Full wwPDB EM Validation Report ⓘ

Jan 11, 2024 – 04:47 PM JST

PDB ID	:	8I9U
EMDB ID	:	EMD-35284
Title	:	Human TRiC-PhLP2A complex in the open state
Authors	:	Roh, S.H.; Park, J.; Kim, H.; Lim, S.
Deposited on	:	2023-02-07
Resolution	:	3.10 Å(reported)
Based on initial model	:	6NR8

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:

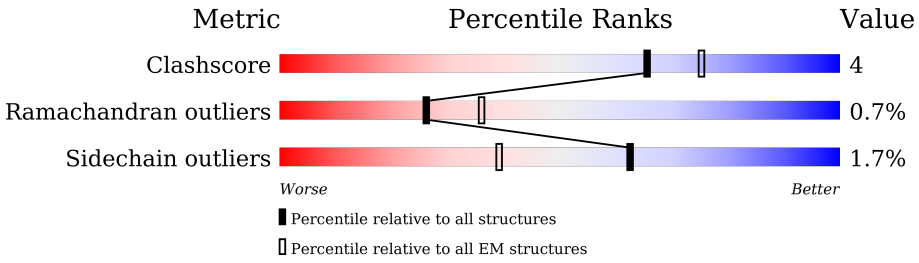
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.10 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	556	40% 81% 13% 6%
1	I	556	49% 80% 14% 6%
2	B	535	38% 83% 10% 7%
2	J	535	43% 83% 10% 7%
3	C	545	23% 81% 11% 7%
3	K	545	33% 81% 11% • 7%
4	D	539	36% 81% 13% • 5%
4	L	539	45% 81% 13% • 5%

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Mol	Chain	Length	Quality of chain
5	E	541	32% 80% 14% 5%
5	M	541	35% 83% 12% 5%
6	F	531	18% 89% 8%
6	N	531	21% 88% 9%
7	G	543	36% 82% 12% 6%
7	O	543	37% 81% 13% 6%
8	H	548	22% 83% 11% 6%
8	P	548	19% 84% 10% 6%
9	Q	239	45% 53% 6% 40%
9	R	239	53% 52% 8% 41%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 65141 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	521	Total	C	N	O	S	0	0
			3956	2479	691	763	23		
1	I	521	Total	C	N	O	S	0	0
			3956	2479	691	763	23		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	499	Total	C	N	O	S	0	0
			3755	2351	660	725	19		
2	J	499	Total	C	N	O	S	0	0
			3755	2351	660	725	19		

- Molecule 3 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	507	Total	C	N	O	S	0	0
			3940	2457	694	759	30		
3	K	507	Total	C	N	O	S	0	0
			3940	2457	694	759	30		

- Molecule 4 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	514	Total	C	N	O	S	0	0
			3880	2426	675	756	23		
4	L	514	Total	C	N	O	S	0	0
			3880	2426	675	756	23		

- Molecule 5 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	513	Total	C	N	O	S	0	0
			3940	2465	688	757	30		
5	M	513	Total	C	N	O	S	0	0
			3940	2465	688	757	30		

- Molecule 6 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	516	Total	C	N	O	S	0	0
			3958	2486	692	759	21		
6	N	516	Total	C	N	O	S	0	0
			3958	2486	692	759	21		

- Molecule 7 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	512	Total	C	N	O	S	0	0
			3936	2485	682	746	23		
7	O	512	Total	C	N	O	S	0	0
			3936	2485	682	746	23		

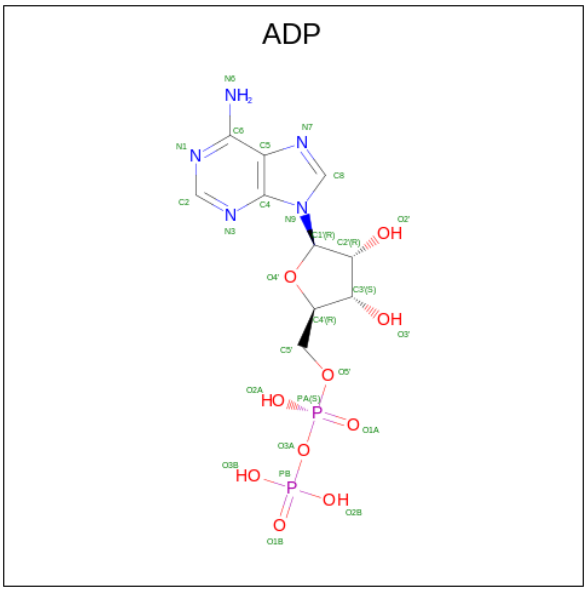
- Molecule 8 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	517	Total	C	N	O	S	0	0
			3942	2485	669	761	27		
8	P	517	Total	C	N	O	S	0	0
			3942	2485	669	761	27		

- Molecule 9 is a protein called Phosducin-like protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	143	Total	C	N	O	S	0	0
			1133	734	188	206	5		
9	R	142	Total	C	N	O	S	0	0
			1124	728	186	205	5		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



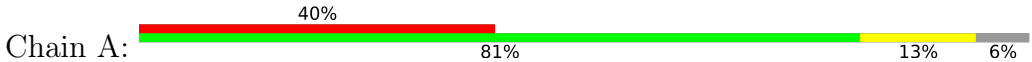
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	N	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	P	1	Total	C	N	O	P	0
			27	10	5	10	2	

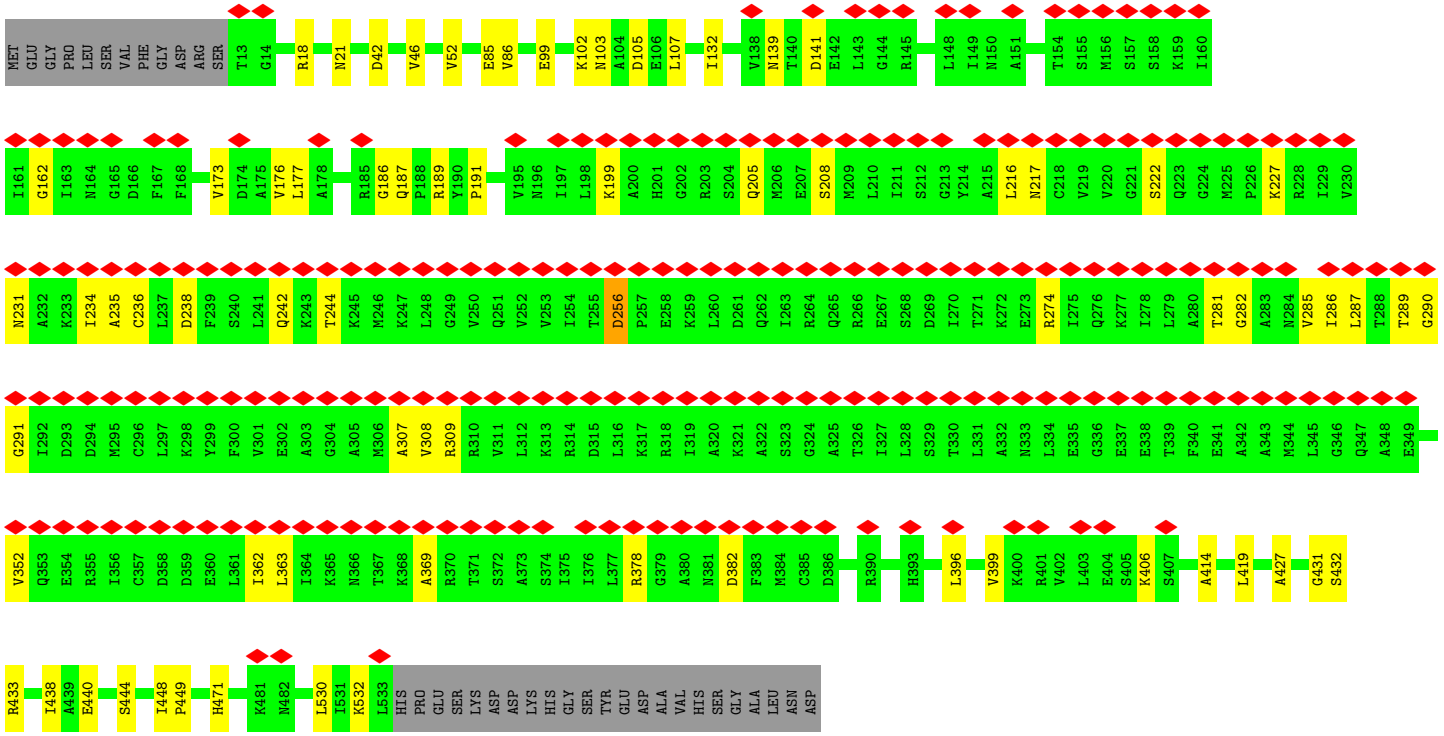
3 Residue-property plots (i)

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: T-complex protein 1 subunit alpha

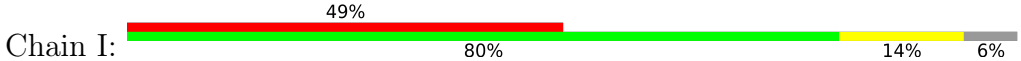
Chain A:

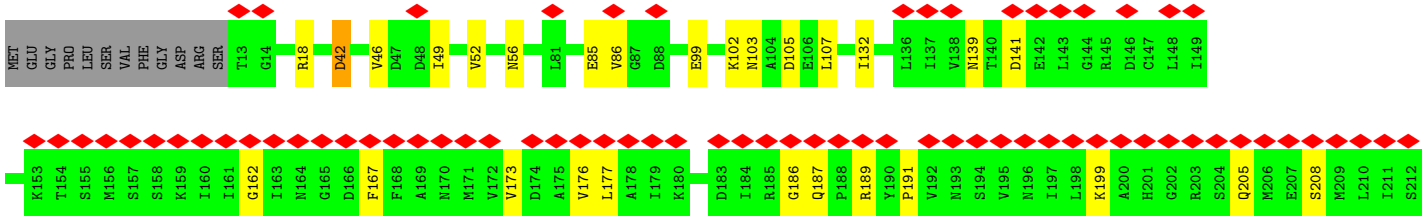




• Molecule 1: T-complex protein 1 subunit alpha

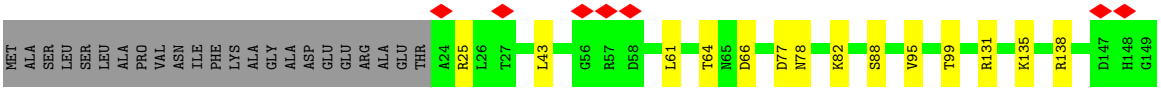
Chain I:

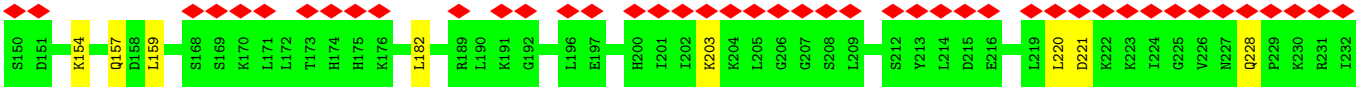


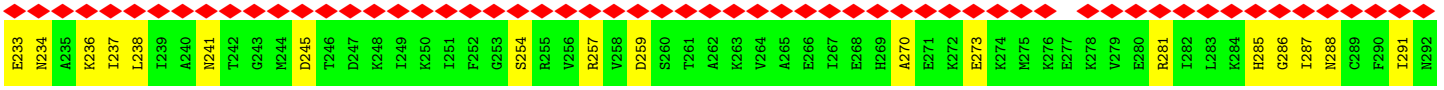


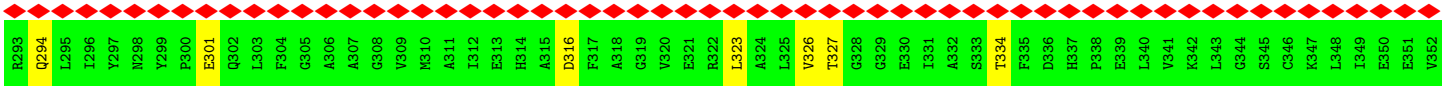
• Molecule 2: T-complex protein 1 subunit beta

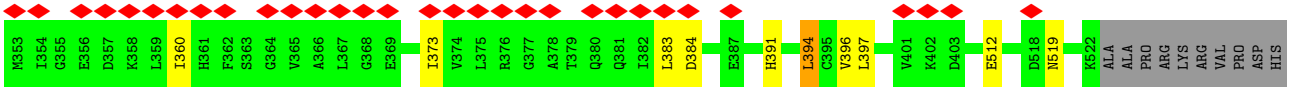
Chain B:





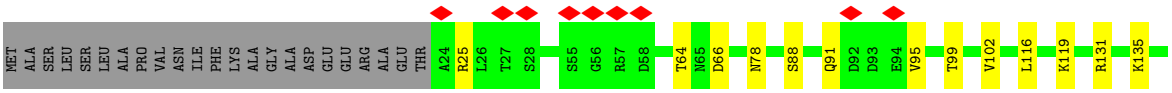


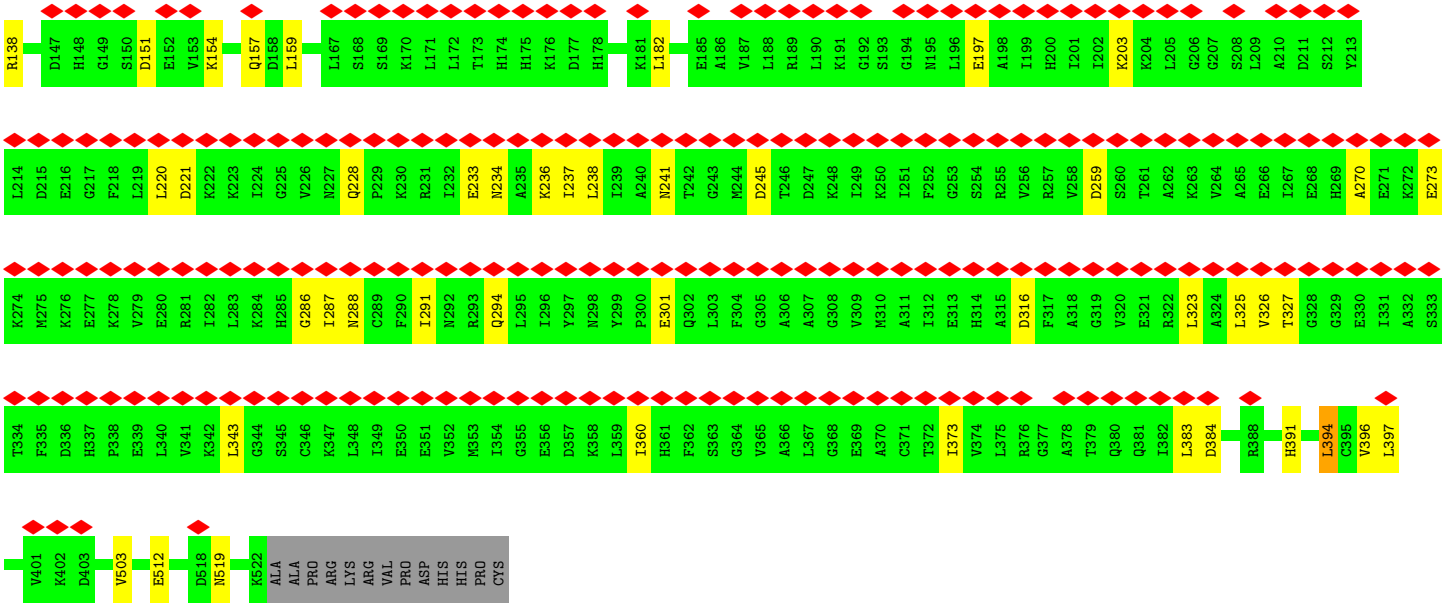




• Molecule 2: T-complex protein 1 subunit beta

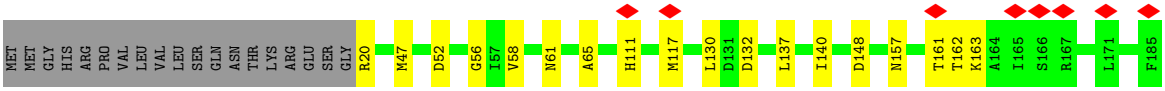
Chain J:





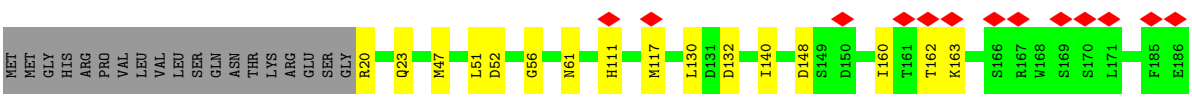
• Molecule 3: T-complex protein 1 subunit gamma

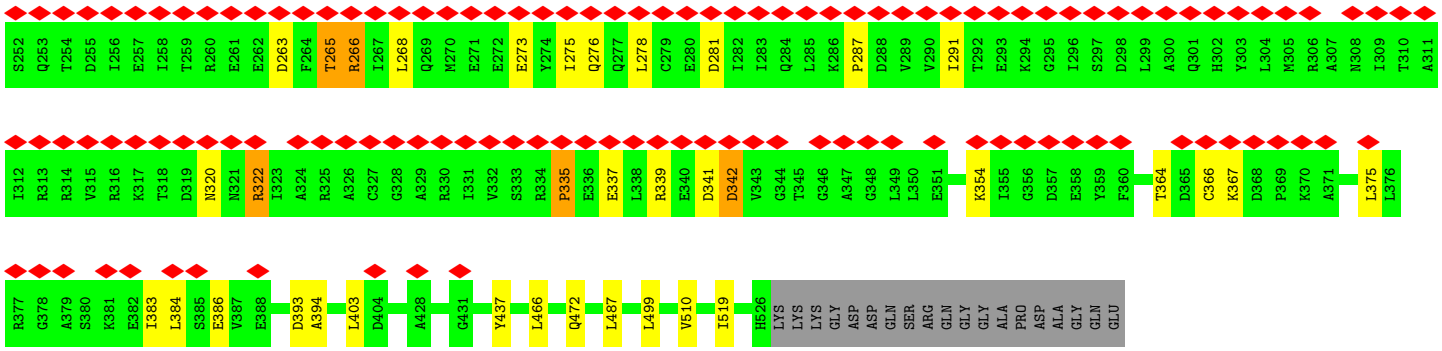
Chain C:



• Molecule 3: T-complex protein 1 subunit gamma

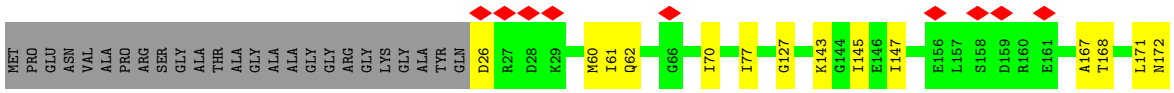
Chain K:

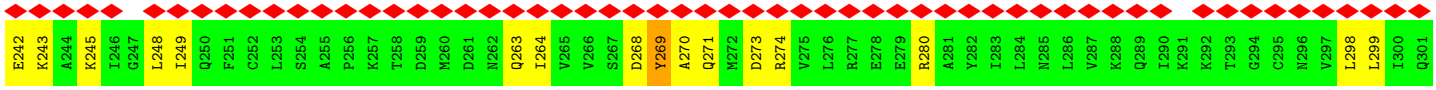


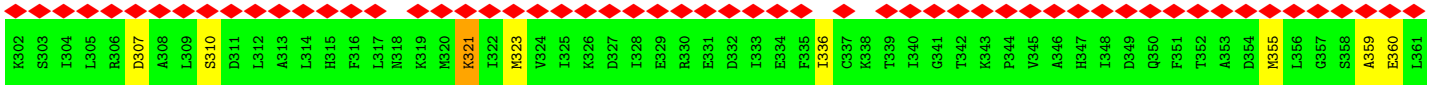


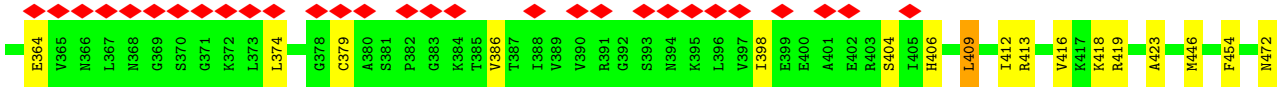
• Molecule 4: T-complex protein 1 subunit delta

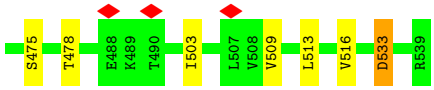
Chain D:





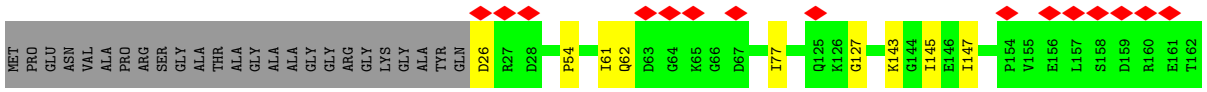


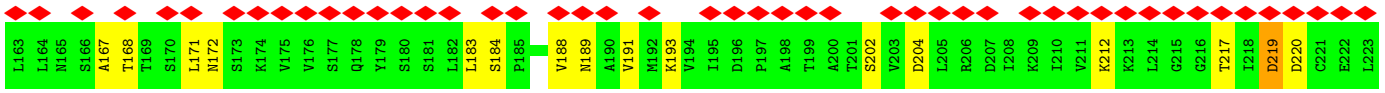


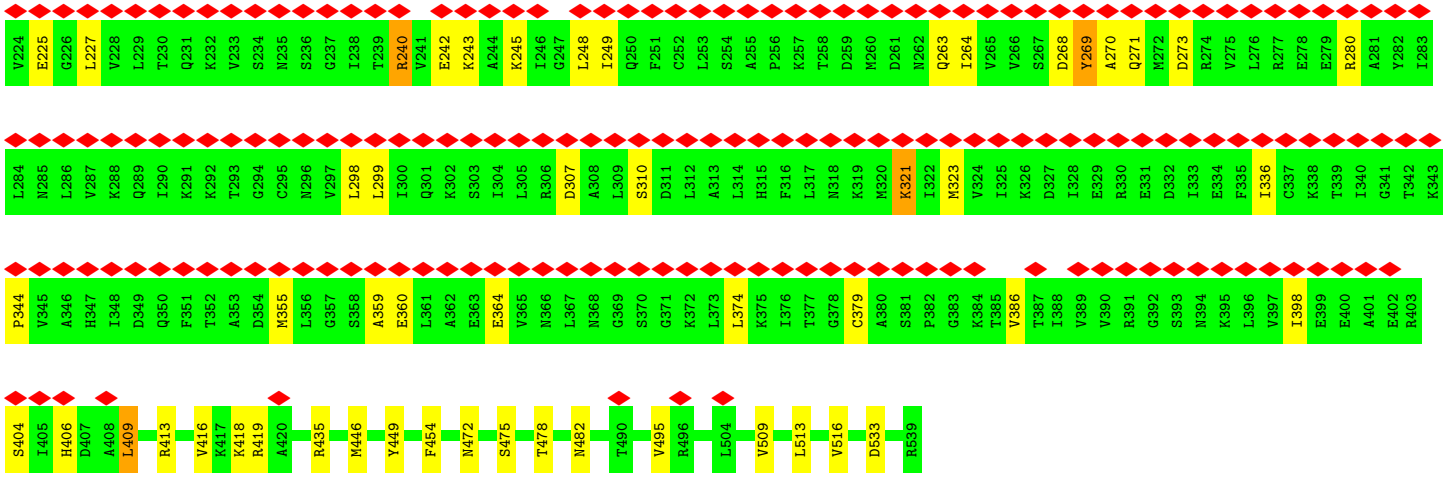


• Molecule 4: T-complex protein 1 subunit delta

Chain L:

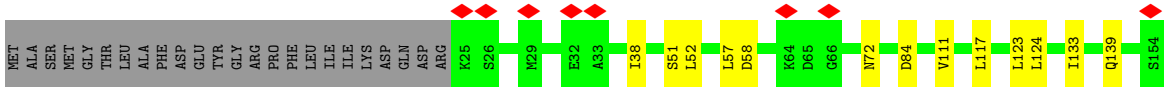






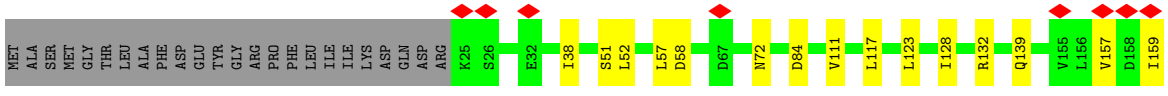
• Molecule 5: T-complex protein 1 subunit epsilon

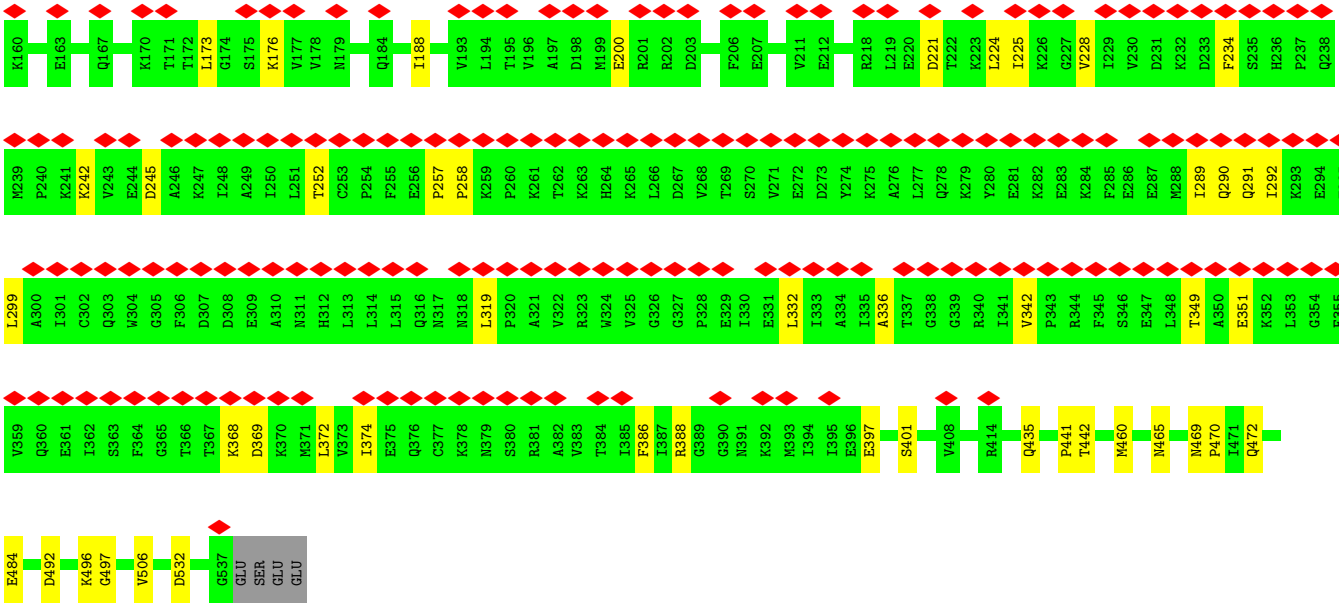
Chain E:



• Molecule 5: T-complex protein 1 subunit epsilon

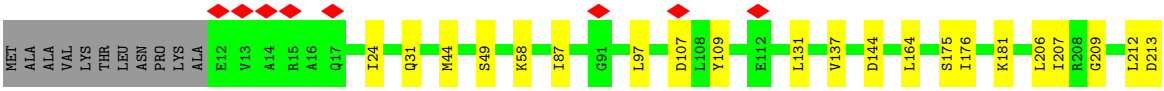
Chain M:

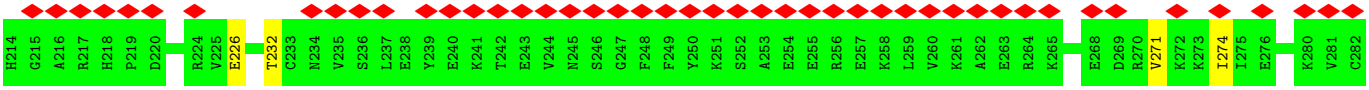


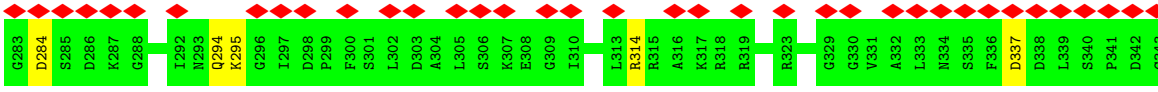


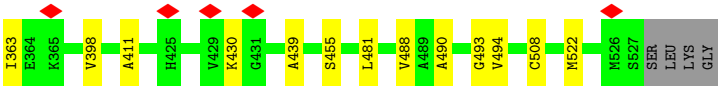
• Molecule 6: T-complex protein 1 subunit zeta

Chain F:



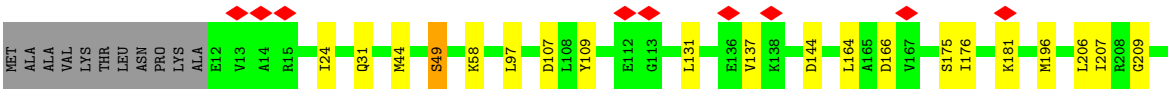


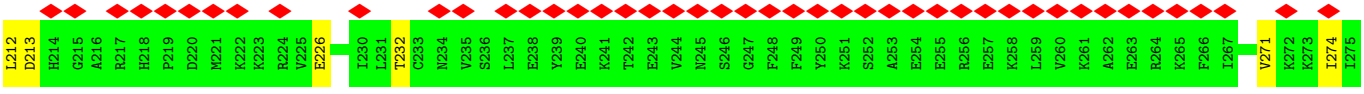


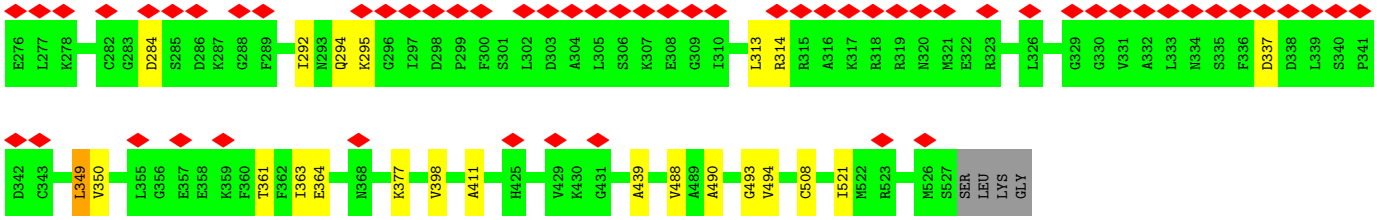


• Molecule 6: T-complex protein 1 subunit zeta

Chain N:

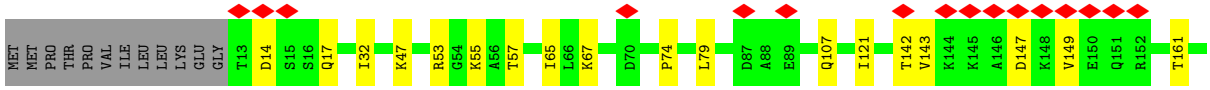


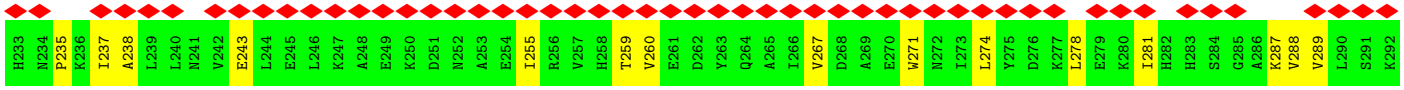


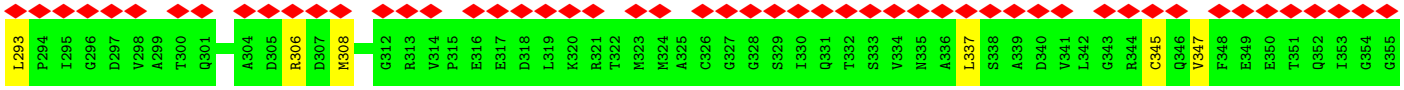


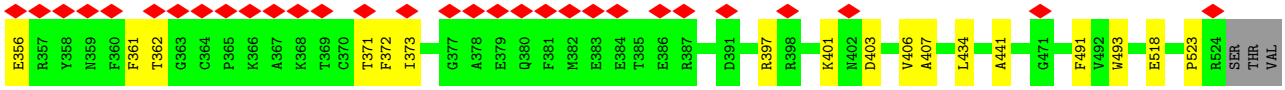
• Molecule 7: T-complex protein 1 subunit eta

Chain G:



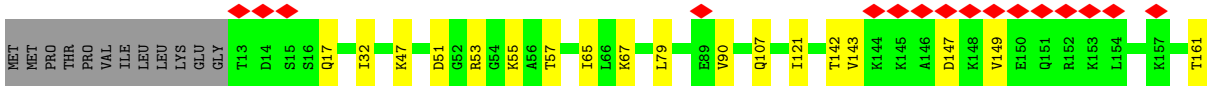


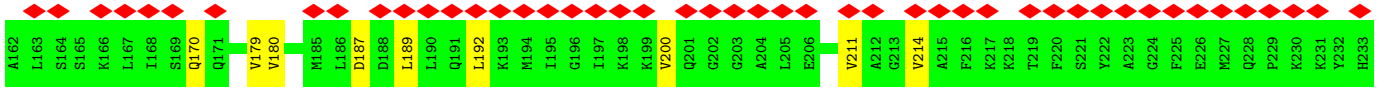


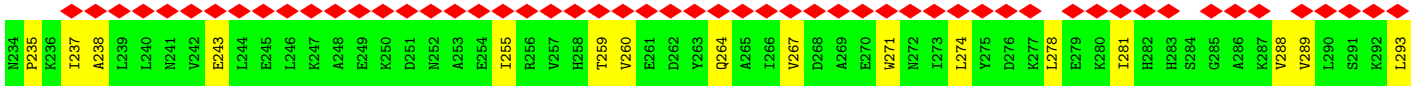


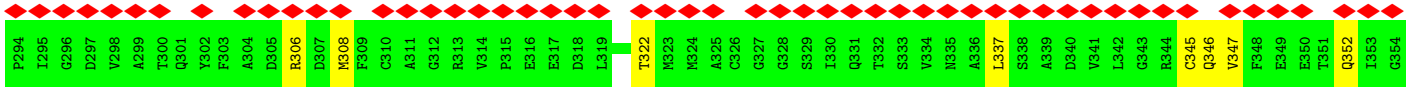
• Molecule 7: T-complex protein 1 subunit eta

Chain O:



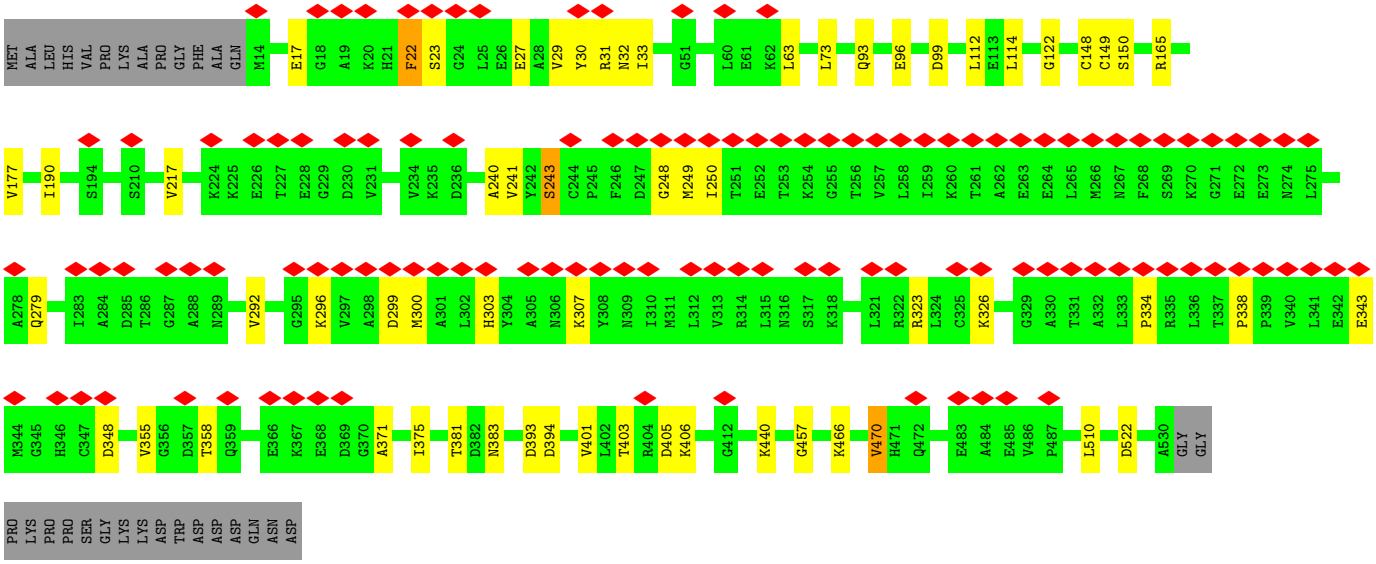






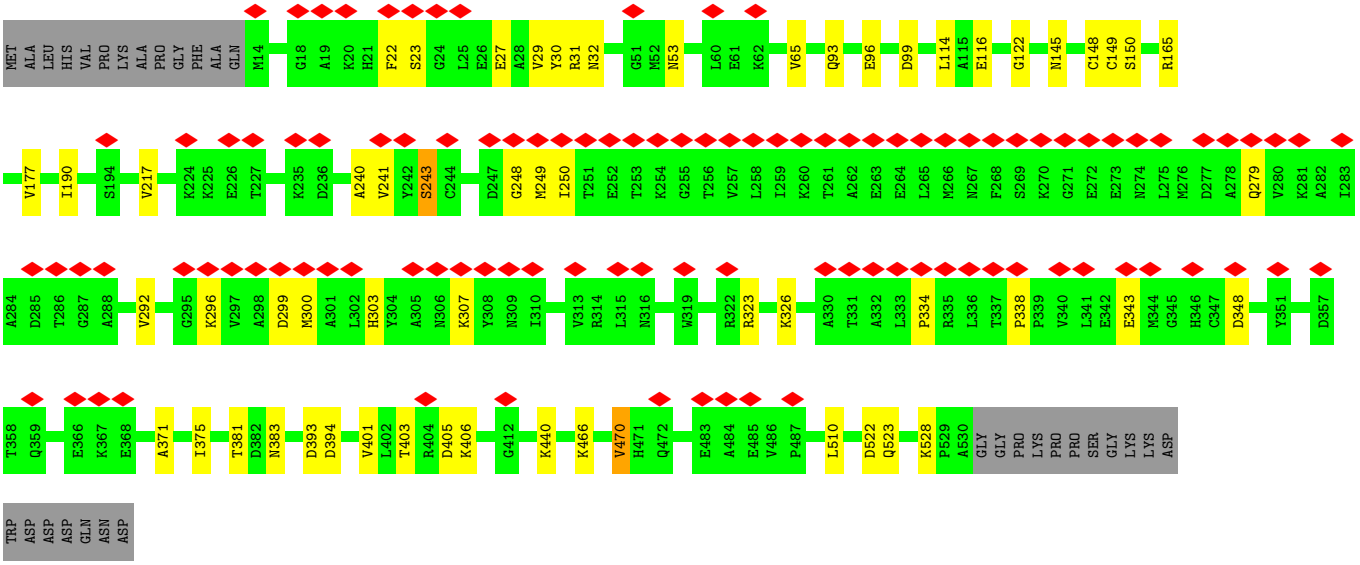
• Molecule 8: T-complex protein 1 subunit theta

Chain H:



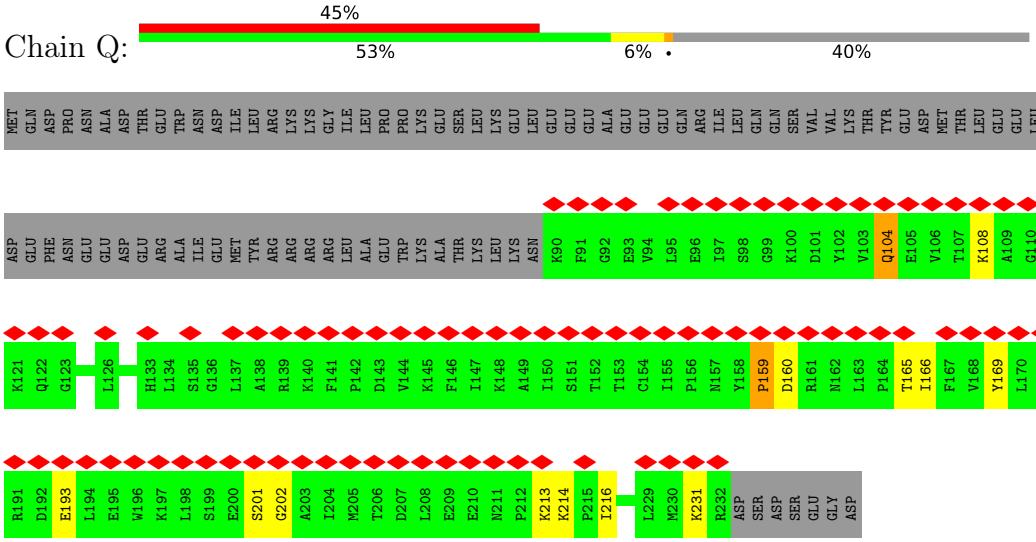
• Molecule 8: T-complex protein 1 subunit theta

Chain P:



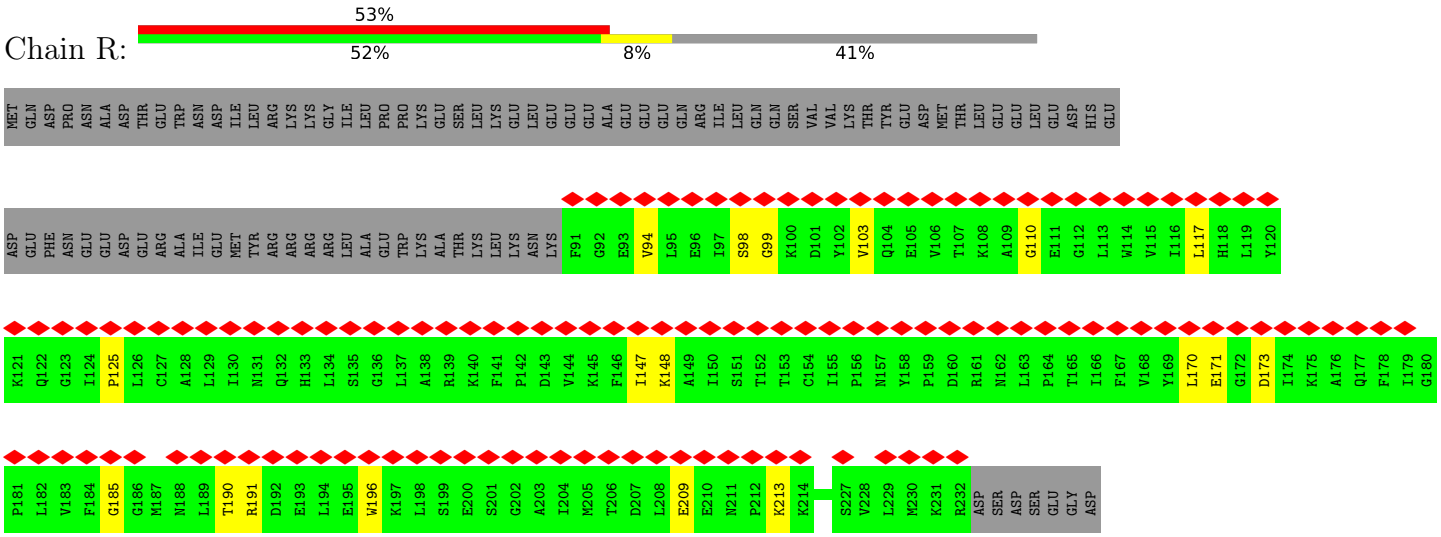
• Molecule 9: Phosducin-like protein 3

Chain Q:



• Molecule 9: Phosducin-like protein 3

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1796900	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction was performed for every micrographs	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	6.752	Depositor
Minimum map value	-3.471	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.165	Depositor
Recommended contour level	0.44	Depositor
Map size (Å)	361.6, 361.6, 361.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.13, 1.13, 1.13	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.23	0/3992	0.39	0/5389
1	I	0.23	0/3992	0.39	0/5389
2	B	0.23	0/3795	0.38	0/5115
2	J	0.23	0/3795	0.38	0/5115
3	C	0.22	0/3985	0.38	0/5378
3	K	0.22	0/3985	0.38	0/5378
4	D	0.23	0/3911	0.40	0/5280
4	L	0.23	0/3911	0.40	0/5280
5	E	0.23	0/3986	0.39	0/5370
5	M	0.23	0/3986	0.39	0/5370
6	F	0.23	0/4004	0.37	0/5397
6	N	0.23	0/4004	0.37	0/5397
7	G	0.23	0/3991	0.38	0/5386
7	O	0.23	0/3991	0.39	0/5386
8	H	0.23	0/3996	0.38	0/5400
8	P	0.23	0/3996	0.38	0/5400
9	Q	0.23	0/1156	0.37	0/1562
9	R	0.23	0/1147	0.38	0/1551
All	All	0.23	0/65623	0.38	0/88543

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3956	0	4124	38	0
1	I	3956	0	4124	39	0
2	B	3755	0	3870	34	0
2	J	3755	0	3870	37	0
3	C	3940	0	4062	35	0
3	K	3940	0	4062	39	0
4	D	3880	0	4090	40	0
4	L	3880	0	4090	39	0
5	E	3940	0	4061	39	0
5	M	3940	0	4061	31	0
6	F	3958	0	4085	21	0
6	N	3958	0	4085	24	0
7	G	3936	0	4029	33	0
7	O	3936	0	4029	37	0
8	H	3942	0	4010	30	0
8	P	3942	0	4010	29	0
9	Q	1133	0	1171	11	0
9	R	1124	0	1158	10	0
10	A	27	0	12	0	0
10	C	27	0	12	0	0
10	D	27	0	12	0	0
10	F	27	0	12	0	0
10	H	27	0	10	0	0
10	I	27	0	12	0	0
10	K	27	0	12	0	0
10	L	27	0	12	0	0
10	N	27	0	12	0	0
10	P	27	0	10	0	0
All	All	65141	0	67107	545	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 (545) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:215:LEU:HD22	3:C:375:LEU:HB2	1.75	0.69
3:K:215:LEU:HD22	3:K:375:LEU:HB2	1.75	0.68
4:D:249:ILE:HD11	4:D:299:LEU:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:249:ILE:HD11	4:L:299:LEU:H	1.59	0.67
5:E:123:LEU:HD21	5:E:446:TYR:HB3	1.75	0.67
8:H:23:SER:HA	8:H:27:GLU:HG2	1.77	0.66
6:F:44:MET:HG2	6:F:58:LYS:HD2	1.79	0.65
7:G:213:GLY:HA3	7:G:361:PHE:O	1.98	0.64
3:K:203:LYS:HG2	3:K:384:LEU:HD12	1.78	0.64
3:C:203:LYS:HG2	3:C:384:LEU:HD12	1.78	0.63
8:H:279:GLN:HG2	8:H:338:PRO:HG3	1.81	0.63
8:P:279:GLN:HG2	8:P:338:PRO:HG3	1.81	0.63
1:I:244:THR:HB	3:K:337:GLU:HB3	1.82	0.62
8:H:148:CYS:SG	8:H:149:CYS:N	2.71	0.62
8:P:148:CYS:SG	8:P:149:CYS:N	2.71	0.62
3:K:20:ARG:HH21	3:K:117:MET:HB3	1.66	0.60
3:K:275:ILE:HD12	3:K:278:LEU:HD12	1.82	0.60
5:E:472:GLN:NE2	4:L:446:MET:SD	2.74	0.60
7:O:259:THR:OG1	7:O:260:VAL:N	2.34	0.60
3:C:20:ARG:HH21	3:C:117:MET:HB3	1.66	0.60
3:C:279:CYS:HA	3:C:283:ILE:HB	1.84	0.60
4:D:446:MET:SD	5:M:472:GLN:NE2	2.74	0.60
3:C:342:ASP:OD1	3:C:342:ASP:N	2.35	0.60
3:C:47:MET:HG2	3:C:61:ASN:HB3	1.84	0.59
1:A:244:THR:HB	3:C:337:GLU:HB3	1.84	0.59
5:E:349:THR:HG23	5:E:351:GLU:H	1.68	0.59
1:I:432:SER:OG	1:I:433:ARG:N	2.36	0.59
5:M:349:THR:HG23	5:M:351:GLU:H	1.68	0.59
8:P:23:SER:HA	8:P:27:GLU:HG2	1.85	0.59
9:R:98:SER:OG	9:R:99:GLY:N	2.34	0.59
3:C:218:VAL:HG22	3:C:322:ARG:HH21	1.68	0.58
1:A:256:ASP:OD2	1:A:256:ASP:N	2.37	0.58
2:B:257:ARG:HG3	5:E:271:VAL:HG13	1.86	0.58
3:K:47:MET:HG2	3:K:61:ASN:HB3	1.85	0.58
1:I:18:ARG:NH2	1:I:105:ASP:OD1	2.37	0.57
7:G:235:PRO:HG2	7:G:345:CYS:HB3	1.86	0.57
1:A:18:ARG:NH2	1:A:105:ASP:OD1	2.37	0.57
7:G:107:GLN:HG3	7:G:441:ALA:HB2	1.86	0.57
1:A:21:ASN:HD21	1:A:530:LEU:HD11	1.70	0.57
2:B:234:ASN:O	2:B:288:ASN:ND2	2.37	0.57
3:K:218:VAL:HG22	3:K:322:ARG:HH21	1.68	0.57
7:O:107:GLN:HG3	7:O:441:ALA:HB2	1.86	0.57
7:O:235:PRO:HG2	7:O:345:CYS:HB3	1.85	0.57
4:D:364:GLU:HB2	4:D:374:LEU:HG	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:212:SER:HA	3:C:375:LEU:O	2.06	0.56
4:L:364:GLU:HB2	4:L:374:LEU:HG	1.88	0.56
5:E:228:VAL:HG11	5:E:332:LEU:HD13	1.88	0.56
3:K:130:LEU:HD22	3:K:510:VAL:HG11	1.88	0.56
3:K:212:SER:HA	3:K:375:LEU:O	2.06	0.56
4:L:418:LYS:HE2	4:L:513:LEU:HB2	1.88	0.56
8:P:32:ASN:ND2	8:P:522:ASP:OD2	2.39	0.56
2:B:131:ARG:NH2	2:B:512:GLU:OE2	2.38	0.56
3:C:130:LEU:HD22	3:C:510:VAL:HG11	1.88	0.56
7:O:347:VAL:HB	7:O:362:THR:O	2.06	0.56
2:J:131:ARG:NH2	2:J:512:GLU:OE2	2.39	0.56
6:N:109:TYR:HE2	6:N:439:ALA:HB2	1.71	0.56
4:D:418:LYS:HE2	4:D:513:LEU:HB2	1.88	0.55
3:K:216:ARG:HE	3:K:364:THR:HG23	1.71	0.55
3:K:239:VAL:H	3:K:287:PRO:HB3	1.71	0.55
5:M:228:VAL:HG11	5:M:332:LEU:HD13	1.88	0.55
3:C:216:ARG:HE	3:C:364:THR:HG23	1.72	0.55
6:F:209:GLY:HA3	6:F:363:ILE:O	2.07	0.55
2:J:234:ASN:O	2:J:288:ASN:ND2	2.38	0.55
1:I:256:ASP:N	1:I:256:ASP:OD2	2.39	0.55
8:H:405:ASP:OD1	8:H:405:ASP:N	2.38	0.55
1:I:132:ILE:HD11	1:I:419:LEU:HD11	1.88	0.55
7:O:161:THR:HG23	7:O:491:PHE:HB3	1.88	0.55
6:F:109:TYR:HE2	6:F:439:ALA:HB2	1.71	0.55
2:J:88:SER:HB3	2:J:99:THR:HG23	1.88	0.55
4:D:263:GLN:HG3	4:D:264:ILE:HG12	1.88	0.55
4:L:263:GLN:HG3	4:L:264:ILE:HG12	1.88	0.55
3:K:244:SER:HB3	3:K:335:PRO:HB3	1.89	0.54
7:G:259:THR:OG1	7:G:260:VAL:N	2.40	0.54
6:F:207:ILE:HG22	6:F:209:GLY:H	1.73	0.54
8:P:299:ASP:N	8:P:299:ASP:OD1	2.40	0.54
1:A:352:VAL:O	1:A:363:LEU:HB2	2.07	0.54
3:K:342:ASP:OD1	3:K:342:ASP:N	2.35	0.54
1:I:242:GLN:NE2	1:I:291:GLY:O	2.41	0.54
1:A:242:GLN:NE2	1:A:291:GLY:O	2.40	0.54
5:E:440:CYS:O	4:L:482:ASN:ND2	2.41	0.54
2:B:236:LYS:NZ	2:B:286:GLY:O	2.41	0.54
1:I:46:VAL:HG22	1:I:52:VAL:HG12	1.90	0.54
6:N:209:GLY:HA3	6:N:363:ILE:O	2.08	0.54
2:J:102:VAL:HG12	2:J:503:VAL:HG13	1.90	0.53
4:L:360:GLU:HG3	4:L:379:CYS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:236:LYS:NZ	2:J:286:GLY:O	2.41	0.53
3:K:204:ILE:HD12	3:K:205:PRO:HD2	1.91	0.53
1:I:414:ALA:O	1:I:471:HIS:NE2	2.41	0.53
6:N:44:MET:HG2	6:N:58:LYS:HD2	1.90	0.53
3:C:204:ILE:HD12	3:C:205:PRO:HD2	1.91	0.53
4:D:360:GLU:HG3	4:D:379:CYS:HB2	1.90	0.53
4:L:61:ILE:HD11	4:L:77:ILE:HG12	1.89	0.53
2:B:228:GLN:NE2	2:B:301:GLU:OE2	2.42	0.53
1:I:352:VAL:O	1:I:363:LEU:HB2	2.08	0.53
2:J:228:GLN:NE2	2:J:301:GLU:OE2	2.42	0.53
4:D:240:ARG:NH1	4:D:242:GLU:OE2	2.42	0.53
7:G:211:VAL:HG12	7:G:371:THR:HB	1.90	0.53
4:L:26:ASP:N	4:L:26:ASP:OD1	2.41	0.53
1:I:532:LYS:HG2	4:L:62:GLN:HB3	1.91	0.52
1:A:414:ALA:O	1:A:471:HIS:NE2	2.43	0.52
5:E:442:THR:HA	4:L:478:THR:HG21	1.90	0.52
5:M:492:ASP:OD1	5:M:492:ASP:N	2.42	0.52
4:D:248:LEU:HB3	4:D:355:MET:HB2	1.92	0.52
9:R:196:TRP:HE1	9:R:209:GLU:HA	1.74	0.52
4:D:26:ASP:OD1	4:D:26:ASP:N	2.41	0.52
5:E:492:ASP:N	5:E:492:ASP:OD1	2.42	0.52
7:G:32:ILE:HD11	7:G:79:LEU:HD23	1.91	0.52
7:G:161:THR:HG23	7:G:491:PHE:HB3	1.92	0.52
6:N:166:ASP:N	6:N:166:ASP:OD1	2.43	0.52
1:A:46:VAL:HG22	1:A:52:VAL:HG12	1.90	0.52
3:C:132:ASP:OD2	3:C:437:TYR:OH	2.26	0.52
8:H:32:ASN:ND2	8:H:522:ASP:OD2	2.43	0.52
8:H:299:ASP:OD1	8:H:299:ASP:N	2.40	0.52
2:J:159:LEU:HD11	2:J:397:LEU:HD21	1.91	0.52
1:A:427:ALA:HB2	1:A:438:ILE:HB	1.91	0.52
1:I:427:ALA:HB2	1:I:438:ILE:HB	1.92	0.52
6:N:207:ILE:HG22	6:N:209:GLY:H	1.74	0.52
1:A:532:LYS:HG2	4:D:62:GLN:HB3	1.91	0.52
4:L:189:ASN:O	4:L:193:LYS:NZ	2.42	0.52
7:O:32:ILE:HD11	7:O:79:LEU:HD23	1.92	0.52
8:P:243:SER:HB2	8:P:334:PRO:HB3	1.91	0.52
1:A:141:ASP:OD1	1:A:141:ASP:N	2.43	0.52
2:J:237:ILE:HD13	2:J:323:LEU:HD21	1.92	0.52
2:J:241:ASN:OD1	2:J:294:GLN:NE2	2.43	0.52
3:K:263:ASP:O	3:K:266:ARG:HB3	2.10	0.52
4:L:240:ARG:NH1	4:L:242:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:243:SER:HB2	8:H:334:PRO:HB3	1.91	0.52
3:K:265:THR:O	3:K:268:LEU:HB3	2.10	0.51
6:F:294:GLN:HG2	6:F:295:LYS:HD2	1.92	0.51
1:I:107:LEU:HD11	1:I:440:GLU:HG3	1.92	0.51
8:H:323:ARG:HA	8:H:326:LYS:HG2	1.92	0.51
9:Q:104:GLN:HE22	9:Q:108:LYS:HD2	1.76	0.51
1:A:289:THR:OG1	1:A:290:GLY:N	2.44	0.51
6:N:294:GLN:HG2	6:N:295:LYS:HD2	1.93	0.51
7:O:121:ILE:HG13	7:O:434:LEU:HD13	1.91	0.51
2:B:88:SER:HB3	2:B:99:THR:HG23	1.91	0.51
6:N:213:ASP:OD1	6:N:213:ASP:N	2.44	0.51
2:B:254:SER:HB3	5:E:271:VAL:HB	1.93	0.51
4:D:168:THR:O	4:D:172:ASN:ND2	2.44	0.51
1:I:243:LYS:HG2	1:I:264:ARG:HB2	1.93	0.51
5:M:58:ASP:OD1	5:M:58:ASP:N	2.44	0.51
8:H:22:PHE:HB3	8:H:31:ARG:HH12	1.76	0.51
5:M:289:ILE:HA	5:M:292:ILE:HG12	1.93	0.51
7:O:346:GLN:HB3	7:O:363:GLY:HA3	1.92	0.51
8:P:240:ALA:HA	8:P:343:GLU:HG3	1.92	0.51
1:A:107:LEU:HD11	1:A:440:GLU:HG3	1.92	0.51
5:M:234:PHE:H	5:M:369:ASP:HB3	1.76	0.51
7:O:179:VAL:HG21	7:O:372:PHE:HB2	1.93	0.51
7:O:211:VAL:HG12	7:O:371:THR:HB	1.91	0.51
1:A:85:GLU:HG3	1:A:86:VAL:HG23	1.93	0.51
1:I:103:ASN:HD22	1:I:444:SER:HB3	1.76	0.51
8:P:323:ARG:HA	8:P:326:LYS:HG2	1.92	0.51
5:M:469:ASN:ND2	5:M:472:GLN:OE1	2.44	0.50
2:B:238:LEU:HD22	2:B:287:ILE:HD12	1.93	0.50
3:C:200:ARG:HH12	3:C:322:ARG:HB2	1.77	0.50
3:C:275:ILE:HG12	3:C:309:ILE:HD13	1.93	0.50
6:F:212:LEU:HB2	6:F:361:THR:HB	1.93	0.50
1:A:432:SER:OG	1:A:433:ARG:N	2.45	0.50
1:I:85:GLU:HG3	1:I:86:VAL:HG23	1.94	0.50
4:D:61:ILE:HD11	4:D:77:ILE:HG12	1.92	0.50
2:J:237:ILE:HG23	2:J:291:ILE:HD11	1.93	0.50
5:M:221:ASP:O	5:M:388:ARG:NH1	2.45	0.50
1:A:173:VAL:HA	1:A:176:VAL:HG22	1.93	0.50
5:M:173:LEU:HG	5:M:401:SER:HB2	1.93	0.50
6:F:87:ILE:HG23	9:Q:231:LYS:HE2	1.94	0.50
1:A:103:ASN:HD22	1:A:444:SER:HB3	1.77	0.50
5:E:221:ASP:O	5:E:388:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:240:ALA:HA	8:H:343:GLU:HG3	1.93	0.50
4:L:248:LEU:HB3	4:L:355:MET:HB2	1.92	0.50
2:B:237:ILE:HG23	2:B:291:ILE:HD11	1.93	0.50
2:B:241:ASN:OD1	2:B:294:GLN:NE2	2.45	0.49
1:I:307:ALA:O	1:I:309:ARG:NH1	2.45	0.49
2:J:197:GLU:HG3	2:J:325:LEU:HD13	1.94	0.49
5:E:188:ILE:HG23	5:E:224:LEU:HB2	1.94	0.49
5:M:188:ILE:HG23	5:M:224:LEU:HB2	1.94	0.49
6:N:212:LEU:HB2	6:N:361:THR:HB	1.93	0.49
7:G:121:ILE:HG13	7:G:434:LEU:HD13	1.93	0.49
1:I:141:ASP:N	1:I:141:ASP:OD1	2.43	0.49
2:J:220:LEU:HD23	2:J:360:ILE:HB	1.95	0.49
1:A:307:ALA:O	1:A:309:ARG:NH1	2.45	0.49
3:C:258:ILE:HG12	3:C:267:ILE:HD11	1.94	0.49
2:J:238:LEU:HD22	2:J:287:ILE:HD12	1.93	0.49
3:K:200:ARG:HH12	3:K:322:ARG:HB2	1.77	0.49
7:O:189:LEU:O	7:O:397:ARG:NH2	2.45	0.49
2:B:25:ARG:NH2	2:B:519:ASN:O	2.46	0.49
4:D:269:TYR:O	4:D:271:GLN:N	2.45	0.49
5:E:173:LEU:HG	5:E:401:SER:HB2	1.93	0.49
5:E:234:PHE:H	5:E:369:ASP:HB3	1.77	0.49
7:G:179:VAL:HG21	7:G:372:PHE:HB2	1.94	0.49
2:B:220:LEU:HD23	2:B:360:ILE:HB	1.95	0.49
6:N:271:VAL:HA	6:N:274:ILE:HG12	1.93	0.49
7:G:187:ASP:OD2	7:G:397:ARG:NH2	2.46	0.49
3:K:52:ASP:HB2	3:K:56:GLY:H	1.78	0.49
3:K:132:ASP:OD2	3:K:437:TYR:OH	2.26	0.49
4:L:472:ASN:ND2	4:L:475:SER:OG	2.46	0.49
3:K:466:LEU:HD13	3:K:487:LEU:HD22	1.95	0.49
9:Q:165:THR:OG1	9:Q:166:ILE:N	2.46	0.48
5:E:139:GLN:NE2	5:E:444:GLU:OE2	2.46	0.48
6:F:271:VAL:HA	6:F:274:ILE:HG12	1.93	0.48
4:L:168:THR:O	4:L:172:ASN:ND2	2.46	0.48
8:P:27:GLU:HB2	8:P:31:ARG:HB2	1.94	0.48
2:B:237:ILE:HD13	2:B:323:LEU:HD21	1.96	0.48
7:G:53:ARG:HH21	7:G:55:LYS:HB3	1.77	0.48
1:I:260:LEU:HD11	3:K:281:ASP:HA	1.95	0.48
6:N:350:VAL:HG22	6:N:363:ILE:HG22	1.95	0.48
2:B:182:LEU:HD21	2:B:373:ILE:HG21	1.95	0.48
3:C:244:SER:HB3	3:C:335:PRO:HB3	1.94	0.48
4:L:269:TYR:O	4:L:271:GLN:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:175:SER:HB2	6:N:206:LEU:HD11	1.96	0.48
7:O:51:ASP:OD1	7:O:51:ASP:N	2.47	0.48
2:J:182:LEU:HD21	2:J:373:ILE:HG21	1.96	0.48
3:K:339:ARG:HG3	3:K:341:ASP:H	1.79	0.48
5:M:57:LEU:O	5:M:72:ASN:ND2	2.41	0.48
6:N:144:ASP:OD1	6:N:144:ASP:N	2.47	0.48
7:O:243:GLU:HG2	7:O:293:LEU:H	1.78	0.48
3:C:162:THR:OG1	3:C:163:LYS:N	2.46	0.48
3:C:393:ASP:OD1	3:C:394:ALA:N	2.46	0.48
8:P:149:CYS:SG	8:P:150:SER:N	2.87	0.48
9:R:170:LEU:HB3	9:R:173:ASP:HB2	1.96	0.48
5:E:52:LEU:O	5:E:465:ASN:ND2	2.47	0.48
5:E:469:ASN:ND2	5:E:472:GLN:OE1	2.46	0.48
1:I:289:THR:OG1	1:I:290:GLY:N	2.47	0.48
6:N:488:VAL:HG12	6:N:490:ALA:H	1.78	0.48
1:A:132:ILE:HD11	1:A:419:LEU:HD11	1.96	0.48
6:F:488:VAL:HG12	6:F:490:ALA:H	1.78	0.48
7:O:187:ASP:OD2	7:O:397:ARG:NH2	2.46	0.48
4:D:189:ASN:O	4:D:193:LYS:NZ	2.47	0.48
8:H:17:GLU:OE2	8:H:23:SER:OG	2.27	0.48
3:K:393:ASP:OD1	3:K:394:ALA:N	2.46	0.48
4:L:307:ASP:OD1	4:L:307:ASP:N	2.44	0.48
1:A:236:CYS:HA	1:A:287:LEU:HB2	1.95	0.47
2:B:159:LEU:HD11	2:B:397:LEU:HD21	1.95	0.47
5:E:289:ILE:HA	5:E:292:ILE:HG12	1.94	0.47
1:I:42:ASP:HA	1:I:56:ASN:HB3	1.95	0.47
5:M:38:ILE:HD12	5:M:117:LEU:HB3	1.95	0.47
9:Q:189:LEU:HD21	9:Q:193:GLU:HB2	1.96	0.47
1:I:236:CYS:HA	1:I:287:LEU:HB2	1.96	0.47
7:O:237:ILE:HA	7:O:288:VAL:HB	1.96	0.47
7:G:237:ILE:HA	7:G:288:VAL:HB	1.97	0.47
8:H:149:CYS:SG	8:H:150:SER:N	2.87	0.47
2:J:66:ASP:OD1	2:J:66:ASP:N	2.47	0.47
4:L:143:LYS:HE2	4:L:147:ILE:HD11	1.97	0.47
4:D:307:ASP:N	4:D:307:ASP:OD1	2.45	0.47
2:J:91:GLN:HE22	2:J:503:VAL:HA	1.79	0.47
1:I:235:ALA:HB3	1:I:286:ILE:HG13	1.95	0.47
1:I:396:LEU:HA	1:I:399:VAL:HG22	1.96	0.47
1:A:227:LYS:NZ	1:A:231:ASN:OD1	2.48	0.47
2:B:316:ASP:OD1	2:B:316:ASP:N	2.47	0.47
4:D:478:THR:HG21	5:M:442:THR:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:243:GLU:HG2	7:G:293:LEU:H	1.79	0.47
1:I:139:ASN:ND2	1:I:141:ASP:O	2.48	0.47
2:J:151:ASP:HB3	2:J:154:LYS:HG2	1.96	0.47
1:I:173:VAL:HA	1:I:176:VAL:HG22	1.96	0.47
3:K:148:ASP:N	3:K:148:ASP:OD1	2.48	0.47
4:L:225:GLU:HG3	4:L:386:VAL:HB	1.96	0.47
5:M:245:ASP:N	5:M:245:ASP:OD1	2.47	0.47
6:N:24:ILE:HG13	6:N:107:ASP:HB2	1.96	0.47
5:E:298:ASN:HB3	5:E:299:LEU:H	1.53	0.47
7:G:17:GLN:HG3	7:G:518:GLU:HB3	1.97	0.47
1:A:396:LEU:HA	1:A:399:VAL:HG22	1.96	0.47
4:D:225:GLU:HG3	4:D:386:VAL:HB	1.97	0.47
5:E:38:ILE:HD12	5:E:117:LEU:HB3	1.96	0.47
7:G:189:LEU:O	7:G:397:ARG:NH2	2.47	0.47
1:I:222:SER:HB2	1:I:309:ARG:HH21	1.80	0.47
4:L:183:LEU:HD22	4:L:404:SER:HB2	1.97	0.47
8:P:93:GLN:HB2	8:P:510:LEU:HD12	1.97	0.47
1:A:222:SER:HB2	1:A:309:ARG:HH21	1.80	0.46
3:C:148:ASP:OD1	3:C:148:ASP:N	2.48	0.46
4:D:202:SER:OG	4:D:204:ASP:OD1	2.33	0.46
6:F:350:VAL:HG22	6:F:363:ILE:HG22	1.95	0.46
4:L:435:ARG:HA	4:L:435:ARG:HD3	1.67	0.46
2:J:64:THR:OG1	2:J:66:ASP:OD1	2.32	0.46
4:L:202:SER:OG	4:L:204:ASP:OD1	2.33	0.46
2:B:64:THR:OG1	2:B:66:ASP:OD1	2.33	0.46
2:B:326:VAL:HG23	2:B:327:THR:HG23	1.97	0.46
1:I:99:GLU:HA	1:I:102:LYS:HE3	1.98	0.46
6:F:213:ASP:N	6:F:213:ASP:OD1	2.44	0.46
8:H:114:LEU:HB3	8:H:440:LYS:HD2	1.96	0.46
8:H:241:VAL:HA	8:H:292:VAL:HB	1.97	0.46
8:P:241:VAL:HA	8:P:292:VAL:HB	1.97	0.46
1:A:235:ALA:HB3	1:A:286:ILE:HG13	1.96	0.46
8:H:217:VAL:HG23	8:H:375:ILE:HG22	1.97	0.46
7:O:200:VAL:HG21	7:O:373:ILE:HG23	1.97	0.46
2:B:66:ASP:OD1	2:B:66:ASP:N	2.49	0.46
5:E:245:ASP:N	5:E:245:ASP:OD1	2.47	0.46
1:A:187:GLN:HE22	1:A:189:ARG:HH11	1.64	0.46
6:N:196:MET:SD	6:N:377:LYS:NZ	2.77	0.46
7:O:142:THR:OG1	7:O:403:ASP:OD1	2.34	0.46
7:O:214:VAL:HG21	7:O:322:THR:HA	1.98	0.46
3:K:162:THR:OG1	3:K:163:LYS:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:176:LYS:NZ	5:M:397:GLU:OE2	2.49	0.46
9:R:117:LEU:HG	9:R:147:ILE:HB	1.98	0.46
8:H:93:GLN:HB2	8:H:510:LEU:HD12	1.98	0.45
8:P:405:ASP:OD1	8:P:405:ASP:N	2.38	0.45
5:M:298:ASN:HB3	5:M:299:LEU:H	1.53	0.45
8:P:217:VAL:HG23	8:P:375:ILE:HG22	1.97	0.45
2:B:270:ALA:O	2:B:273:GLU:HG3	2.16	0.45
4:D:143:LYS:HE2	4:D:147:ILE:HD11	1.97	0.45
2:J:270:ALA:O	2:J:273:GLU:HG3	2.15	0.45
1:I:187:GLN:HE22	1:I:189:ARG:HH11	1.64	0.45
8:P:401:VAL:HG11	8:P:406:LYS:HG2	1.99	0.45
1:A:99:GLU:HA	1:A:102:LYS:HE3	1.98	0.45
5:E:481:GLN:NE2	5:E:489:LEU:O	2.49	0.45
5:M:123:LEU:HG	5:M:128:ILE:HD12	1.99	0.45
2:B:233:GLU:O	2:B:288:ASN:ND2	2.49	0.45
5:E:442:THR:HG23	5:E:443:LEU:HD23	1.98	0.45
6:F:175:SER:HB2	6:F:206:LEU:HD11	1.98	0.45
1:I:245:LYS:HA	1:I:250:VAL:HG21	1.98	0.45
7:O:407:ALA:HA	7:O:493:TRP:HD1	1.81	0.45
6:F:24:ILE:HG13	6:F:107:ASP:HB2	1.98	0.45
6:N:292:ILE:HD13	6:N:313:LEU:HB2	1.98	0.45
8:H:401:VAL:HG11	8:H:406:LYS:HG2	1.99	0.44
1:I:199:LYS:HE2	1:I:382:ASP:HA	1.99	0.44
3:K:273:GLU:HA	3:K:276:GLN:HB2	1.98	0.44
5:M:52:LEU:O	5:M:465:ASN:ND2	2.50	0.44
7:O:238:ALA:HB3	7:O:289:VAL:HA	1.99	0.44
2:B:259:ASP:OD1	2:B:259:ASP:N	2.51	0.44
5:E:176:LYS:NZ	5:E:397:GLU:OE2	2.50	0.44
3:K:51:LEU:HD23	6:N:521:ILE:HG22	1.98	0.44
2:J:135:LYS:HD3	2:J:138:ARG:HH21	1.81	0.44
3:K:366:CYS:HB3	3:K:367:LYS:H	1.64	0.44
1:A:139:ASN:ND2	1:A:141:ASP:O	2.50	0.44
2:B:135:LYS:HD3	2:B:138:ARG:HH21	1.82	0.44
8:H:190:ILE:HG23	8:H:371:ALA:HB3	2.00	0.44
4:L:268:ASP:OD2	4:L:268:ASP:N	2.46	0.44
4:D:60:MET:HG3	4:D:70:ILE:HG12	1.99	0.44
1:I:308:VAL:HG11	1:I:362:ILE:HD11	1.99	0.44
7:G:47:LYS:HD2	7:G:65:ILE:HD13	1.99	0.44
7:G:238:ALA:HB3	7:G:289:VAL:HA	1.99	0.44
5:E:52:LEU:HD11	5:E:111:VAL:HG21	2.00	0.44
2:J:233:GLU:O	2:J:288:ASN:ND2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:316:ASP:N	2:J:316:ASP:OD1	2.50	0.44
1:A:406:LYS:HD2	1:A:406:LYS:HA	1.73	0.43
3:C:52:ASP:HB2	3:C:56:GLY:H	1.83	0.43
3:C:354:LYS:HD2	3:C:354:LYS:HA	1.77	0.43
4:D:212:LYS:HB3	4:D:398:ILE:HD11	1.99	0.43
7:G:74:PRO:HB3	8:H:63:LEU:HD11	1.99	0.43
7:G:147:ASP:N	7:G:147:ASP:OD1	2.50	0.43
1:I:406:LYS:HD2	1:I:406:LYS:HA	1.73	0.43
7:O:67:LYS:HB2	7:O:67:LYS:HE3	1.81	0.43
8:P:348:ASP:OD1	8:P:348:ASP:N	2.51	0.43
9:Q:201:SER:OG	9:Q:202:GLY:N	2.51	0.43
9:R:110:GLY:H	9:R:171:GLU:HB3	1.83	0.43
3:C:239:VAL:H	3:C:287:PRO:HB3	1.83	0.43
6:F:144:ASP:N	6:F:144:ASP:OD1	2.49	0.43
2:J:154:LYS:O	2:J:157:GLN:HG3	2.18	0.43
4:L:212:LYS:HB3	4:L:398:ILE:HD11	2.00	0.43
5:M:368:LYS:HD2	5:M:368:LYS:HA	1.76	0.43
8:P:190:ILE:HG23	8:P:371:ALA:HB3	2.00	0.43
7:G:200:VAL:HG21	7:G:373:ILE:HG23	2.01	0.43
8:H:355:VAL:O	8:H:358:THR:OG1	2.25	0.43
8:H:401:VAL:HG13	8:H:403:THR:H	1.83	0.43
3:K:52:ASP:N	3:K:56:GLY:O	2.46	0.43
5:M:252:THR:OG1	5:M:342:VAL:O	2.37	0.43
6:N:31:GLN:HG3	6:N:97:LEU:HA	2.00	0.43
1:I:49:ILE:HA	9:R:125:PRO:HB3	2.00	0.43
4:L:280:ARG:HE	4:L:280:ARG:HB2	1.70	0.43
7:O:17:GLN:HG3	7:O:518:GLU:HB3	1.98	0.43
7:O:281:ILE:HA	7:O:337:LEU:HD21	2.00	0.43
1:A:199:LYS:HE2	1:A:382:ASP:HA	1.99	0.43
5:E:445:GLN:HB3	5:E:449:ARG:HH21	1.83	0.43
8:H:381:THR:HG23	8:H:383:ASN:H	1.83	0.43
2:J:288:ASN:N	2:J:288:ASN:OD1	2.51	0.43
3:K:354:LYS:HD2	3:K:354:LYS:HA	1.77	0.43
4:L:243:LYS:C	4:L:245:LYS:H	2.22	0.43
2:B:61:LEU:HD23	2:B:61:LEU:HA	1.88	0.43
3:C:137:LEU:HD12	3:C:137:LEU:HA	1.84	0.43
5:E:460:MET:HG3	5:E:470:PRO:HB2	2.00	0.43
7:G:142:THR:OG1	7:G:403:ASP:OD1	2.36	0.43
7:G:218:LYS:HD3	7:G:356:GLU:HA	2.01	0.43
8:P:381:THR:HG23	8:P:383:ASN:H	1.83	0.43
5:E:84:ASP:OD1	5:E:84:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:271:TRP:HD1	7:G:274:LEU:HD12	1.84	0.43
7:G:407:ALA:HA	7:G:493:TRP:HD1	1.82	0.43
8:H:348:ASP:N	8:H:348:ASP:OD1	2.51	0.43
2:J:259:ASP:OD1	2:J:259:ASP:N	2.50	0.43
3:C:197:LYS:HE2	3:C:197:LYS:HB2	1.90	0.43
7:G:306:ARG:HB3	7:G:308:MET:HG2	2.00	0.43
3:K:383:ILE:O	3:K:386:GLU:HG3	2.19	0.43
7:O:47:LYS:HD2	7:O:65:ILE:HD13	2.01	0.43
9:R:94:VAL:HG11	9:R:148:LYS:HE2	2.00	0.43
3:C:58:VAL:HG21	9:Q:216:ILE:HG13	2.00	0.43
5:E:252:THR:OG1	5:E:342:VAL:O	2.36	0.43
7:O:306:ARG:HB3	7:O:308:MET:HG2	2.00	0.43
7:O:352:GLN:HB3	7:O:357:ARG:HG3	2.01	0.43
7:O:401:LYS:HD3	7:O:401:LYS:HA	1.89	0.43
3:C:234:LYS:HA	3:C:234:LYS:HD2	1.84	0.43
3:C:282:ILE:HD11	3:C:338:LEU:H	1.84	0.43
9:Q:119:LEU:HD13	9:Q:119:LEU:HA	1.92	0.43
7:G:14:ASP:OD1	7:G:14:ASP:N	2.47	0.42
7:G:67:LYS:HB2	7:G:67:LYS:HE3	1.81	0.42
4:L:406:HIS:O	4:L:409:LEU:HD23	2.19	0.42
6:N:349:LEU:HB3	6:N:364:GLU:HG2	2.00	0.42
7:O:53:ARG:HH21	7:O:55:LYS:HB3	1.83	0.42
7:O:147:ASP:N	7:O:147:ASP:OD1	2.51	0.42
2:B:154:LYS:O	2:B:157:GLN:HG3	2.18	0.42
2:B:288:ASN:N	2:B:288:ASN:OD1	2.51	0.42
1:I:216:LEU:HB2	1:I:362:ILE:HD12	2.02	0.42
3:K:234:LYS:HA	3:K:234:LYS:HD2	1.84	0.42
8:P:401:VAL:HG13	8:P:403:THR:H	1.84	0.42
9:Q:213:LYS:O	9:Q:214:LYS:HG2	2.20	0.42
4:D:243:LYS:C	4:D:245:LYS:H	2.22	0.42
4:L:321:LYS:HE3	4:L:323:MET:HB2	2.01	0.42
6:N:131:LEU:HD23	6:N:131:LEU:HA	1.91	0.42
7:G:401:LYS:HD3	7:G:401:LYS:HA	1.90	0.42
8:P:303:HIS:CE1	8:P:307:LYS:HD2	2.55	0.42
1:A:216:LEU:HB2	1:A:362:ILE:HD12	2.01	0.42
3:C:130:LEU:HB2	3:C:510:VAL:HG21	2.02	0.42
6:F:411:ALA:HB2	6:F:494:VAL:HG11	2.02	0.42
7:G:287:LYS:HB2	7:G:287:LYS:HE3	1.80	0.42
1:I:216:LEU:HB3	1:I:217:ASN:H	1.71	0.42
3:K:403:LEU:HD23	3:K:403:LEU:HA	1.92	0.42
5:M:52:LEU:HD11	5:M:111:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:ALA:HB1	9:Q:216:ILE:HG21	2.01	0.42
3:C:383:ILE:O	3:C:386:GLU:HG3	2.19	0.42
6:F:31:GLN:HG3	6:F:97:LEU:HA	2.00	0.42
7:G:255:ILE:HD12	7:G:255:ILE:HA	1.92	0.42
2:J:391:HIS:O	2:J:394:LEU:HD23	2.20	0.42
7:O:271:TRP:HD1	7:O:274:LEU:HD12	1.85	0.42
7:O:356:GLU:OE2	7:O:375:ARG:NH1	2.43	0.42
3:C:366:CYS:HB3	3:C:367:LYS:H	1.64	0.42
4:D:167:ALA:O	4:D:171:LEU:HB2	2.18	0.42
7:G:281:ILE:HA	7:G:337:LEU:HD21	2.02	0.42
8:H:165:ARG:HE	8:H:177:VAL:HG13	1.84	0.42
2:J:25:ARG:NH2	2:J:519:ASN:O	2.52	0.42
4:D:268:ASP:OD2	4:D:268:ASP:N	2.46	0.42
4:D:321:LYS:HE3	4:D:323:MET:HB2	2.01	0.42
4:D:472:ASN:ND2	4:D:475:SER:OG	2.49	0.42
7:G:278:LEU:HA	7:G:281:ILE:HG12	2.01	0.42
1:A:448:ILE:HB	1:A:449:PRO:HD3	2.02	0.42
2:B:391:HIS:O	2:B:394:LEU:HD23	2.20	0.42
4:D:406:HIS:O	4:D:409:LEU:HD23	2.20	0.42
4:D:412:ILE:HD13	4:D:412:ILE:HA	1.94	0.42
2:J:91:GLN:O	2:J:95:VAL:HG22	2.19	0.42
8:P:145:ASN:HD22	8:P:145:ASN:HA	1.75	0.42
4:D:202:SER:HB3	4:D:413:ARG:HG3	2.02	0.42
4:D:274:ARG:HA	4:D:274:ARG:HD3	1.69	0.42
5:E:58:ASP:OD1	5:E:58:ASP:N	2.49	0.42
6:F:284:ASP:N	6:F:284:ASP:OD1	2.53	0.42
8:H:33:ILE:HG23	8:H:112:LEU:HB3	2.02	0.42
8:H:393:ASP:OD1	8:H:394:ASP:N	2.52	0.42
9:R:213:LYS:HA	9:R:213:LYS:HD2	1.81	0.42
1:A:234:ILE:HG22	1:A:285:VAL:HB	2.01	0.41
5:E:368:LYS:HD2	5:E:368:LYS:HA	1.77	0.41
8:H:303:HIS:CE1	8:H:307:LYS:HD2	2.55	0.41
3:K:243:SER:HB2	3:K:291:ILE:HG12	2.02	0.41
5:M:132:ARG:NH1	7:O:454:GLY:O	2.45	0.41
2:B:245:ASP:OD1	2:B:245:ASP:N	2.54	0.41
5:E:57:LEU:O	5:E:72:ASN:ND2	2.49	0.41
3:K:187:GLU:H	3:K:187:GLU:HG3	1.70	0.41
6:N:49:SER:HB3	8:P:528:LYS:HB2	2.02	0.41
6:N:411:ALA:HB2	6:N:494:VAL:HG11	2.01	0.41
1:A:205:GLN:HA	1:A:378:ARG:HG3	2.02	0.41
1:A:308:VAL:HG11	1:A:362:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:116:LEU:HD12	2:J:116:LEU:HA	1.95	0.41
3:K:160:ILE:HD12	3:K:160:ILE:HA	1.87	0.41
5:M:84:ASP:N	5:M:84:ASP:OD1	2.52	0.41
7:O:278:LEU:HA	7:O:281:ILE:HG12	2.01	0.41
1:A:216:LEU:HB3	1:A:217:ASN:H	1.71	0.41
4:D:217:THR:HG22	4:D:219:ASP:H	1.85	0.41
4:D:242:GLU:HB3	4:D:359:ALA:HB1	2.02	0.41
5:E:485:MET:HB3	5:E:486:ASN:H	1.71	0.41
1:I:205:GLN:HA	1:I:378:ARG:HG3	2.03	0.41
4:L:242:GLU:HB3	4:L:359:ALA:HB1	2.02	0.41
5:M:336:ALA:HB1	5:M:374:ILE:HG21	2.02	0.41
9:Q:159:PRO:HB2	9:Q:160:ASP:H	1.67	0.41
2:B:221:ASP:OD1	2:B:221:ASP:N	2.54	0.41
4:D:183:LEU:HD22	4:D:404:SER:HB2	2.02	0.41
2:J:135:LYS:HB2	2:J:135:LYS:HE2	1.88	0.41
6:N:284:ASP:OD1	6:N:284:ASP:N	2.53	0.41
8:P:53:ASN:HB3	8:P:65:VAL:HB	2.02	0.41
8:P:393:ASP:OD1	8:P:394:ASP:N	2.53	0.41
4:L:188:VAL:HA	4:L:191:VAL:HG12	2.03	0.41
7:O:255:ILE:HD12	7:O:255:ILE:HA	1.93	0.41
7:G:347:VAL:HB	7:G:362:THR:O	2.21	0.41
2:J:245:ASP:N	2:J:245:ASP:OD1	2.54	0.41
4:L:167:ALA:O	4:L:171:LEU:HB2	2.20	0.41
5:M:496:LYS:HB3	5:M:497:GLY:H	1.68	0.41
8:P:165:ARG:HE	8:P:177:VAL:HG13	1.84	0.41
5:E:225:ILE:HD11	5:E:386:PHE:HB2	2.02	0.41
2:J:221:ASP:OD1	2:J:221:ASP:N	2.54	0.41
2:B:203:LYS:HD3	2:B:383:LEU:HD22	2.03	0.41
2:B:220:LEU:HB3	2:B:221:ASP:H	1.60	0.41
4:D:145:ILE:HD12	4:D:516:VAL:HG22	2.02	0.41
4:D:533:ASP:OD1	4:D:533:ASP:N	2.54	0.41
5:E:336:ALA:HB1	5:E:374:ILE:HG21	2.02	0.41
6:F:131:LEU:HD23	6:F:131:LEU:HA	1.91	0.41
8:H:466:LYS:O	8:H:470:VAL:HG23	2.21	0.41
4:L:145:ILE:HD12	4:L:516:VAL:HG22	2.02	0.41
7:O:90:VAL:HG11	7:O:498:VAL:HG13	2.03	0.41
9:R:98:SER:HG	9:R:99:GLY:H	1.65	0.41
4:D:249:ILE:HD13	4:D:298:LEU:HD22	2.02	0.41
4:D:280:ARG:HE	4:D:280:ARG:HB2	1.71	0.41
1:I:208:SER:HA	1:I:378:ARG:HH21	1.86	0.41
2:J:203:LYS:HD3	2:J:383:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:130:LEU:HB2	3:K:510:VAL:HG21	2.02	0.41
3:K:339:ARG:HB3	3:K:342:ASP:HB3	2.03	0.41
5:M:157:VAL:HG23	5:M:159:ILE:H	1.86	0.41
7:O:170:GLN:H	7:O:170:GLN:HG2	1.66	0.41
2:B:43:LEU:HD23	2:B:43:LEU:HA	1.92	0.40
3:C:157:ASN:O	3:C:161:THR:OG1	2.33	0.40
5:E:257:PRO:HA	5:E:258:PRO:HD3	1.89	0.40
1:I:448:ILE:HB	1:I:449:PRO:HD3	2.02	0.40
2:J:119:LYS:HD3	2:J:119:LYS:HA	1.82	0.40
4:L:54:PRO:HG2	4:L:495:VAL:HG11	2.03	0.40
5:M:242:LYS:HA	5:M:242:LYS:HD3	1.88	0.40
8:P:114:LEU:HB3	8:P:440:LYS:HD2	2.02	0.40
9:R:190:THR:OG1	9:R:191:ARG:N	2.53	0.40
1:A:208:SER:HA	1:A:378:ARG:HH21	1.87	0.40
3:C:243:SER:HB2	3:C:291:ILE:HG12	2.03	0.40
5:E:133:ILE:HG22	5:E:447:ALA:HB2	2.03	0.40
5:E:157:VAL:HG23	5:E:159:ILE:H	1.86	0.40
8:H:73:LEU:HD23	8:H:73:LEU:HA	1.96	0.40
2:J:220:LEU:HB3	2:J:221:ASP:H	1.60	0.40
2:J:238:LEU:HA	2:J:343:LEU:HD13	2.03	0.40
4:L:249:ILE:HD13	4:L:298:LEU:HD22	2.02	0.40
6:N:176:ILE:HG13	6:N:398:VAL:HG11	2.04	0.40
8:P:29:VAL:HG12	8:P:116:GLU:HG3	2.03	0.40
1:A:238:ASP:N	1:A:238:ASP:OD1	2.45	0.40
1:A:431:GLY:HA3	7:O:466:ALA:HB2	2.04	0.40
4:D:188:VAL:HA	4:D:191:VAL:HG12	2.02	0.40
6:F:176:ILE:HG13	6:F:398:VAL:HG11	2.02	0.40
3:K:23:GLN:NE2	3:K:519:ILE:O	2.55	0.40
4:L:202:SER:HB3	4:L:413:ARG:HG3	2.03	0.40
5:M:257:PRO:HA	5:M:258:PRO:HD3	1.89	0.40
8:P:249:MET:HG3	8:P:250:ILE:HG13	2.03	0.40
8:P:466:LYS:O	8:P:470:VAL:HG23	2.21	0.40
9:Q:169:TYR:HE1	9:Q:174:ILE:HG12	1.86	0.40
2:B:77:ASP:HA	2:B:82:LYS:HE3	2.03	0.40
4:D:208:ILE:HD13	4:D:208:ILE:HA	1.98	0.40
4:D:423:ALA:HB1	4:D:503:ILE:HG21	2.04	0.40
6:F:455:SER:HB2	6:F:481:LEU:HD22	2.03	0.40
1:I:234:ILE:HG22	1:I:285:VAL:HB	2.02	0.40
4:L:533:ASP:OD1	4:L:533:ASP:N	2.54	0.40
2:B:281:ARG:O	2:B:285:HIS:ND1	2.44	0.40
3:C:334:ARG:HH21	3:C:338:LEU:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:323:ARG:HB3	5:E:324:TRP:H	1.71	0.40
5:E:535:LYS:HB2	5:E:536:PRO:HD3	2.03	0.40
6:F:430:LYS:HA	6:F:430:LYS:HD2	1.98	0.40
8:H:249:MET:HG3	8:H:250:ILE:HG13	2.03	0.40
2:J:326:VAL:HG23	2:J:327:THR:HG23	2.02	0.40
4:L:217:THR:HG22	4:L:219:ASP:H	1.85	0.40
4:L:248:LEU:HD21	4:L:344:PRO:HA	2.03	0.40
5:M:225:ILE:HD11	5:M:386:PHE:HB2	2.02	0.40
5:M:460:MET:HG3	5:M:470:PRO:HB2	2.02	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	519/556 (93%)	456 (88%)	57 (11%)	6 (1%)	13	44
1	I	519/556 (93%)	459 (88%)	54 (10%)	6 (1%)	13	44
2	B	497/535 (93%)	441 (89%)	55 (11%)	1 (0%)	47	79
2	J	497/535 (93%)	450 (90%)	47 (10%)	0	100	100
3	C	505/545 (93%)	419 (83%)	84 (17%)	2 (0%)	34	69
3	K	505/545 (93%)	420 (83%)	82 (16%)	3 (1%)	25	59
4	D	512/539 (95%)	429 (84%)	78 (15%)	5 (1%)	15	49
4	L	512/539 (95%)	432 (84%)	76 (15%)	4 (1%)	19	54
5	E	511/541 (94%)	447 (88%)	59 (12%)	5 (1%)	15	49
5	M	511/541 (94%)	443 (87%)	65 (13%)	3 (1%)	25	59
6	F	514/531 (97%)	457 (89%)	54 (10%)	3 (1%)	25	59
6	N	514/531 (97%)	454 (88%)	57 (11%)	3 (1%)	25	59
7	G	510/543 (94%)	466 (91%)	41 (8%)	3 (1%)	25	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	O	510/543 (94%)	467 (92%)	41 (8%)	2 (0%)	34 69
8	H	515/548 (94%)	443 (86%)	64 (12%)	8 (2%)	9 37
8	P	515/548 (94%)	441 (86%)	67 (13%)	7 (1%)	11 40
9	Q	141/239 (59%)	120 (85%)	20 (14%)	1 (1%)	22 57
9	R	140/239 (59%)	118 (84%)	21 (15%)	1 (1%)	22 57
All	All	8447/9154 (92%)	7362 (87%)	1022 (12%)	63 (1%)	26 57

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	THR
4	D	270	ALA
5	E	532	ASP
7	G	149	VAL
4	L	270	ALA
5	M	532	ASP
7	O	149	VAL
9	Q	159	PRO
1	A	186	GLY
1	A	369	ALA
3	C	472	GLN
4	D	321	LYS
5	E	317	ASN
5	E	423	GLY
6	F	226	GLU
1	I	186	GLY
1	I	281	THR
1	I	369	ALA
3	K	472	GLN
4	L	321	LYS
5	M	319	LEU
6	N	226	GLU
4	D	269	TYR
6	F	49	SER
7	G	217	LYS
8	H	30	TYR
8	H	96	GLU
8	H	470	VAL
4	L	269	TYR
8	P	96	GLU

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Mol	Chain	Res	Type
8	P	470	VAL
4	D	533	ASP
5	E	319	LEU
5	E	441	PRO
5	M	441	PRO
6	N	49	SER
8	P	523	GLN
1	A	162	GLY
3	C	140	ILE
8	H	243	SER
1	I	162	GLY
3	K	140	ILE
8	P	30	TYR
8	P	243	SER
2	B	95	VAL
8	H	122	GLY
9	R	185	GLY
6	F	493	GLY
7	G	523	PRO
3	K	335	PRO
4	L	127	GLY
6	N	493	GLY
8	P	122	GLY
8	H	457	GLY
1	I	282	GLY
1	A	282	GLY
4	D	127	GLY
8	H	248	GLY
7	O	523	PRO
8	P	248	GLY
1	A	191	PRO
8	H	29	VAL
1	I	191	PRO

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	434/463 (94%)	430 (99%)	4 (1%)	78	91
1	I	434/463 (94%)	428 (99%)	6 (1%)	67	86
2	B	399/427 (93%)	394 (99%)	5 (1%)	69	87
2	J	399/427 (93%)	395 (99%)	4 (1%)	76	90
3	C	439/469 (94%)	431 (98%)	8 (2%)	59	82
3	K	439/469 (94%)	430 (98%)	9 (2%)	53	79
4	D	439/452 (97%)	427 (97%)	12 (3%)	44	74
4	L	439/452 (97%)	425 (97%)	14 (3%)	39	69
5	E	432/456 (95%)	423 (98%)	9 (2%)	53	79
5	M	432/456 (95%)	423 (98%)	9 (2%)	53	79
6	F	431/442 (98%)	423 (98%)	8 (2%)	57	81
6	N	431/442 (98%)	423 (98%)	8 (2%)	57	81
7	G	420/443 (95%)	414 (99%)	6 (1%)	67	86
7	O	420/443 (95%)	414 (99%)	6 (1%)	67	86
8	H	428/452 (95%)	424 (99%)	4 (1%)	78	91
8	P	428/452 (95%)	424 (99%)	4 (1%)	78	91
9	Q	126/215 (59%)	125 (99%)	1 (1%)	81	92
9	R	125/215 (58%)	124 (99%)	1 (1%)	81	92
All	All	7095/7638 (93%)	6977 (98%)	118 (2%)	62	83

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	177	LEU
1	A	256	ASP
1	A	274	ARG
2	B	78	ASN
2	B	334	THR
2	B	384	ASP
2	B	394	LEU
2	B	396	VAL
3	C	111	HIS
3	C	188	ASN
3	C	228	ARG
3	C	266	ARG
3	C	320	ASN

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Mol	Chain	Res	Type
3	C	322	ARG
3	C	342	ASP
3	C	499	LEU
4	D	219	ASP
4	D	220	ASP
4	D	227	LEU
4	D	240	ARG
4	D	273	ASP
4	D	310	SER
4	D	336	ILE
4	D	409	LEU
4	D	416	VAL
4	D	419	ARG
4	D	454	PHE
4	D	509	VAL
5	E	51	SER
5	E	124	LEU
5	E	200	GLU
5	E	290	GLN
5	E	291	GLN
5	E	372	LEU
5	E	435	GLN
5	E	484	GLU
5	E	506	VAL
6	F	137	VAL
6	F	164	LEU
6	F	181	LYS
6	F	232	THR
6	F	314	ARG
6	F	337	ASP
6	F	508	CYS
6	F	522	MET
7	G	57	THR
7	G	143	VAL
7	G	184	MET
7	G	192	LEU
7	G	267	VAL
7	G	406	VAL
8	H	22	PHE
8	H	99	ASP
8	H	296	LYS
8	H	300	MET

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Mol	Chain	Res	Type
1	I	42	ASP
1	I	167	PHE
1	I	177	LEU
1	I	231	ASN
1	I	274	ARG
1	I	409	VAL
2	J	78	ASN
2	J	384	ASP
2	J	394	LEU
2	J	396	VAL
3	K	111	HIS
3	K	188	ASN
3	K	228	ARG
3	K	265	THR
3	K	266	ARG
3	K	320	ASN
3	K	322	ARG
3	K	342	ASP
3	K	499	LEU
4	L	184	SER
4	L	219	ASP
4	L	220	ASP
4	L	227	LEU
4	L	240	ARG
4	L	273	ASP
4	L	310	SER
4	L	336	ILE
4	L	409	LEU
4	L	416	VAL
4	L	419	ARG
4	L	449	TYR
4	L	454	PHE
4	L	509	VAL
5	M	51	SER
5	M	139	GLN
5	M	200	GLU
5	M	290	GLN
5	M	291	GLN
5	M	372	LEU
5	M	435	GLN
5	M	484	GLU
5	M	506	VAL

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Mol	Chain	Res	Type
6	N	137	VAL
6	N	164	LEU
6	N	181	LYS
6	N	232	THR
6	N	314	ARG
6	N	337	ASP
6	N	349	LEU
6	N	508	CYS
7	O	57	THR
7	O	143	VAL
7	O	180	VAL
7	O	192	LEU
7	O	264	GLN
7	O	267	VAL
8	P	22	PHE
8	P	99	ASP
8	P	296	LYS
8	P	300	MET
9	Q	104	GLN
9	R	103	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	242	GLN
2	B	294	GLN
3	C	320	ASN
4	D	368	ASN
4	D	472	ASN
4	D	482	ASN
5	E	46	ASN
5	E	264	HIS
5	E	503	GLN
5	E	516	GLN
6	F	23	ASN
6	F	105	GLN
7	G	25	ASN
7	G	241	ASN
7	G	432	GLN
7	G	462	ASN
7	G	501	ASN

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Mol	Chain	Res	Type
8	H	67	ASN
8	H	95	GLN
8	H	145	ASN
8	H	185	GLN
8	H	309	ASN
1	I	20	GLN
2	J	91	GLN
2	J	294	GLN
3	K	320	ASN
4	L	368	ASN
4	L	472	ASN
4	L	482	ASN
5	M	46	ASN
5	M	503	GLN
5	M	516	GLN
6	N	23	ASN
6	N	105	GLN
7	O	25	ASN
7	O	432	GLN
7	O	448	GLN
7	O	462	ASN
7	O	501	ASN
8	P	67	ASN
8	P	95	GLN
8	P	145	ASN
8	P	185	GLN
8	P	309	ASN
9	R	132	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	ADP	N	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.40	4 (13%)
10	ADP	H	601	8	24,29,29	0.96	1 (4%)	29,45,45	1.41	4 (13%)
10	ADP	A	601	-	24,29,29	0.95	1 (4%)	29,45,45	1.44	4 (13%)
10	ADP	C	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
10	ADP	L	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.42	4 (13%)
10	ADP	I	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
10	ADP	P	601	8	24,29,29	0.97	1 (4%)	29,45,45	1.41	4 (13%)
10	ADP	K	601	-	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)
10	ADP	D	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.43	4 (13%)
10	ADP	F	601	-	24,29,29	0.95	1 (4%)	29,45,45	1.40	4 (13%)

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
10	ADP	N	601	-	-	2/12/32/32	0/3/3/3
10	ADP	H	601	8	-	2/12/32/32	0/3/3/3
10	ADP	A	601	-	-	2/12/32/32	0/3/3/3
10	ADP	C	601	-	-	1/12/32/32	0/3/3/3
10	ADP	L	601	-	-	3/12/32/32	0/3/3/3
10	ADP	I	601	-	-	1/12/32/32	0/3/3/3
10	ADP	P	601	8	-	2/12/32/32	0/3/3/3
10	ADP	K	601	-	-	2/12/32/32	0/3/3/3
10	ADP	D	601	-	-	2/12/32/32	0/3/3/3
10	ADP	F	601	-	-	2/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	601	ADP	C5-C4	2.52	1.47	1.40
10	K	601	ADP	C5-C4	2.52	1.47	1.40
10	I	601	ADP	C5-C4	2.51	1.47	1.40
10	D	601	ADP	C5-C4	2.51	1.47	1.40
10	L	601	ADP	C5-C4	2.51	1.47	1.40
10	A	601	ADP	C5-C4	2.50	1.47	1.40
10	C	601	ADP	C5-C4	2.50	1.47	1.40
10	H	601	ADP	C5-C4	2.49	1.47	1.40
10	N	601	ADP	C5-C4	2.49	1.47	1.40
10	F	601	ADP	C5-C4	2.49	1.47	1.40

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	601	ADP	PA-O3A-PB	-3.50	120.82	132.83
10	I	601	ADP	PA-O3A-PB	-3.49	120.84	132.83
10	C	601	ADP	PA-O3A-PB	-3.49	120.85	132.83
10	A	601	ADP	PA-O3A-PB	-3.48	120.87	132.83
10	L	601	ADP	PA-O3A-PB	-3.28	121.56	132.83
10	D	601	ADP	PA-O3A-PB	-3.28	121.57	132.83
10	P	601	ADP	PA-O3A-PB	-3.25	121.67	132.83
10	H	601	ADP	PA-O3A-PB	-3.25	121.68	132.83
10	C	601	ADP	C3'-C2'-C1'	3.24	105.86	100.98
10	F	601	ADP	N3-C2-N1	-3.21	123.66	128.68
10	K	601	ADP	C3'-C2'-C1'	3.21	105.81	100.98
10	L	601	ADP	N3-C2-N1	-3.21	123.66	128.68
10	D	601	ADP	C3'-C2'-C1'	3.21	105.81	100.98
10	N	601	ADP	N3-C2-N1	-3.21	123.66	128.68
10	D	601	ADP	N3-C2-N1	-3.21	123.66	128.68
10	P	601	ADP	N3-C2-N1	-3.21	123.67	128.68
10	I	601	ADP	C3'-C2'-C1'	3.21	105.81	100.98
10	L	601	ADP	C3'-C2'-C1'	3.20	105.80	100.98
10	I	601	ADP	N3-C2-N1	-3.20	123.67	128.68
10	A	601	ADP	C3'-C2'-C1'	3.20	105.79	100.98
10	C	601	ADP	N3-C2-N1	-3.18	123.70	128.68
10	H	601	ADP	N3-C2-N1	-3.17	123.72	128.68
10	N	601	ADP	C3'-C2'-C1'	3.16	105.74	100.98
10	K	601	ADP	N3-C2-N1	-3.16	123.74	128.68
10	F	601	ADP	C3'-C2'-C1'	3.16	105.73	100.98
10	A	601	ADP	N3-C2-N1	-3.15	123.75	128.68
10	H	601	ADP	C3'-C2'-C1'	3.14	105.70	100.98
10	P	601	ADP	C3'-C2'-C1'	3.09	105.64	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	N	601	ADP	PA-O3A-PB	-3.00	122.52	132.83
10	F	601	ADP	PA-O3A-PB	-2.99	122.55	132.83
10	I	601	ADP	C4-C5-N7	-2.75	106.53	109.40
10	K	601	ADP	C4-C5-N7	-2.73	106.55	109.40
10	A	601	ADP	C4-C5-N7	-2.73	106.56	109.40
10	H	601	ADP	C4-C5-N7	-2.72	106.57	109.40
10	L	601	ADP	C4-C5-N7	-2.72	106.57	109.40
10	D	601	ADP	C4-C5-N7	-2.72	106.57	109.40
10	C	601	ADP	C4-C5-N7	-2.71	106.57	109.40
10	P	601	ADP	C4-C5-N7	-2.71	106.58	109.40
10	N	601	ADP	C4-C5-N7	-2.67	106.62	109.40
10	F	601	ADP	C4-C5-N7	-2.65	106.64	109.40

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	F	601	ADP	C3'-C4'-C5'-O5'
10	N	601	ADP	C3'-C4'-C5'-O5'
10	F	601	ADP	O4'-C4'-C5'-O5'
10	N	601	ADP	O4'-C4'-C5'-O5'
10	D	601	ADP	PB-O3A-PA-O1A
10	D	601	ADP	PB-O3A-PA-O2A
10	H	601	ADP	PB-O3A-PA-O1A
10	H	601	ADP	PB-O3A-PA-O2A
10	L	601	ADP	PB-O3A-PA-O2A
10	P	601	ADP	PB-O3A-PA-O2A
10	L	601	ADP	PB-O3A-PA-O1A
10	P	601	ADP	PB-O3A-PA-O1A
10	A	601	ADP	C5'-O5'-PA-O1A
10	K	601	ADP	C5'-O5'-PA-O1A
10	L	601	ADP	C5'-O5'-PA-O1A
10	A	601	ADP	O4'-C4'-C5'-O5'
10	C	601	ADP	O4'-C4'-C5'-O5'
10	I	601	ADP	O4'-C4'-C5'-O5'
10	K	601	ADP	O4'-C4'-C5'-O5'

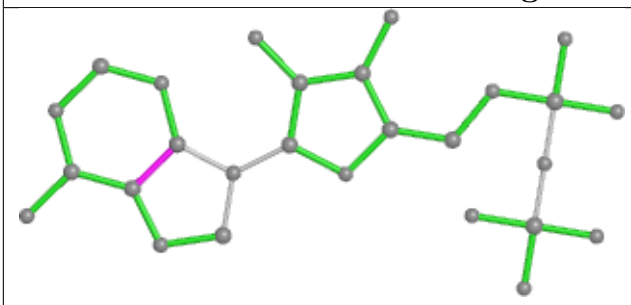
There are no ring outliers.

No monomer is involved in short contacts.

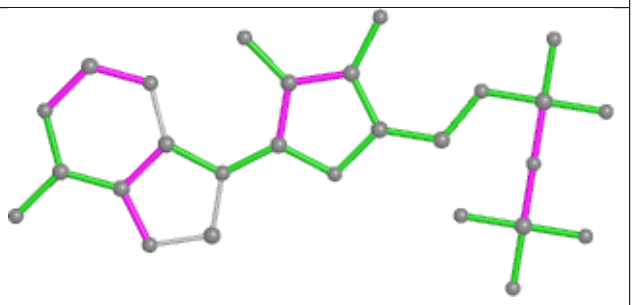
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

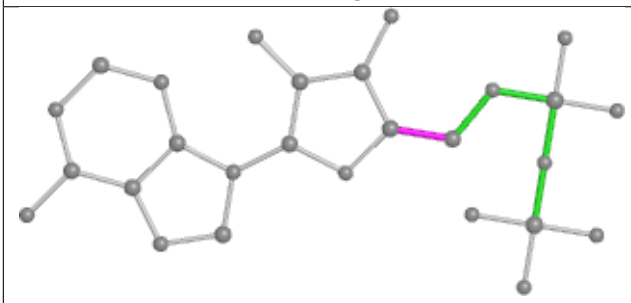
Ligand ADP N 601



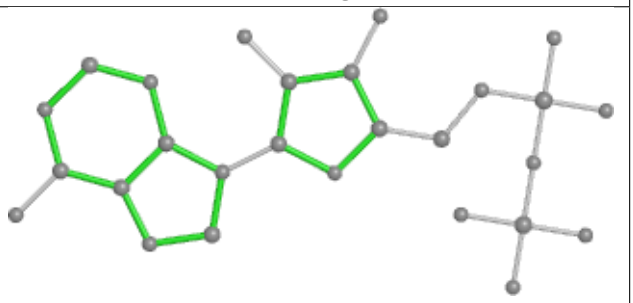
Bond lengths



Bond angles

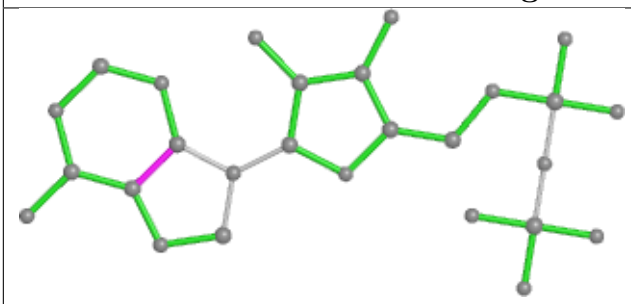


Torsions



Rings

Ligand ADP H 601



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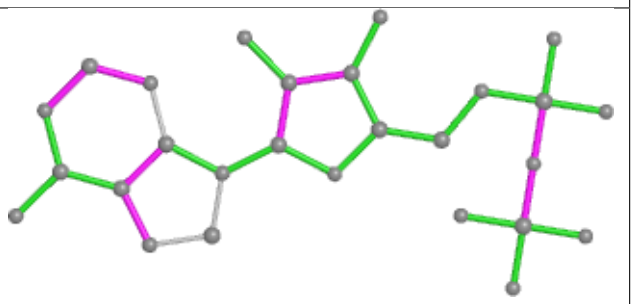

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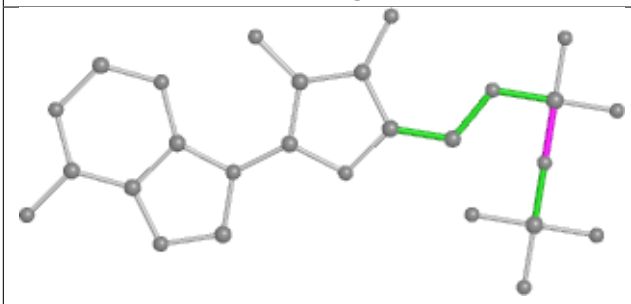

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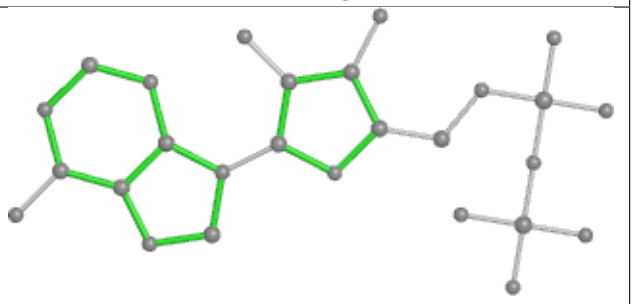
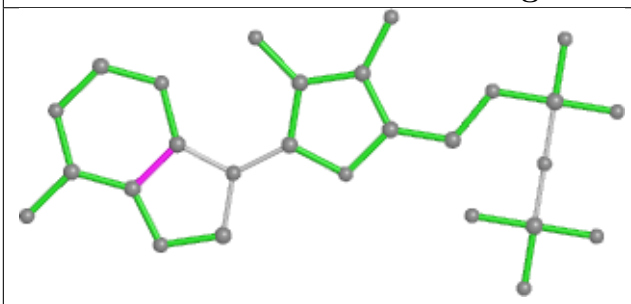


Rings

Ligand ADP A 601



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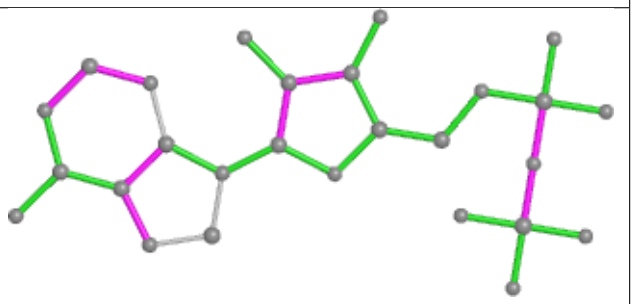

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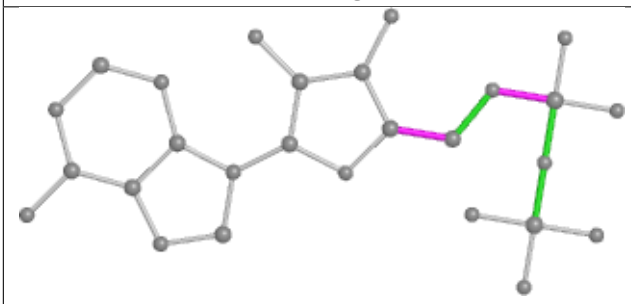

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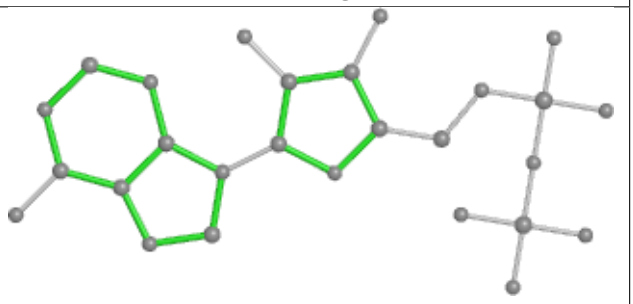
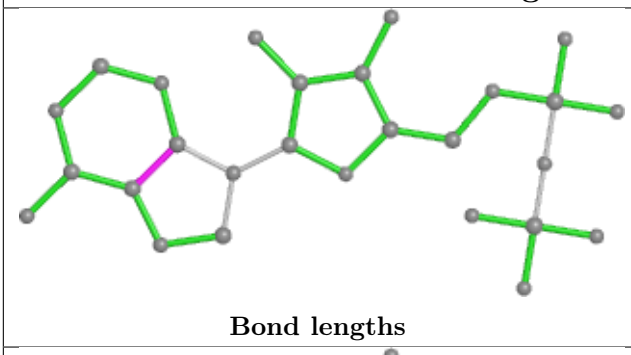


Rings

Ligand ADP C 601



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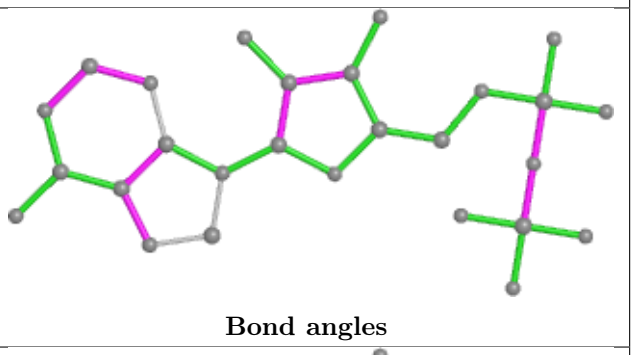

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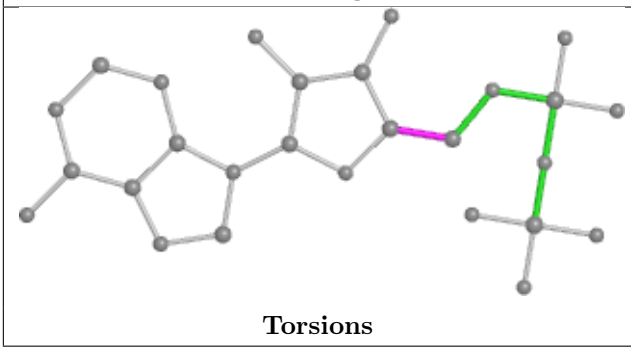

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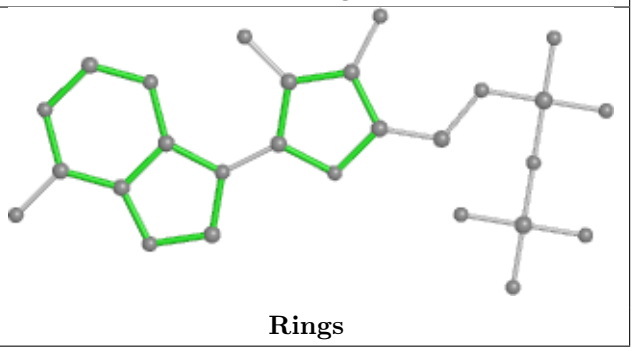
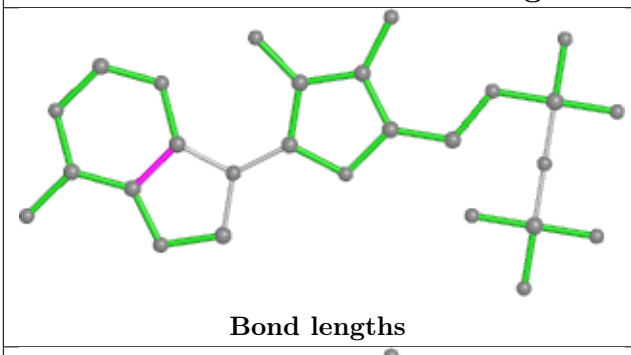
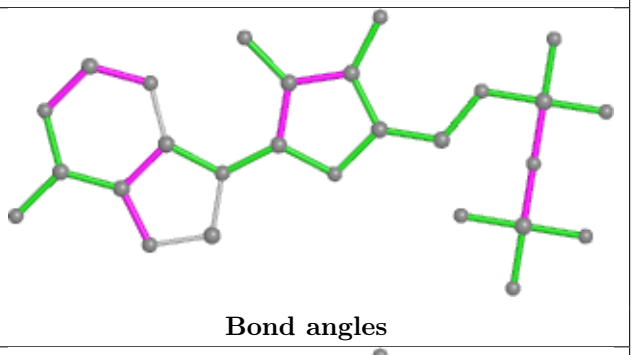


Rings

Ligand ADP L 601



Bond lengths



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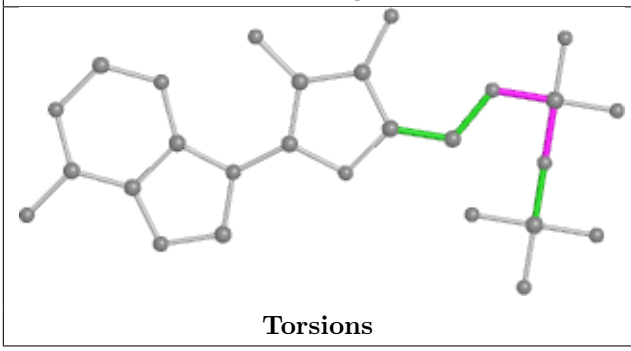

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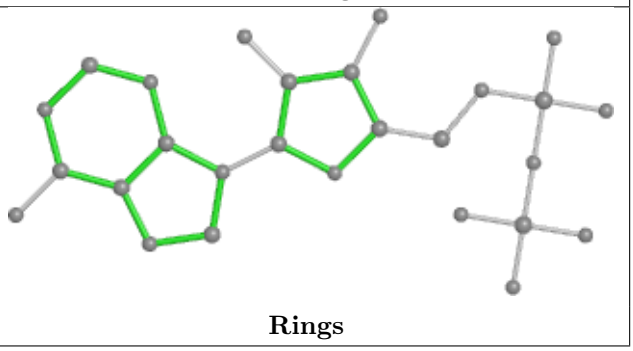

Rings

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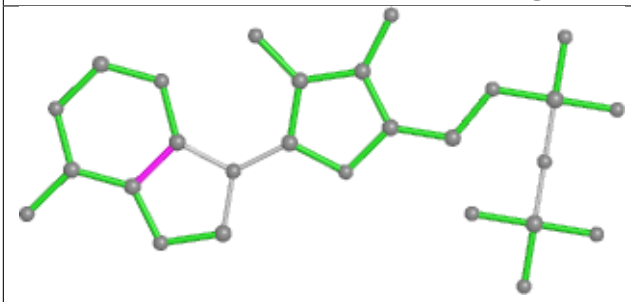
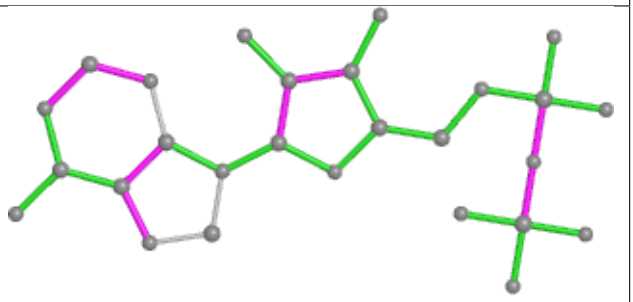
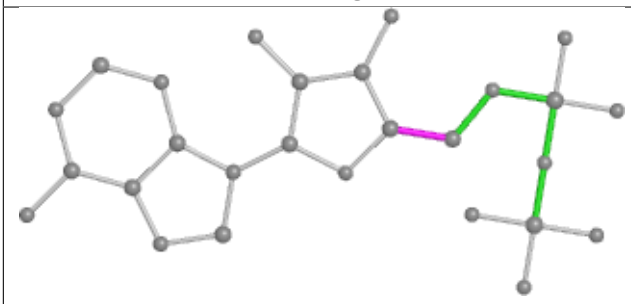
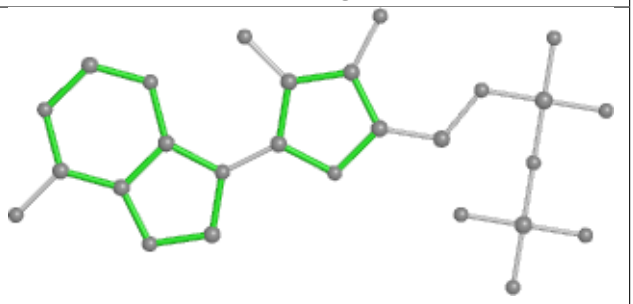
 Bond lengths	 Bond angles
 Torsions	 Rings

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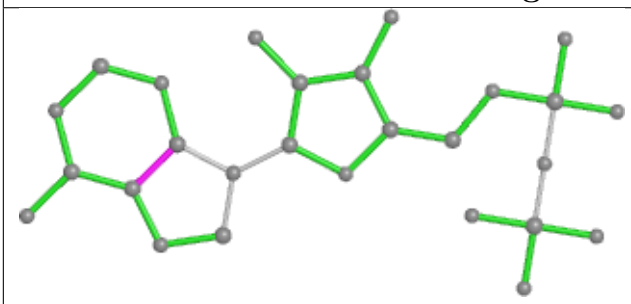
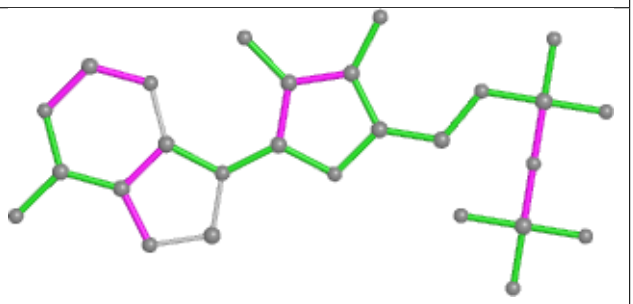
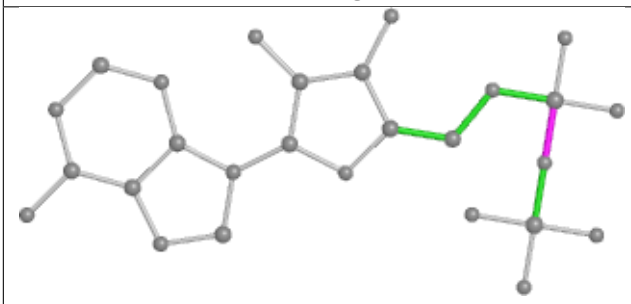
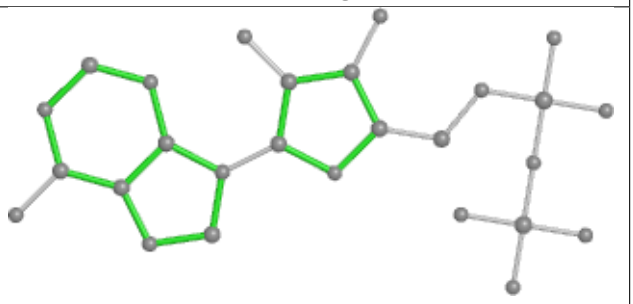
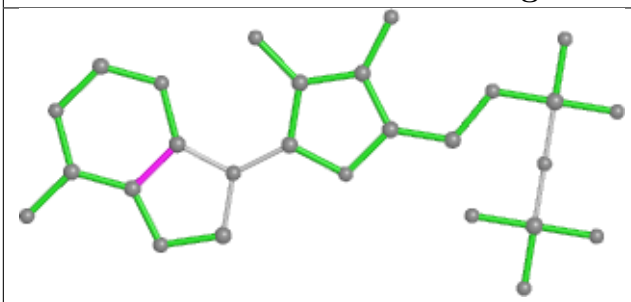
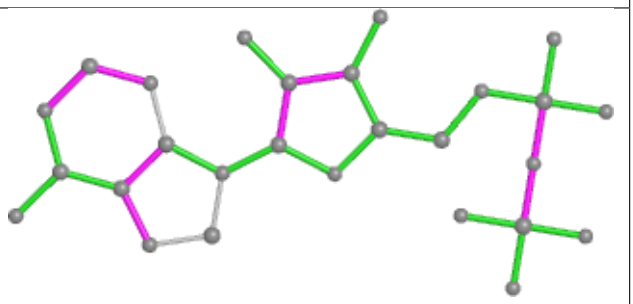
 Bond lengths	 Bond angles
 Torsions	 Rings

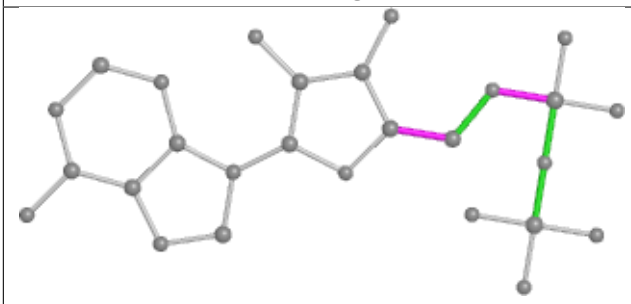
Ligand ADP K 601



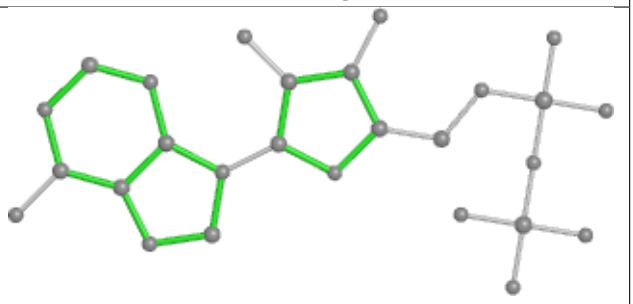
Bond lengths



Bond angles

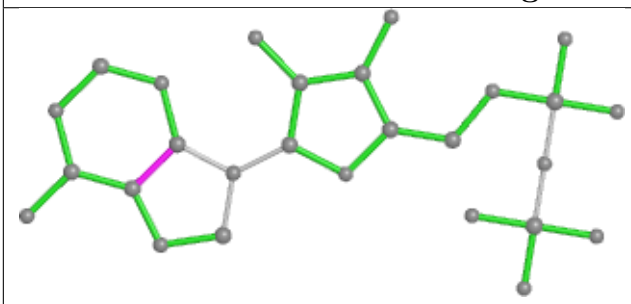


Torsions

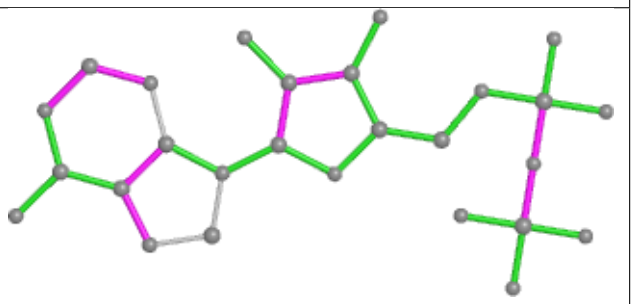


Rings

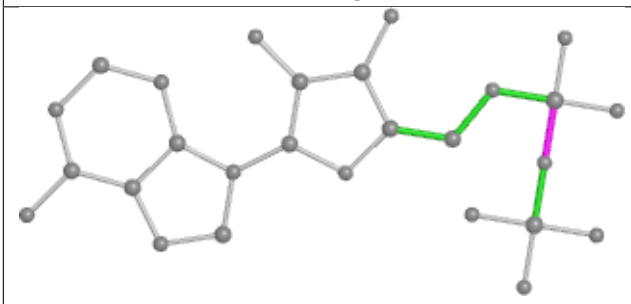
Ligand ADP D 601



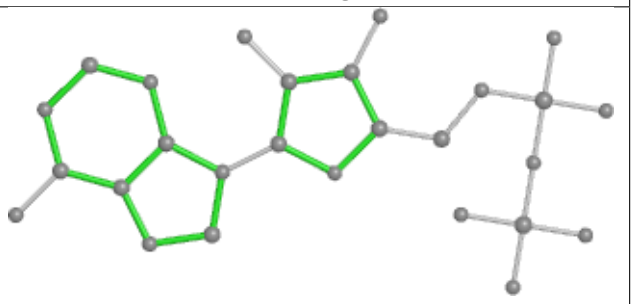
Bond lengths



Bond angles

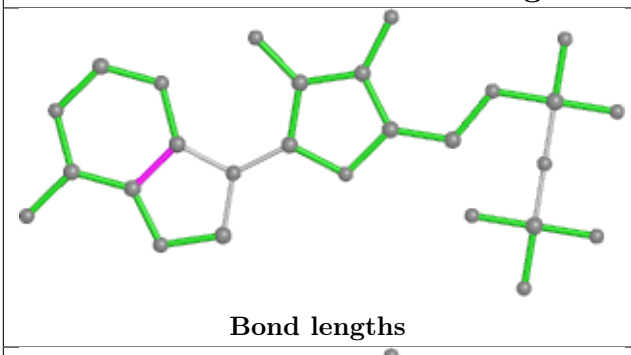


Torsions

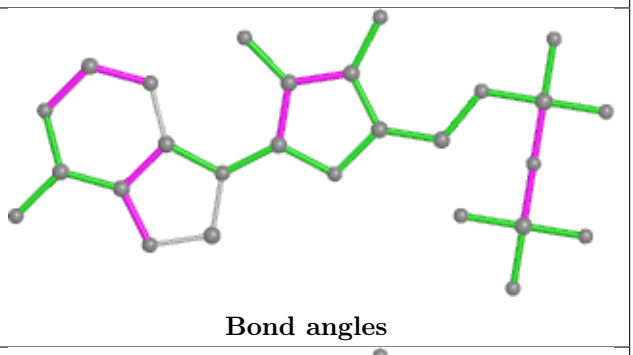


Rings

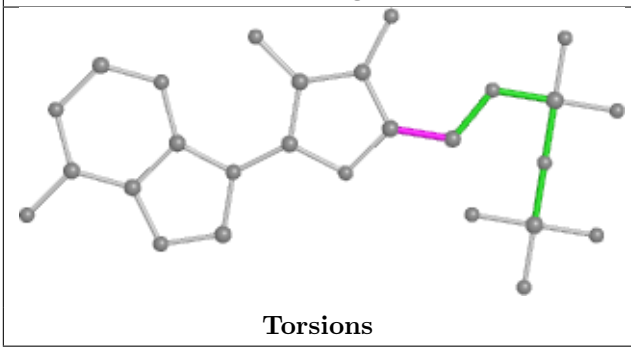
Ligand ADP F 601



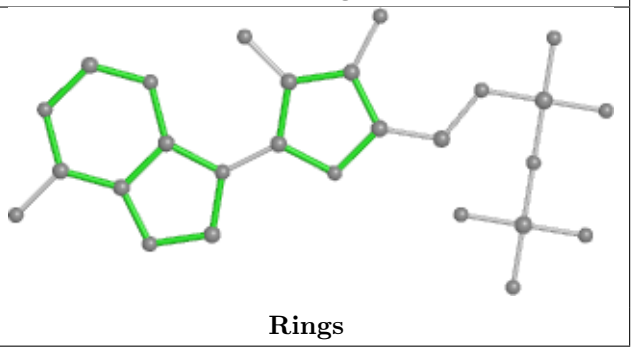
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

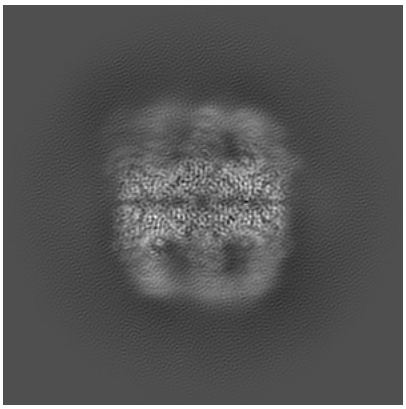
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35284. These allow visual inspection of the internal detail of the map and identification of artifacts.

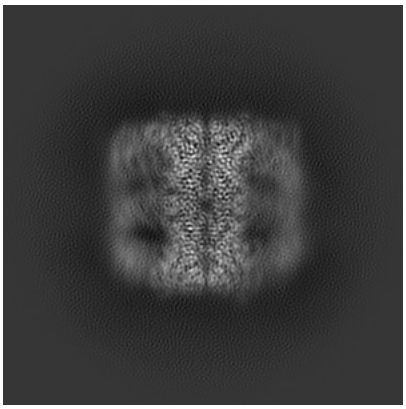
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

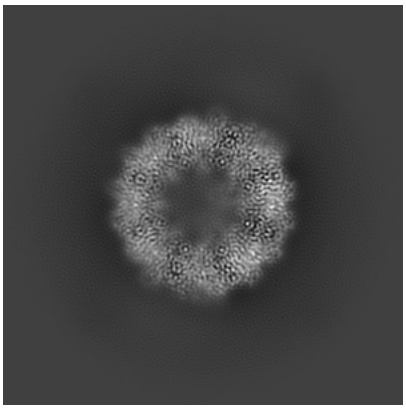
6.1.1 Primary map



X

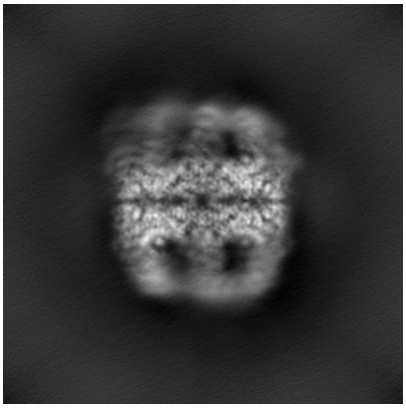


Y

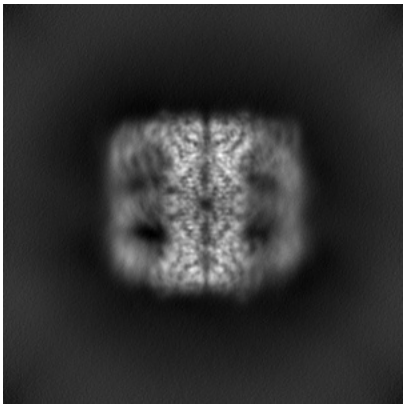


Z

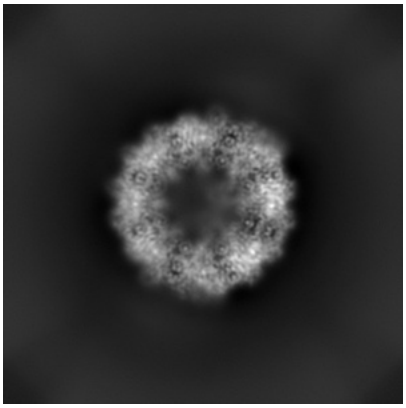
6.1.2 Raw map



X



Y

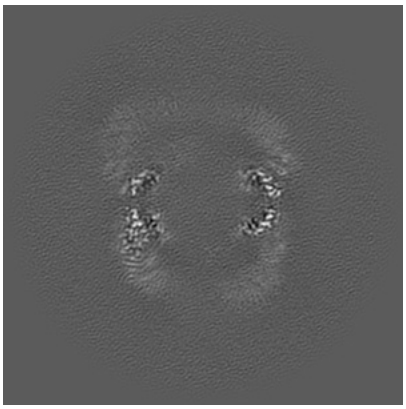


Z

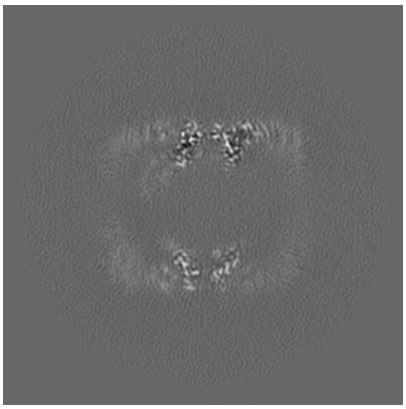
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

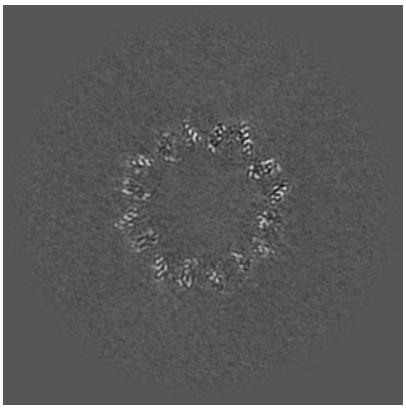
6.2.1 Primary map



X Index: 160

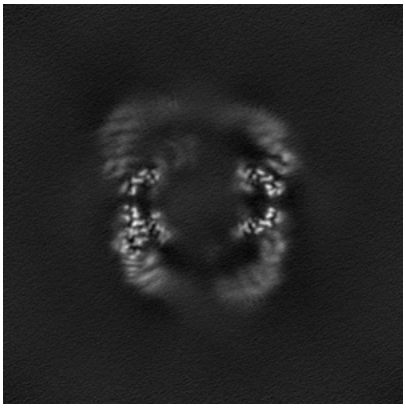


Y Index: 160

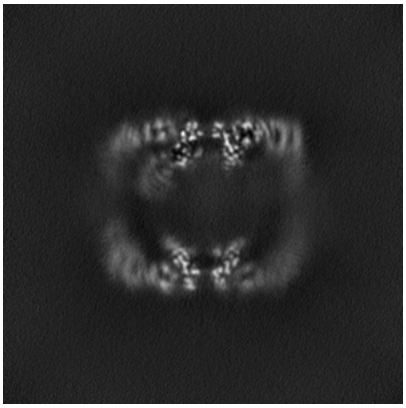


Z Index: 160

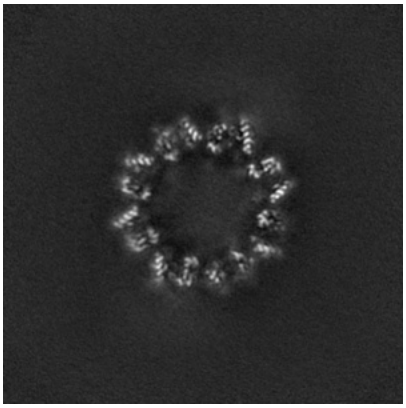
6.2.2 Raw map



X Index: 160



Y Index: 160

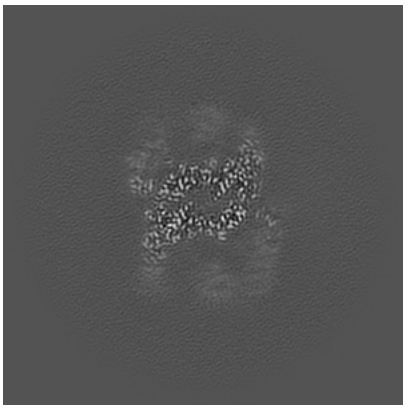


Z Index: 160

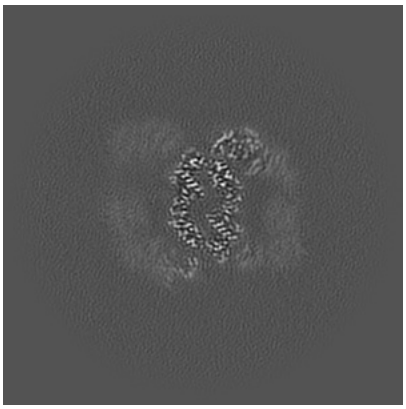
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

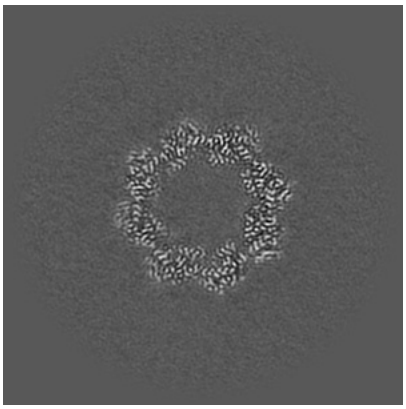
6.3.1 Primary map



X Index: 204

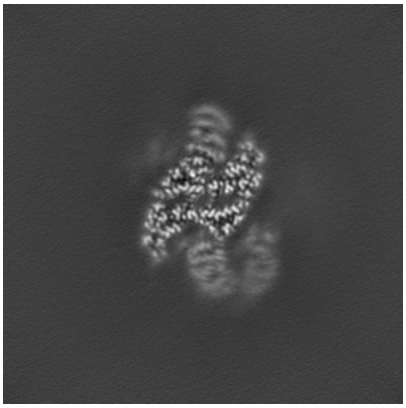


Y Index: 202

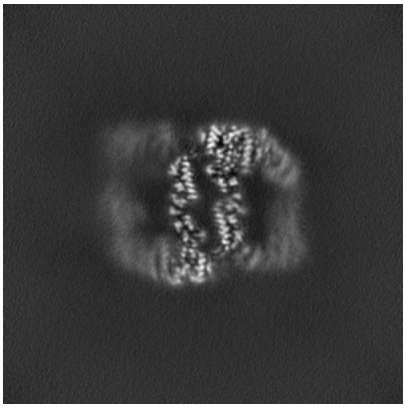


Z Index: 150

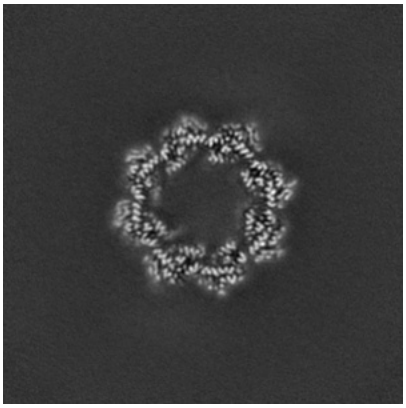
6.3.2 Raw map



X Index: 213



Y Index: 195

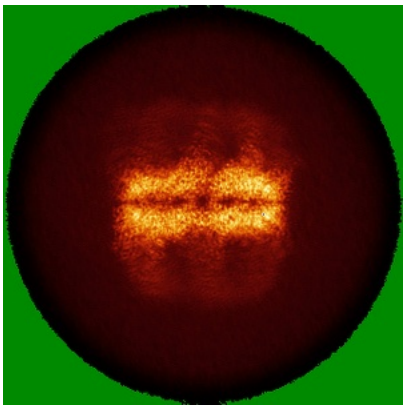


Z Index: 151

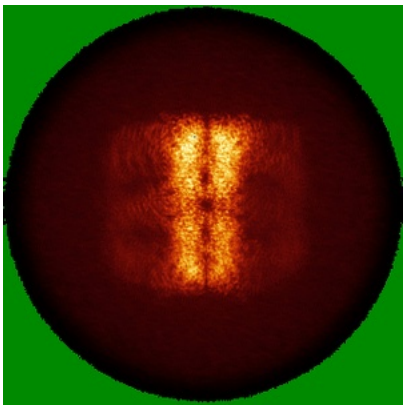
The images above show the largest variance slices of the map in three orthogonal directions.

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

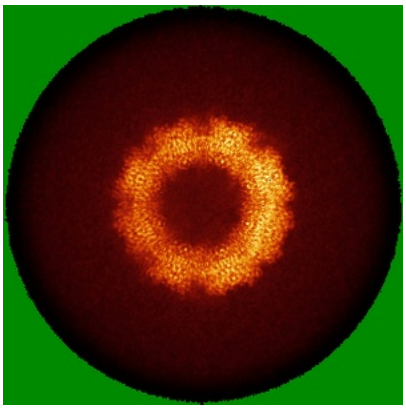
6.4.1 Primary map



X

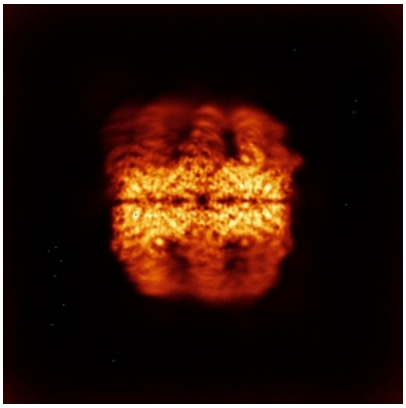


Y

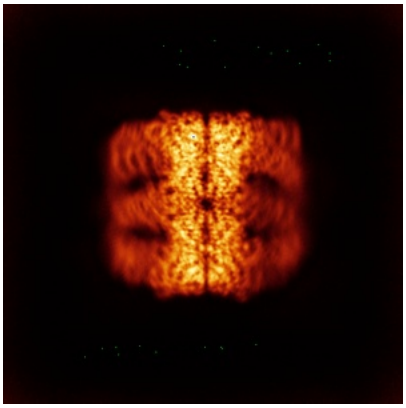


Z

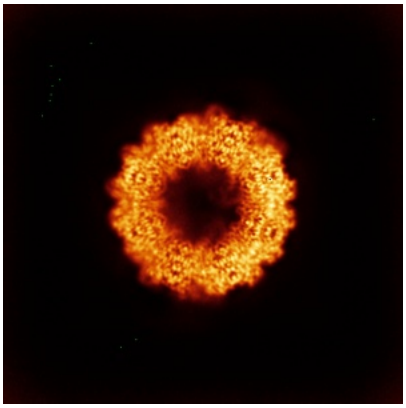
6.4.2 Raw map



X



Y

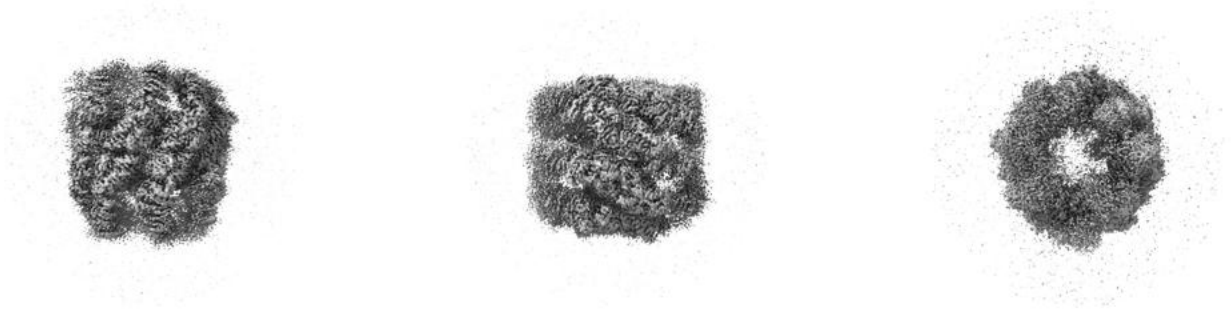


Z

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

6.5 Orthogonal surface views (i)

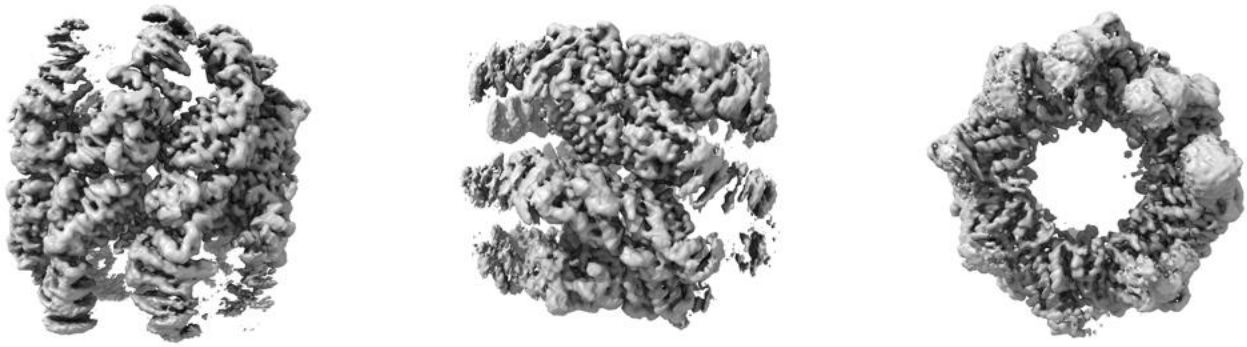
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.44. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

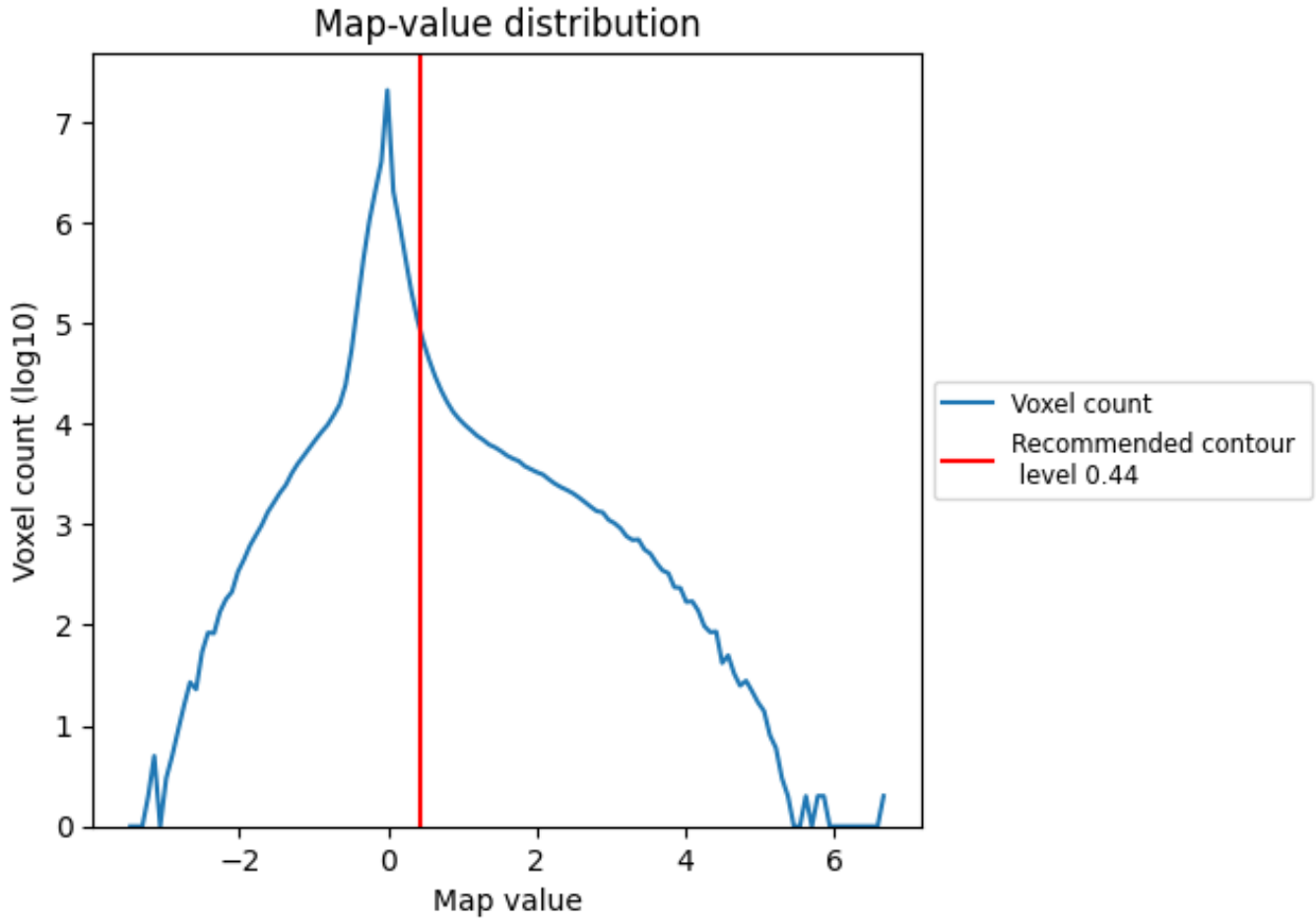
6.6 Mask visualisation (i)

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

7 Map analysis

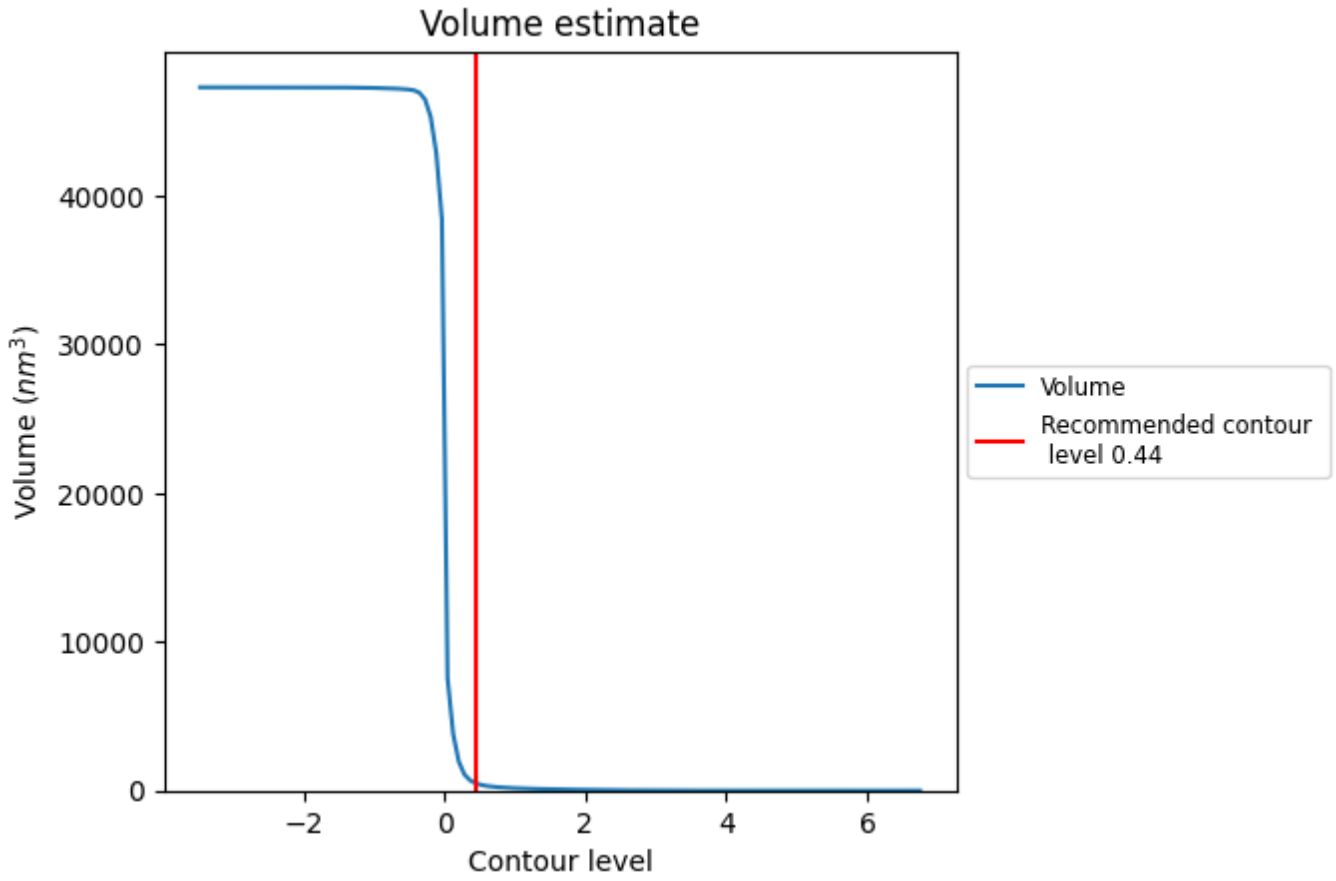
This section contains the results of statistical analysis of the map.

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.

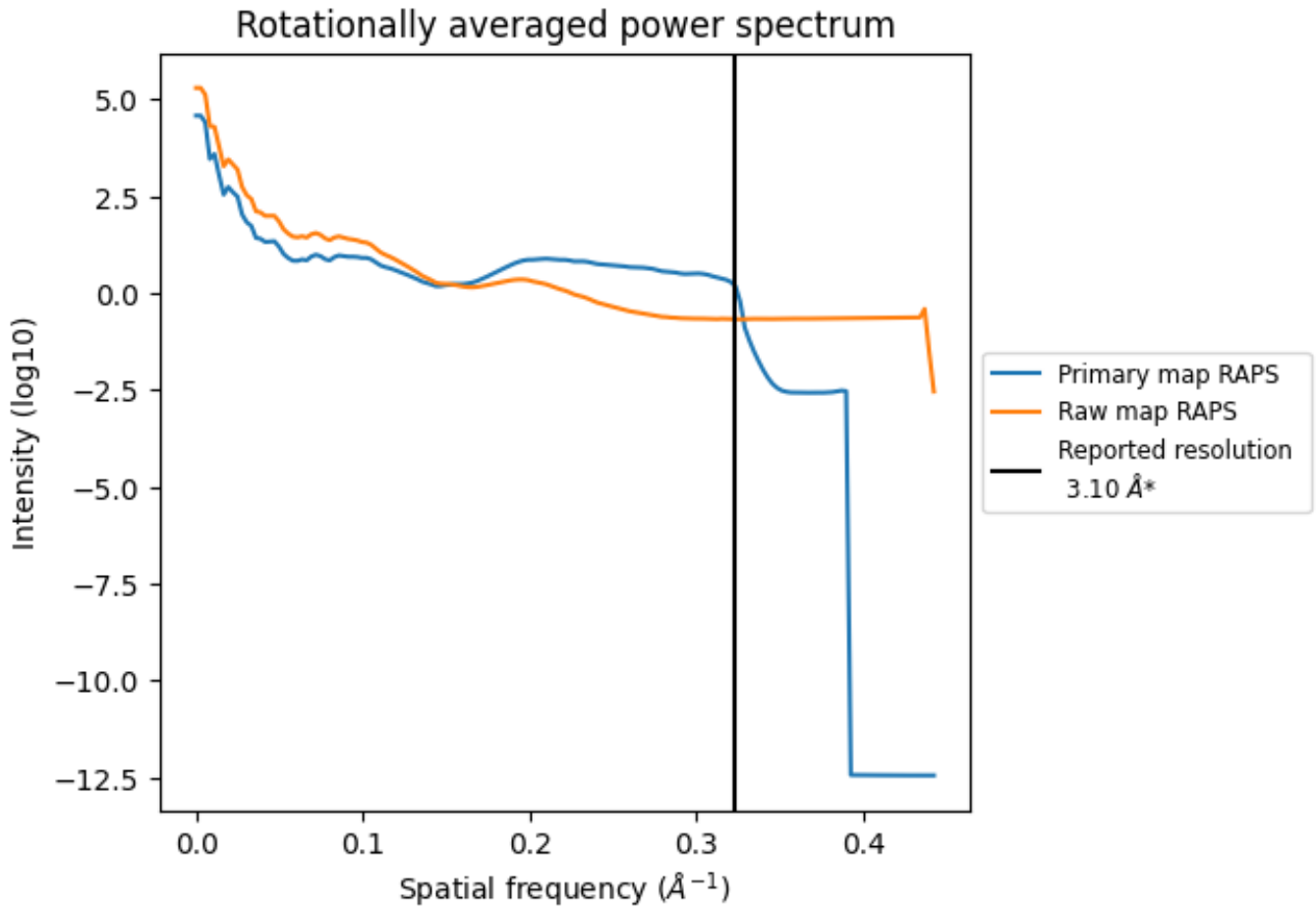
7.2 Volume estimate



The volume at the recommended contour level is 499 nm^3; this corresponds to an approximate mass of 451 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)

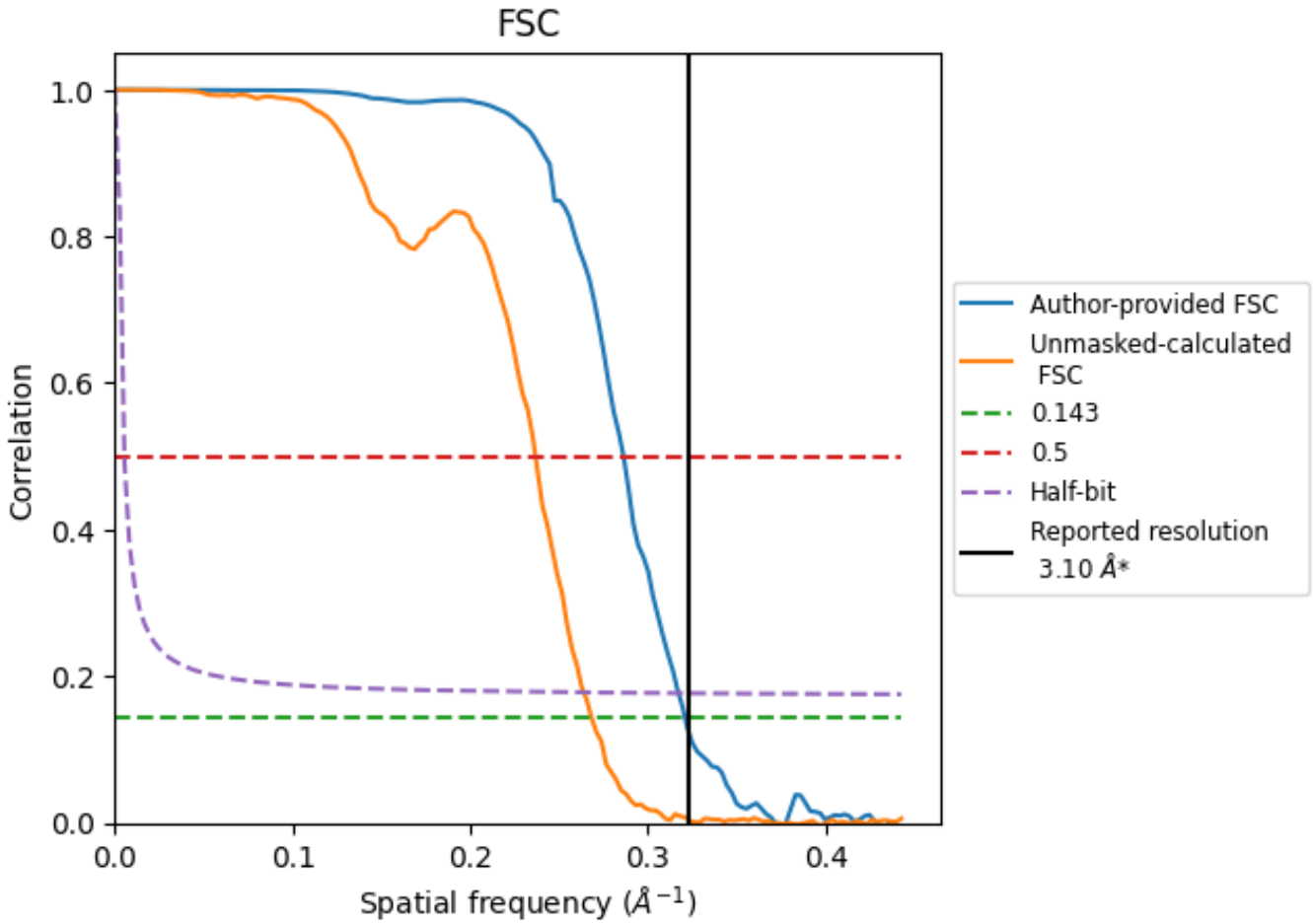


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

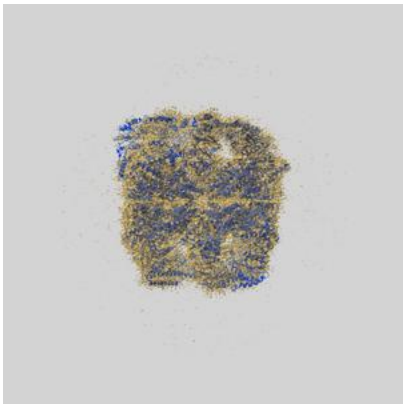
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.49	3.15
Unmasked-calculated*	3.73	4.22	3.79

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.73 differs from the reported value 3.1 by more than 10 %

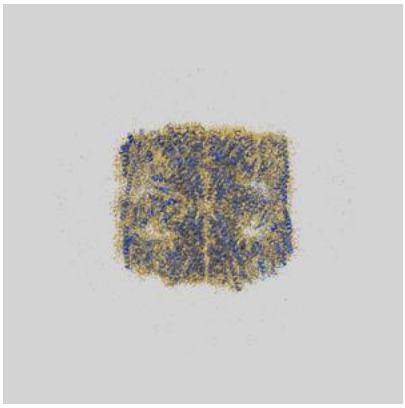
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35284 and PDB model 8I9U. Per-residue inclusion information can be found in section 3 on page 7.

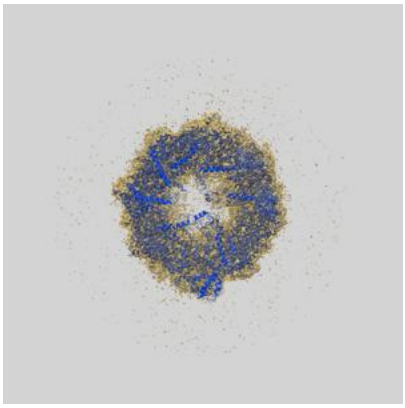
9.1 Map-model overlay



X



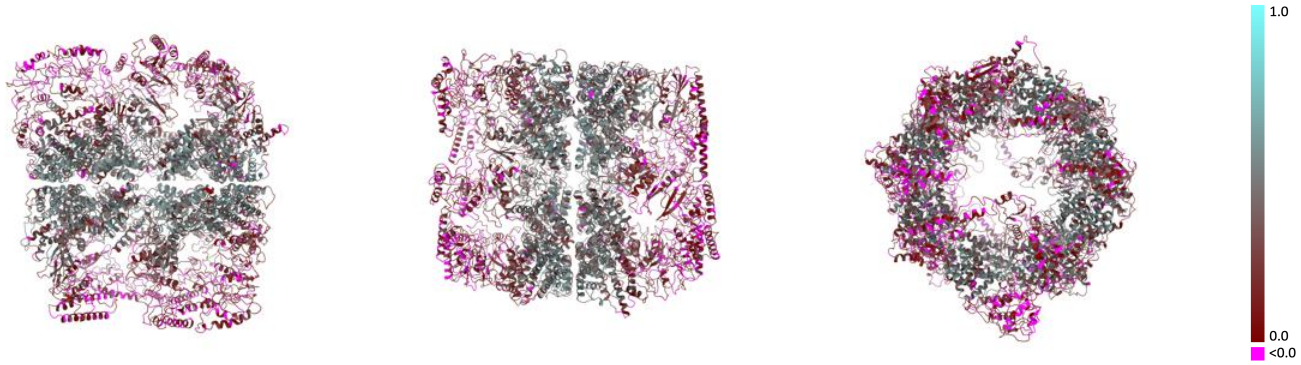
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.44 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.

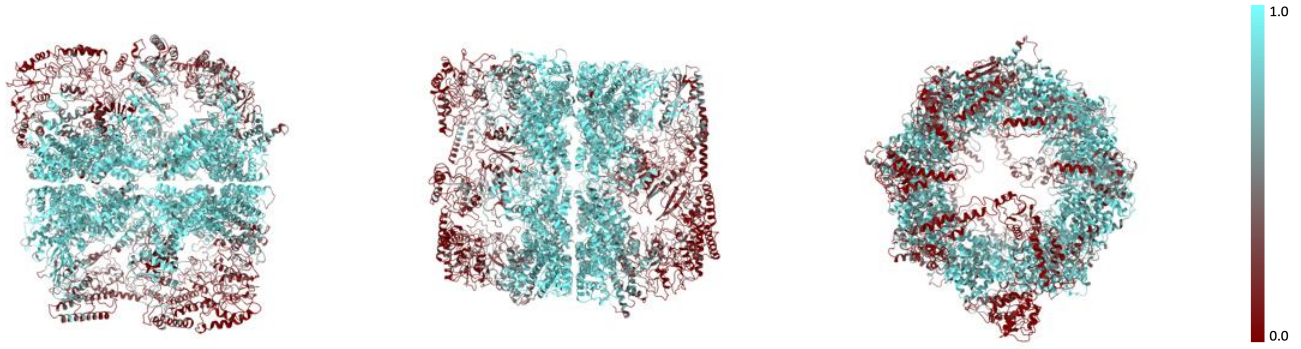
9.2 Q-score mapped to coordinate model (i)



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.

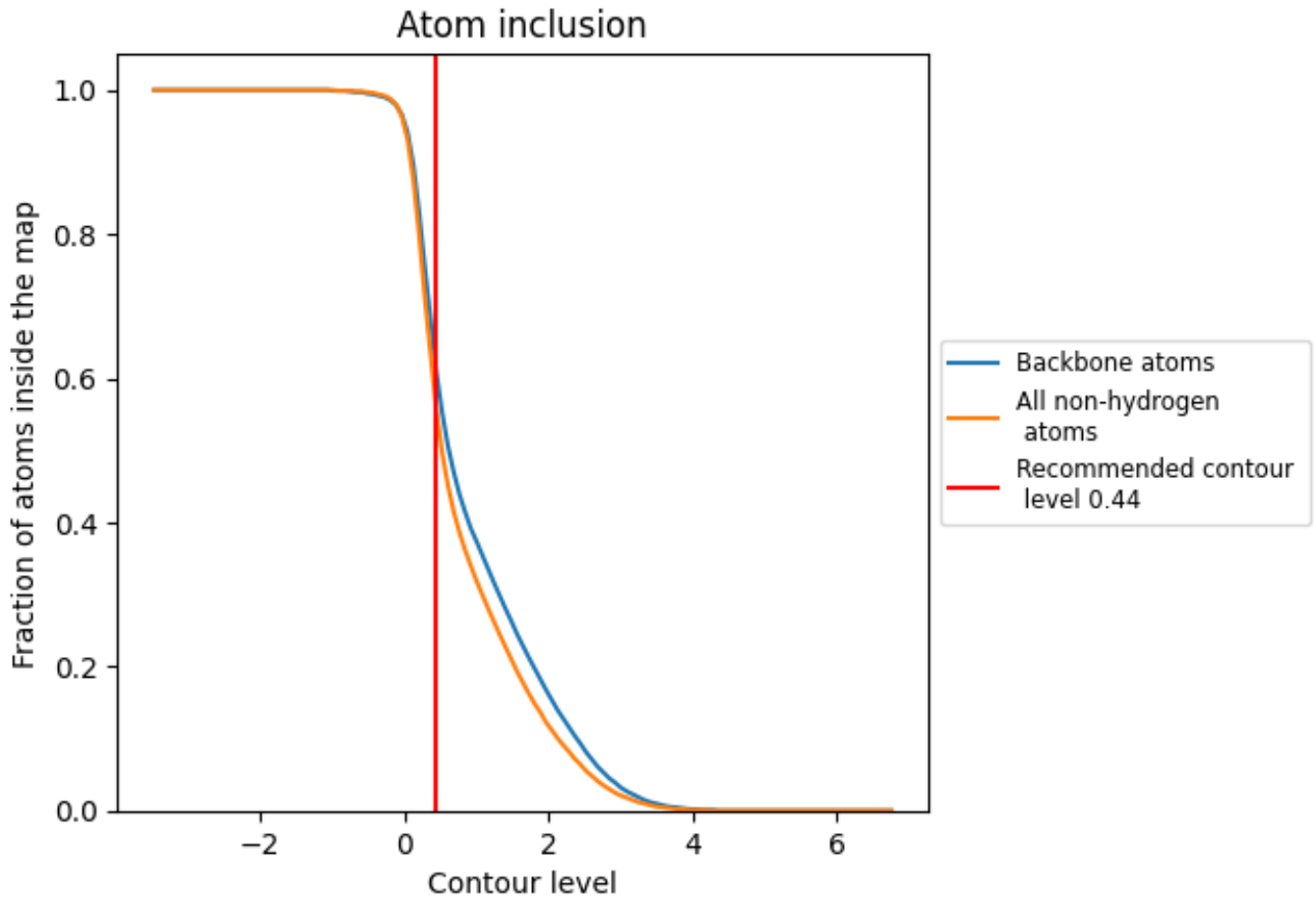
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.44).

9.4 Atom inclusion (i)



At the recommended contour level, 61% 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 (0.44) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5560	0.2860
A	0.5110	0.2830
B	0.5440	0.3010
C	0.6540	0.3210
D	0.5430	0.2860
E	0.5530	0.2340
F	0.6990	0.3290
G	0.5550	0.2510
H	0.6740	0.3180
I	0.4260	0.2370
J	0.4750	0.2620
K	0.5730	0.2920
L	0.4480	0.2310
M	0.5300	0.2790
N	0.6760	0.3360
O	0.5460	0.2970
P	0.6950	0.3390
Q	0.2370	0.2860
R	0.1170	0.2180