Full wwPDB EM Validation Report (i)

Aug 27, 2026 – 02:31 PM EDT

PDB ID	:	9YA8 / pdb_00009ya8
EMDB ID	:	EMD-72724
Title	:	The structure of the cardiac native crossbridge in the rigor state, myosin heads bound to actin molecules 6 and 7
Authors	:	Galkin, V.E.; Risi, C.M.
Deposited on	:	2025-09-15
Resolution	:	4.32 Å(reported)
Based on initial models	:	7KO5, 7JH7, 5H53, 8DD0, 6SFA

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 (i) 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 (1)) were used in the production of this report:

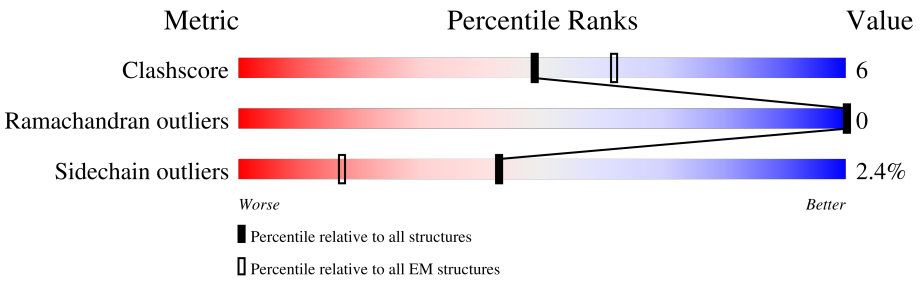
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

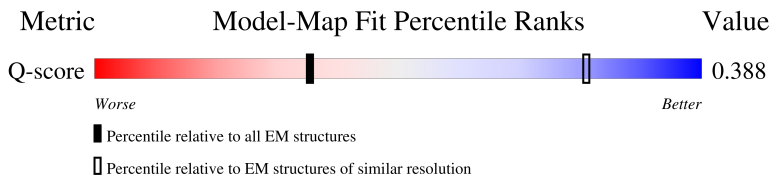
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.32 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3853 (3.83 - 4.82)

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	377	88% 11%
1	B	377	82% 16%
1	C	377	86% 12%
1	D	377	84% 15%

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Mol	Chain	Length	Quality of chain
2	E	284	32% 7% 60%
2	F	284	30% 10% 60%
2	G	284	15% 9% 75%
2	H	284	18% 7% 75%
3	I	285	18% 6% 76%
4	J	1935	36% 6% 58%
4	K	1935	36% 5% 58%
5	L	196	60% 17% 22%
5	M	196	60% 17% 22%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 30831 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 Actin, alpha cardiac muscle 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	375	2932	1854	493	565	20	0	0
1	B	375	2932	1854	493	565	20	0	0
1	C	375	2932	1854	493	565	20	0	0
1	D	375	2932	1854	493	565	20	0	0

- Molecule 2 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	115	930	573	149	206	2	0	0
2	F	115	930	573	149	206	2	0	0
2	G	70	562	343	98	118	3	0	0
2	H	70	562	343	98	118	3	0	0

- Molecule 3 is a protein called Troponin T2, cardiac type.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	68	595	359	121	114	1	0	0

- Molecule 4 is a protein called Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	807	6489	4134	1116	1207	32	0	0

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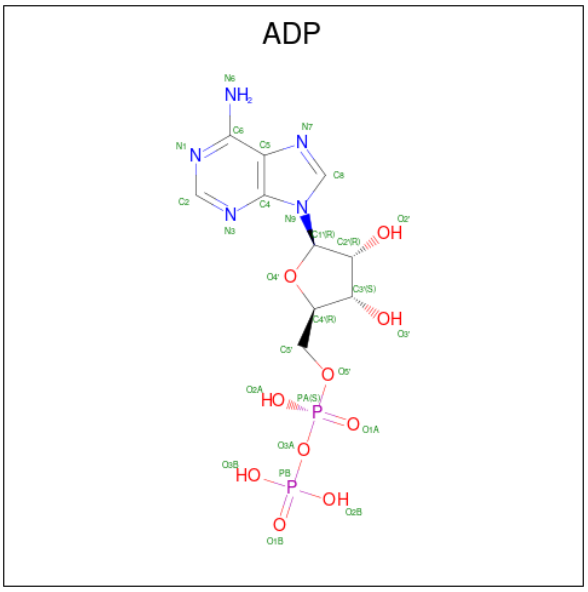
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	807	6489	4134	1116	1207	32	0	0

- Molecule 5 is a protein called Myosin light chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	153	1217	766	202	238	11	0	0
			Total	C	N	O	S		
5	M	153	1217	766	202	238	11	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	27	10	5	10	2	0
			Total	C	N	O	P	
6	B	1	27	10	5	10	2	0
			Total	C	N	O	P	
6	C	1	27	10	5	10	2	0
			Total	C	N	O	P	
6	D	1	27	10	5	10	2	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

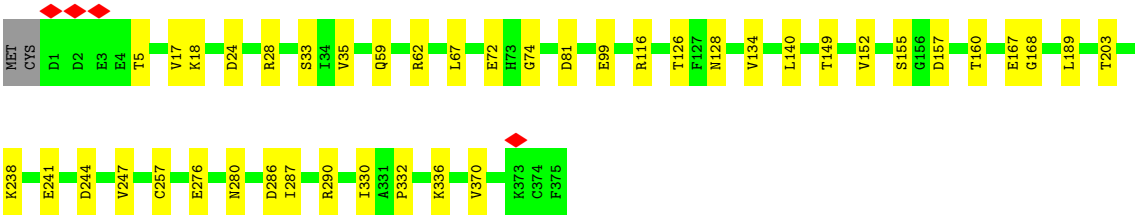
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
7	A	1	1	1	0
7	B	1	1	1	0
7	C	1	1	1	0
7	D	1	1	1	0

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.

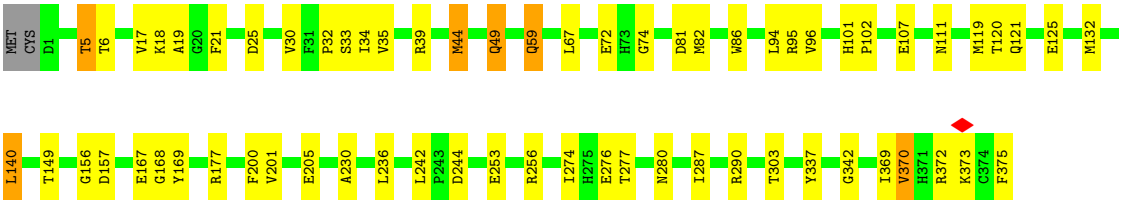
• Molecule 1: Actin, alpha cardiac muscle 1

Chain A:



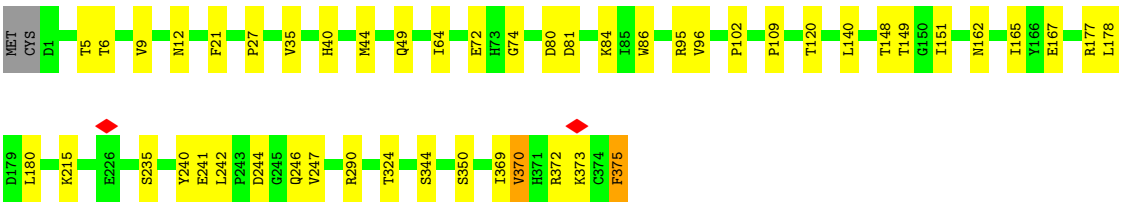
• Molecule 1: Actin, alpha cardiac muscle 1

Chain B:



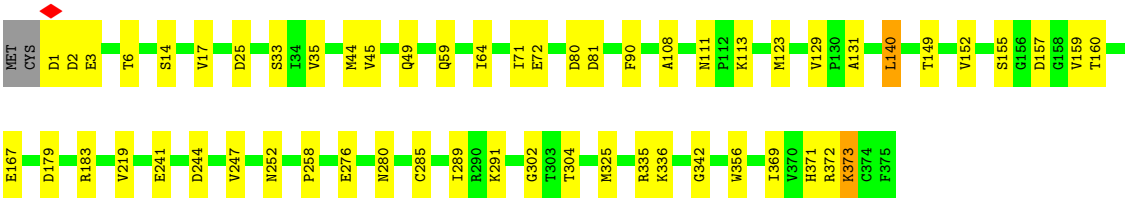
• Molecule 1: Actin, alpha cardiac muscle 1

Chain C:



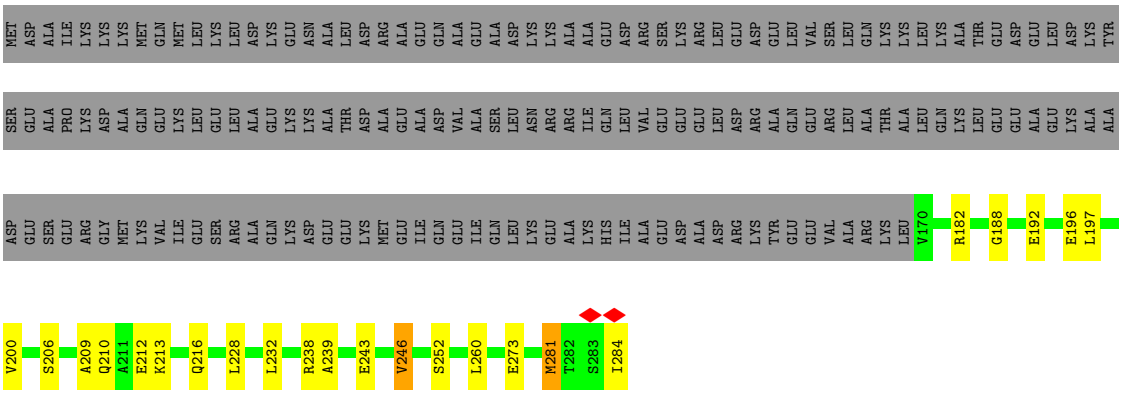
• Molecule 1: Actin, alpha cardiac muscle 1

Chain D:



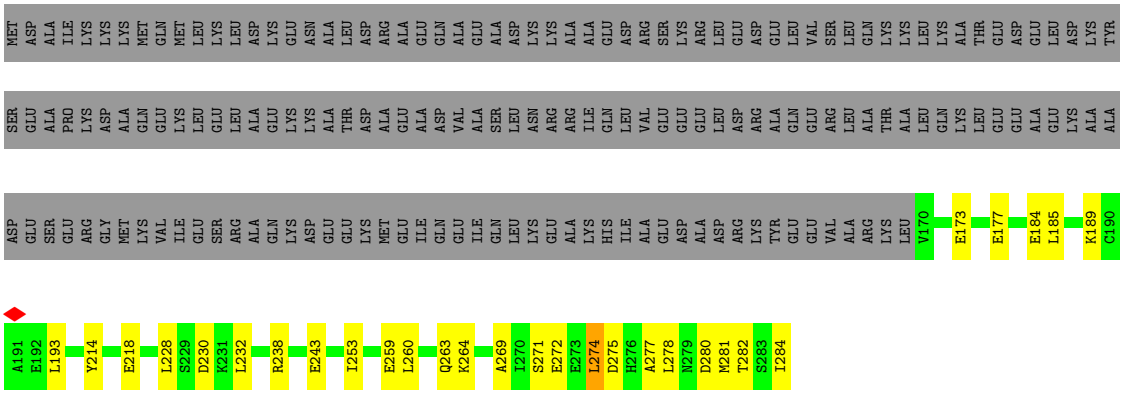
- Molecule 2: Tropomyosin alpha-1 chain

Chain E:



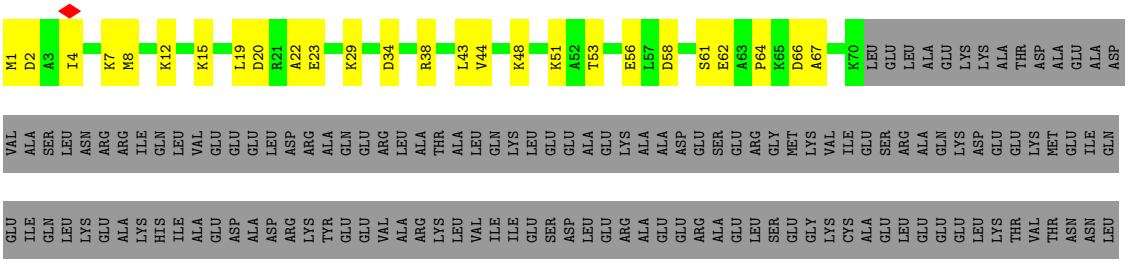
- Molecule 2: Tropomyosin alpha-1 chain

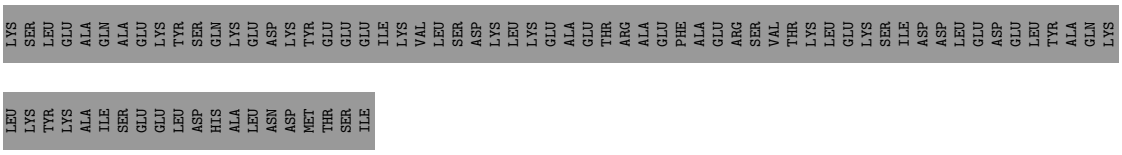
Chain F:



- Molecule 2: Tropomyosin alpha-1 chain

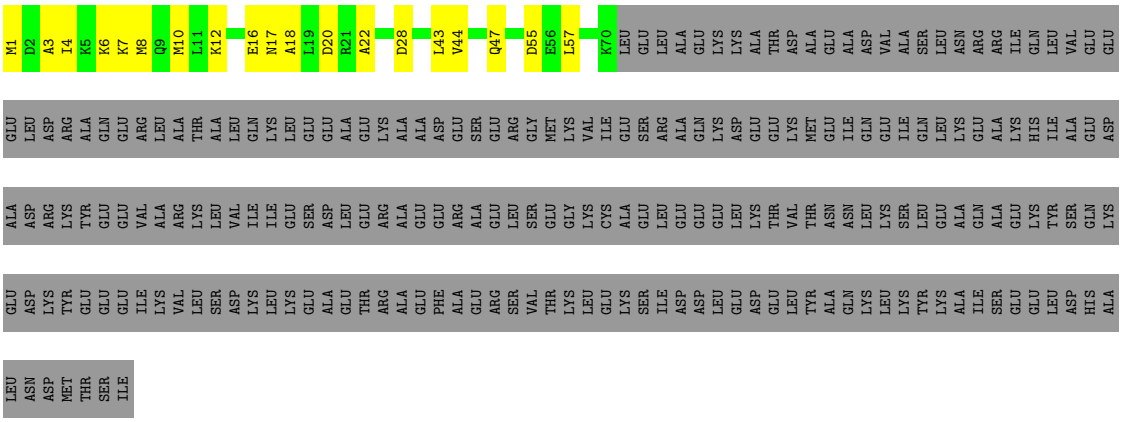
Chain G:





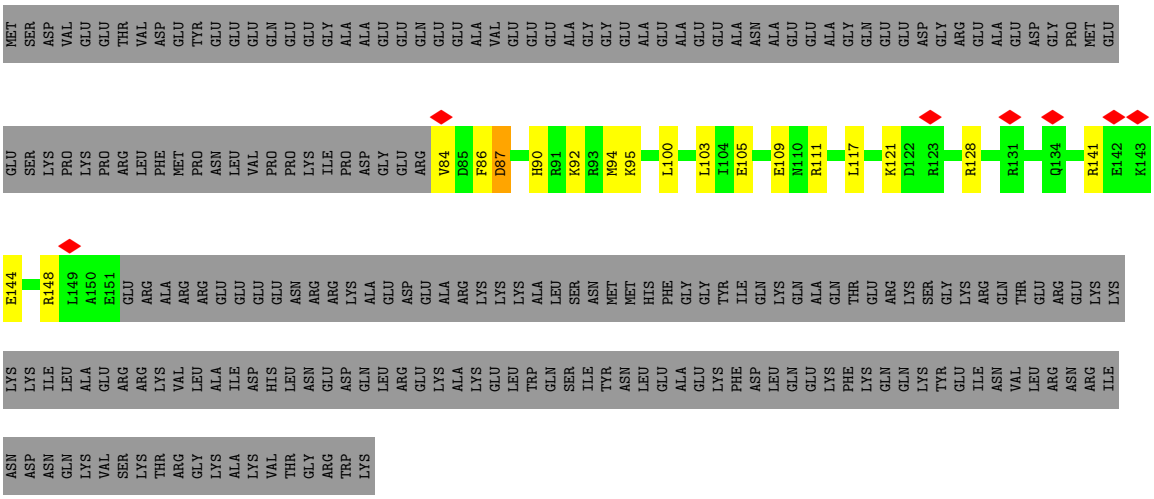
• Molecule 2: Tropomyosin alpha-1 chain

Chain H:



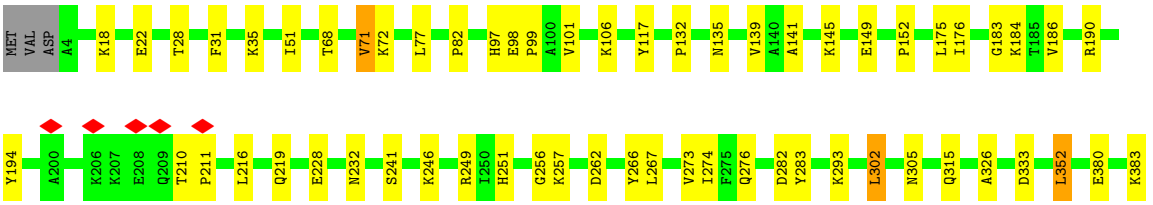
• Molecule 3: Troponin T2, cardiac type

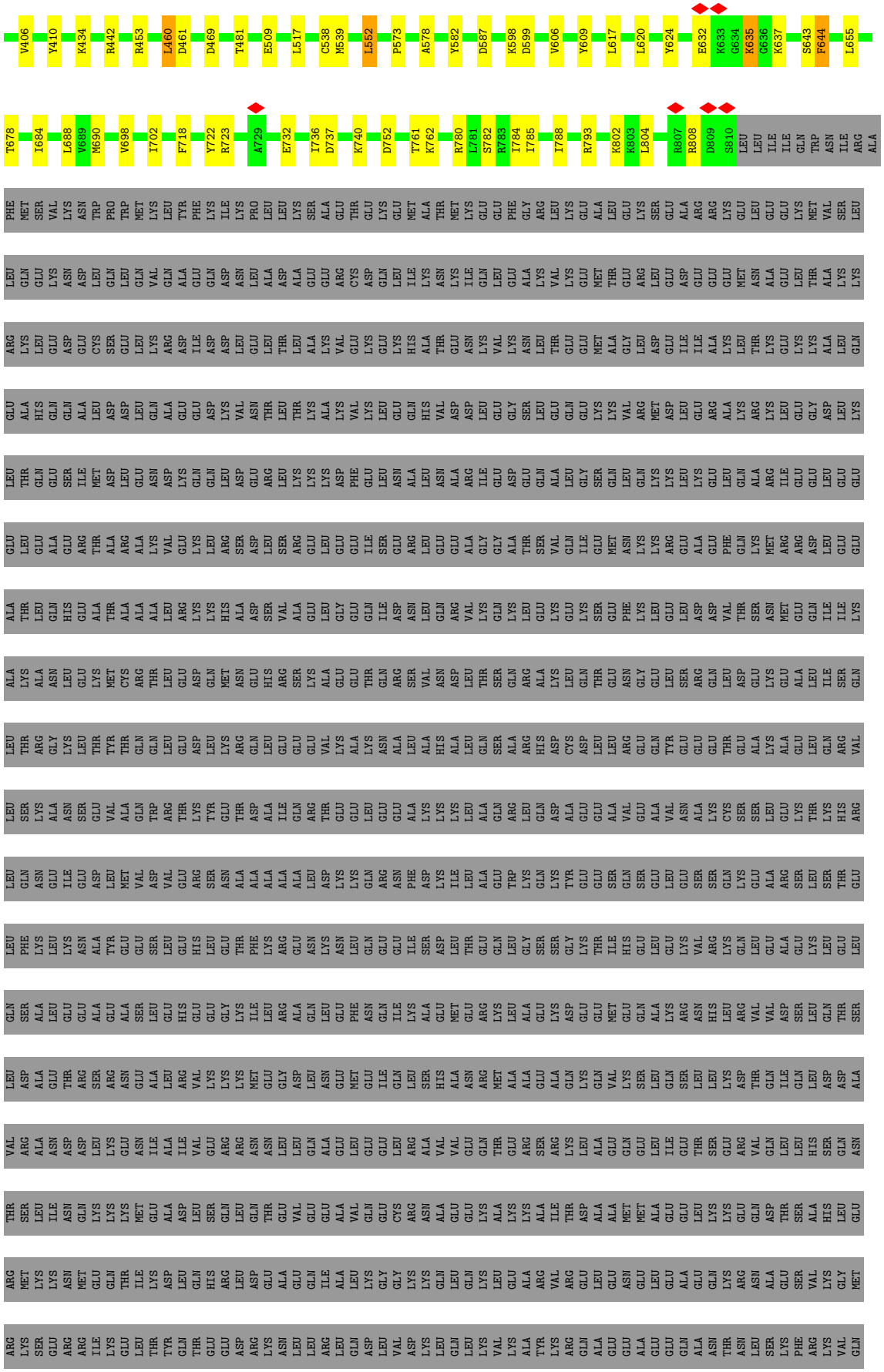
Chain I:

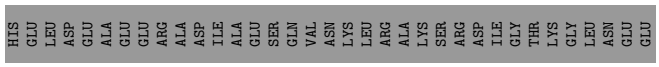


• Molecule 4: Myosin-7

Chain J:

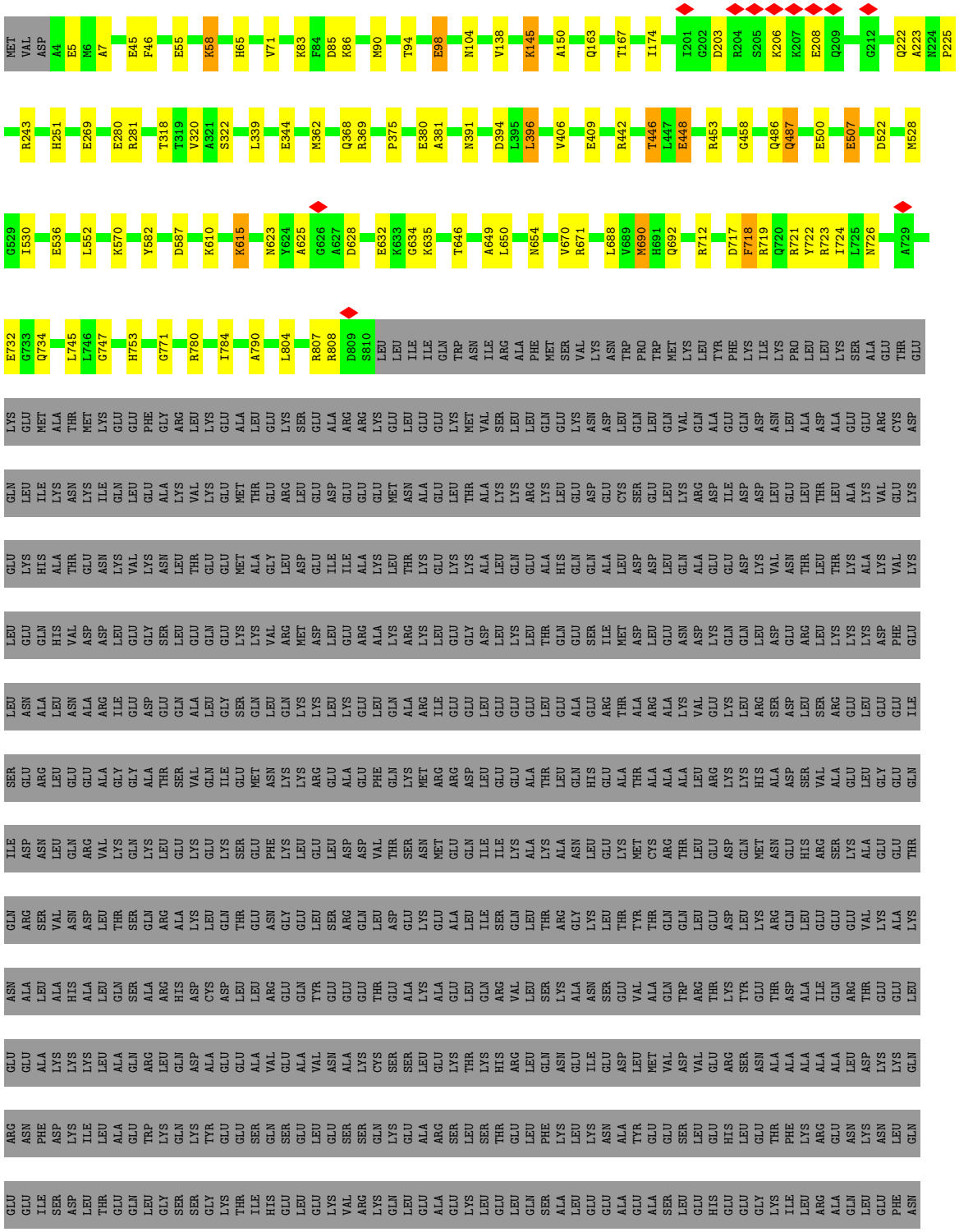



V406 Y410 K434 R442 R453 L460 D461 D469 T481 E509 L517 C538 M539 L552 P573 A578 Y582 D587 K598 D599 V606 Y609 L617 L620 Y624 E632 K633 G634 K635 G636 K637 S643 F644 L655
T678 I684 L688 V689 M690 V698 I702 F718 Y722 R723 A729 E732 I736 D737 K740 D752 T761 K762 R780 L781 S782 R783 I784 I785 I788 R793 K802 K803 L804 R807 R808 D809 S810 LEU LEU ILE ILE ILE GLN TRP ASN ILE ARG ALA



- Molecule 4: Myosin-7

Chain K:



GLN ILE LYS ALA GLU MET GLU ARG LYS LEU ALA GLU LYS ASP GLU GLU MET GLU GLN ALA LYS ARG ASN HIS LEU ARG VAL VAL ASP SER LEU GLN THR SER LEU ASP ALA GLU THR ARG SER ARG ASN GLU ALA LEU ARG VAL LYS LYS MET GLU GLY ASP LEU ASN GLU MET GLU

ILE GLN LEU SER HIS ALA ASN ARG MET ALA ALA GLU ALA GLN LYS GLN VAL LYS SER LEU GLN SER LEU LEU LYS ASP THR GLN ILE GLN LEU ASP ASP ALA VAL ARG ALA ASN ASP ASP LEU LYS GLU ASN ILE ALA ILE VAL GLU ARG ARG ASN ASN LEU LEU GLN ALA GLU LEU GLU

GLU LEU ARG ALA VAL VAL GLU GLN THR GLU ARG SER ARG LYS LEU ALA GLU GLN GLU GLU ILE GLU THR SER GLU ARG VAL GLN LEU LEU HIS SER GLN ASN THR SER LEU ILE ASN GLN LYS LYS LYS MET GLU ALA ASP LEU GLN THR GLU VAL GLU GLU ALA VAL GLN

GLU CYS ARG ASN ALA GLU GLU LYS ALA LYS ALA ALA ILE THR ASP ALA ALA MET MET ALA GLU GLU LEU LYS LYS GLU GLN ASP THR SER ALA HIS LEU GLU ARG MET LYS LYS ASN MET GLU GLN THR ILE LYS ASP LEU GLU ASP GLN HIS ARG LEU ASP GLU GLN ILE ALA LEU LYS

GLY GLY LYS LYS GLN LEU GLN LYS LEU GLU ALA ARG VAL ARG GLU LEU GLU ASN GLU LEU GLU ALA GLU GLN LYS ARG ASN ALA GLU SER VAL LYS GLY MET ARG LYS SER GLU ARG ARG ILE GLU LYS GLU THR TYR GLN THR GLU GLU ASP ARG LYS ASN LEU LEU ARG LEU GLN ASP

LEU VAL ASP LYS LEU GLN LEU LYS VAL LYS ALA TYR LYS ARG GLN ALA GLU GLU ALA GLU GLN ALA GLU GLU LEU ASP GLU ALA GLU GLU ARG ALA ASP ILE ALA GLU SER GLN VAL ASN LYS LEU ARG ALA LYS SER ARG ASP

ILE GLY THR LYS GLY LEU ASN GLU GLU

- Molecule 5: Myosin light chain 3

Chain L:

MET ALA PRO LYS LYS PRO GLU PRO LYS LYS ASP ASP ALA LYS ALA ALA ALA LYS ALA ALA PRO ALA PRO ALA PRO ALA PRO ALA PRO ALA PRO GLU PRO LYS GLU PRO GLU PHE ASP ALA SER LYS I43 K44 I45 I52 K56 E57 A58 F59 M60 L61 R64 T65 P66 K67 C68

E69 M70 K71 I72 L84 V93 V96 K99 E104 K108 F112 L116 I122 E136 R139 D142 V149 H156 L161 G162 E163 E171 M174 A175 E178 D179 G182 C183 Y186 V190 I193 M194 A195 SER

- Molecule 5: Myosin light chain 3

Chain M:

MET ALA PRO LYS LYS PRO GLU PRO LYS LYS ASP ASP ALA LYS ALA ALA ALA LYS ALA ALA PRO ALA PRO ALA PRO ALA PRO ALA PRO ALA PRO GLU PRO LYS GLU PRO GLU PHE ASP ALA SER LYS I43 T48 E57 L61 F62 D63 R64 T65 Y74 G75 Q76 L81

Q86 N87 P88 T89 Q90 V93 L105 M109 M118 D133 E136 G137 K143 T148 V149 M150 L154 V157 L158 A159 T160 R164 V170 G182 C183 Y186 E187 A188 F189 I193 M194 A195 SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86644	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	34	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	14.519	Depositor
Minimum map value	-6.759	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.198	Depositor
Recommended contour level	1.2	Depositor
Map size (Å)	536.97595, 536.97595, 536.97595	wwPDB
Map dimensions	396, 396, 396	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3559998, 1.3559998, 1.3559998	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: MG, 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	0.09	0/2995	0.28	0/4057
1	B	0.10	0/2995	0.27	0/4057
1	C	0.09	0/2995	0.28	0/4057
1	D	0.10	0/2995	0.27	0/4057
2	E	0.16	0/935	0.22	0/1249
2	F	0.16	0/935	0.25	0/1249
2	G	0.12	0/563	0.23	0/744
2	H	0.14	0/563	0.28	0/744
3	I	0.11	0/598	0.24	0/791
4	J	0.12	0/6623	0.31	0/8918
4	K	0.12	0/6623	0.34	2/8918 (0.0%)
5	L	0.11	0/1236	0.36	2/1658 (0.1%)
5	M	0.11	0/1236	0.41	2/1658 (0.1%)
All	All	0.11	0/31292	0.30	6/42157 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	628	ASP	CA-C-N	7.91	135.94	121.70
4	K	628	ASP	C-N-CA	7.91	135.94	121.70
5	M	182	GLY	CA-C-N	7.26	134.78	121.70
5	M	182	GLY	C-N-CA	7.26	134.78	121.70
5	L	182	GLY	CA-C-N	6.49	133.38	121.70
5	L	182	GLY	C-N-CA	6.49	133.38	121.70

There are no chirality outliers.

There are no planarity outliers.

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	2932	0	2894	24	0
1	B	2932	0	2894	44	0
1	C	2932	0	2894	33	0
1	D	2932	0	2894	36	0
2	E	930	0	917	21	0
2	F	930	0	917	27	0
2	G	562	0	580	20	0
2	H	562	0	580	25	0
3	I	595	0	603	21	0
4	J	6489	0	6484	66	0
4	K	6489	0	6484	59	0
5	L	1217	0	1199	26	0
5	M	1217	0	1199	24	0
6	A	27	0	12	2	0
6	B	27	0	12	1	0
6	C	27	0	12	0	0
6	D	27	0	12	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	30831	0	30587	353	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 6.

All (353) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:176:ILE:HG22	4:J:184:LYS:HZ2	1.40	0.86
1:C:149:THR:HG22	1:C:167:GLU:H	1.48	0.77
2:H:6:LYS:NZ	2:H:10:MET:SD	2.58	0.76
4:J:517:LEU:HD21	4:J:582:TYR:HB3	1.70	0.72
2:H:20:ASP:OD1	4:K:368:GLN:NE2	2.23	0.72
1:C:290:ARG:NH1	1:D:244:ASP:OD2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:62:PHE:O	5:M:76:GLN:NE2	2.24	0.71
1:B:149:THR:HG22	1:B:167:GLU:H	1.57	0.70
4:K:723:ARG:NH1	5:M:136:GLU:OE1	2.26	0.69
1:A:17:VAL:HG23	1:A:33:SER:HB3	1.75	0.68
3:I:144:GLU:OE2	3:I:148:ARG:NH1	2.26	0.68
1:B:32:PRO:HG2	1:B:59:GLN:HG3	1.73	0.68
4:K:718:PHE:HA	4:K:722:TYR:HB2	1.75	0.68
2:F:275:ASP:HB2	3:I:111:ARG:HH22	1.59	0.68
4:K:719:ARG:NH1	4:K:734:GLN:OE1	2.27	0.67
2:H:16:GLU:HG2	4:K:369:ARG:HH12	1.58	0.66
3:I:87:ASP:N	3:I:87:ASP:OD1	2.29	0.66
2:G:53:THR:HG23	2:H:57:LEU:HD12	1.77	0.65
1:D:17:VAL:HG23	1:D:33:SER:HB3	1.79	0.64
4:K:203:ASP:OD2	4:K:206:LYS:NZ	2.28	0.64
5:M:65:THR:HG21	5:M:109:MET:HE1	1.79	0.63
1:C:120:THR:HG21	1:C:370:VAL:HG21	1.79	0.62
1:D:276:GLU:O	1:D:280:ASN:ND2	2.31	0.62
4:J:141:ALA:O	4:J:145:LYS:NZ	2.33	0.62
1:D:108:ALA:HB3	1:D:111:ASN:HD21	1.63	0.62
1:B:95:ARG:NH1	4:J:632:GLU:O	2.28	0.62
1:C:350:SER:N	4:K:536:GLU:OE1	2.31	0.62
4:J:793:ARG:NH1	5:L:163:GLU:OE1	2.27	0.62
1:C:178:LEU:HG	1:C:180:LEU:H	1.65	0.62
4:J:228:GLU:OE1	4:J:232:ASN:ND2	2.33	0.62
5:M:160:THR:O	5:M:164:ARG:NH1	2.33	0.61
4:J:256:GLY:O	4:J:257:LYS:NZ	2.32	0.61
1:A:149:THR:HG22	1:A:167:GLU:H	1.66	0.61
1:B:369:ILE:HD12	1:B:372:ARG:HD2	1.82	0.61
1:A:59:GLN:O	1:A:62:ARG:NH1	2.33	0.60
1:B:169:TYR:OH	1:C:49:GLN:NE2	2.29	0.60
2:H:8:MET:HE3	2:H:12:LYS:HZ3	1.66	0.60
4:K:55:GLU:HG2	4:K:58:LYS:HE3	1.84	0.60
4:J:132:PRO:O	4:J:135:ASN:ND2	2.27	0.60
4:K:281:ARG:NH1	4:K:318:THR:O	2.35	0.59
1:C:35:VAL:HG21	1:C:81:ASP:HB3	1.84	0.59
4:J:293:LYS:HD3	4:J:326:ALA:HB1	1.84	0.59
4:J:761:THR:HG23	4:J:762:LYS:HG3	1.84	0.59
4:K:804:LEU:HD11	5:M:64:ARG:HH22	1.67	0.59
1:C:95:ARG:NH1	4:K:632:GLU:O	2.36	0.58
4:K:804:LEU:HD11	4:K:807:ARG:HH21	1.69	0.58
4:J:266:TYR:HB3	4:J:267:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:74:TYR:HB3	5:M:105:LEU:HA	1.86	0.58
5:M:186:TYR:O	5:M:187:GLU:HG3	2.04	0.58
5:M:159:ALA:HB2	5:M:170:VAL:HG21	1.85	0.57
1:D:159:VAL:HG23	1:D:179:ASP:HA	1.85	0.57
4:K:320:VAL:HG22	4:K:322:SER:H	1.70	0.57
5:L:65:THR:HG22	5:L:67:LYS:H	1.70	0.57
1:C:21:PHE:HZ	1:C:96:VAL:HG11	1.70	0.57
1:A:168:GLY:HA2	1:B:44:MET:HG3	1.86	0.57
2:F:274:LEU:HD22	2:G:1:MET:HE1	1.87	0.57
4:J:22:GLU:N	4:J:22:GLU:OE1	2.38	0.57
1:D:1:ASP:O	1:D:6:THR:OG1	2.22	0.56
4:J:539:MET:HE2	4:J:644:PHE:HB3	1.87	0.56
4:K:145:LYS:HE3	4:K:150:ALA:HB2	1.85	0.56
5:M:86:GLN:OE1	5:M:87:ASN:N	2.37	0.56
4:J:578:ALA:HA	4:J:587:ASP:HA	1.88	0.56
4:K:790:ALA:HB2	5:M:89:THR:HB	1.88	0.56
1:C:369:ILE:HD12	1:C:372:ARG:HD2	1.88	0.56
5:L:67:LYS:HB3	5:L:69:GLU:HG2	1.88	0.56
1:B:6:THR:OG1	1:B:101:HIS:ND1	2.30	0.56
1:D:369:ILE:HD11	1:D:373:LYS:HE2	1.88	0.56
4:J:785:ILE:HA	4:J:788:ILE:HG22	1.86	0.55
5:M:81:LEU:HD11	5:M:118:MET:HE2	1.88	0.55
1:A:286:ASP:OD2	1:B:39:ARG:NH2	2.39	0.55
1:B:156:GLY:O	1:B:303:THR:OG1	2.24	0.55
1:C:148:THR:HG23	1:C:149:THR:HG23	1.88	0.55
4:J:804:LEU:HB3	4:J:808:ARG:HH11	1.71	0.55
4:K:85:ASP:OD2	4:K:86:LYS:NZ	2.36	0.54
1:D:123:MET:HE3	1:D:129:VAL:HG11	1.88	0.54
2:F:281:MET:HE3	2:H:7:LYS:HD3	1.88	0.54
1:A:116:ARG:HD3	1:A:134:VAL:HG11	1.89	0.54
1:B:34:ILE:HD12	1:B:67:LEU:HD13	1.88	0.54
2:H:4:ILE:HA	2:H:7:LYS:HD2	1.90	0.54
4:K:780:ARG:NH2	5:M:133:ASP:OD1	2.38	0.54
1:A:99:GLU:OE1	1:A:128:ASN:ND2	2.40	0.54
4:J:98:GLU:HB3	4:J:690:MET:HE1	1.90	0.54
3:I:86:PHE:O	3:I:90:HIS:ND1	2.40	0.54
4:J:276:GLN:HG2	4:J:315:GLN:HB2	1.89	0.53
4:K:409:GLU:N	4:K:409:GLU:OE1	2.41	0.53
1:B:17:VAL:HG23	1:B:33:SER:HB3	1.91	0.53
4:J:469:ASP:HB3	4:J:573:PRO:HD2	1.90	0.53
5:M:189:PHE:O	5:M:193:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ASP:OD2	1:C:84:LYS:NZ	2.42	0.53
1:C:27:PRO:HG2	4:K:406:VAL:HG23	1.90	0.53
4:K:368:GLN:O	4:K:369:ARG:HG2	2.09	0.52
4:J:249:ARG:NH2	4:J:262:ASP:OD2	2.43	0.52
2:E:239:ALA:HB1	2:F:238:ARG:HH11	1.74	0.52
4:J:509:GLU:OE1	4:J:509:GLU:N	2.42	0.52
4:K:646:THR:HG23	4:K:649:ALA:H	1.75	0.52
4:J:723:ARG:NH2	5:L:136:GLU:OE1	2.41	0.52
1:B:18:LYS:HG2	1:B:30:VAL:HG22	1.92	0.52
1:B:107:GLU:OE1	1:B:111:ASN:ND2	2.42	0.52
2:E:252:SER:HB2	3:I:128:ARG:HH22	1.75	0.52
2:F:173:GLU:O	2:F:177:GLU:HG2	2.09	0.51
1:B:230:ALA:HB2	1:B:236:LEU:HD12	1.92	0.51
2:E:273:GLU:OE2	2:H:1:MET:N	2.38	0.51
4:J:788:ILE:HD11	5:L:193:ILE:HD13	1.92	0.51
1:B:86:TRP:HH2	1:B:119:MET:HG3	1.76	0.51
4:J:273:VAL:HG23	4:J:274:ILE:HG12	1.92	0.51
4:K:784:ILE:HG21	5:M:137:GLY:HA3	1.92	0.51
5:L:182:GLY:HA2	5:L:183:CYS:HB2	1.93	0.51
5:M:186:TYR:C	5:M:188:ALA:H	2.18	0.51
1:B:337:TYR:CZ	4:J:406:VAL:HG21	2.46	0.51
5:L:59:PHE:HE1	5:L:72:ILE:HG12	1.76	0.51
2:F:269:ALA:O	2:F:272:GLU:HG3	2.10	0.51
1:D:35:VAL:HG21	1:D:81:ASP:HB3	1.92	0.51
2:E:284:ILE:HG12	2:H:12:LYS:HZ2	1.76	0.50
2:G:22:ALA:HB2	2:H:22:ALA:HA	1.92	0.50
2:G:56:GLU:HB2	2:H:57:LEU:HD11	1.92	0.50
2:H:10:MET:HA	3:I:92:LYS:NZ	2.26	0.50
4:K:375:PRO:HG3	4:K:396:LEU:HD21	1.93	0.50
2:E:260:LEU:HA	2:F:260:LEU:HD13	1.93	0.50
1:D:90:PHE:HZ	1:D:123:MET:HE1	1.76	0.50
2:H:3:ALA:HA	3:I:103:LEU:HD22	1.93	0.50
1:B:35:VAL:HG21	1:B:81:ASP:HB3	1.93	0.50
1:C:241:GLU:HG2	1:C:247:VAL:HG12	1.93	0.50
1:D:302:GLY:HA2	1:D:336:LYS:HG2	1.92	0.50
4:J:637:LYS:H	4:J:637:LYS:HD3	1.76	0.50
2:E:281:MET:HG3	2:G:7:LYS:HG2	1.94	0.50
2:G:8:MET:HG2	2:G:12:LYS:HE3	1.93	0.50
5:M:89:THR:O	5:M:93:VAL:HG23	2.12	0.50
1:C:290:ARG:HB2	1:D:244:ASP:HB3	1.93	0.49
2:H:3:ALA:HB2	3:I:103:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:186:VAL:O	4:J:190:ARG:HG2	2.12	0.49
1:A:290:ARG:NH1	1:B:244:ASP:OD2	2.44	0.49
1:D:149:THR:HG22	1:D:167:GLU:H	1.76	0.49
4:J:780:ARG:O	4:J:784:ILE:HG12	2.12	0.49
4:J:149:GLU:N	4:J:149:GLU:OE1	2.46	0.49
4:J:782:SER:HA	4:J:785:ILE:HG22	1.94	0.49
2:E:209:ALA:O	2:E:213:LYS:HG2	2.13	0.49
1:B:169:TYR:CD1	1:C:40:HIS:HB2	2.47	0.49
2:F:260:LEU:HG	3:I:121:LYS:NZ	2.27	0.49
5:L:174:MET:O	5:L:178:GLU:N	2.45	0.49
5:M:182:GLY:N	5:M:183:CYS:HB3	2.28	0.49
2:E:238:ARG:NH2	2:F:243:GLU:OE1	2.46	0.49
1:A:67:LEU:H	1:A:203:THR:HG21	1.77	0.48
5:M:150:MET:SD	5:M:150:MET:N	2.87	0.48
1:A:157:ASP:OD1	6:A:401:ADP:O3'	2.32	0.48
4:K:723:ARG:HE	4:K:732:GLU:CD	2.20	0.48
1:A:244:ASP:OD1	1:A:244:ASP:N	2.44	0.48
2:H:10:MET:HA	3:I:92:LYS:HZ1	1.79	0.48
4:K:5:GLU:N	4:K:5:GLU:OE1	2.47	0.48
1:A:24:ASP:OD2	1:A:28:ARG:NH2	2.47	0.48
2:G:58:ASP:O	2:G:62:GLU:HG2	2.14	0.48
1:B:21:PHE:HZ	1:B:96:VAL:HG11	1.77	0.48
1:C:151:ILE:HD11	1:C:162:ASN:HD21	1.78	0.48
2:G:34:ASP:O	2:G:38:ARG:HG2	2.13	0.48
4:K:808:ARG:NH1	5:M:61:LEU:O	2.47	0.48
1:B:25:ASP:OD1	4:J:643:SER:OG	2.26	0.47
1:D:244:ASP:OD1	1:D:244:ASP:N	2.39	0.47
4:J:302:LEU:HD13	4:J:383:LYS:HG2	1.96	0.47
1:A:72:GLU:O	1:A:74:GLY:N	2.47	0.47
1:D:369:ILE:HA	1:D:372:ARG:HD3	1.95	0.47
2:F:264:LYS:HG3	3:I:121:LYS:HZ1	1.79	0.47
4:J:785:ILE:HG21	5:L:161:LEU:HB3	1.95	0.47
1:D:113:LYS:HE2	1:D:371:HIS:CE1	2.49	0.47
2:E:228:LEU:HB3	2:F:228:LEU:HD23	1.97	0.47
4:K:45:GLU:O	4:K:46:PHE:HB2	2.14	0.47
2:E:281:MET:SD	2:G:4:ILE:HA	2.55	0.47
4:J:481:THR:HG22	4:J:655:LEU:HD13	1.96	0.47
1:B:253:GLU:HA	1:B:256:ARG:HB2	1.95	0.47
1:D:25:ASP:OD1	1:D:25:ASP:N	2.46	0.47
4:K:90:MET:HE1	4:K:104:ASN:HB3	1.96	0.47
1:D:113:LYS:HB3	1:D:371:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:SER:HB2	2:G:2:ASP:CG	2.41	0.46
2:F:275:ASP:HB2	3:I:111:ARG:NH2	2.28	0.46
1:B:290:ARG:NH1	1:C:244:ASP:OD2	2.48	0.46
1:C:5:THR:O	1:C:102:PRO:HD2	2.14	0.46
2:E:212:GLU:O	2:E:216:GLN:HG2	2.16	0.46
4:K:486:GLN:HG3	4:K:582:TYR:CZ	2.50	0.46
1:C:72:GLU:O	1:C:74:GLY:N	2.49	0.46
2:F:214:TYR:O	2:F:218:GLU:HG2	2.15	0.46
2:H:7:LYS:O	2:H:10:MET:HG2	2.16	0.46
4:K:442:ARG:O	4:K:446:THR:OG1	2.25	0.46
1:C:165:ILE:HG21	1:D:44:MET:HE3	1.96	0.46
1:C:244:ASP:OD2	1:C:246:GLN:NE2	2.48	0.46
1:A:35:VAL:HG21	1:A:81:ASP:HB3	1.96	0.46
4:J:606:VAL:HG11	4:J:624:TYR:CD2	2.51	0.46
4:J:723:ARG:HD2	4:J:732:GLU:HG2	1.97	0.46
1:B:276:GLU:O	1:B:280:ASN:ND2	2.43	0.46
5:L:139:ARG:NH1	5:L:142:ASP:OD2	2.49	0.46
5:M:57:GLU:O	5:M:61:LEU:HG	2.16	0.46
1:B:5:THR:O	1:B:102:PRO:HD2	2.15	0.45
1:B:21:PHE:CZ	1:B:96:VAL:HG11	2.51	0.45
2:E:243:GLU:O	2:E:246:VAL:HG12	2.16	0.45
4:J:282:ASP:OD1	4:J:283:TYR:N	2.39	0.45
4:J:609:TYR:CD1	4:J:617:LEU:HD21	2.52	0.45
2:F:281:MET:HG2	2:H:7:LYS:HE2	1.97	0.45
4:K:724:ILE:HA	5:M:136:GLU:HG3	1.97	0.45
1:C:167:GLU:HB3	1:D:64:ILE:HD13	1.98	0.45
1:D:14:SER:OG	1:D:71:ILE:O	2.29	0.45
4:K:500:GLU:OE1	4:K:712:ARG:NH2	2.47	0.45
5:L:45:ILE:HG21	5:L:116:LEU:HD13	1.98	0.45
1:D:131:ALA:HB1	1:D:356:TRP:HB3	1.99	0.45
2:F:185:LEU:O	2:F:189:LYS:HG2	2.17	0.45
4:J:737:ASP:OD2	4:J:740:LYS:NZ	2.44	0.45
4:K:634:GLY:HA3	4:K:635:LYS:HA	1.71	0.45
1:A:116:ARG:HB3	1:A:370:VAL:HG11	1.97	0.45
4:K:251:HIS:CG	4:K:453:ARG:HD3	2.51	0.45
1:C:12:ASN:HD21	1:C:86:TRP:HZ2	1.65	0.45
4:K:174:ILE:N	4:K:458:GLY:O	2.50	0.45
1:B:132:MET:HE2	1:B:132:MET:HB2	1.93	0.45
2:E:182:ARG:HH22	2:F:184:GLU:HG3	1.82	0.45
2:F:264:LYS:HG3	3:I:121:LYS:NZ	2.32	0.45
4:J:538:CYS:SG	4:J:598:LYS:HG3	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:507:GLU:H	4:K:507:GLU:HG3	1.55	0.45
2:E:188:GLY:O	2:E:192:GLU:HG2	2.16	0.45
2:F:264:LYS:HE3	3:I:117:LEU:HB3	1.98	0.45
4:J:183:GLY:HA2	4:J:186:VAL:HG22	1.98	0.45
4:K:280:GLU:N	4:K:280:GLU:OE1	2.50	0.45
5:M:154:LEU:HA	5:M:157:VAL:HG22	1.99	0.45
1:D:219:VAL:HG22	1:D:258:PRO:HB2	1.98	0.44
3:I:105:GLU:O	3:I:109:GLU:HG2	2.17	0.44
4:J:28:THR:HG21	5:L:156:HIS:HE1	1.82	0.44
4:K:223:ALA:HB2	4:K:339:LEU:HD21	2.00	0.44
4:K:688:LEU:O	4:K:692:GLN:HG2	2.18	0.44
1:A:276:GLU:O	1:A:280:ASN:ND2	2.50	0.44
1:C:9:VAL:HG21	1:C:344:SER:HA	2.00	0.44
1:D:304:THR:O	1:D:335:ARG:NH1	2.50	0.44
4:J:249:ARG:HB2	4:J:262:ASP:OD1	2.18	0.44
4:K:530:ILE:HA	4:K:552:LEU:HD11	1.99	0.44
1:B:120:THR:HG21	1:B:370:VAL:HG21	1.99	0.44
4:K:98:GLU:CG	4:K:690:MET:HE1	2.47	0.44
5:L:67:LYS:HE2	5:L:67:LYS:HB2	1.76	0.44
1:D:72:GLU:OE1	1:D:183:ARG:NH1	2.51	0.44
1:D:241:GLU:HA	1:D:247:VAL:HG12	2.00	0.44
1:B:72:GLU:O	1:B:74:GLY:N	2.50	0.44
1:D:49:GLN:OE1	1:D:49:GLN:N	2.45	0.44
5:L:45:ILE:HG12	5:L:116:LEU:HB3	2.00	0.44
1:A:189:LEU:HD13	1:A:257:CYS:HB2	2.00	0.44
5:L:57:GLU:O	5:L:61:LEU:HD23	2.18	0.44
2:H:3:ALA:O	2:H:7:LYS:HG3	2.18	0.43
3:I:141:ARG:HD3	3:I:141:ARG:HA	1.86	0.43
1:C:109:PRO:O	1:C:177:ARG:NH1	2.50	0.43
4:K:587:ASP:OD1	4:K:587:ASP:N	2.51	0.43
1:B:157:ASP:HB2	6:B:401:ADP:H4'	2.00	0.43
4:K:222:GLN:O	4:K:225:PRO:HD2	2.18	0.43
4:K:362:MET:HE1	4:K:381:ALA:HB2	2.00	0.43
1:D:157:ASP:OD1	6:D:401:ADP:O3'	2.36	0.43
5:L:149:VAL:HG13	5:L:186:TYR:CE2	2.53	0.43
1:A:330:ILE:HG22	1:A:332:PRO:HD3	1.99	0.43
2:E:196:GLU:O	2:E:200:VAL:HG23	2.19	0.43
2:G:66:ASP:OD1	2:G:66:ASP:N	2.51	0.43
5:L:69:GLU:O	5:L:71:LYS:NZ	2.44	0.43
1:C:215:LYS:HD2	1:C:240:TYR:HE1	1.83	0.43
1:D:2:ASP:OD1	1:D:3:GLU:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:163:GLN:O	4:K:167:THR:HG22	2.18	0.43
4:K:7:ALA:HB2	4:K:138:VAL:HG12	2.01	0.43
4:K:615:LYS:H	4:K:615:LYS:HD3	1.82	0.43
1:B:274:ILE:HA	1:B:277:THR:HG22	2.01	0.43
2:F:259:GLU:O	2:F:263:GLN:HG2	2.19	0.43
4:K:717:ASP:OD2	4:K:721:ARG:NH2	2.51	0.43
1:B:5:THR:HG23	1:B:6:THR:H	1.84	0.43
1:B:121:GLN:NE2	1:B:125:GLU:OE1	2.44	0.43
2:G:15:LYS:HG3	2:H:18:ALA:HB2	2.01	0.43
5:M:143:LYS:HE3	5:M:143:LYS:HB2	1.85	0.43
1:A:18:LYS:NZ	6:A:401:ADP:O2B	2.43	0.43
1:B:111:ASN:OD1	1:B:177:ARG:NH1	2.50	0.43
1:B:140:LEU:O	1:B:342:GLY:HA3	2.19	0.43
4:K:487:GLN:HE21	4:K:487:GLN:HB3	1.61	0.43
5:L:104:GLU:OE1	5:L:108:LYS:HG2	2.19	0.43
1:A:241:GLU:HA	1:A:247:VAL:HG12	2.00	0.42
2:F:278:LEU:O	2:F:282:THR:HG23	2.19	0.42
1:A:155:SER:HB2	1:A:160:THR:HG23	2.00	0.42
1:D:80:ASP:OD1	1:D:80:ASP:N	2.50	0.42
2:E:197:LEU:HD22	2:F:193:LEU:HD23	2.01	0.42
4:J:117:TYR:CZ	4:J:152:PRO:HA	2.55	0.42
4:J:175:LEU:HD22	4:J:460:LEU:HD22	2.01	0.42
4:K:83:LYS:HE3	4:K:83:LYS:HB3	1.77	0.42
4:J:251:HIS:CD2	4:J:453:ARG:HB2	2.53	0.42
4:J:434:LYS:HB3	4:J:620:LEU:HD22	2.01	0.42
4:J:71:VAL:HG12	4:J:72:LYS:H	1.85	0.42
4:K:391:ASN:HB2	4:K:394:ASP:HB3	2.01	0.42
4:K:610:LYS:HD2	4:K:625:ALA:HB3	2.00	0.42
4:K:724:ILE:HG22	4:K:780:ARG:HG2	2.02	0.42
2:E:284:ILE:HG12	2:H:12:LYS:NZ	2.33	0.42
5:L:93:VAL:HA	5:L:96:VAL:HG22	2.02	0.42
5:L:190:VAL:HA	5:L:193:ILE:HD12	2.01	0.42
1:D:140:LEU:O	1:D:342:GLY:HA3	2.20	0.42
1:D:291:LYS:NZ	1:D:325:MET:SD	2.81	0.42
2:H:8:MET:HE3	2:H:12:LYS:NZ	2.33	0.42
1:B:168:GLY:HA2	1:C:44:MET:HG3	2.01	0.42
2:E:228:LEU:HD23	2:F:228:LEU:HB3	2.02	0.42
4:J:31:PHE:CG	4:J:82:PRO:HD3	2.54	0.42
1:B:167:GLU:HB3	1:C:64:ILE:HD13	2.02	0.42
4:K:94:THR:HG21	4:K:771:GLY:N	2.34	0.42
1:B:49:GLN:H	1:B:49:GLN:NE2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:51:LYS:HD3	2:G:51:LYS:HA	1.92	0.42
4:J:698:VAL:O	4:J:702:ILE:HG12	2.20	0.42
1:B:95:ARG:O	4:J:635:LYS:N	2.53	0.41
1:C:375:PHE:HD1	1:C:375:PHE:HA	1.73	0.41
4:J:246:LYS:HZ3	4:J:461:ASP:CG	2.28	0.41
5:L:52:ILE:HD12	5:L:52:ILE:HA	1.87	0.41
4:K:448:GLU:CD	4:K:453:ARG:HH22	2.26	0.41
1:D:155:SER:HB2	1:D:160:THR:HG23	2.01	0.41
2:G:64:PRO:HA	2:G:67:ALA:HB3	2.03	0.41
2:H:44:VAL:HA	2:H:47:GLN:HE21	1.86	0.41
4:K:650:LEU:O	4:K:654:ASN:ND2	2.42	0.41
2:G:44:VAL:HG12	2:G:48:LYS:NZ	2.36	0.41
4:J:552:LEU:HD13	4:J:552:LEU:HA	1.81	0.41
5:M:89:THR:OG1	5:M:90:GLN:N	2.53	0.41
1:A:238:LYS:HA	1:A:238:LYS:HD3	1.84	0.41
1:A:287:ILE:HD11	1:B:242:LEU:HD23	2.02	0.41
1:A:336:LYS:HB3	1:A:336:LYS:HE2	1.88	0.41
2:E:232:LEU:HD13	2:F:232:LEU:HA	2.02	0.41
2:E:281:MET:SD	2:G:4:ILE:HD13	2.60	0.41
4:J:802:LYS:HA	4:J:802:LYS:HD3	1.83	0.41
4:J:97:HIS:HB3	4:J:99:PRO:HD2	2.03	0.41
2:G:19:LEU:O	2:G:23:GLU:HG2	2.20	0.41
4:K:670:VAL:C	4:K:671:ARG:HE	2.29	0.41
5:L:122:ILE:HD13	5:L:122:ILE:HA	1.89	0.41
5:L:171:GLU:O	5:L:175:ALA:N	2.54	0.41
1:B:19:ALA:HB1	1:B:94:LEU:HD11	2.03	0.41
1:B:200:PHE:HD1	1:B:205:GLU:HB3	1.86	0.41
1:B:287:ILE:HD11	1:C:242:LEU:HD23	2.03	0.41
1:D:285:CYS:HB3	1:D:289:ILE:HD11	2.01	0.41
2:F:274:LEU:HD13	2:F:274:LEU:HA	1.92	0.41
2:H:17:ASN:HD22	3:I:84:VAL:HG13	1.86	0.41
4:J:718:PHE:O	4:J:722:TYR:HB2	2.20	0.41
4:K:747:GLY:HA2	4:K:753:HIS:CE1	2.56	0.41
1:C:5:THR:O	1:C:6:THR:C	2.63	0.41
3:I:100:LEU:O	3:I:103:LEU:HG	2.21	0.41
4:J:106:LYS:HE3	4:J:684:ILE:HB	2.03	0.41
4:J:736:ILE:HG12	4:J:737:ASP:H	1.86	0.41
1:D:252:ASN:OD1	1:D:252:ASN:N	2.52	0.40
4:J:210:THR:HA	4:J:211:PRO:HD3	1.91	0.40
4:J:352:LEU:HD13	4:J:352:LEU:HA	1.93	0.40
2:G:61:SER:C	2:G:64:PRO:HD2	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:380:GLU:HA	4:J:383:LYS:HE2	2.03	0.40
4:J:752:ASP:OD1	4:J:752:ASP:N	2.54	0.40
4:K:243:ARG:HG3	4:K:269:GLU:HB2	2.04	0.40
5:L:179:ASP:HB3	5:L:182:GLY:HA3	2.03	0.40
2:F:260:LEU:C	3:I:121:LYS:HZ3	2.29	0.40
2:F:271:SER:O	3:I:111:ARG:NH2	2.55	0.40
2:G:29:LYS:HG3	2:H:28:ASP:C	2.47	0.40
2:G:43:LEU:HA	2:H:43:LEU:HD11	2.02	0.40
3:I:94:MET:SD	3:I:95:LYS:N	2.95	0.40
4:J:35:LYS:HA	4:J:51:ILE:HB	2.03	0.40
4:J:139:VAL:HG13	4:J:194:TYR:CD1	2.56	0.40
5:L:56:LYS:NZ	5:L:112:PHE:HB3	2.36	0.40
5:L:99:LYS:HD3	5:L:99:LYS:HA	1.94	0.40
1:B:82:MET:HA	1:B:82:MET:HE3	2.03	0.40
2:E:206:SER:O	2:E:210:GLN:HG2	2.21	0.40
1:D:276:GLU:HG2	1:D:280:ASN:HD21	1.86	0.40
2:F:277:ALA:HA	2:F:280:ASP:OD2	2.22	0.40
4:J:77:LEU:HD13	4:J:97:HIS:HB3	2.03	0.40
4:J:251:HIS:HD2	4:J:453:ARG:HB2	1.87	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	373/377 (99%)	358 (96%)	15 (4%)	0	100	100
1	B	373/377 (99%)	354 (95%)	19 (5%)	0	100	100
1	C	373/377 (99%)	355 (95%)	18 (5%)	0	100	100
1	D	373/377 (99%)	361 (97%)	12 (3%)	0	100	100
2	E	113/284 (40%)	113 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	113/284 (40%)	113 (100%)	0	0	100	100
2	G	68/284 (24%)	67 (98%)	1 (2%)	0	100	100
2	H	68/284 (24%)	68 (100%)	0	0	100	100
3	I	66/285 (23%)	66 (100%)	0	0	100	100
4	J	805/1935 (42%)	775 (96%)	30 (4%)	0	100	100
4	K	805/1935 (42%)	770 (96%)	35 (4%)	0	100	100
5	L	151/196 (77%)	145 (96%)	6 (4%)	0	100	100
5	M	151/196 (77%)	142 (94%)	9 (6%)	0	100	100
All	All	3832/7191 (53%)	3687 (96%)	145 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	318/320 (99%)	314 (99%)	4 (1%)	61	72
1	B	318/320 (99%)	309 (97%)	9 (3%)	38	59
1	C	318/320 (99%)	313 (98%)	5 (2%)	55	69
1	D	318/320 (99%)	313 (98%)	5 (2%)	55	69
2	E	103/245 (42%)	101 (98%)	2 (2%)	50	66
2	F	103/245 (42%)	99 (96%)	4 (4%)	28	50
2	G	60/245 (24%)	59 (98%)	1 (2%)	53	67
2	H	60/245 (24%)	59 (98%)	1 (2%)	53	67
3	I	64/249 (26%)	63 (98%)	1 (2%)	55	69
4	J	697/1697 (41%)	677 (97%)	20 (3%)	37	58
4	K	697/1697 (41%)	675 (97%)	22 (3%)	34	55
5	L	133/163 (82%)	132 (99%)	1 (1%)	73	77
5	M	133/163 (82%)	129 (97%)	4 (3%)	36	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3322/6229 (53%)	3243 (98%)	79 (2%)	43	63

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	126	THR
1	A	140	LEU
1	A	152	VAL
1	B	5	THR
1	B	44	MET
1	B	49	GLN
1	B	59	GLN
1	B	140	LEU
1	B	201	VAL
1	B	370	VAL
1	B	373	LYS
1	B	375	PHE
1	C	140	LEU
1	C	324	THR
1	C	370	VAL
1	C	373	LYS
1	C	375	PHE
1	D	45	VAL
1	D	59	GLN
1	D	140	LEU
1	D	152	VAL
1	D	373	LYS
2	E	246	VAL
2	E	281	MET
2	F	230	ASP
2	F	253	ILE
2	F	274	LEU
2	F	284	ILE
2	G	20	ASP
2	H	55	ASP
3	I	87	ASP
4	J	18	LYS
4	J	68	THR
4	J	71	VAL
4	J	101	VAL
4	J	216	LEU

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Mol	Chain	Res	Type
4	J	219	GLN
4	J	241	SER
4	J	302	LEU
4	J	305	ASN
4	J	333	ASP
4	J	352	LEU
4	J	410	TYR
4	J	442	ARG
4	J	460	LEU
4	J	552	LEU
4	J	599	ASP
4	J	635	LYS
4	J	644	PHE
4	J	678	THR
4	J	688	LEU
4	K	58	LYS
4	K	65	HIS
4	K	71	VAL
4	K	98	GLU
4	K	145	LYS
4	K	208	GLU
4	K	344	GLU
4	K	380	GLU
4	K	396	LEU
4	K	446	THR
4	K	448	GLU
4	K	487	GLN
4	K	507	GLU
4	K	522	ASP
4	K	528	MET
4	K	570	LYS
4	K	615	LYS
4	K	623	ASN
4	K	690	MET
4	K	718	PHE
4	K	726	ASN
4	K	745	LEU
5	L	67	LYS
5	M	48	THR
5	M	86	GLN
5	M	93	VAL
5	M	148	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	115	ASN
1	B	40	HIS
1	B	49	GLN
1	B	59	GLN
1	B	73	HIS
1	B	92	ASN
1	B	275	HIS
1	B	353	GLN
1	B	371	HIS
1	C	40	HIS
1	C	59	GLN
1	C	92	ASN
1	C	115	ASN
1	D	59	GLN
1	D	73	HIS
1	D	92	ASN
1	D	314	GLN
1	D	371	HIS
2	E	263	GLN
2	E	279	ASN
2	F	279	ASN
2	G	9	GLN
2	H	17	ASN
2	H	47	GLN
4	J	27	GLN
4	J	153	HIS
4	J	193	GLN
4	J	251	HIS
4	J	347	ASN
4	J	368	GLN
4	J	419	GLN
4	J	692	GLN
4	K	27	GLN
4	K	75	GLN
4	K	172	GLN
4	K	187	ASN
4	K	238	ASN
4	K	284	HIS
4	K	347	ASN
4	K	415	GLN

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Mol	Chain	Res	Type
4	K	416	ASN
4	K	418	GLN
4	K	437	ASN
4	K	487	GLN
4	K	581	HIS
4	K	595	GLN
4	K	666	HIS
5	L	156	HIS
5	M	121	HIS
5	M	125	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
6	ADP	A	401	7	28,29,29	1.39	4 (14%)	43,45,45	1.83	10 (23%)
6	ADP	B	401	7	28,29,29	1.41	4 (14%)	43,45,45	1.82	9 (20%)
6	ADP	D	401	7	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ADP	C	401	7	28,29,29	1.40	4 (14%)	43,45,45	1.84	10 (23%)

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
6	ADP	A	401	7	-	7/16/32/32	0/3/3/3
6	ADP	B	401	7	-	4/16/32/32	0/3/3/3
6	ADP	D	401	7	-	1/16/32/32	0/3/3/3
6	ADP	C	401	7	-	4/16/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	401	ADP	C5-C4	4.68	1.47	1.39
6	D	401	ADP	C5-C4	4.66	1.47	1.39
6	C	401	ADP	C5-C4	4.65	1.47	1.39
6	A	401	ADP	C5-C4	4.64	1.47	1.39
6	B	401	ADP	C5-C6	2.71	1.48	1.41
6	A	401	ADP	C5-C6	2.70	1.48	1.41
6	D	401	ADP	C5-C6	2.66	1.48	1.41
6	C	401	ADP	C5-C6	2.65	1.48	1.41
6	D	401	ADP	C5-N7	-2.35	1.34	1.39
6	B	401	ADP	C5-N7	-2.33	1.34	1.39
6	C	401	ADP	C5-N7	-2.32	1.34	1.39
6	A	401	ADP	C5-N7	-2.30	1.34	1.39
6	D	401	ADP	C8-N7	2.26	1.36	1.31
6	B	401	ADP	C8-N7	2.24	1.36	1.31
6	C	401	ADP	C8-N7	2.24	1.36	1.31
6	A	401	ADP	C8-N7	2.22	1.36	1.31

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	401	ADP	C5-C4-N3	-5.98	118.49	126.72
6	C	401	ADP	C5-C4-N3	-5.85	118.66	126.72
6	A	401	ADP	C5-C4-N3	-5.84	118.67	126.72
6	B	401	ADP	C5-C4-N3	-5.79	118.74	126.72
6	D	401	ADP	N3-C4-N9	4.77	135.29	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	401	ADP	N3-C4-N9	4.71	135.17	127.17
6	A	401	ADP	N3-C4-N9	4.66	135.10	127.17
6	B	401	ADP	N3-C4-N9	4.65	135.08	127.17
6	B	401	ADP	C2-N3-C4	3.68	120.83	111.83
6	A	401	ADP	C2-N3-C4	3.68	120.82	111.83
6	C	401	ADP	C2-N3-C4	3.67	120.81	111.83
6	D	401	ADP	C2-N3-C4	3.67	120.79	111.83
6	C	401	ADP	C4-C5-N7	-3.38	106.72	110.58
6	A	401	ADP	C4-C5-N7	-3.38	106.72	110.58
6	B	401	ADP	C4-C5-N7	-3.37	106.72	110.58
6	D	401	ADP	C4-C5-N7	-3.35	106.75	110.58
6	B	401	ADP	N3-C2-N1	-3.21	123.72	128.58
6	C	401	ADP	N3-C2-N1	-3.17	123.78	128.58
6	A	401	ADP	N3-C2-N1	-3.17	123.78	128.58
6	D	401	ADP	N3-C2-N1	-3.06	123.95	128.58
6	C	401	ADP	C4-N9-C8	2.70	108.57	105.74
6	B	401	ADP	C4-N9-C8	2.69	108.56	105.74
6	A	401	ADP	C4-N9-C8	2.60	108.47	105.74
6	D	401	ADP	C4-N9-C8	2.56	108.43	105.74
6	B	401	ADP	C5-N7-C8	2.49	107.36	103.45
6	C	401	ADP	C5-N7-C8	2.49	107.36	103.45
6	A	401	ADP	C5-N7-C8	2.46	107.32	103.45
6	D	401	ADP	C5-N7-C8	2.44	107.28	103.45
6	C	401	ADP	C3'-C2'-C1'	2.38	105.97	101.46
6	D	401	ADP	C3'-C2'-C1'	2.34	105.88	101.46
6	B	401	ADP	C2'-C1'-N9	-2.33	107.52	113.30
6	A	401	ADP	C3'-C2'-C1'	2.26	105.74	101.46
6	A	401	ADP	C2'-C1'-N9	-2.25	107.72	113.30
6	C	401	ADP	C2'-C1'-N9	-2.23	107.76	113.30
6	B	401	ADP	C6-C5-N7	2.06	136.05	132.09
6	D	401	ADP	C2'-C1'-N9	-2.02	108.29	113.30
6	A	401	ADP	C6-C5-N7	2.00	135.95	132.09
6	C	401	ADP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	ADP	PA-O3A-PB-O2B
6	A	401	ADP	C5'-O5'-PA-O2A
6	A	401	ADP	C5'-O5'-PA-O3A
6	B	401	ADP	C5'-O5'-PA-O1A

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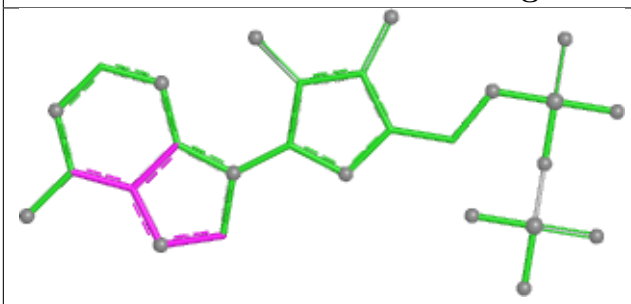
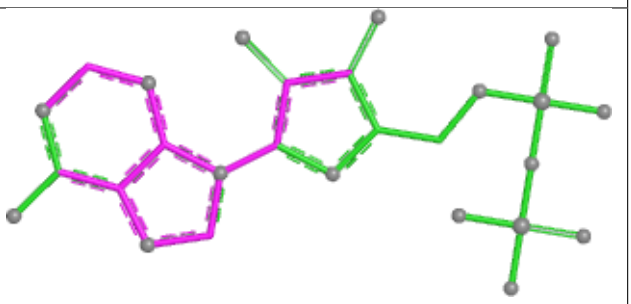
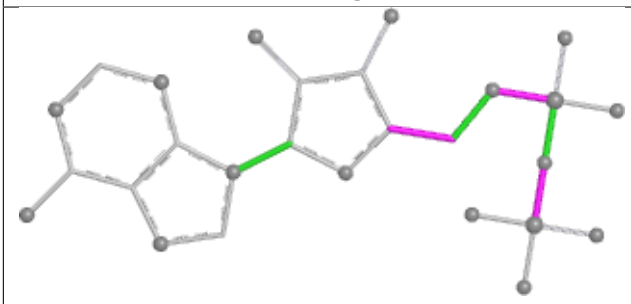
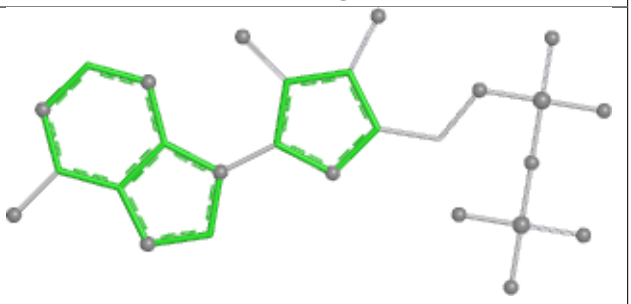
Mol	Chain	Res	Type	Atoms
6	B	401	ADP	C5'-O5'-PA-O3A
6	C	401	ADP	C5'-O5'-PA-O3A
6	D	401	ADP	C5'-O5'-PA-O2A
6	B	401	ADP	C3'-C4'-C5'-O5'
6	C	401	ADP	C3'-C4'-C5'-O5'
6	B	401	ADP	O4'-C4'-C5'-O5'
6	C	401	ADP	O4'-C4'-C5'-O5'
6	A	401	ADP	C3'-C4'-C5'-O5'
6	A	401	ADP	C5'-O5'-PA-O1A
6	C	401	ADP	C5'-O5'-PA-O1A
6	A	401	ADP	PA-O3A-PB-O1B
6	A	401	ADP	O4'-C4'-C5'-O5'

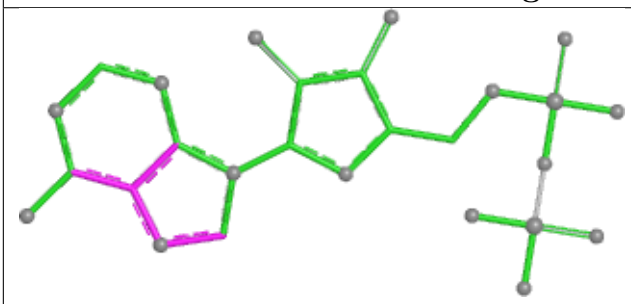
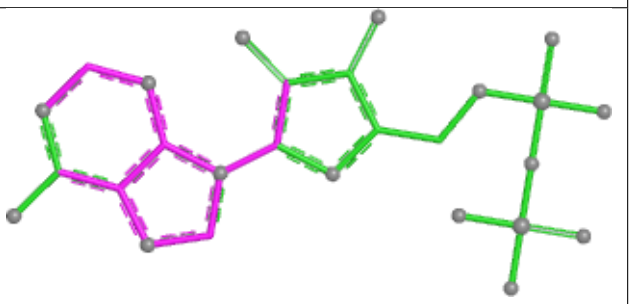
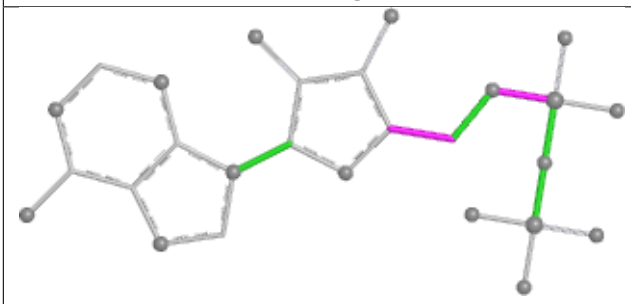
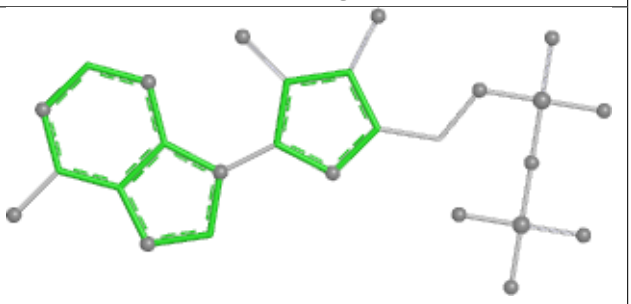
There are no ring outliers.

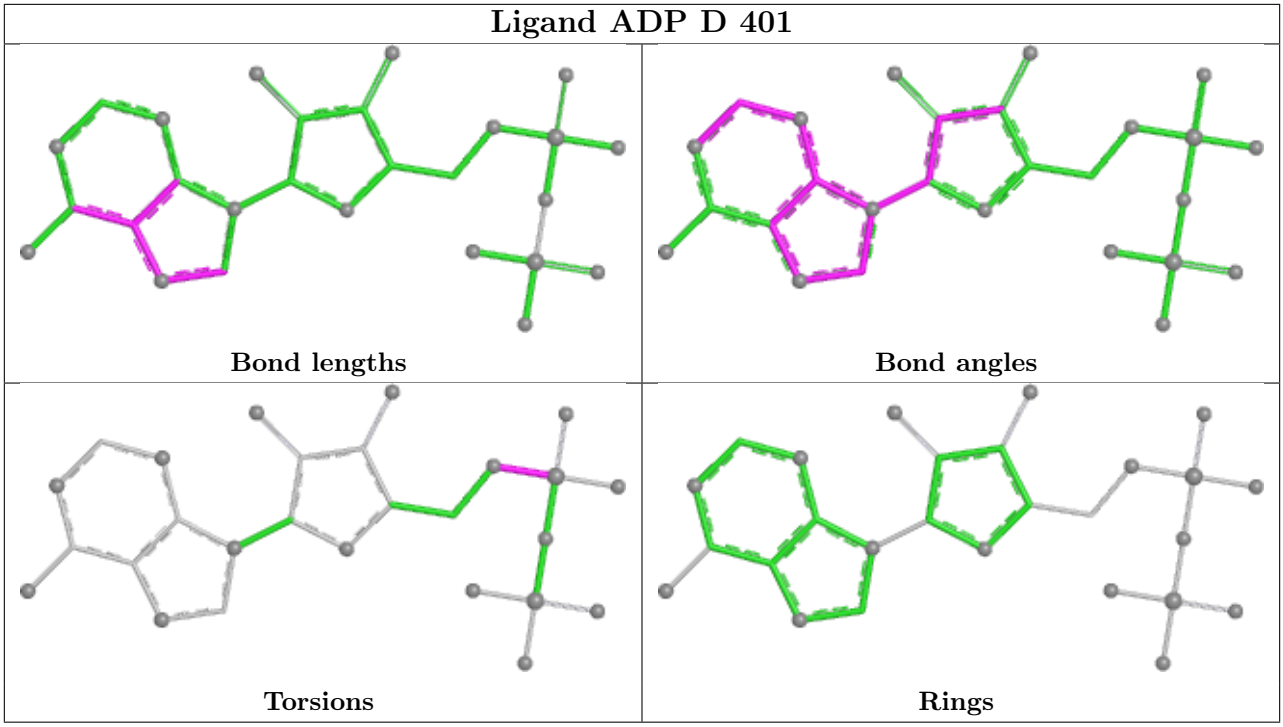
3 monomers are involved in 4 short contacts:

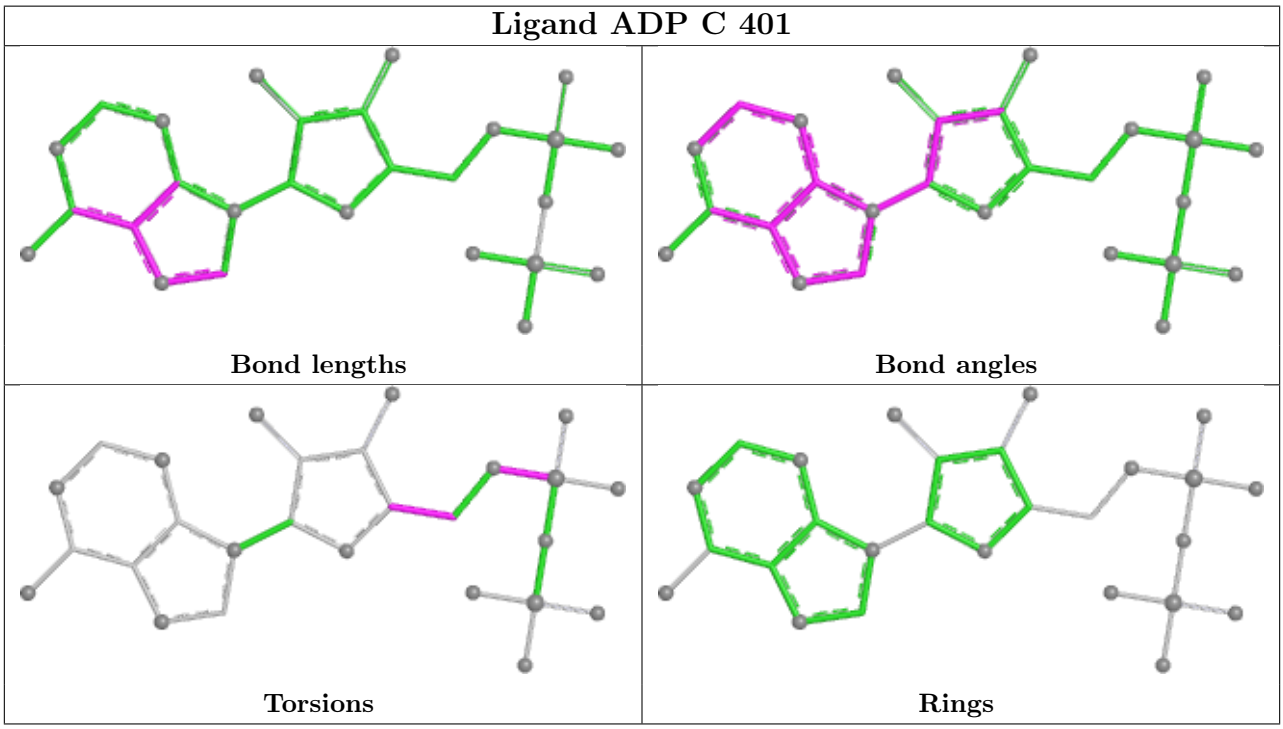
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	ADP	2	0
6	B	401	ADP	1	0
6	D	401	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 A 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 401	
 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.

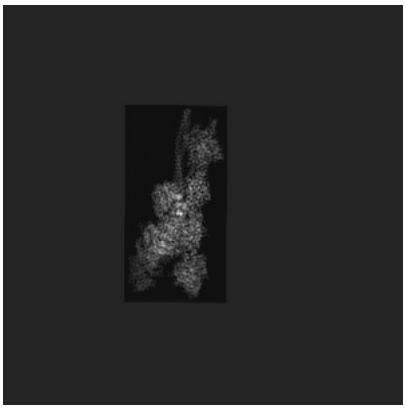
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-72724. These allow visual inspection of the internal detail of the map and identification of artifacts.

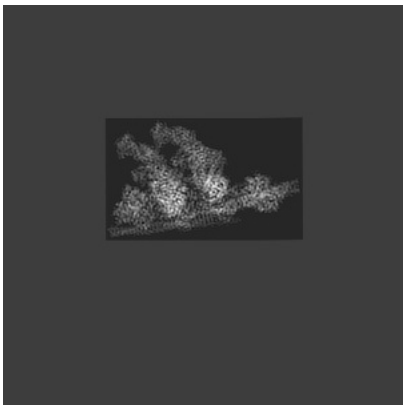
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

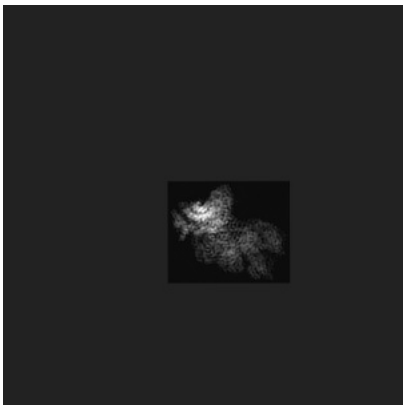
6.1.1 Primary map



X

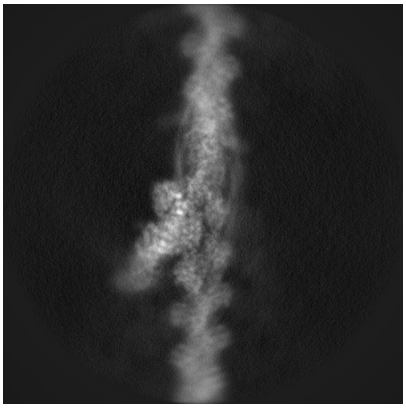


Y

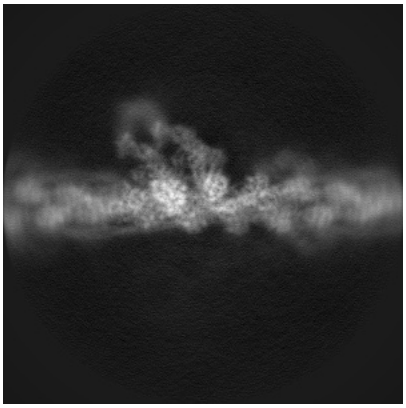


Z

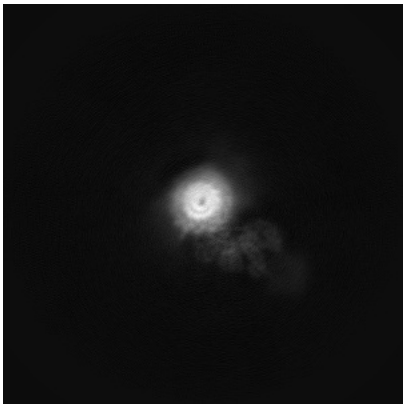
6.1.2 Raw map



X



Y



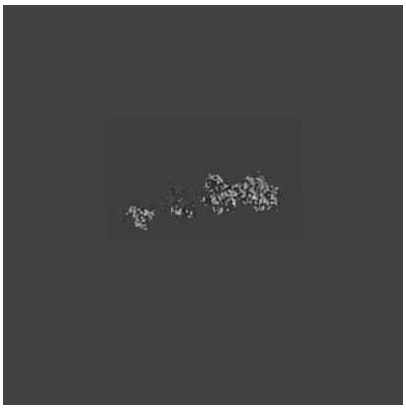
Z

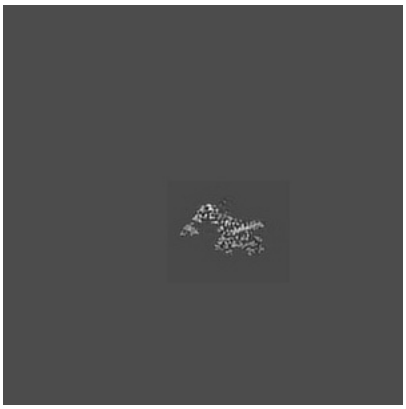
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

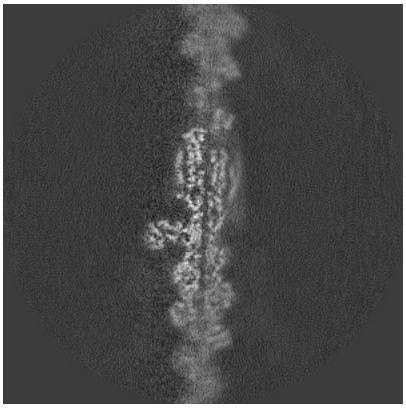
6.2.1 Primary map

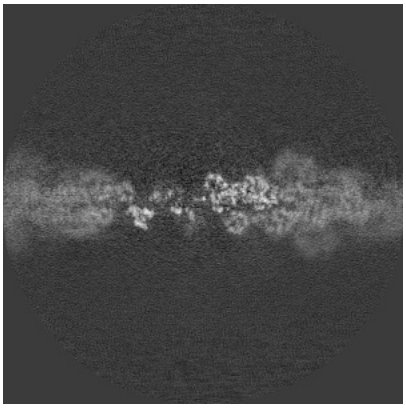
X Index: 198


Y Index: 198


Z Index: 198

6.2.2 Raw map


X Index: 198


Y Index: 198

Z Index: 198

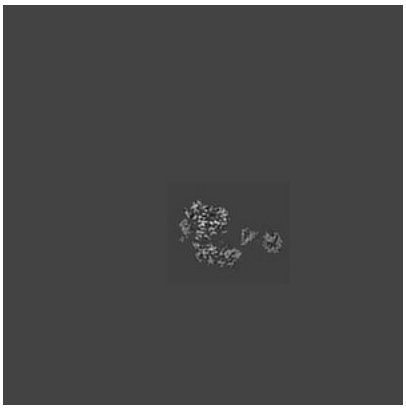
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

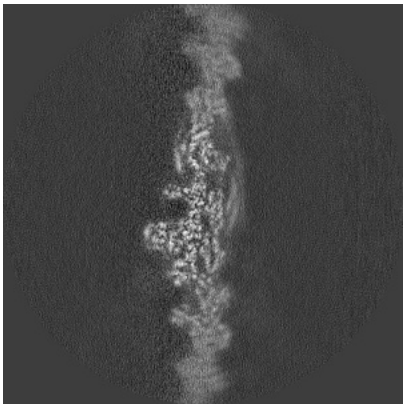
6.3.1 Primary map

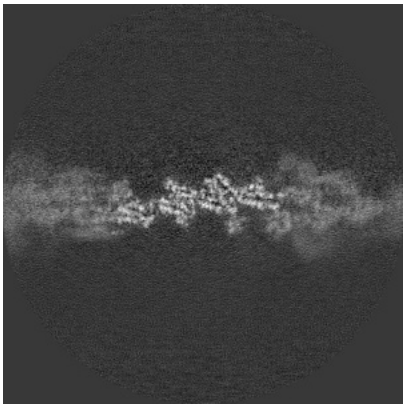
X Index: 207

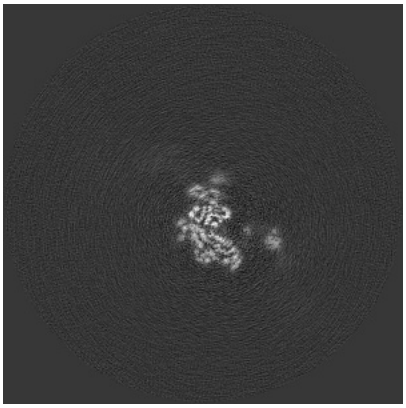
Y Index: 187


Z Index: 171

6.3.2 Raw map


X Index: 204

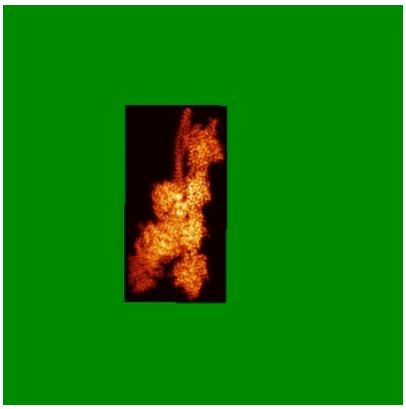

Y Index: 193

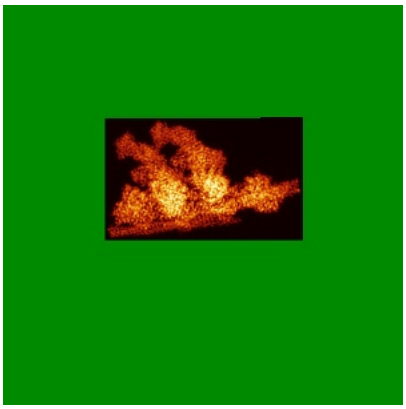

Z Index: 165

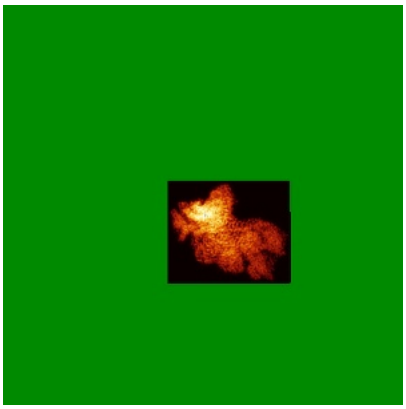
The images above show the largest variance slices of the map in three orthogonal directions.

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

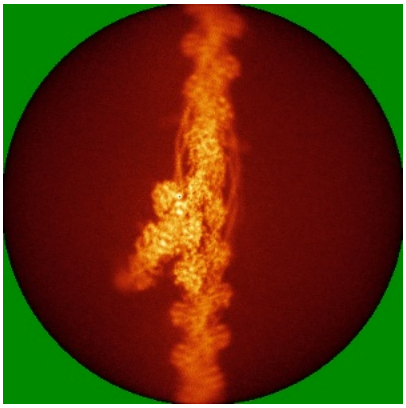
6.4.1 Primary map

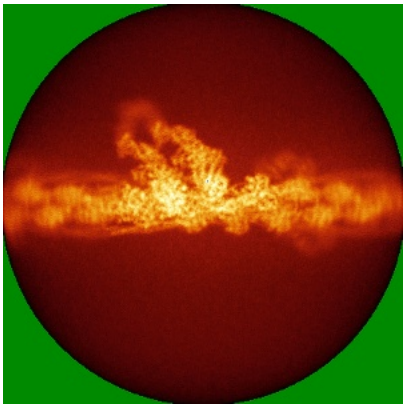

X

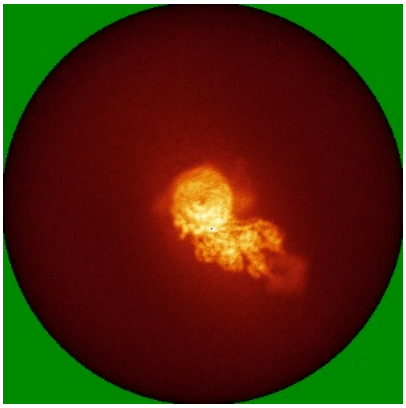

Y


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 1.2. 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.

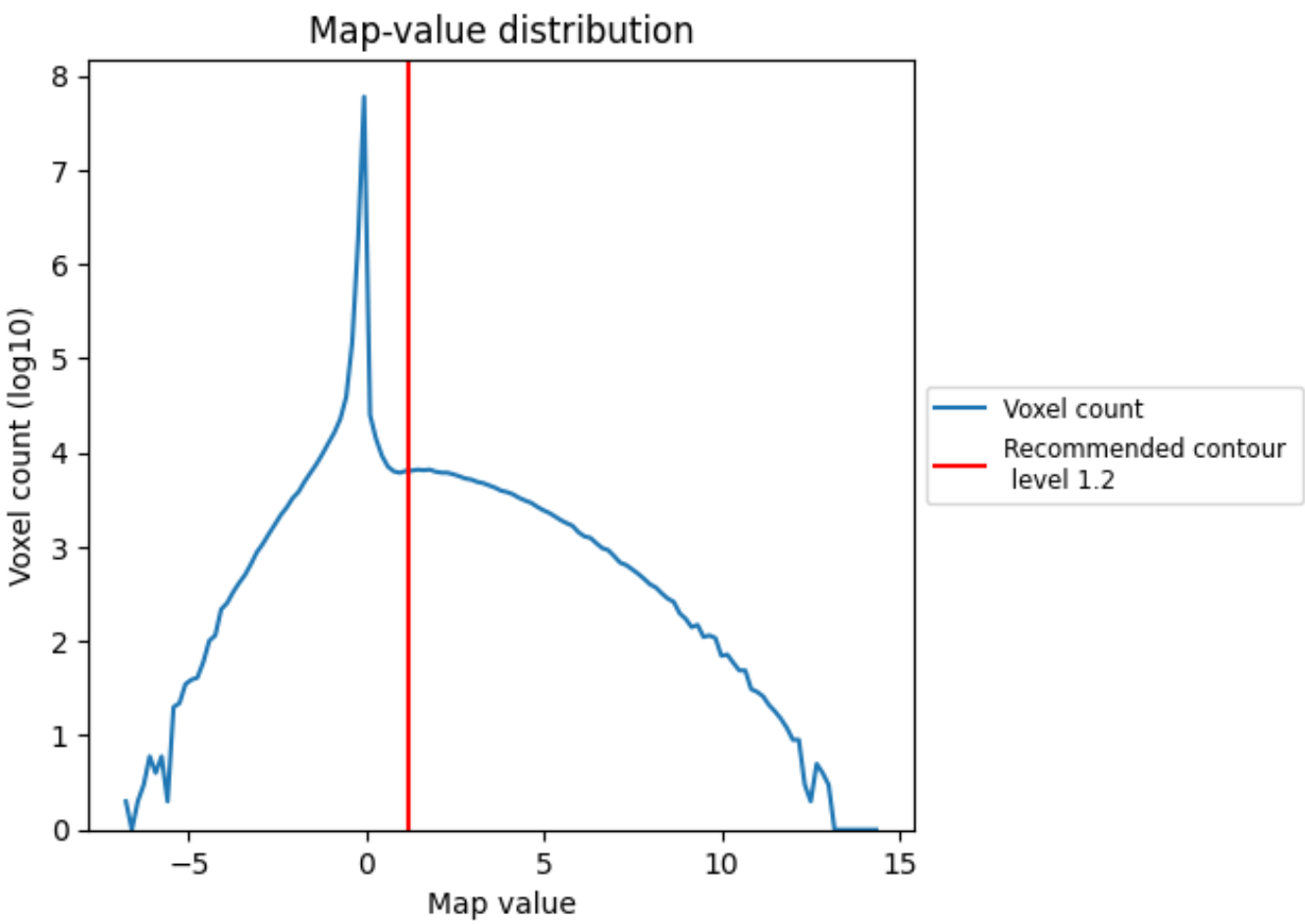
6.6 Mask visualisation (i)

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

7 Map analysis (i)

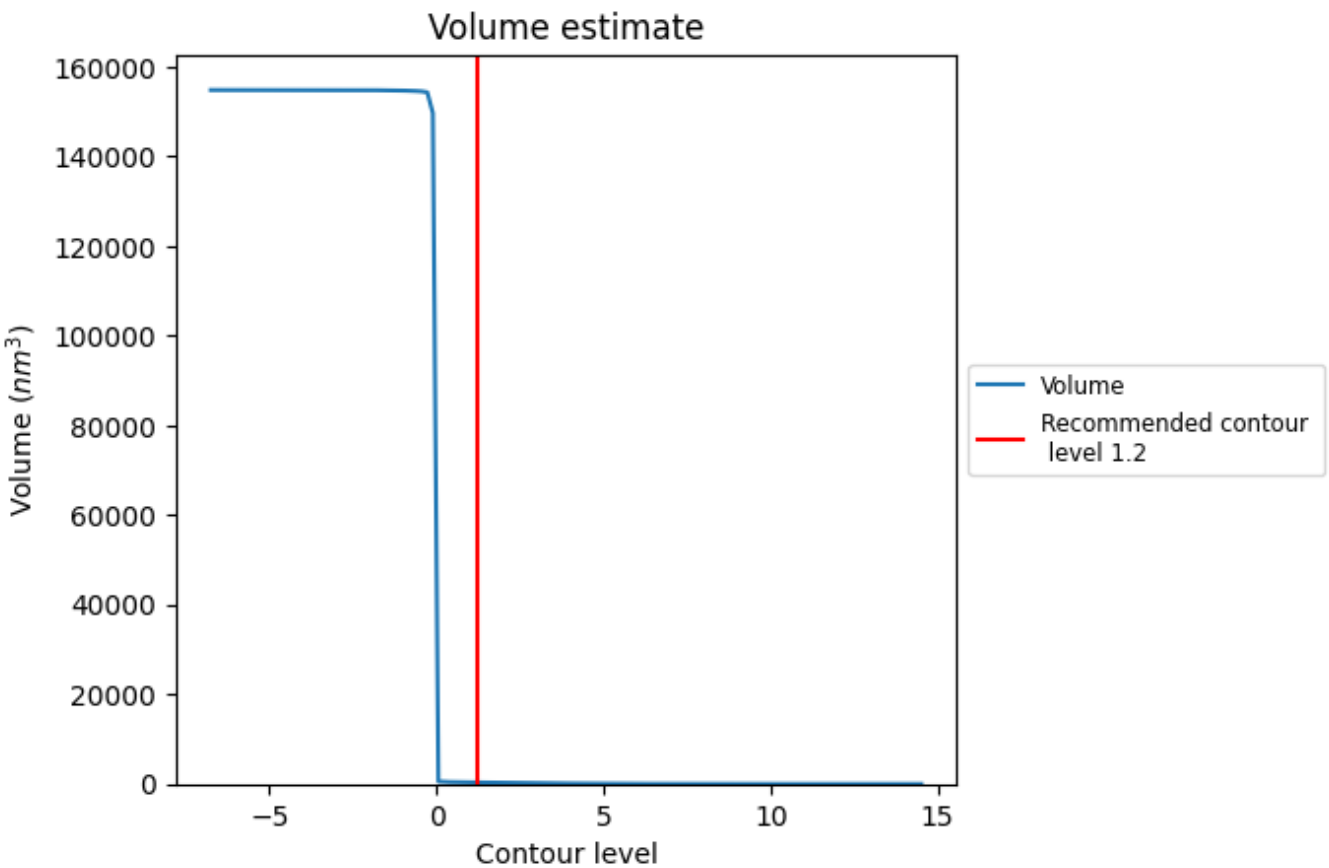
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

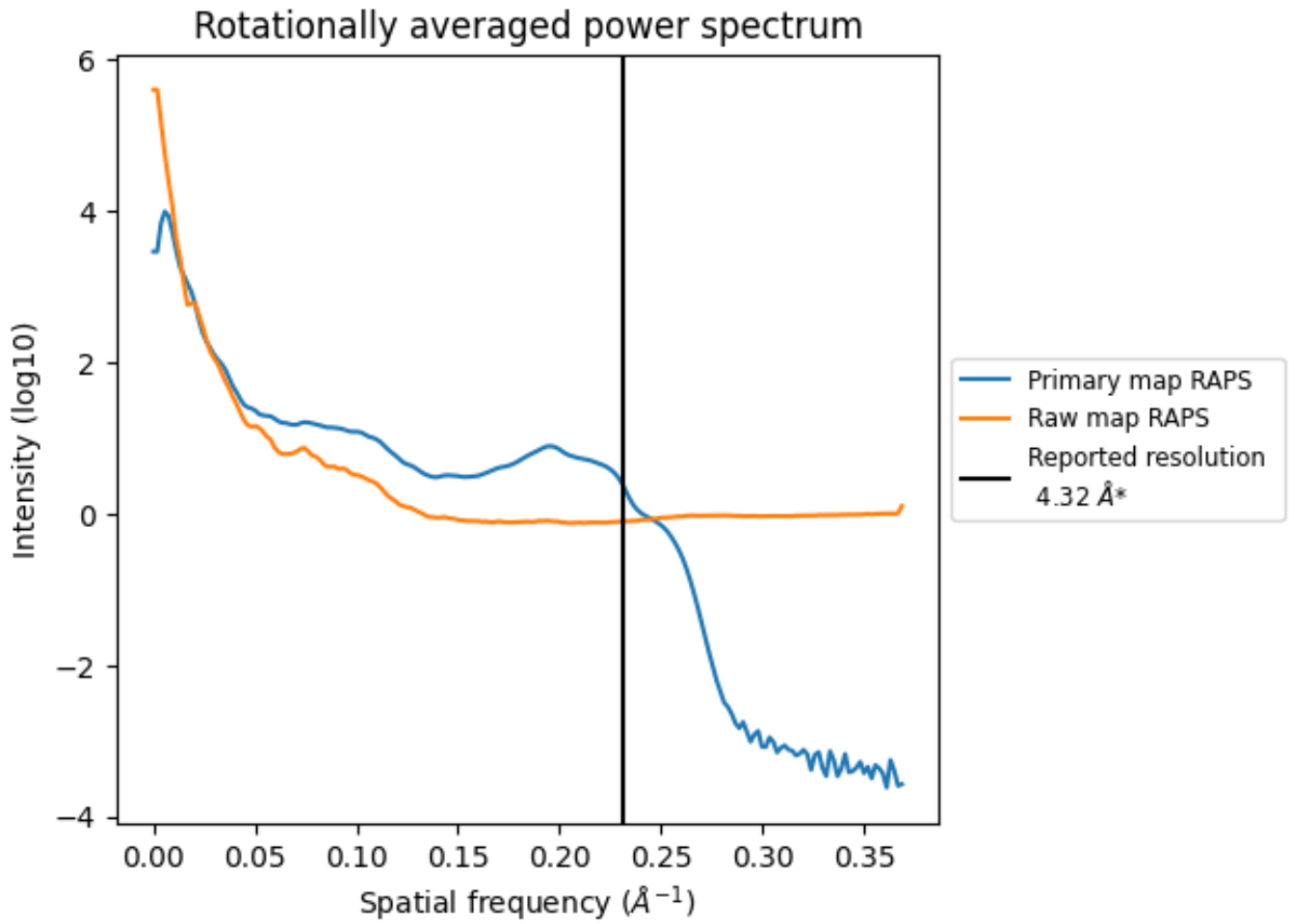
7.2 Volume estimate (i)



The volume at the recommended contour level is 344 nm^3; this corresponds to an approximate mass of 310 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)

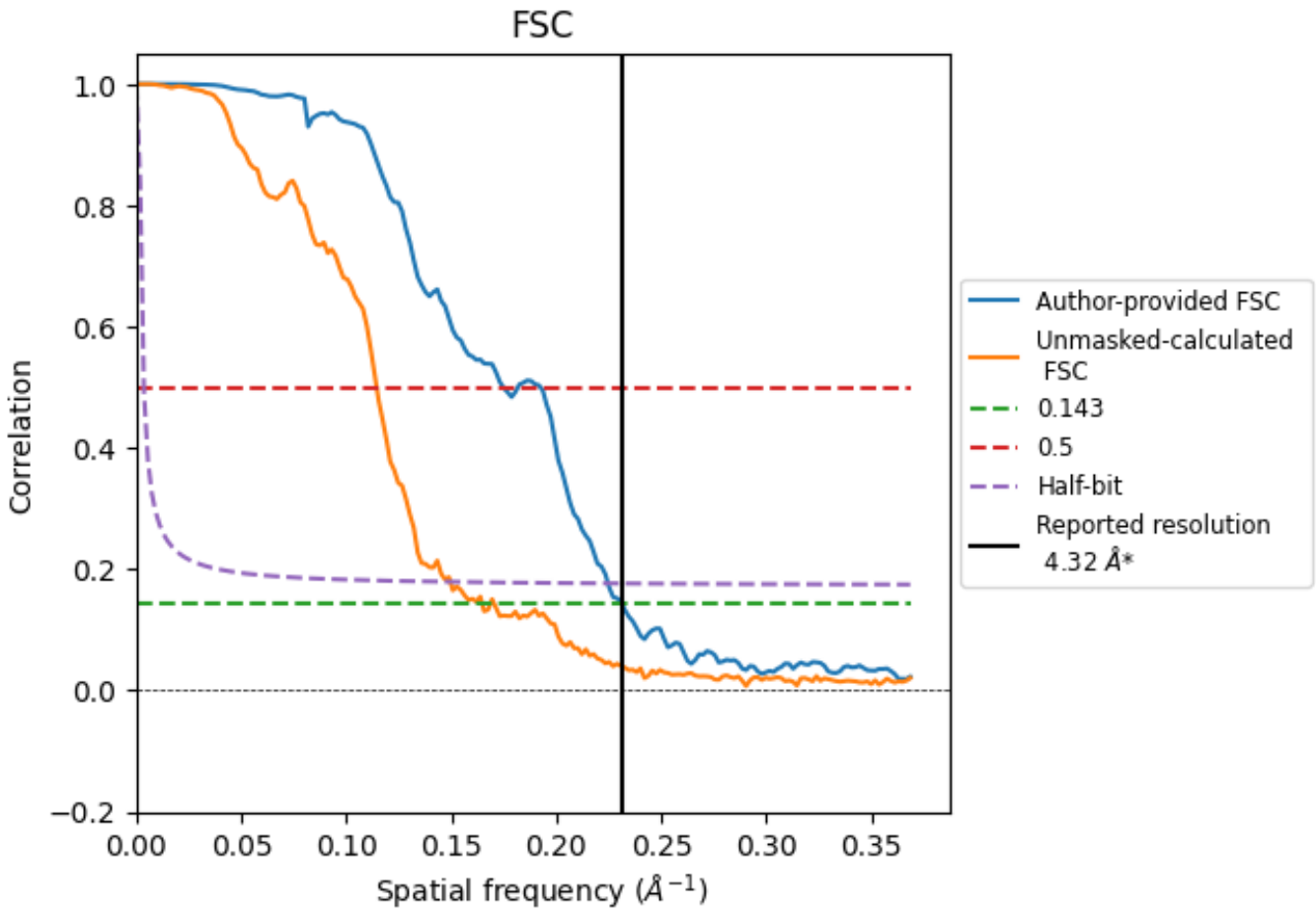


*Reported resolution corresponds to spatial frequency of 0.231 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.231 Å^{-1}

8.2 Resolution estimates (i)

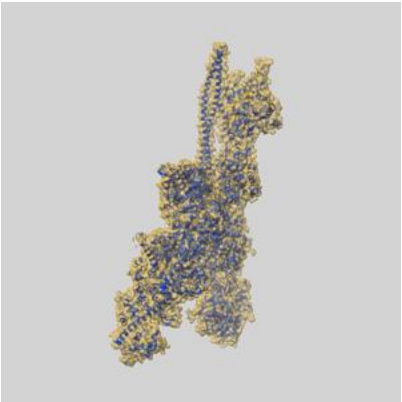
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.32	-	-
Author-provided FSC curve	4.32	5.72	4.45
Unmasked-calculated*	6.07	8.73	6.68

*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 6.07 differs from the reported value 4.32 by more than 10 %

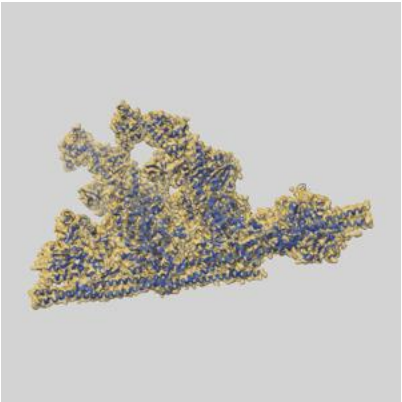
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-72724 and PDB model 9YA8. Per-residue inclusion information can be found in section 3 on page 7.

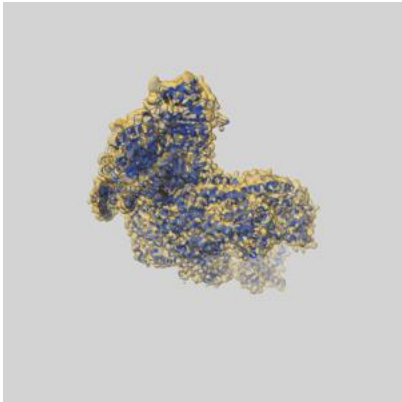
9.1 Map-model overlay (i)



X



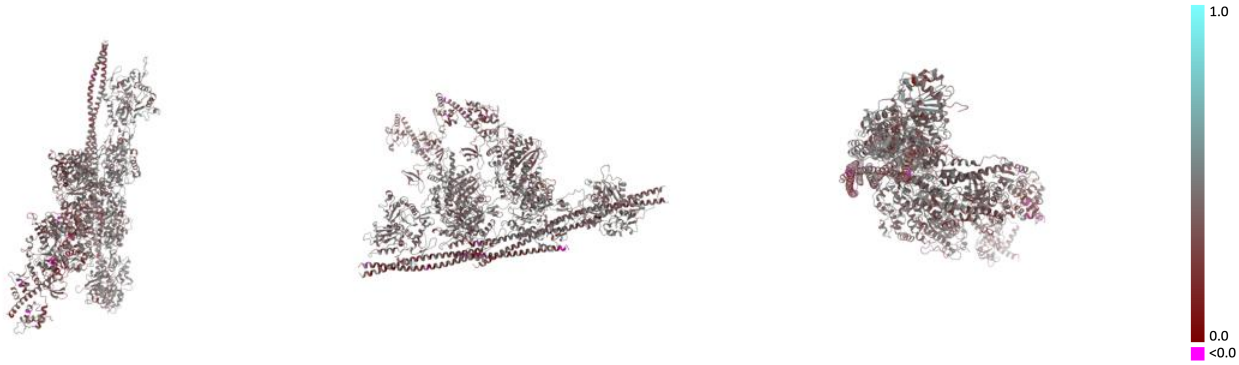
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.2 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.

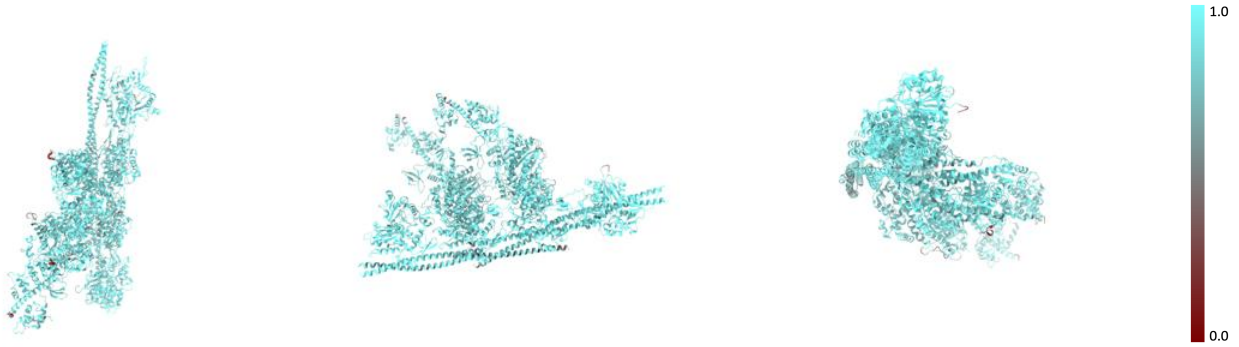
9.2 Q-score mapped to coordinate model (i)



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.

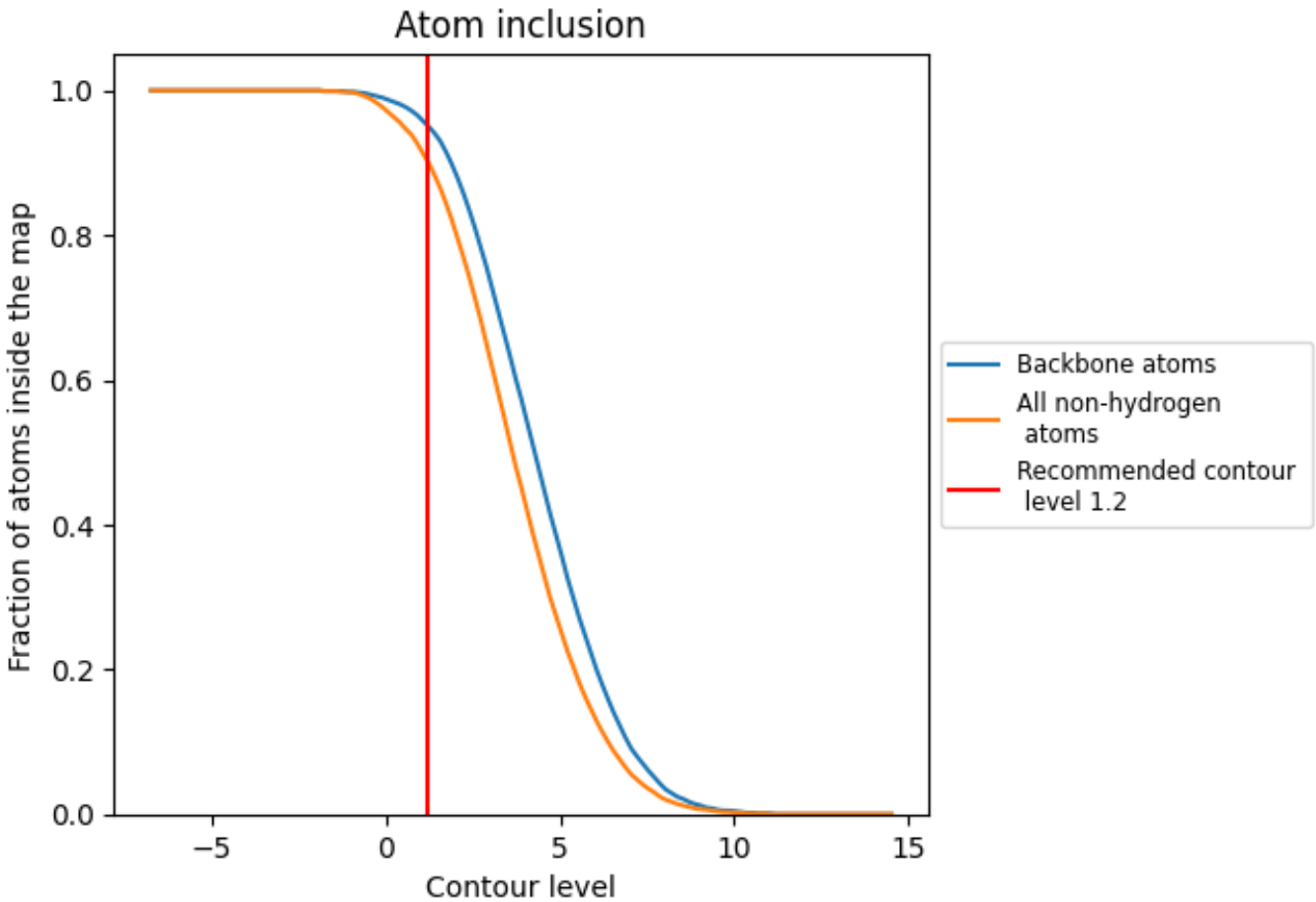
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.2).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9010	0.3880
A	0.9320	0.4230
B	0.9170	0.4340
C	0.9000	0.4090
D	0.9350	0.4200
E	0.9190	0.3500
F	0.8900	0.3270
G	0.8560	0.2900
H	0.8900	0.2940
I	0.6970	0.2500
J	0.9090	0.3870
K	0.8970	0.3900
L	0.8440	0.3220
M	0.8720	0.3560