	L	19	0	0	0	0
22	M	14	0	0	1	0
22	N	3	0	0	0	0
22	O	2	0	0	0	0
22	P	2	0	0	0	0
22	R	2	0	0	0	0
22	S	23	0	0	0	0
All	All	54473	0	53742	426	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 4.

All (426) 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)
11:L:279:ILE:HD13	11:L:304:LEU:HD22	1.74	0.70
4:E:1178:ARG:HA	5:F:492:ARG:HH22	1.56	0.69
1:A:51:ARG:HH21	2:C:933:ARG:HA	1.57	0.69
2:C:692:LYS:HD2	2:C:807:ARG:HD2	1.74	0.69
4:E:206:LEU:HD21	4:E:1153:LEU:HD13	1.75	0.69
4:E:440:LYS:HB3	4:E:1132:PHE:HB2	1.73	0.69
4:E:1182:ILE:HB	4:E:1183:PRO:HD2	1.72	0.69
5:F:138:ARG:NH2	5:F:170:LEU:O	2.25	0.68
11:L:286:ASN:ND2	11:L:319:GLU:OE2	2.25	0.68
14:O:141:GLU:OE1	14:O:144:ARG:NH2	2.27	0.67
17:S:380:PRO:HD2	17:S:383:LEU:HD12	1.77	0.67
4:E:228:VAL:HG21	4:E:246:LEU:HD21	1.77	0.66
4:E:455:ASP:HB2	4:E:474:SER:HB2	1.76	0.66
4:E:1006:TYR:HE2	8:I:250:GLU:HG3	1.62	0.65
5:F:408:LYS:NZ	5:F:421:GLN:O	2.28	0.65
10:K:419:ARG:NH2	10:K:458:SER:O	2.30	0.65
5:F:811:ILE:HD13	5:F:842:TYR:HB3	1.80	0.64
5:F:410:ARG:HD3	5:F:816:VAL:HG21	1.81	0.63
6:G:621:MET:HA	6:G:624:ASN:HD22	1.63	0.63
3:D:624:TYR:HB3	12:M:282:LEU:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:415:TYR:HB2	9:J:227:THR:HG21	1.81	0.62
4:E:493:ILE:O	7:H:380:ARG:NH1	2.33	0.61
8:I:129:PHE:HD2	8:I:209:ASN:HB2	1.65	0.61
10:K:312:GLU:OE1	10:K:315:ARG:NH2	2.33	0.61
9:J:185:GLY:O	12:M:264:ARG:NH1	2.33	0.60
16:R:38:ARG:HG2	16:R:44:ARG:HG2	1.83	0.60
4:E:572:ARG:NH1	4:E:573:ARG:O	2.34	0.60
5:F:346:ARG:HA	5:F:349:LYS:HD3	1.83	0.60
1:B:21:ARG:HH22	16:R:69:GLU:HG2	1.66	0.60
9:J:297:GLN:OE1	9:J:300:ARG:NH1	2.35	0.60
2:C:129:SER:HA	2:C:313:ARG:HD3	1.83	0.60
3:D:294:GLU:OE1	3:D:297:ARG:NH2	2.34	0.60
8:I:187:ARG:NH1	8:I:189:GLU:OE2	2.35	0.60
4:E:209:VAL:HG13	4:E:210:VAL:HG13	1.83	0.59
4:E:479:LEU:HD23	4:E:1104:ALA:HB2	1.84	0.59
5:F:452:ARG:NH2	15:Q:657:ASP:OD1	2.35	0.59
3:D:361:GLU:HG2	4:E:1293:THR:HB	1.84	0.59
2:C:1000:VAL:HG12	3:D:508:GLU:HB3	1.85	0.59
2:C:562:LYS:HG3	2:C:647:VAL:HB	1.85	0.59
4:E:574:ARG:NH1	4:E:804:GLU:OE1	2.36	0.59
14:P:144:ARG:NH1	17:S:385:GLN:HB2	2.17	0.59
1:B:26:ARG:NH1	1:B:131:ASP:OD2	2.36	0.58
1:A:289:LYS:NZ	1:A:310:GLU:OE2	2.29	0.58
8:I:59:LEU:HD22	8:I:71:LEU:HB3	1.85	0.58
10:K:323:ALA:HB1	10:K:328:GLN:HB3	1.84	0.58
4:E:614:ILE:HG12	4:E:840:VAL:HG22	1.85	0.57
5:F:323:LYS:HE2	5:F:327:LEU:HD11	1.86	0.57
5:F:478:ARG:NH1	5:F:481:GLU:OE1	2.36	0.57
11:L:199:LEU:O	11:L:450:ARG:NH2	2.37	0.57
14:O:167:ARG:NH1	14:O:169:GLU:OE2	2.37	0.57
3:D:548:ARG:NH1	12:M:310:GLU:OE2	2.37	0.57
4:E:161:ILE:HD12	4:E:180:ILE:HG23	1.87	0.57
4:E:1262:GLU:OE1	5:F:343:ARG:NH1	2.37	0.57
11:L:330:ASN:ND2	11:L:347:ASP:OD2	2.37	0.57
4:E:982:THR:HB	7:H:166:ILE:HD12	1.86	0.57
11:L:359:LEU:HB2	11:L:401:THR:HB	1.86	0.57
12:M:210:ILE:HG23	12:M:215:ASP:HB2	1.86	0.57
2:C:424:ILE:HD11	4:E:178:TYR:HE2	1.70	0.56
5:F:225:ASP:OD2	5:F:228:ASN:ND2	2.32	0.56
8:I:181:LEU:HD11	8:I:255:LEU:HD21	1.86	0.56
10:K:383:THR:HG1	10:K:386:THR:HG1	1.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:407:ARG:NH1	15:Q:672:GLU:OE2	2.38	0.56
3:D:663:ARG:NH1	3:D:666:GLU:OE1	2.38	0.56
4:E:1006:TYR:CE2	8:I:250:GLU:HG3	2.41	0.56
5:F:388:LEU:HD22	5:F:398:ILE:HD11	1.87	0.56
3:D:221:GLN:NE2	3:D:225:GLU:OE2	2.40	0.55
15:Q:585:ALA:HB1	15:Q:710:GLU:HG3	1.87	0.55
2:C:504:ARG:NH1	4:E:1126:GLY:O	2.39	0.55
2:C:1055:LEU:HD13	3:D:12:ILE:HG23	1.87	0.55
4:E:1194:ILE:HD13	4:E:1251:LEU:HD22	1.88	0.55
11:L:443:LEU:O	16:R:38:ARG:NH2	2.40	0.55
16:R:75:ILE:HG23	16:R:80:LYS:HB2	1.89	0.55
5:F:107:ARG:HG2	5:F:140:LEU:HD11	1.88	0.55
7:H:295:ILE:HD11	7:H:340:LEU:HD13	1.89	0.55
17:S:360:LEU:HD22	17:S:364:LYS:HE2	1.88	0.55
4:E:804:GLU:OE2	7:H:399:SER:N	2.39	0.54
4:E:1033:LEU:HD23	4:E:1039:LEU:HD13	1.89	0.54
7:H:70:GLU:OE1	7:H:74:ARG:NH2	2.40	0.54
10:K:388:ASP:HB2	10:K:435:ILE:HD13	1.90	0.54
4:E:104:TRP:CD1	4:E:164:PRO:HG3	2.43	0.54
9:J:263:MET:SD	9:J:295:ARG:NH2	2.80	0.54
2:C:440:ILE:HD12	2:C:523:PHE:HB3	1.90	0.54
4:E:63:LEU:HD11	9:J:285:ARG:HD2	1.89	0.54
6:G:564:GLU:OE2	6:G:667:ARG:NH1	2.41	0.54
6:G:529:ASN:ND2	6:G:562:THR:OG1	2.39	0.53
1:A:100:LEU:HD13	17:S:575:SER:HB3	1.91	0.53
1:B:113:PRO:HD3	1:B:142:PRO:HA	1.91	0.53
16:R:120:GLY:O	16:R:123:LYS:NZ	2.41	0.53
2:C:1056:ASN:OD1	2:C:1069:ARG:NH1	2.42	0.53
3:D:302:ARG:NH1	3:D:330:GLU:OE1	2.42	0.53
11:L:327:GLY:HA2	11:L:346:TRP:CE2	2.44	0.53
11:L:298:ARG:NH1	11:L:301:ASP:OD2	2.41	0.52
15:Q:690:ARG:NH1	15:Q:759:GLU:OE1	2.35	0.52
17:S:292:SER:HB3	17:S:336:VAL:HG21	1.90	0.52
17:S:583:GLY:O	17:S:588:LYS:NZ	2.42	0.52
2:C:102:GLY:HA3	2:C:361:LEU:HB3	1.92	0.52
3:D:302:ARG:HD3	3:D:327:LEU:HB3	1.91	0.52
6:G:587:LYS:NZ	6:G:620:GLU:OE2	2.42	0.52
3:D:16:SER:HB3	3:D:263:TRP:CZ2	2.45	0.52
11:L:355:SER:OG	11:L:420:GLU:OE1	2.22	0.52
1:A:64:ARG:HG2	1:A:150:LYS:HB2	1.92	0.52
2:C:458:VAL:H	2:C:467:ARG:HH12	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1129:LEU:HG	4:E:1130:VAL:HG23	1.92	0.51
5:F:218:GLU:HG2	5:F:222:LYS:HE2	1.92	0.51
5:F:408:LYS:HB3	5:F:423:GLU:HG2	1.92	0.51
1:A:70:ILE:HD11	1:A:77:ILE:HG12	1.93	0.51
2:C:851:ASP:OD2	22:C:1101:HOH:O	2.18	0.51
4:E:1093:ILE:HB	4:E:1100:VAL:HB	1.92	0.51
5:F:293:THR:HG22	5:F:331:CYS:HB2	1.92	0.51
10:K:124:MET:HG2	10:K:127:TRP:CZ2	2.45	0.51
1:A:234:GLU:HG2	1:A:235:GLU:HG3	1.91	0.51
8:I:58:PRO:HG2	8:I:61:ALA:HB2	1.92	0.51
1:A:102:GLY:O	1:A:104:ARG:NE	2.44	0.51
2:C:929:ILE:HG13	2:C:938:PHE:HD2	1.76	0.51
10:K:131:GLU:OE2	10:K:134:ARG:NH1	2.43	0.51
1:B:124:PRO:HG2	1:B:127:VAL:HG21	1.93	0.51
2:C:633:CYS:SG	14:O:124:GLU:HG2	2.50	0.51
11:L:358:HIS:CE1	11:L:360:ASN:HB2	2.46	0.51
3:D:206:LEU:HD22	3:D:211:ILE:HD11	1.93	0.51
1:A:321:LEU:O	1:A:325:GLU:N	2.39	0.50
2:C:328:ALA:HB2	2:C:364:THR:HG21	1.94	0.50
3:D:185:GLU:OE2	3:D:188:ARG:NH2	2.38	0.50
5:F:107:ARG:NH2	5:F:142:GLU:OE2	2.44	0.50
7:H:543:GLU:OE1	7:H:546:ARG:NH2	2.40	0.50
1:B:123:LEU:HD11	1:B:129:ILE:HD12	1.93	0.50
4:E:1008:GLN:NE2	8:I:244:SER:OG	2.33	0.50
14:P:100:ILE:HD11	14:P:181:ILE:HD11	1.93	0.50
1:A:248:LEU:HD12	17:S:564:ILE:HD13	1.93	0.50
2:C:418:TYR:OH	4:E:183:TYR:OH	2.25	0.50
4:E:575:ASN:HB3	4:E:876:LEU:HB3	1.93	0.50
1:A:73:ASP:N	1:A:73:ASP:OD1	2.39	0.49
1:A:123:LEU:HD11	1:A:129:ILE:HD12	1.94	0.49
3:D:11:ARG:HH12	3:D:258:ASN:HD21	1.59	0.49
3:D:62:GLY:O	3:D:100:ARG:NH1	2.44	0.49
18:T:83:ASP:OD1	18:T:116:LYS:N	2.41	0.49
6:G:712:ASP:OD1	6:G:714:HIS:ND1	2.35	0.49
6:G:762:ARG:NH2	6:G:785:THR:O	2.45	0.49
11:L:129:THR:OG1	11:L:139:PHE:O	2.23	0.49
8:I:129:PHE:CD2	8:I:209:ASN:HB2	2.48	0.49
11:L:246:ASP:OD1	11:L:249:ARG:N	2.44	0.49
2:C:882:ARG:NH2	2:C:908:GLU:OE2	2.46	0.49
2:C:120:ARG:HD2	2:C:369:PHE:HB3	1.94	0.49
2:C:616:SER:OG	2:C:620:THR:OG1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:35:GLY:HA2	3:D:60:ILE:HG23	1.93	0.49
1:A:304:GLU:O	1:A:308:LYS:NZ	2.33	0.48
2:C:674:LEU:HD11	2:C:836:LEU:HG	1.95	0.48
12:M:285:ARG:NH2	22:M:401:HOH:O	2.46	0.48
3:D:669:ILE:HD12	4:E:7:LEU:HD11	1.94	0.48
4:E:928:PHE:HZ	4:E:1122:ILE:HD11	1.78	0.48
5:F:78:LEU:HG	5:F:90:VAL:HG13	1.94	0.48
6:G:751:VAL:HB	6:G:790:GLY:HA3	1.94	0.48
5:F:66:LEU:HD21	6:G:793:MET:HE2	1.94	0.48
1:A:83:SER:O	1:A:87:ILE:HG12	2.14	0.48
2:C:595:GLU:HG2	2:C:612:MET:SD	2.53	0.48
5:F:373:ARG:NH2	5:F:461:ASP:OD2	2.39	0.48
13:N:213:VAL:HG23	13:N:214:TRP:CD1	2.49	0.48
3:D:11:ARG:HB3	4:E:1306:ILE:HG12	1.95	0.47
3:D:306:LEU:HD11	3:D:325:GLU:HG2	1.96	0.47
10:K:159:LYS:HD3	10:K:186:ASP:HB2	1.96	0.47
11:L:372:PRO:HA	11:L:375:TYR:CZ	2.48	0.47
9:J:390:PRO:HG2	9:J:393:ASN:ND2	2.29	0.47
2:C:66:GLU:OE1	2:C:108:ASN:ND2	2.47	0.47
2:C:675:ILE:HG22	2:C:852:MET:HG2	1.96	0.47
5:F:83:ARG:NH1	11:L:408:PRO:O	2.37	0.47
4:E:389:VAL:HB	4:E:400:VAL:HG23	1.97	0.47
1:B:213:GLU:O	1:B:217:GLU:HG2	2.13	0.47
9:J:245:TRP:CH2	9:J:247:ARG:HB2	2.50	0.47
10:K:361:LEU:HD21	10:K:378:GLU:HG2	1.96	0.47
3:D:209:ARG:O	3:D:213:GLU:HG2	2.14	0.47
3:D:216:LEU:HG	3:D:220:LYS:HZ2	1.79	0.47
4:E:57:LEU:HD13	4:E:128:VAL:HG22	1.95	0.47
4:E:470:LEU:HD13	4:E:1113:ALA:HB3	1.96	0.47
11:L:87:ARG:O	11:L:87:ARG:NH1	2.38	0.47
1:A:273:PHE:HA	1:A:294:THR:HA	1.97	0.47
2:C:305:ASP:O	2:C:311:ASN:ND2	2.44	0.47
2:C:320:LEU:HD21	2:C:374:LEU:HD12	1.96	0.47
2:C:689:HIS:CD2	2:C:814:ARG:HD2	2.49	0.47
5:F:289:ILE:O	5:F:293:THR:HG23	2.15	0.47
3:D:481:LEU:HD13	3:D:529:SER:HB3	1.97	0.47
13:N:267:GLN:HG2	13:N:270:GLN:HE21	1.80	0.47
4:E:154:SER:HA	4:E:160:MET:HA	1.97	0.47
5:F:608:THR:HG22	5:F:612:LYS:HD2	1.97	0.47
7:H:462:LYS:HE3	7:H:464:ILE:HD11	1.96	0.47
17:S:489:ALA:HB2	17:S:533:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:20:ILE:HD13	3:D:270:PRO:HD3	1.96	0.46
8:I:158:THR:O	8:I:162:GLU:HG2	2.16	0.46
10:K:110:HIS:CG	10:K:130:PRO:HG3	2.50	0.46
6:G:785:THR:OG1	6:G:788:ASN:O	2.33	0.46
9:J:306:GLU:HB3	9:J:310:ALA:HB3	1.98	0.46
4:E:1175:CYS:SG	5:F:745:PRO:HG3	2.55	0.46
2:C:733:TRP:HB2	2:C:786:ARG:NH2	2.31	0.46
4:E:304:TYR:O	4:E:1219:ARG:HD3	2.16	0.46
11:L:298:ARG:HD2	11:L:301:ASP:OD1	2.15	0.46
3:D:542:LEU:HD13	4:E:49:GLN:HG3	1.98	0.46
11:L:418:VAL:HG13	11:L:474:LEU:HB3	1.96	0.46
14:P:147:GLN:HG2	17:S:316:SER:OG	2.16	0.46
1:A:61:CYS:SG	1:A:174:ALA:HB1	2.56	0.46
4:E:568:LEU:HD13	7:H:503:LEU:HG	1.98	0.46
1:B:70:ILE:HA	1:B:168:ARG:HH22	1.80	0.45
2:C:860:PRO:HG2	4:E:131:MET:SD	2.56	0.45
17:S:346:THR:HG23	17:S:348:HIS:H	1.81	0.45
3:D:12:ILE:HD11	4:E:1300:ALA:HB3	1.97	0.45
4:E:475:HIS:ND1	7:H:96:ARG:HD2	2.31	0.45
4:E:573:ARG:HB2	4:E:576:ARG:HG3	1.98	0.45
5:F:413:VAL:HG12	5:F:817:ILE:HD11	1.97	0.45
15:Q:586:PHE:HB3	15:Q:709:GLU:O	2.16	0.45
2:C:1046:ARG:NH2	3:D:102:TYR:HB3	2.32	0.45
4:E:1030:ILE:HD13	7:H:202:LEU:HD23	1.98	0.45
10:K:383:THR:OG1	10:K:386:THR:OG1	2.20	0.45
2:C:383:PRO:HG3	2:C:579:VAL:HG21	1.98	0.45
2:C:453:PRO:O	2:C:524:GLN:NE2	2.49	0.45
4:E:1206:GLN:NE2	4:E:1218:ASN:OD1	2.43	0.45
2:C:450:LEU:O	2:C:473:PRO:HD3	2.16	0.45
2:C:733:TRP:HB2	2:C:786:ARG:HH21	1.80	0.45
11:L:121:GLU:OE2	11:L:298:ARG:NH2	2.43	0.45
11:L:260:ARG:HD3	11:L:283:ASP:HB2	1.98	0.45
2:C:611:ILE:HG23	2:C:614:GLN:HG3	1.99	0.45
4:E:1033:LEU:HD22	4:E:1048:TRP:CG	2.52	0.45
1:A:80:ILE:HG12	1:A:139:LEU:HD23	1.99	0.45
3:D:344:PRO:HB2	3:D:352:VAL:HG13	1.99	0.45
4:E:27:ILE:HG13	4:E:35:THR:HG21	1.98	0.45
4:E:271:ILE:HG21	12:M:209:PRO:HB2	1.99	0.45
4:E:395:ASP:OD1	4:E:395:ASP:N	2.45	0.45
5:F:153:SER:HA	5:F:188:THR:HG21	1.98	0.45
7:H:200:GLU:O	7:H:204:LYS:NZ	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:10:LEU:HD23	4:E:1318:LEU:HD21	1.97	0.45
3:D:159:ARG:NH2	15:Q:680:ASP:OD1	2.50	0.45
3:D:528:ILE:HG13	3:D:529:SER:N	2.32	0.45
4:E:1314:GLU:OE1	4:E:1314:GLU:N	2.34	0.45
7:H:414:GLU:HG3	7:H:472:LEU:HD22	1.98	0.45
2:C:316:SER:OG	2:C:317:VAL:N	2.50	0.45
6:G:508:GLU:N	6:G:508:GLU:OE1	2.50	0.45
7:H:334:TYR:CZ	7:H:365:ARG:HD3	2.52	0.45
9:J:397:ALA:HB3	9:J:400:ALA:HB2	1.98	0.45
11:L:128:ILE:HB	11:L:278:MET:HB2	1.99	0.45
9:J:246:SER:O	9:J:247:ARG:HB3	2.17	0.45
17:S:353:LYS:HA	17:S:353:LYS:HD2	1.83	0.45
7:H:418:LEU:HD13	7:H:481:ARG:HB2	1.99	0.44
3:D:668:ALA:HA	16:R:71:GLN:OE1	2.16	0.44
4:E:296:THR:HG21	4:E:1230:SER:HB2	1.98	0.44
3:D:42:THR:HG23	3:D:297:ARG:HD3	1.99	0.44
3:D:644:LYS:NZ	12:M:238:LEU:O	2.50	0.44
4:E:383:CYS:O	4:E:405:LYS:N	2.50	0.44
7:H:505:ARG:NH1	7:H:508:GLU:OE1	2.51	0.44
2:C:68:ASP:O	2:C:72:GLU:HG2	2.18	0.44
4:E:1187:LEU:O	4:E:1191:GLU:HG2	2.18	0.44
14:P:120:MET:HG2	14:P:174:LEU:HD11	1.99	0.44
2:C:456:GLU:HB2	2:C:469:LEU:HD22	1.99	0.44
3:D:391:SER:HB2	3:D:394:ARG:HG3	1.99	0.44
11:L:425:CYS:HA	11:L:428:MET:HE2	1.98	0.44
3:D:245:VAL:HG21	4:E:1245:PRO:HG2	1.99	0.44
6:G:463:GLU:O	6:G:467:GLN:HG2	2.17	0.44
1:B:131:ASP:HB3	1:B:134:GLN:HG3	2.00	0.44
3:D:197:GLY:O	3:D:201:GLU:HG2	2.18	0.44
1:B:85:HIS:O	1:B:89:MET:HG2	2.18	0.44
2:C:943:ILE:HG22	4:E:56:SER:OG	2.17	0.44
3:D:15:VAL:HG21	3:D:23:TRP:HH2	1.82	0.44
3:D:541:VAL:HG11	4:E:53:THR:HG21	1.99	0.44
4:E:62:LEU:HD23	4:E:128:VAL:HG21	1.97	0.44
4:E:362:ILE:HD13	4:E:391:ILE:HG12	2.00	0.44
6:G:629:ILE:HG22	6:G:653:VAL:HG13	1.99	0.44
2:C:15:PHE:HB2	2:C:387:ILE:HD11	2.00	0.44
2:C:586:GLU:OE2	14:O:74:ARG:NH2	2.40	0.44
4:E:155:ASP:HB2	4:E:156:PRO:HD2	1.98	0.44
8:I:174:SER:HB3	8:I:213:TRP:CE2	2.52	0.44
4:E:980:LEU:HD22	4:E:1040:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:503:GLY:HA2	6:G:715:ARG:HG2	1.99	0.43
1:B:145:LEU:HD21	1:B:147:ILE:HD11	2.01	0.43
4:E:102:GLU:OE1	4:E:375:ARG:NH2	2.45	0.43
5:F:83:ARG:HG2	11:L:408:PRO:HD2	2.00	0.43
7:H:402:PRO:HG3	18:T:76:LEU:HD13	2.00	0.43
9:J:206:ASP:OD1	9:J:211:ARG:NH2	2.50	0.43
10:K:206:LYS:HG2	14:O:145:ASP:HB3	1.99	0.43
11:L:73:GLU:OE2	16:R:48:ARG:NH2	2.37	0.43
11:L:104:ILE:HD12	11:L:285:LEU:HG	2.00	0.43
15:Q:605:SER:O	15:Q:608:GLU:HG2	2.18	0.43
6:G:437:GLU:O	6:G:441:LYS:HG2	2.18	0.43
9:J:257:THR:HG23	9:J:276:PRO:HG2	2.00	0.43
4:E:92:HIS:CE1	4:E:94:VAL:HB	2.53	0.43
5:F:115:ALA:O	5:F:119:ASN:ND2	2.47	0.43
6:G:525:ARG:HD3	6:G:557:ASP:O	2.18	0.43
12:M:149:CYS:HB3	12:M:258:LYS:HE2	2.01	0.43
2:C:597:ILE:HD11	2:C:626:PRO:HB3	1.99	0.43
5:F:414:SER:OG	5:F:813:ASP:OD1	2.33	0.43
6:G:684:ARG:O	6:G:687:ARG:HG2	2.19	0.43
9:J:261:LYS:O	9:J:265:GLU:HG2	2.17	0.43
14:P:160:ASP:OD1	14:P:162:SER:OG	2.25	0.43
16:R:70:GLU:HG2	16:R:73:ARG:HH12	1.84	0.43
1:A:19:GLU:OE1	1:A:31:ARG:NH1	2.42	0.43
2:C:592:THR:HG22	2:C:597:ILE:HG23	2.01	0.43
10:K:252:LYS:HD3	10:K:252:LYS:HA	1.84	0.43
12:M:172:THR:HG23	12:M:178:ILE:O	2.19	0.43
14:O:128:ASN:OD1	14:O:128:ASN:N	2.49	0.43
1:A:113:PRO:HD3	1:A:142:PRO:HG3	2.00	0.43
1:A:191:ASN:OD1	1:A:191:ASN:N	2.52	0.43
1:A:304:GLU:O	1:A:308:LYS:HG2	2.19	0.43
2:C:77:SER:OG	2:C:103:ASN:HB3	2.18	0.43
5:F:161:LEU:HD21	5:F:197:VAL:HG13	2.01	0.43
8:I:102:GLU:CD	8:I:102:GLU:H	2.22	0.43
10:K:97:GLY:HA3	10:K:140:PRO:HG2	2.01	0.43
1:B:173:ASP:OD1	1:B:173:ASP:N	2.51	0.43
11:L:438:GLN:HA	11:L:441:LYS:HE3	2.01	0.43
3:D:180:THR:HG23	15:Q:702:ARG:HH12	1.84	0.43
4:E:290:PRO:O	4:E:1226:ARG:NH1	2.48	0.43
4:E:609:PHE:HE1	4:E:857:ALA:HB2	1.83	0.43
3:D:160:LEU:HD21	15:Q:764:LEU:HD12	1.99	0.43
4:E:571:LYS:HD2	4:E:571:LYS:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:101:LYS:HG2	10:K:102:GLU:OE1	2.19	0.42
3:D:6:LYS:HB2	4:E:1330:LYS:HE2	2.01	0.42
3:D:535:MET:SD	4:E:43:LYS:HG3	2.59	0.42
7:H:205:ASP:OD1	7:H:207:LYS:NZ	2.52	0.42
10:K:302:LEU:HD22	10:K:356:VAL:HG21	2.01	0.42
1:A:225:LEU:HD22	1:B:45:ILE:HD11	2.01	0.42
2:C:362:THR:O	2:C:366:GLU:HG2	2.19	0.42
4:E:70:TRP:CZ2	9:J:278:LEU:HD12	2.54	0.42
4:E:489:ILE:HD12	4:E:938:LEU:HD13	2.01	0.42
4:E:1089:GLY:HA2	4:E:1104:ALA:HB3	2.00	0.42
4:E:1241:ASN:HB2	5:F:337:VAL:HG22	2.01	0.42
16:R:36:ILE:HG12	16:R:44:ARG:NH2	2.34	0.42
3:D:19:GLN:HE21	3:D:23:TRP:HE1	1.66	0.42
3:D:124:SER:HB3	3:D:127:ALA:HB3	2.00	0.42
4:E:1038:ASN:OD1	4:E:1038:ASN:N	2.51	0.42
5:F:414:SER:OG	5:F:414:SER:O	2.37	0.42
6:G:427:ILE:HG22	6:G:460:GLY:HA3	2.01	0.42
6:G:586:MET:HB3	6:G:593:PRO:HG3	2.01	0.42
8:I:174:SER:HB3	8:I:213:TRP:CD2	2.55	0.42
11:L:202:GLU:OE2	11:L:218:ARG:NE	2.53	0.42
4:E:886:LYS:HB3	18:T:79:ASP:HB3	2.01	0.42
6:G:432:LYS:HE3	6:G:432:LYS:HB3	1.79	0.42
6:G:477:ALA:O	6:G:481:MET:HG3	2.20	0.42
11:L:110:ILE:HB	11:L:314:ILE:HB	2.00	0.42
5:F:469:ASN:OD1	5:F:469:ASN:N	2.53	0.42
5:F:809:PRO:HG2	5:F:840:LEU:HD11	2.02	0.42
7:H:370:ASN:ND2	7:H:373:GLU:HG3	2.35	0.42
10:K:134:ARG:HG2	10:K:359:GLY:HA3	2.01	0.42
2:C:579:VAL:HG12	2:C:643:GLY:HA3	2.01	0.42
6:G:674:ASP:HA	6:G:719:GLY:HA3	2.02	0.42
10:K:457:PRO:HA	10:K:460:TRP:CE2	2.55	0.42
11:L:440:GLN:HB2	11:L:461:MET:HE1	2.02	0.42
15:Q:538:LEU:O	15:Q:542:ASN:ND2	2.48	0.42
1:A:131:ASP:HB3	1:A:134:GLN:HG3	2.01	0.42
6:G:580:ARG:NH2	6:G:613:ASP:OD2	2.41	0.42
6:G:785:THR:HG22	6:G:793:MET:SD	2.60	0.42
11:L:300:LYS:HE3	11:L:300:LYS:HB2	1.89	0.42
14:P:95:ARG:HG3	14:P:97:VAL:H	1.85	0.42
6:G:575:LEU:HB3	6:G:578:GLU:HB2	2.01	0.42
7:H:308:ASN:HD22	7:H:308:ASN:HA	1.66	0.42
18:T:53:VAL:HG21	18:T:111:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:MET:HG2	1:A:201:ILE:HD13	2.02	0.41
2:C:35:LEU:HD23	2:C:329:LEU:HD11	2.02	0.41
3:D:619:PRO:HG3	3:D:634:TYR:CZ	2.55	0.41
4:E:1262:GLU:OE1	4:E:1262:GLU:N	2.53	0.41
5:F:410:ARG:HD2	5:F:414:SER:O	2.20	0.41
18:T:50:GLU:O	18:T:53:VAL:HG22	2.19	0.41
2:C:659:VAL:HG22	2:C:852:MET:HB2	2.01	0.41
3:D:161:ARG:NH1	15:Q:768:HIS:O	2.50	0.41
7:H:418:LEU:HD11	7:H:477:ALA:HB1	2.02	0.41
10:K:344:LYS:HE2	10:K:344:LYS:HB2	1.89	0.41
11:L:349:ILE:HD13	11:L:349:ILE:HA	1.97	0.41
9:J:260:LEU:HD23	9:J:260:LEU:HA	1.93	0.41
15:Q:354:THR:HB	15:Q:545:ASN:HD22	1.86	0.41
2:C:826:HIS:NE2	2:C:870:GLU:OE1	2.44	0.41
4:E:257:ILE:HD12	4:E:262:VAL:HG11	2.01	0.41
9:J:213:HIS:ND1	9:J:214:PRO:O	2.48	0.41
11:L:361:SER:HB3	11:L:481:LEU:HD11	2.00	0.41
14:O:175:GLN:NE2	14:O:179:ASP:OD1	2.53	0.41
2:C:881:ASP:OD1	9:J:398:PRO:HG2	2.20	0.41
7:H:168:PRO:HB3	7:H:273:TYR:HB2	2.03	0.41
3:D:130:LEU:HD23	3:D:206:LEU:HD11	2.01	0.41
3:D:172:LYS:HE3	3:D:173:TYR:CE2	2.55	0.41
5:F:398:ILE:HA	5:F:399:PRO:HD3	1.95	0.41
5:F:775:GLU:HG2	5:F:779:LYS:HE2	2.02	0.41
6:G:733:SER:HB3	6:G:818:ILE:HD11	2.02	0.41
7:H:325:VAL:HG21	7:H:342:LEU:HD13	2.02	0.41
1:A:72:HIS:HB3	2:C:731:GLY:HA2	2.02	0.41
2:C:79:GLU:N	2:C:79:GLU:OE1	2.53	0.41
2:C:661:TYR:HB2	2:C:943:ILE:HG23	2.02	0.41
2:C:868:ILE:HG23	2:C:943:ILE:CD1	2.51	0.41
4:E:92:HIS:CE1	4:E:95:GLU:HG3	2.55	0.41
5:F:77:GLU:OE2	5:F:81:ARG:NE	2.52	0.41
6:G:561:ARG:O	6:G:565:ALA:N	2.50	0.41
8:I:205:ILE:HG21	8:I:249:ALA:HB2	2.03	0.41
11:L:327:GLY:HA2	11:L:346:TRP:CD2	2.55	0.41
1:A:117:THR:OG1	1:A:119:ARG:HG2	2.20	0.41
3:D:479:HIS:CD2	3:D:481:LEU:H	2.39	0.41
3:D:516:HIS:CE1	16:R:83:THR:HG23	2.56	0.41
4:E:369:VAL:HB	4:E:381:PHE:HB3	2.03	0.41
5:F:413:VAL:HG21	5:F:809:PRO:HB3	2.03	0.41
7:H:337:ARG:HA	7:H:363:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:131:GLU:HB3	10:K:300:GLN:NE2	2.36	0.41
10:K:197:LYS:HE3	10:K:208:GLU:OE2	2.21	0.41
10:K:416:VAL:O	10:K:420:GLN:HG2	2.21	0.41
11:L:446:LEU:HD22	11:L:449:ALA:HB2	2.02	0.41
18:T:41:LEU:HD11	18:T:102:ARG:HB2	2.02	0.41
18:T:53:VAL:HG23	18:T:109:GLY:O	2.21	0.41
18:T:57:ARG:HH21	18:T:61:LEU:HD21	1.86	0.41
3:D:622:VAL:HB	12:M:284:ILE:HB	2.02	0.41
5:F:435:ARG:HA	5:F:438:GLU:HG2	2.03	0.41
6:G:467:GLN:CD	6:G:502:ARG:HH12	2.25	0.41
10:K:200:PHE:CE1	10:K:205:MET:HG3	2.56	0.41
11:L:472:LYS:HB3	11:L:472:LYS:HE2	1.85	0.41
16:R:95:ASN:HB3	16:R:98:GLU:HG3	2.02	0.41
1:A:43:ASP:HB2	1:B:51:ARG:NH2	2.35	0.40
3:D:10:LEU:HD21	4:E:1318:LEU:HD11	2.03	0.40
6:G:567:LEU:HD11	6:G:601:MET:HE3	2.03	0.40
9:J:305:LYS:HB2	9:J:305:LYS:HE2	1.90	0.40
13:N:252:GLU:H	13:N:252:GLU:HG3	1.70	0.40
1:B:104:ARG:NH2	17:S:507:ASP:OD2	2.54	0.40
3:D:15:VAL:HG21	3:D:23:TRP:CH2	2.57	0.40
3:D:234:ASP:N	3:D:234:ASP:OD1	2.55	0.40
7:H:312:TRP:CZ2	8:I:261:PRO:HG3	2.56	0.40
9:J:280:GLU:HG3	12:M:331:SER:HB2	2.04	0.40
11:L:373:GLU:CD	11:L:373:GLU:H	2.24	0.40
14:O:98:PRO:HB3	14:O:185:MET:HB3	2.04	0.40
3:D:399:ARG:NH2	16:R:157:LEU:HD12	2.36	0.40
4:E:255:ILE:HD11	4:E:285:ILE:HG23	2.04	0.40
4:E:615:PHE:CD1	4:E:841:LEU:HG	2.56	0.40
4:E:1015:ILE:HG23	7:H:156:SER:HB3	2.03	0.40
6:G:782:PHE:HB3	6:G:792:ILE:HG22	2.04	0.40
2:C:127:LEU:HD12	2:C:315:ARG:HD3	2.04	0.40
4:E:141:SER:O	4:E:145:GLN:HG2	2.21	0.40
7:H:315:HIS:O	7:H:318:ARG:NH2	2.55	0.40
11:L:160:ARG:HE	11:L:223:ARG:HD3	1.86	0.40
11:L:166:LEU:HD23	11:L:166:LEU:HA	1.94	0.40
13:N:175:TRP:CE2	13:N:211:PRO:HD3	2.57	0.40
16:R:134:ASN:HA	16:R:138:PHE:O	2.22	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%)	283 (96%)	12 (4%)	0	100	100
1	B	212/327 (65%)	207 (98%)	5 (2%)	0	100	100
2	C	625/1072 (58%)	614 (98%)	11 (2%)	0	100	100
3	D	525/680 (77%)	512 (98%)	13 (2%)	0	100	100
4	E	874/1373 (64%)	846 (97%)	27 (3%)	1 (0%)	51	73
5	F	529/911 (58%)	510 (96%)	19 (4%)	0	100	100
6	G	379/862 (44%)	363 (96%)	16 (4%)	0	100	100
7	H	432/675 (64%)	422 (98%)	10 (2%)	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	372/460 (81%)	362 (97%)	10 (3%)	0	100	100
11	L	402/483 (83%)	394 (98%)	7 (2%)	1 (0%)	47	68
12	M	202/334 (60%)	200 (99%)	2 (1%)	0	100	100
13	N	211/297 (71%)	207 (98%)	4 (2%)	0	100	100
14	O	112/185 (60%)	110 (98%)	2 (2%)	0	100	100
14	P	106/185 (57%)	105 (99%)	1 (1%)	0	100	100
15	Q	214/768 (28%)	210 (98%)	4 (2%)	0	100	100
16	R	108/162 (67%)	107 (99%)	1 (1%)	0	100	100
17	S	382/611 (62%)	367 (96%)	15 (4%)	0	100	100
18	T	102/140 (73%)	99 (97%)	3 (3%)	0	100	100
All	All	6525/10644 (61%)	6345 (97%)	178 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	1183	PRO

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Mol	Chain	Res	Type
11	L	405	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%)	270 (98%)	5 (2%)	59 81
1	B	191/301 (64%)	190 (100%)	1 (0%)	88 96
2	C	564/931 (61%)	560 (99%)	4 (1%)	84 94
3	D	492/608 (81%)	487 (99%)	5 (1%)	76 90
4	E	805/1230 (65%)	801 (100%)	4 (0%)	88 96
5	F	457/782 (58%)	453 (99%)	4 (1%)	78 92
6	G	331/740 (45%)	327 (99%)	4 (1%)	71 88
7	H	394/609 (65%)	392 (100%)	2 (0%)	88 96
8	I	187/230 (81%)	187 (100%)	0	100 100
9	J	212/469 (45%)	211 (100%)	1 (0%)	88 96
10	K	329/401 (82%)	326 (99%)	3 (1%)	78 92
11	L	362/431 (84%)	359 (99%)	3 (1%)	81 93
12	M	195/299 (65%)	194 (100%)	1 (0%)	88 96
13	N	185/259 (71%)	183 (99%)	2 (1%)	73 89
14	O	103/169 (61%)	101 (98%)	2 (2%)	57 80
14	P	97/169 (57%)	96 (99%)	1 (1%)	76 90
15	Q	190/661 (29%)	190 (100%)	0	100 100
16	R	101/144 (70%)	98 (97%)	3 (3%)	41 68
17	S	336/532 (63%)	333 (99%)	3 (1%)	78 92
18	T	93/126 (74%)	93 (100%)	0	100 100
All	All	5899/9392 (63%)	5851 (99%)	48 (1%)	82 93

All (48) 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	129	ILE
1	A	154	ASN
1	B	132	ASN
2	C	320	LEU
2	C	476	ASP
2	C	542	ASN
2	C	923	TYR
3	D	235	ARG
3	D	514	PHE
3	D	517	MET
3	D	624	TYR
3	D	631	HIS
4	E	396	ILE
4	E	864	THR
4	E	869	ARG
4	E	1204	LYS
5	F	207	ARG
5	F	241	ARG
5	F	270	ASN
5	F	492	ARG
6	G	624	ASN
6	G	636	MET
6	G	642	ASP
6	G	747	VAL
7	H	181	LYS
7	H	204	LYS
9	J	287	ARG
10	K	265	PHE
10	K	314	ARG
10	K	383	THR
11	L	87	ARG
11	L	109	ASP
11	L	204	ASP
12	M	139	ASP
13	N	214	TRP
13	N	252	GLU
14	O	85	GLN
14	O	128	ASN
14	P	174	LEU
16	R	50	THR

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Mol	Chain	Res	Type
16	R	54	LYS
16	R	73	ARG
17	S	298	LYS
17	S	562	ASN
17	S	570	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	196	GLN
1	A	303	GLN
1	B	196	GLN
2	C	505	GLN
2	C	542	ASN
2	C	623	HIS
3	D	258	ASN
3	D	324	GLN
3	D	417	GLN
3	D	479	HIS
3	D	583	ASN
4	E	863	ASN
4	E	1032	ASN
4	E	1282	GLN
4	E	1291	GLN
5	F	838	HIS
6	G	529	ASN
6	G	624	ASN
6	G	754	GLN
7	H	308	ASN
9	J	329	GLN
10	K	255	GLN
10	K	331	ASN
11	L	132	GLN
11	L	438	GLN
14	O	88	GLN
14	P	88	GLN
15	Q	751	HIS
17	S	277	GLN
17	S	361	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	$\#\|Z\| > 2$
21	SAH	L	8001	11	24,28,28	1.19	3 (12%)	25,40,40	1.74	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
21	SAH	L	8001	11	-	4/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	8001	SAH	C2-N3	3.80	1.38	1.32
21	L	8001	SAH	C2-N1	2.28	1.38	1.33
21	L	8001	SAH	OXT-C	-2.19	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	L	8001	SAH	N3-C2-N1	-5.41	120.22	128.68
21	L	8001	SAH	C5'-SD-CG	-3.48	91.82	102.27
21	L	8001	SAH	C3'-C2'-C1'	3.15	105.71	100.98
21	L	8001	SAH	OXT-C-O	-2.70	117.96	124.09
21	L	8001	SAH	OXT-C-CA	2.21	120.90	113.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

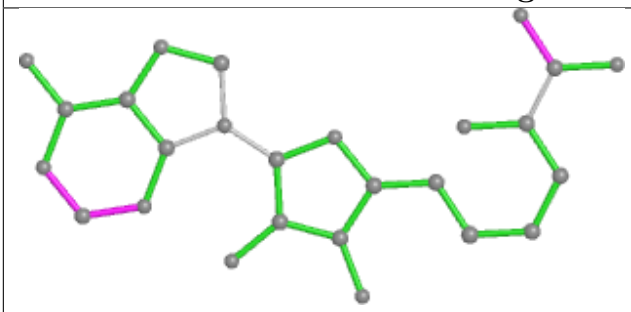
Mol	Chain	Res	Type	Atoms
21	L	8001	SAH	C3'-C4'-C5'-SD
21	L	8001	SAH	O4'-C4'-C5'-SD
21	L	8001	SAH	C-CA-CB-CG
21	L	8001	SAH	CB-CG-SD-C5'

There are no ring outliers.

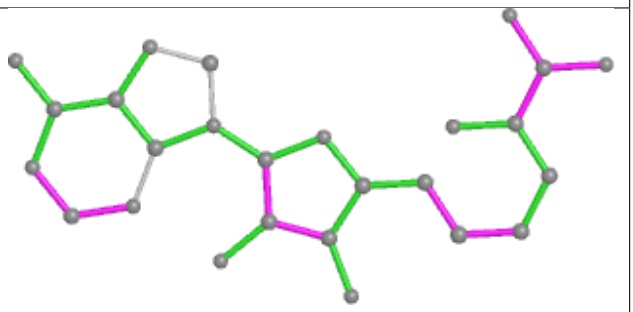
No monomer is involved in short contacts.

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 then 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.

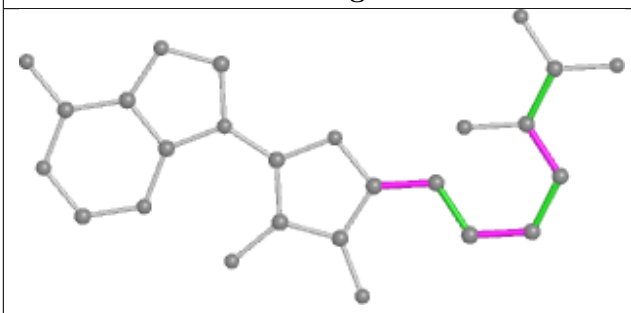
Ligand SAH L 8001



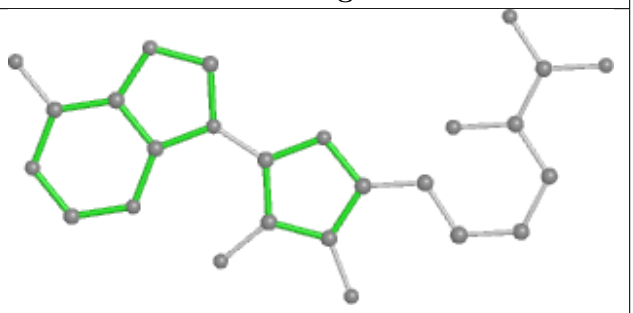
Bond lengths



Bond angles



Torsions



Rings

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.

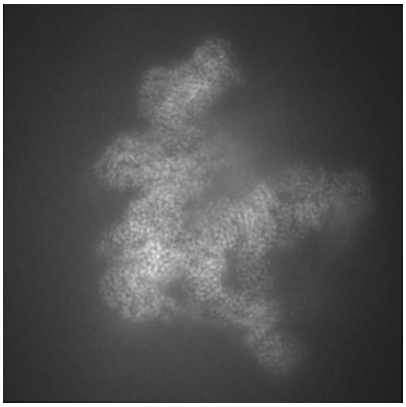
6 Map visualisation

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.

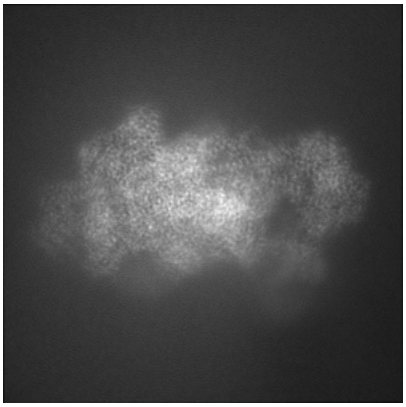
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

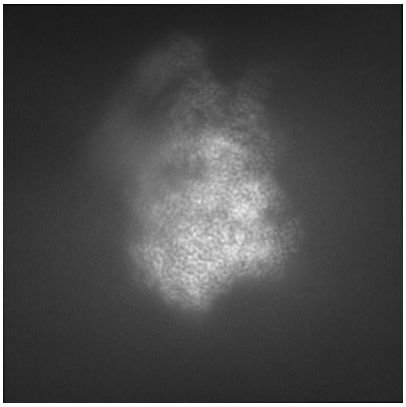
6.1.1 Primary map



X



Y

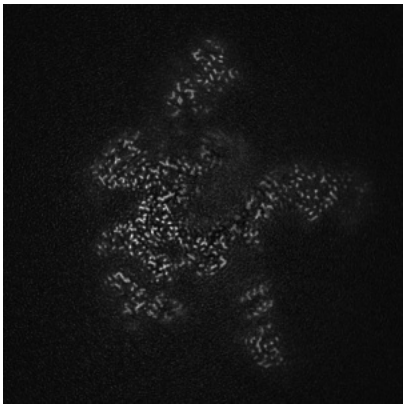


Z

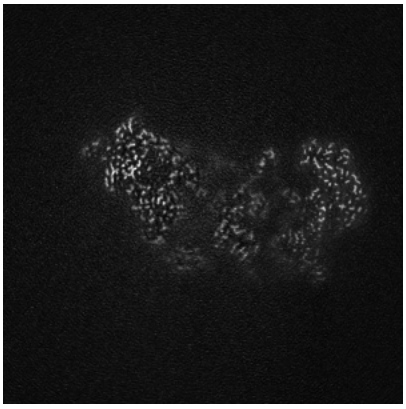
The images above show the map projected in three orthogonal directions.

6.2 Central slices

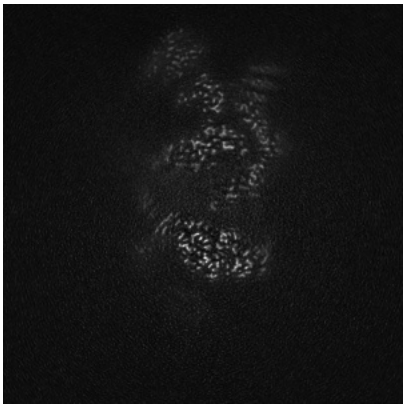
6.2.1 Primary map



X Index: 300



Y Index: 300

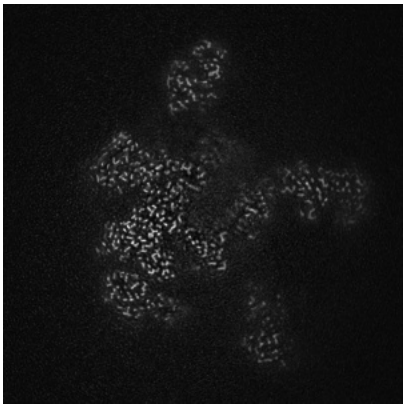


Z Index: 300

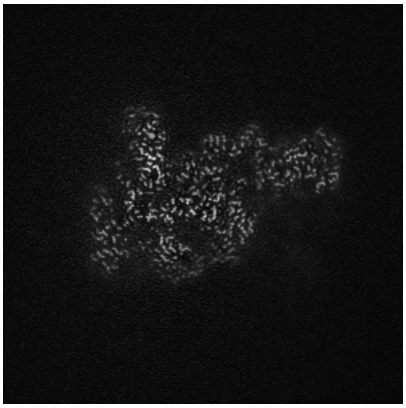
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

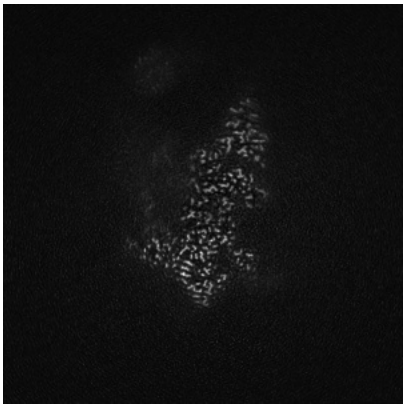
6.3.1 Primary map



X Index: 289



Y Index: 232

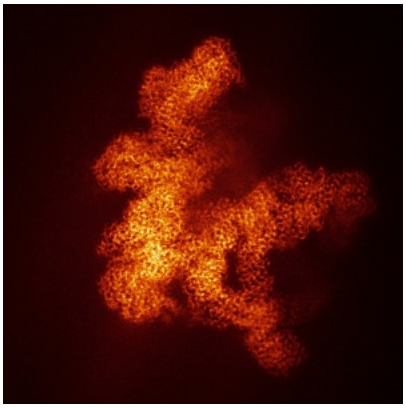


Z Index: 253

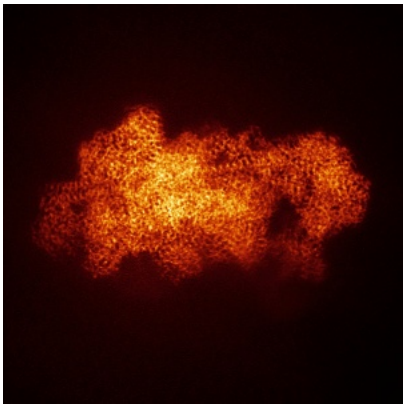
The images above show the largest variance slices of the map in three orthogonal directions.

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

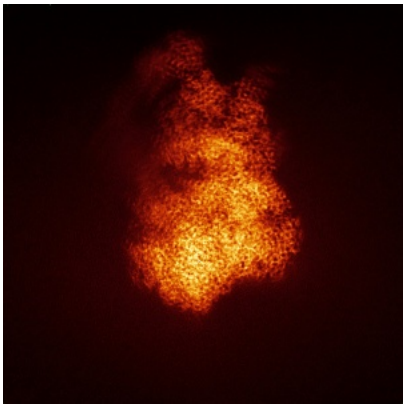
6.4.1 Primary map



X



Y

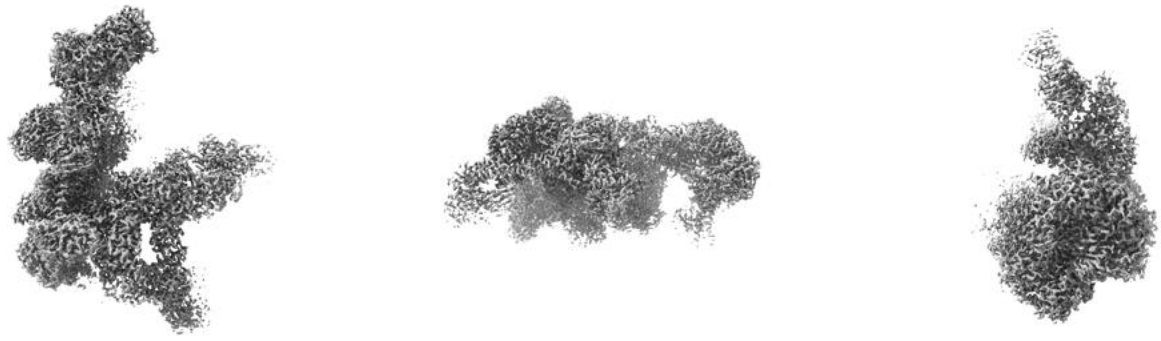


Z

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



X Y Z

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.

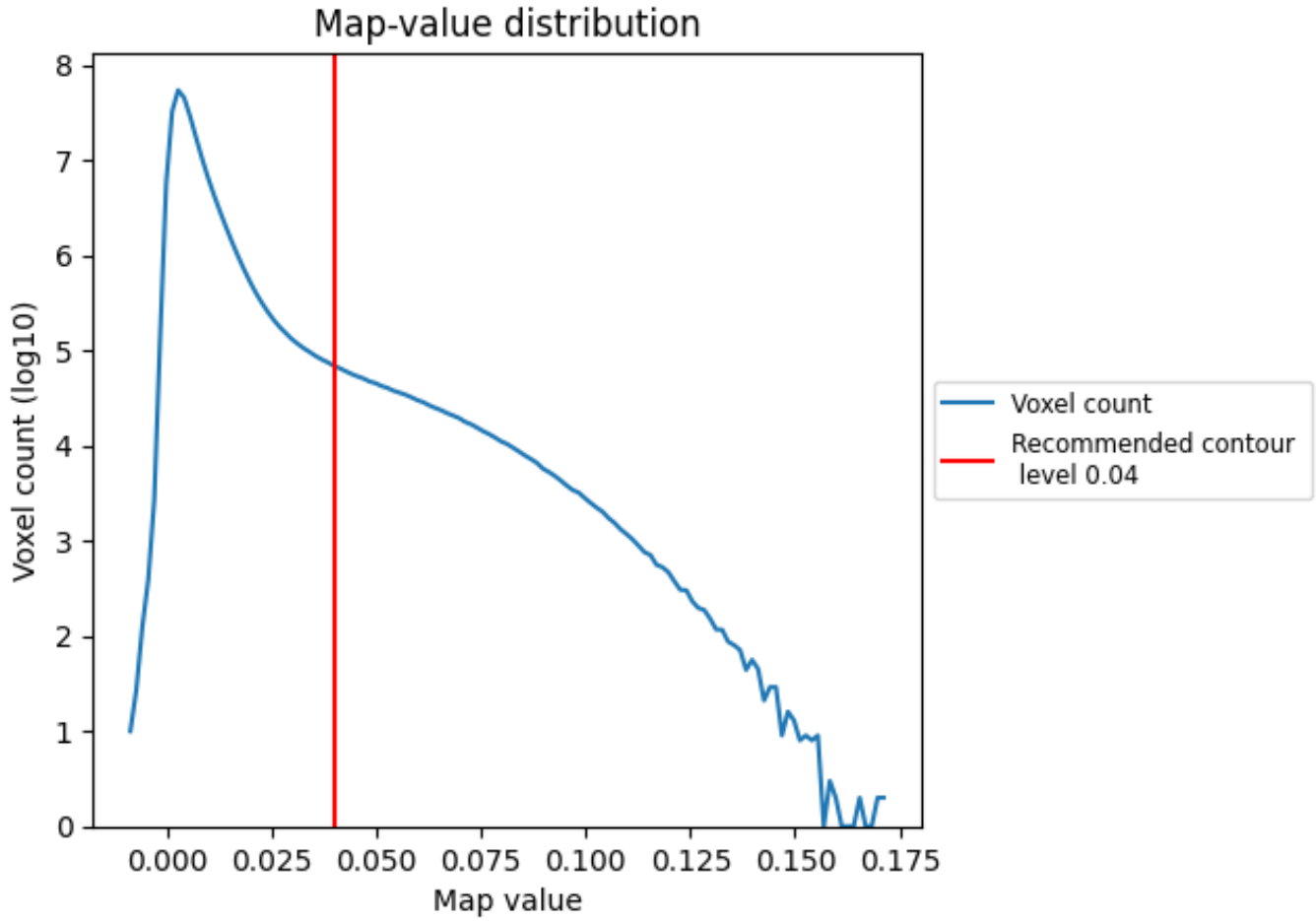
6.6 Mask visualisation (i)

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

7 Map analysis

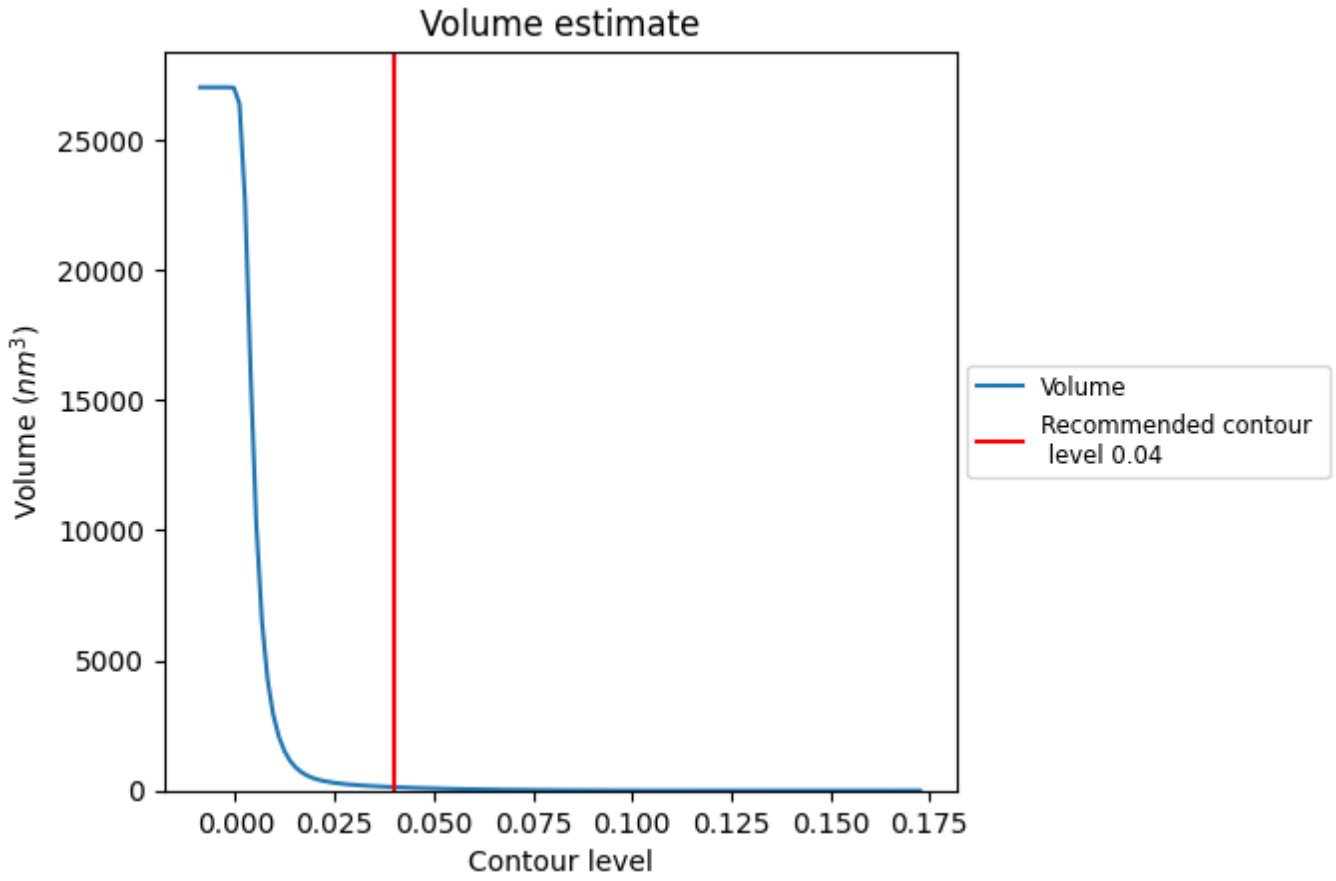
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

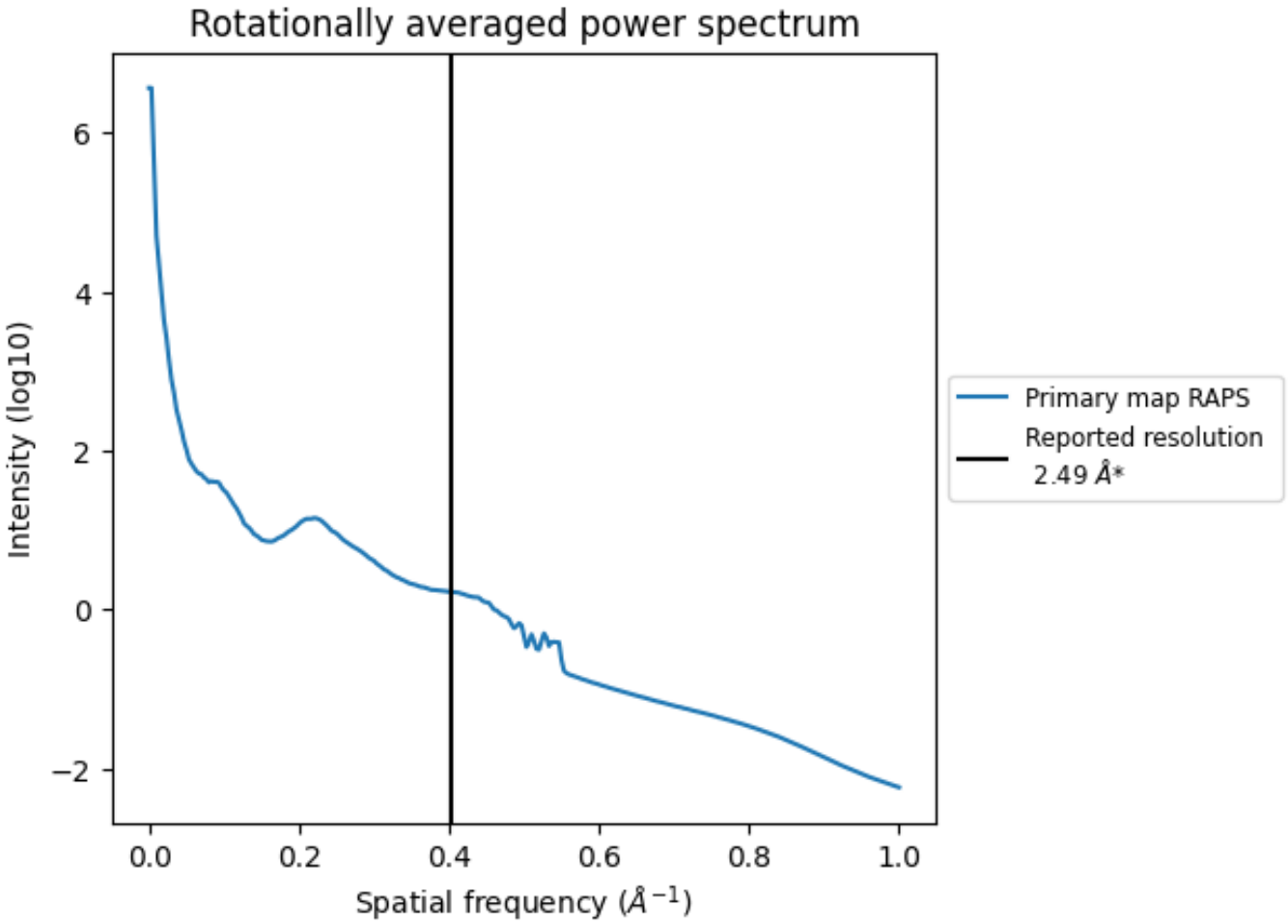
7.2 Volume estimate



The volume at the recommended contour level is 132 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 $Å^{-1}$

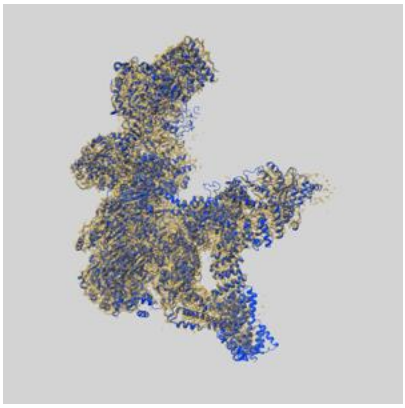
8 Fourier-Shell correlation (i)

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

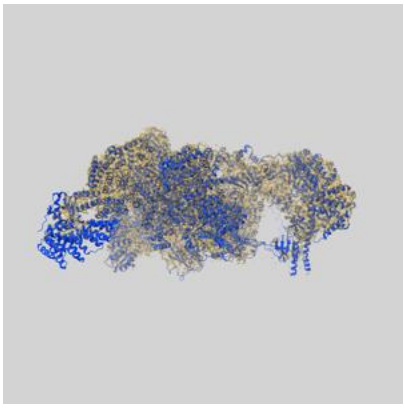
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18935 and PDB model 8R5O. Per-residue inclusion information can be found in section 3 on page 9.

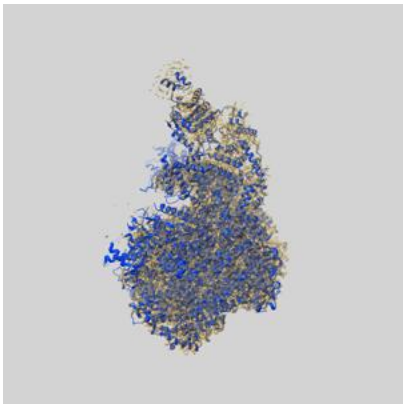
9.1 Map-model overlay



X



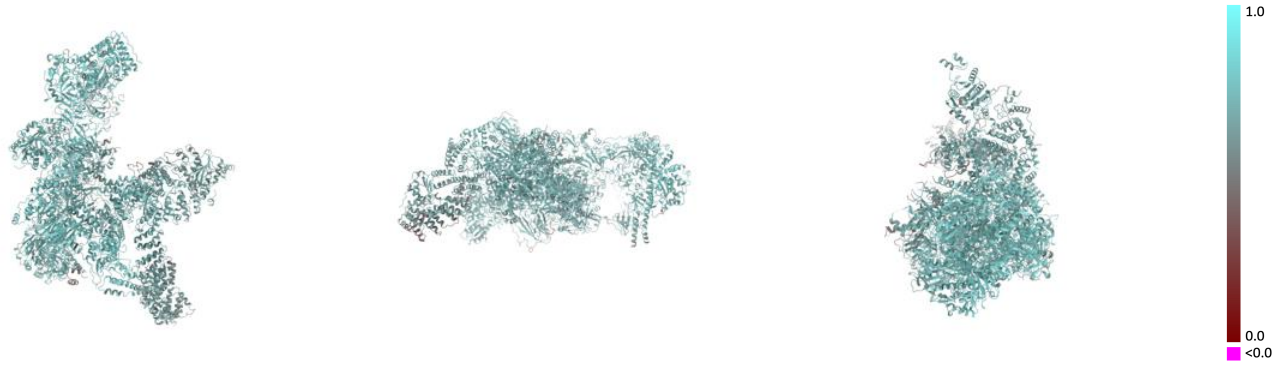
Y



Z

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.

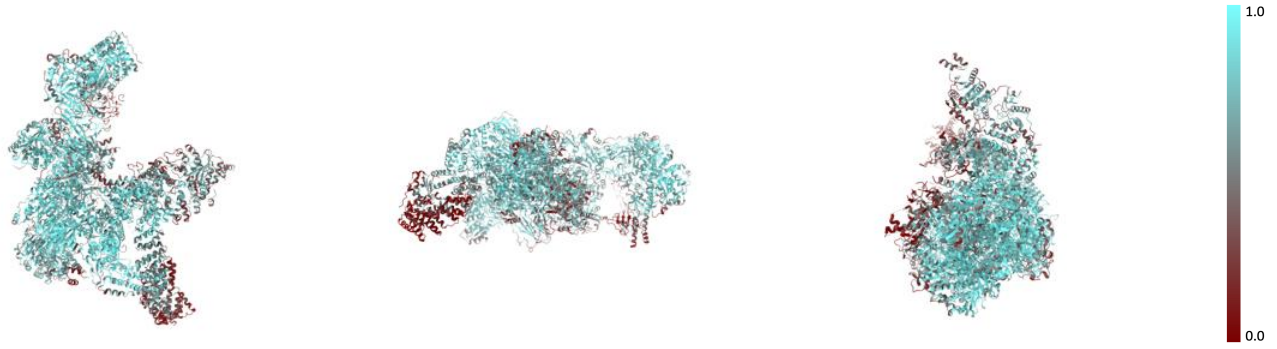
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

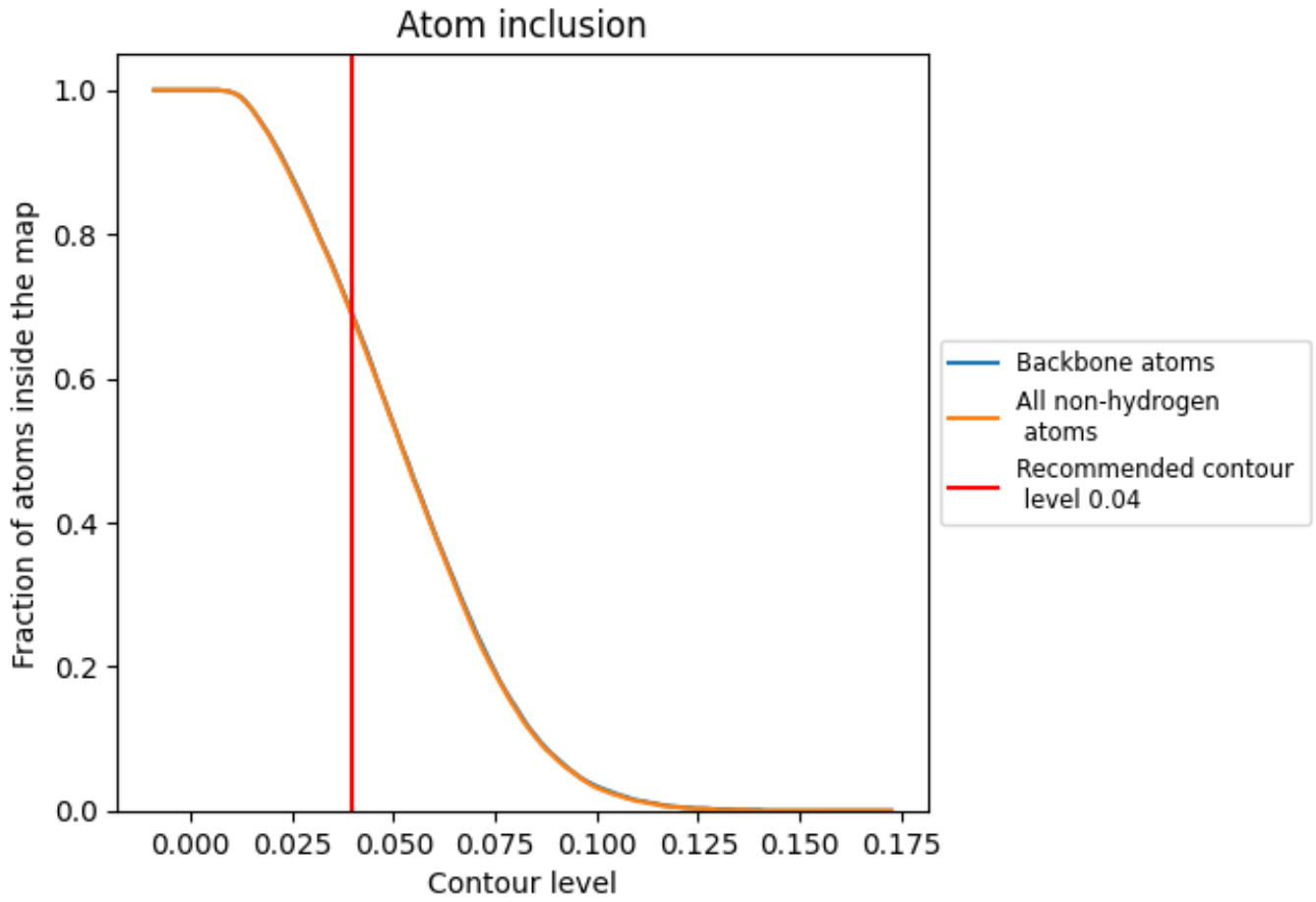
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 69% of all backbone atoms, 68% 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	0.6850	0.6890
A	0.7030	0.6900
B	0.7760	0.7060
C	0.7440	0.7100
D	0.6400	0.6560
E	0.6920	0.6960
F	0.6470	0.6580
G	0.2060	0.5690
H	0.6740	0.7000
I	0.8050	0.7130
J	0.8200	0.7330
K	0.8120	0.7330
L	0.8220	0.7110
M	0.8300	0.7160
N	0.7320	0.6940
O	0.6940	0.7060
P	0.6270	0.6670
Q	0.4930	0.6330
R	0.7180	0.6810
S	0.7840	0.7170
T	0.7280	0.7150