Full wwPDB EM Validation Report (i)

Aug 27, 2026 – 02:31 PM EDT

PDB ID	:	9YJP / pdb_00009yjp
EMDB ID	:	EMD-73030
Title	:	The structure of the cardiac native crossbridge in the rigor state, myosin heads bound to actin molecules 2 and 3
Authors	:	Galkin, V.E.; Risi, C.M.
Deposited on	:	2025-10-03
Resolution	:	4.80 Å(reported)
Based on initial models	:	5H53, 8DD0, 6SFA, 7KO5, 7JH7

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:

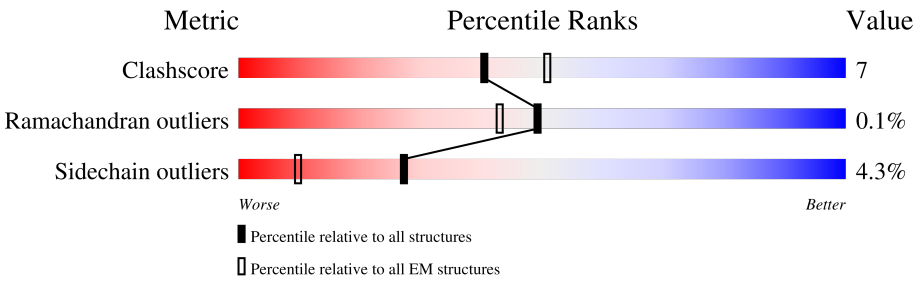
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

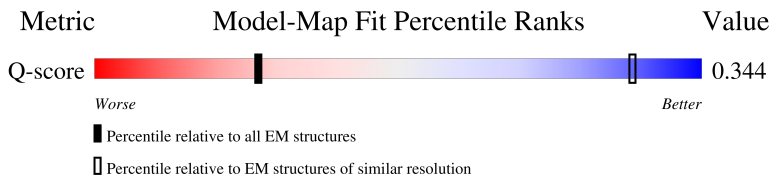
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.80 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	1575 (4.30 - 5.30)

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	84% 14% ••
1	B	377	75% 24% ••
1	C	377	88% 11% ••
1	D	377	77% 21% ••

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Mol	Chain	Length	Quality of chain
2	E	284	55% 10% 35%
2	F	284	54% 11% 35%
3	G	161	68% 29%
4	H	211	45% 18% 36%
5	I	285	17% 8% 74%
6	J	1935	35% 6% 58%
6	K	1935	35% 6% 58%
7	L	196	47% 30% 22%
7	M	196	53% 23% 22%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 33211 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	186	1495	912	254	326	3	0	0
2	F	186	1495	912	254	326	3	0	0

- Molecule 3 is a protein called Troponin C, slow skeletal and cardiac muscles.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	160	1274	789	195	278	12	0	0

- Molecule 4 is a protein called Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	134	1077	667	208	197	5	0	0

- Molecule 5 is a protein called Troponin T2, cardiac type.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	I	74	643	401	123	119	0	0

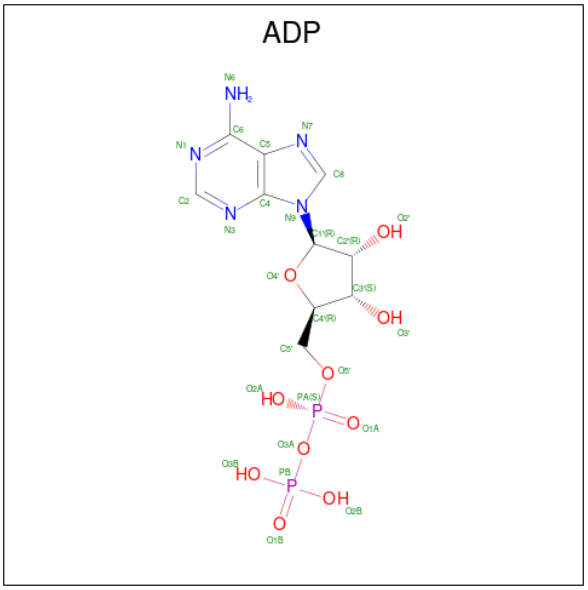
- Molecule 6 is a protein called Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	805	6475	4127	1114	1202	32	0	0
6	K	805	6475	4127	1114	1202	32	0	0

- Molecule 7 is a protein called Myosin light chain 3.

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

- Molecule 8 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	
8	A	1	27	10	5	10	2	0
8	B	1	27	10	5	10	2	0

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

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

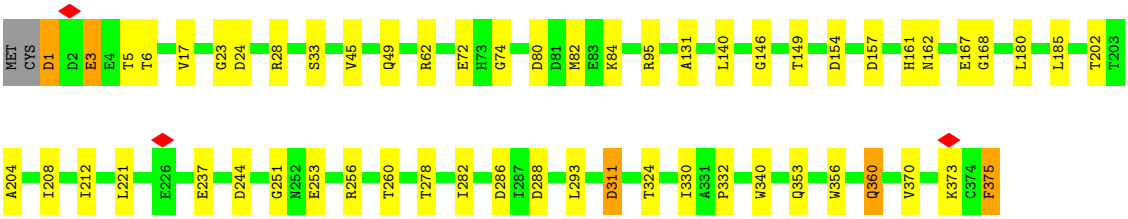
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
10	G	3	3	3	0

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.

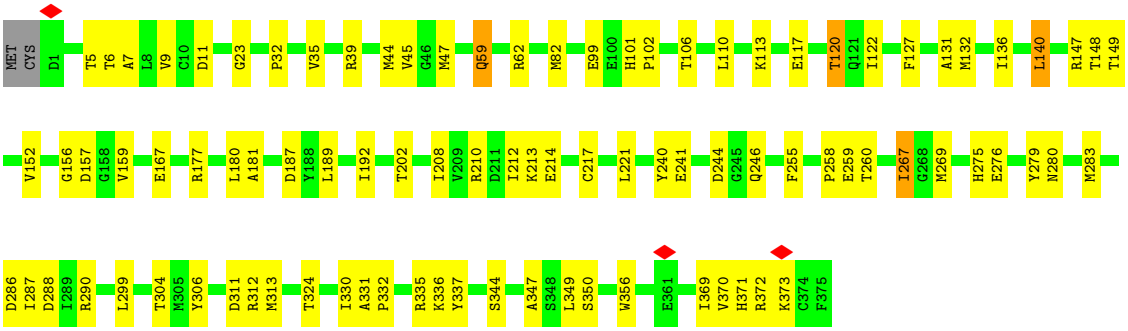
• Molecule 1: Actin, alpha cardiac muscle 1

Chain A:



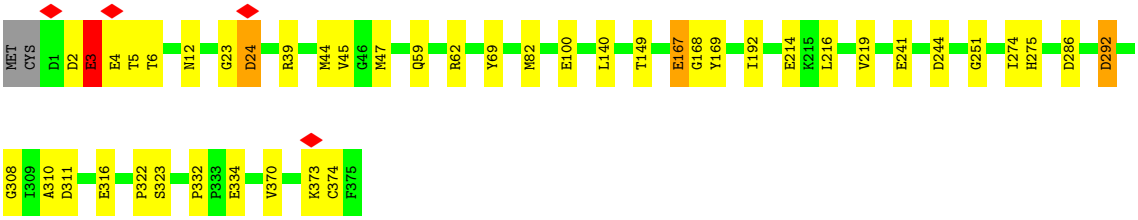
• Molecule 1: Actin, alpha cardiac muscle 1

Chain B:



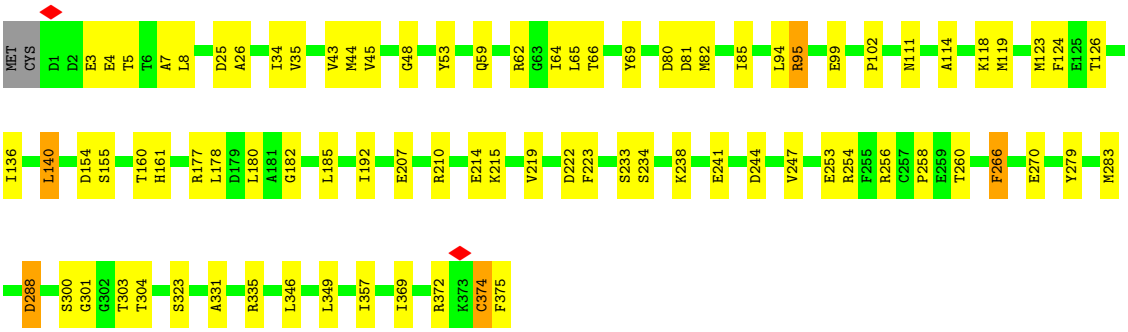
• Molecule 1: Actin, alpha cardiac muscle 1

Chain C:



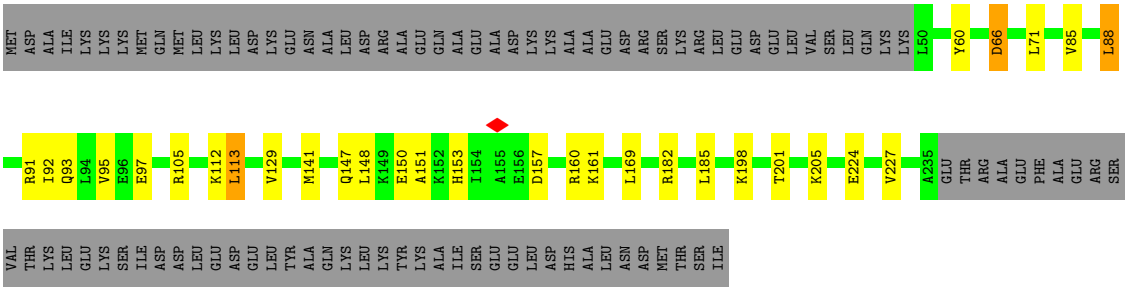
• Molecule 1: Actin, alpha cardiac muscle 1

Chain D:



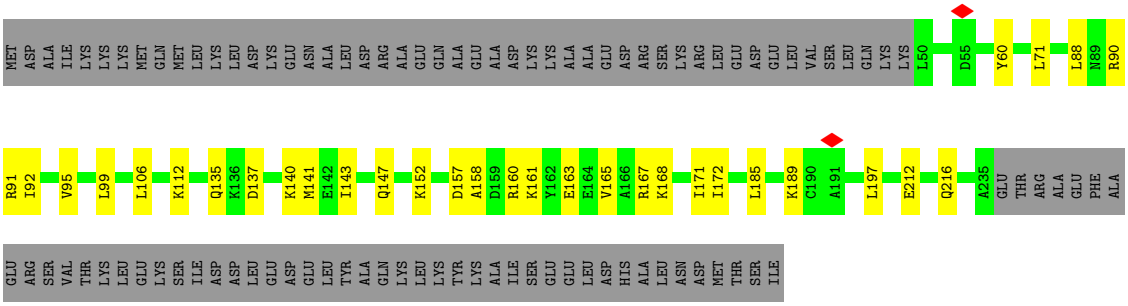
• Molecule 2: Tropomyosin alpha-1 chain

Chain E:



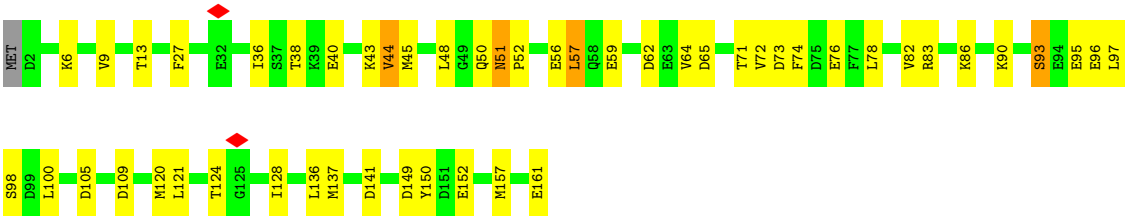
• Molecule 2: Tropomyosin alpha-1 chain

Chain F:



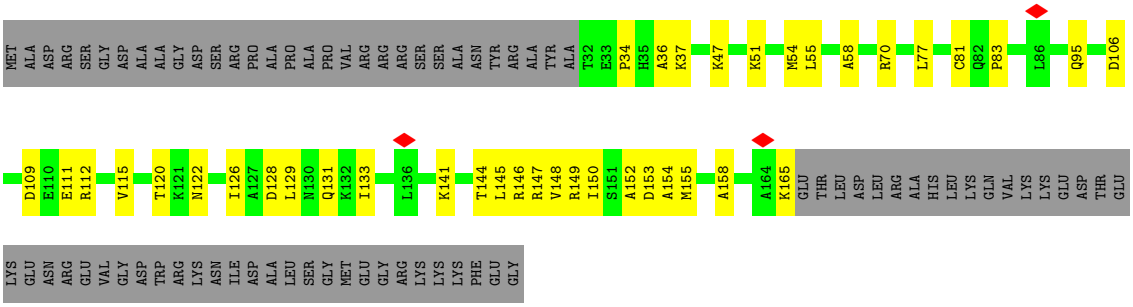
• Molecule 3: Troponin C, slow skeletal and cardiac muscles

Chain G:



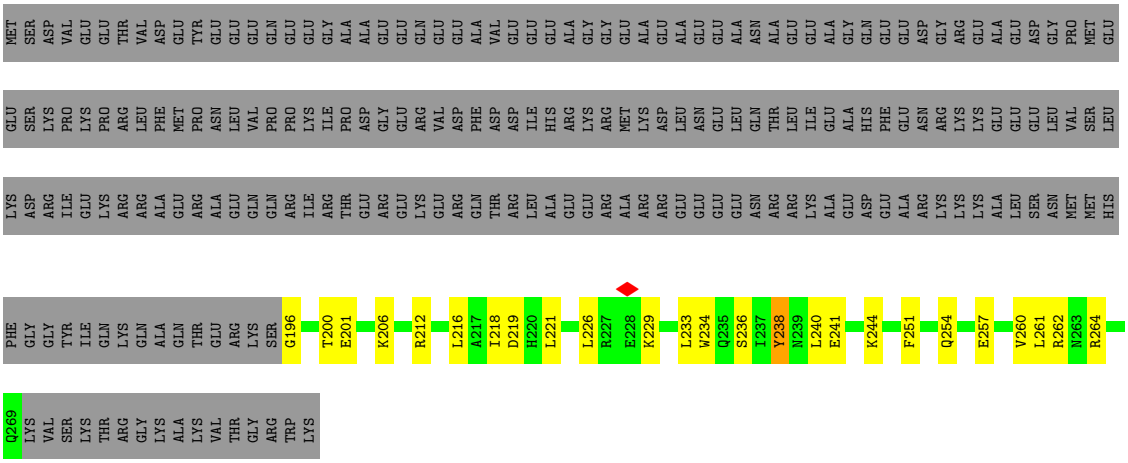
- Molecule 4: Troponin I, cardiac muscle

Chain H:



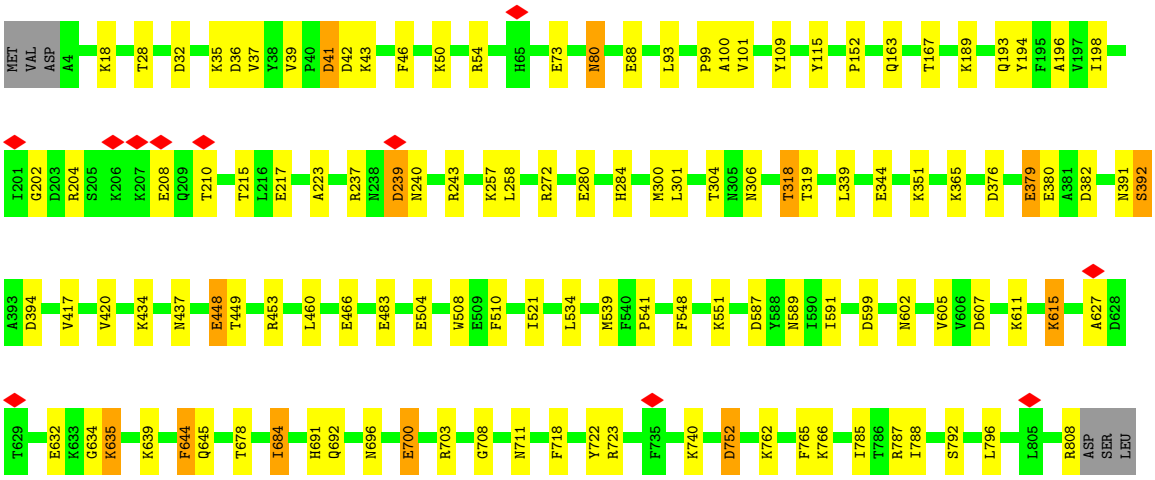
- Molecule 5: Troponin T2, cardiac type

Chain I:



- Molecule 6: Myosin-7

Chain J:



LEU ILE ILE GLN TRP ASN ILE ARG ALA PHE MET SER VAL LYS ASN TRP PRO TRP MET LYS LEU TYR PHE LYS ILE LYS PRO LEU LEU LYS SER ALA GLU THR GLU LYS GLU MET ALA THR MET LYS GLU GLU PHE GLY ARG LEU LYS GLU ALA LEU GLU LYS SER GLU ALA ARG ARG LYS

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

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

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

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

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

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

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

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

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

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

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

GLN LEU GLU ALA GLU LYS LEU GLU LEU GLN SER ALA LEU GLU GLU ALA GLU ALA SER LEU GLU HIS GLU GLU GLY LYS ILE LEU ARG ALA GLN LEU GLU PHE ASN 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 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 LEU ILE GLU THR SER GLU

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

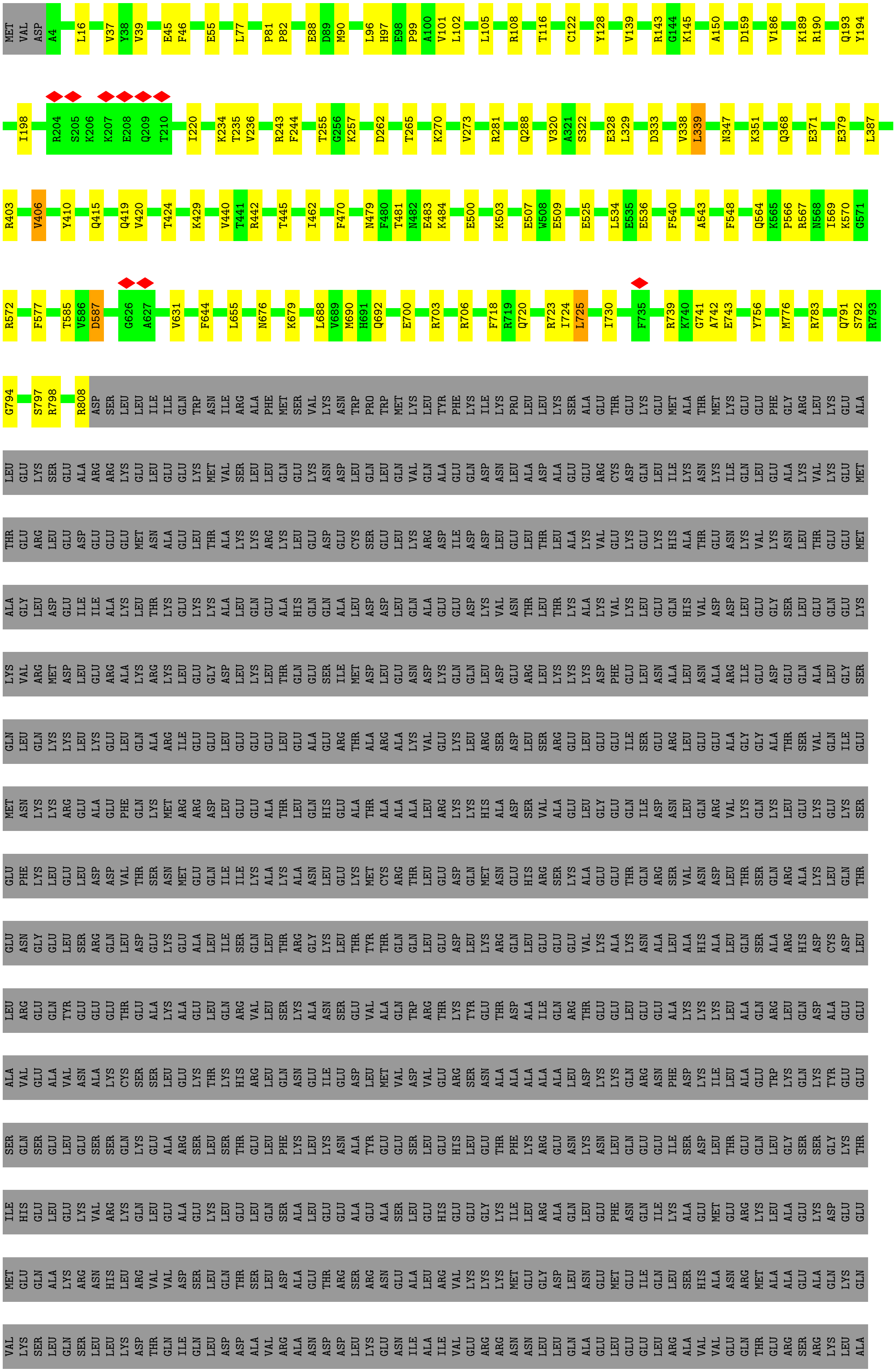
GLU GLN ASP THR SER ALA HIS LEU GLU ARG MET LYS LYS ASN MET GLU GLN THR ILE LYS ASP LEU GLN HIS ARG LEU ASP GLU ALA GLU GLN ILE ALA LEU LYS GLY GLY LYS LYS GLN LEU GLN LYS LEU GLU ALA ARG VAL ARG GLU LEU GLU ASN GLU LEU GLU ALA GLU GLN LYS

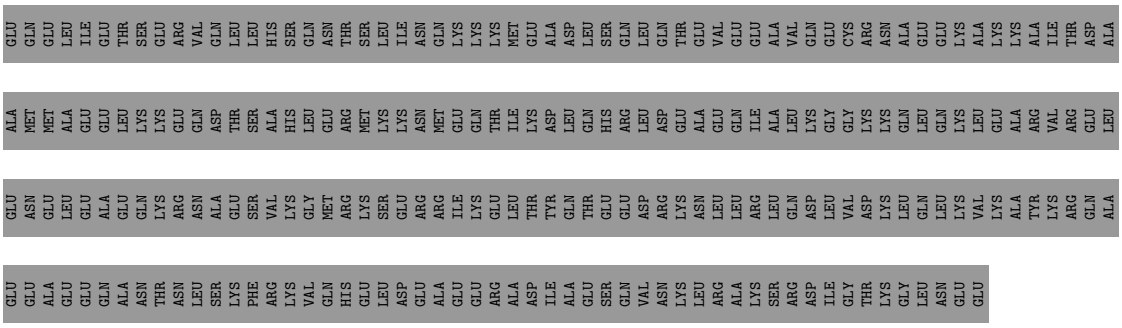
ARG ASN ALA GLU SER VAL LYS GLY MET ARG LYS SER GLU ARG ARG ILE LYS GLU LEU THR TYR GLN THR GLU GLU ASP ARG LYS ASN LEU LEU ARG LEU GLN ASP LEU VAL ASP LYS LEU GLN LEU LYS VAL LYS ALA TYR LYS ARG GLN ALA GLU GLU ALA GLU GLU GLN ALA ASN THR

ASN LEU SER LYS PHE ARG LYS VAL GLN HIS 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 6: Myosin-7

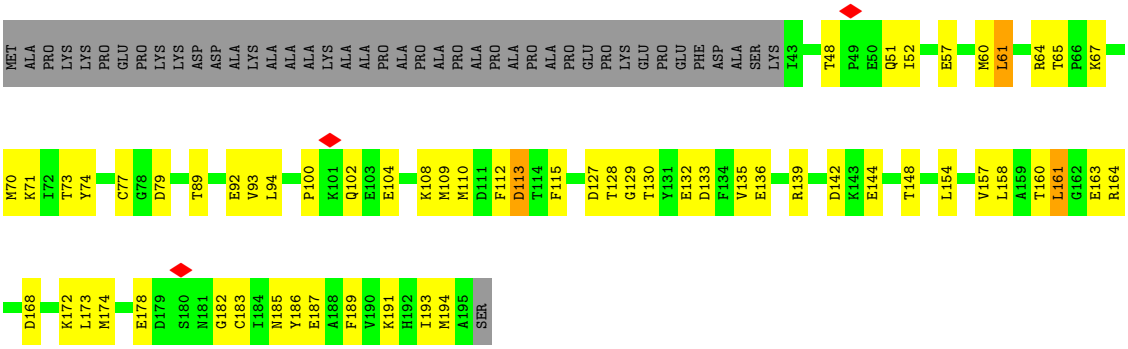
Chain K: 35% 6% 58%


MET VAL ASP A4 L16 V37 Y38 V39 E45 F46 E55 L77 P81 P82 E88 D89 M90 L96 H97 E98 P99 A100 V101 L102 L105 R108 T116 C122 Y128 V139 R143 G144 K145 A150 D159 V186 K189 R190 Q193 Y194
I198 R204 S205 K206 K207 E208 Q209 T210 I220 K234 T235 V236 R243 F244 T255 G256 K257 D262 T265 K270 V273 R281 Q288 V320 A321 S322 E328 L329 D333 V338 L339 N347 K351 Q368 E371 E379 L387
R403 V406 Y410 Q415 Q419 V420 T424 K429 V440 T441 R442 T445 I462 F470 N479 F480 T481 N482 E483 K484 E500 K503 E507 W508 E509 E525 L534 E535 E536 F540 A543 F548 Q564 K565 P566 R567 N568 I569 K570 G571
R572 F577 T585 V586 D587 G626 A627 V631 F644 L655 N676 K679 L688 V689 M690 H691 Q692 E700 R703 R706 F718 R719 Q720 R723 I724 L725 I730 F735 R739 K740 G741 A742 E743 Y756 M776 R783 Q791 S792 R793
G794 S797 R798 R808 ASP SER LEU LEU ILE ILE GLN TRP ASN ILE ARG ALA PHE MET SER VAL LYS ASN TRP PRO TRP MET LYS LEU TYR PHE LYS ILE LYS PRO LEU LEU LYS SER ALA GLU THR GLU LYS GLU MET ALA THR MET LYS GLU GLU PHE GLY ARG LEU LYS GLU ALA
LEU GLU LYS SER GLU ALA ARG ARG LYS GLU LEU GLU GLU LYS MET VAL SER LEU LEU GLN GLU LYS ASN ASP LEU GLN LEU GLN VAL GLN ALA GLU GLN ASP ASN LEU ALA ASP ALA GLU GLU ARG CYS ASP GLN LEU ILE LYS ASN LYS ILE GLN LEU GLU ALA LYS VAL LYS GLU MET
THR GLU ARG LEU GLU ASP GLU GLU GLU MET ASN ALA GLU LEU THR ALA LYS LYS ARG LYS LEU GLU ASP GLU CYS SER GLU LEU LYS ARG ASP ILE ASP ASP LEU GLU LEU THR LEU ALA LYS VAL GLU LYS GLU LYS HIS ALA THR GLU ASN LYS VAL LYS ASN LEU THR GLU GLU MET
ALA GLY LEU ASP GLU ILE ILE ALA LYS LEU THR LYS GLU LYS LYS ALA LEU GLN GLU ALA HIS GLN GLN ALA LEU ASP ASP LEU GLN ALA GLU GLU ASP LYS VAL ASN THR LEU THR LYS ALA LYS VAL LYS LEU GLU GLN HIS VAL ASP ASP LEU GLU GLY SER LEU GLU GLN GLU LYS
LYS VAL ARG MET ASP LEU GLU ARG ALA LYS ARG LYS LEU GLU GLY ASP LEU LYS LEU THR GLN GLU SER ILE MET ASP LEU GLU ASN ASP LYS GLN GLN LEU ASP GLU ARG LEU LYS LYS LYS ASP PHE GLU LEU ASN ALA LEU ASN ALA ARG ILE GLU ASP GLU GLN ALA LEU GLY SER
GLN LEU GLN LYS LYS LEU LYS GLU LEU GLN ALA ARG ILE GLU GLU LEU GLU GLU GLU LEU GLU ALA GLU ARG THR ALA ARG ALA LYS VAL GLU LYS LEU ARG SER ASP LEU SER ARG GLU LEU GLU GLU ILE SER GLU ARG LEU GLU GLU ALA GLY GLY ALA THR SER VAL GLN ILE GLU
MET ASN LYS LYS ARG GLU ALA GLU PHE GLN LYS MET ARG ARG ASP LEU GLU GLU ALA THR LEU GLN HIS GLU ALA THR ALA ALA ALA LEU ARG LYS LYS HIS ALA ASP SER VAL ALA GLU LEU GLY GLU GLN ILE ASP ASN LEU GLN ARG VAL LYS GLN LYS LEU GLU LYS GLU LYS SER
GLU PHE LYS LEU GLU LEU ASP ASP VAL THR SER ASN MET GLU GLN ILE ILE LYS ALA LYS ALA ASN LEU GLU LYS MET CYS ARG THR LEU GLU ASP GLN MET ASN GLU HIS ARG SER LYS ALA GLU GLU THR GLN ARG SER VAL ASN ASP LEU THR SER GLN ARG ALA LYS LEU GLN THR
GLU ASN GLY GLU LEU SER ARG GLN LEU ASP GLU LYS GLU ALA LEU ILE SER GLN LEU THR ARG GLY LYS LEU THR TYR THR GLN GLN LEU GLU ASP LEU LYS ARG GLN LEU GLU GLU GLU VAL LYS ALA LYS ASN ALA LEU ALA HIS ALA LEU GLN SER ALA ARG HIS ASP CYS ASP LEU
LEU ARG GLU GLN TYR GLU GLU GLU THR GLU ALA LYS ALA GLU LEU GLN ARG VAL LEU SER LYS ALA ASN SER GLU VAL ALA GLN TRP ARG THR LYS TYR GLU THR ASP ALA ILE GLN ARG THR GLU GLU LEU GLU GLU ALA LYS LYS LEU ALA GLN ARG LEU GLN ASP ALA GLU GLU
ALA VAL GLU ALA VAL ASN ALA LYS CYS SER SER LEU GLU LYS THR LYS HIS ARG LEU GLN ASN GLU ILE GLU ASP LEU MET VAL ASP VAL GLU ARG SER ASN ALA ALA ALA ALA ALA LEU ASP LYS LYS GLN ARG ASN PHE ASP LYS ILE LEU ALA GLU TRP LYS GLN LYS TYR GLU GLU
SER GLN SER GLU LEU GLU SER SER GLN LYS GLU ALA ARG SER LEU SER THR GLU LEU PHE LYS LEU LYS ASN ALA TYR GLU GLU SER LEU GLU HIS LEU GLU THR PHE LYS ARG GLU ASN LYS ASN LEU GLN GLU GLU ILE SER ASP LEU THR GLU GLN LEU GLY SER SER GLY LYS THR
ILE HIS GLU LEU GLU LYS VAL ARG LYS GLN LEU GLU ALA GLU LYS LEU GLU LEU GLN SER ALA LEU GLU GLU ALA GLU ALA SER LEU GLU HIS GLU GLU GLY LYS ILE LEU ARG ALA GLN LEU GLU PHE ASN 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 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



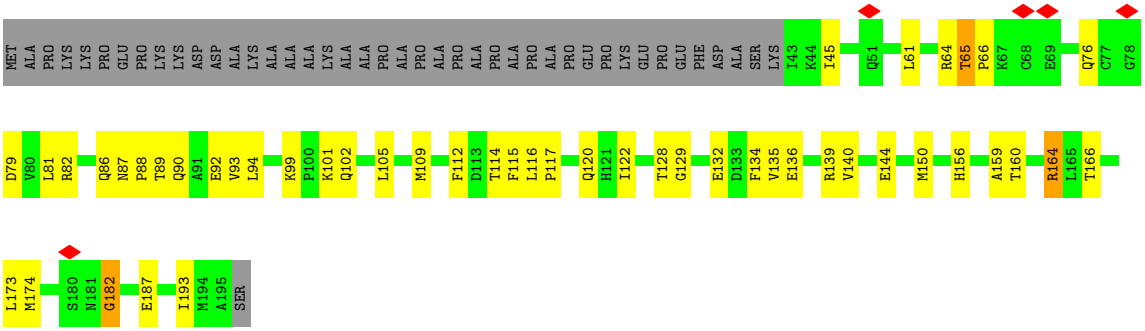
- Molecule 7: Myosin light chain 3

Chain L:



- Molecule 7: Myosin light chain 3

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31180	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	11.968	Depositor
Minimum map value	-5.440	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.196	Depositor
Recommended contour level	1.4	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: ADP, MG, CA

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	0.19	0/2995	0.42	2/4057 (0.0%)
1	B	0.20	0/2995	0.34	0/4057
1	C	1.02	1/2995 (0.0%)	1.49	13/4057 (0.3%)
1	D	0.20	0/2995	0.32	0/4057
2	E	0.22	0/1500	0.29	0/2001
2	F	0.20	0/1500	0.28	0/2001
3	G	0.21	0/1287	0.34	0/1720
4	H	0.92	0/1085	1.64	8/1445 (0.6%)
5	I	0.20	0/649	0.33	0/861
6	J	0.20	0/6609	0.39	0/8899
6	K	0.20	0/6609	0.38	0/8899
7	L	0.20	0/1236	0.44	2/1658 (0.1%)
7	M	0.20	0/1236	0.41	2/1658 (0.1%)
All	All	0.39	1/33691 (0.0%)	0.64	27/45370 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	6	THR	C-O	-5.63	1.16	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	152	ALA	CA-C-N	9.47	133.91	120.28
4	H	152	ALA	C-N-CA	9.47	133.91	120.28
1	A	1	ASP	CA-C-N	7.82	135.78	121.70
1	A	1	ASP	C-N-CA	7.82	135.78	121.70
1	C	12	ASN	CA-CB-CG	-7.56	105.04	112.60
7	L	182	GLY	CA-C-N	7.03	134.35	121.70
7	L	182	GLY	C-N-CA	7.03	134.35	121.70
4	H	106	ASP	CA-CB-CG	6.83	119.43	112.60
7	M	182	GLY	CA-C-N	6.62	133.61	121.70
7	M	182	GLY	C-N-CA	6.62	133.61	121.70
1	C	332	PRO	O-C-N	-6.53	118.08	121.15
1	C	3	GLU	N-CA-CB	6.23	121.02	110.49
1	C	24	ASP	CA-C-N	6.03	128.85	120.29
1	C	24	ASP	C-N-CA	6.03	128.85	120.29
4	H	70	ARG	CA-C-N	5.92	126.67	119.99
4	H	70	ARG	C-N-CA	5.92	126.67	119.99
4	H	158	ALA	N-CA-C	5.82	117.43	111.14
1	C	292	ASP	CA-CB-CG	-5.61	106.99	112.60
1	C	332	PRO	CA-C-O	-5.45	116.42	120.73
1	C	286	ASP	CA-CB-CG	-5.43	107.17	112.60
1	C	310	ALA	CA-C-N	5.36	127.41	120.44
1	C	310	ALA	C-N-CA	5.36	127.41	120.44
1	C	251	GLY	CA-C-N	5.22	127.80	120.28
1	C	251	GLY	C-N-CA	5.22	127.80	120.28
4	H	120	THR	N-CA-CB	5.22	117.80	110.12
4	H	141	LYS	N-CA-C	5.18	116.92	108.63
1	C	274	ILE	N-CA-C	5.09	115.81	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	69	TYR	Sidechain

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	35	0
1	B	2932	0	2892	58	0
1	C	2932	0	2894	29	0
1	D	2932	0	2894	48	0
2	E	1495	0	1490	27	0
2	F	1495	0	1490	30	0
3	G	1274	0	1203	42	0
4	H	1077	0	1141	42	0
5	I	643	0	663	28	0
6	J	6475	0	6475	76	0
6	K	6475	0	6473	86	0
7	L	1217	0	1199	38	0
7	M	1217	0	1199	27	0
8	A	27	0	12	0	0
8	B	27	0	12	1	0
8	C	27	0	12	1	0
8	D	27	0	12	1	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	G	3	0	0	1	0
All	All	33211	0	32955	466	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (466) 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)
6:K:569:ILE:HG12	6:K:572:ARG:CD	1.50	1.39
6:J:627:ALA:HB2	6:J:639:LYS:NZ	1.43	1.33
1:D:48:GLY:HA2	4:H:131:GLN:OE1	1.35	1.25
6:K:564:GLN:OE1	6:K:567:ARG:NH1	1.83	1.11
6:K:569:ILE:HG12	6:K:572:ARG:HD3	1.39	1.04
6:K:569:ILE:HG12	6:K:572:ARG:HD2	1.33	1.02
6:K:569:ILE:CG1	6:K:572:ARG:CD	2.42	0.98
6:J:627:ALA:CB	6:J:639:LYS:NZ	2.30	0.95
4:H:147:ARG:HG2	4:H:148:VAL:H	1.32	0.94
6:K:569:ILE:CG1	6:K:572:ARG:HD2	1.99	0.91
6:J:627:ALA:HB2	6:J:639:LYS:HZ1	1.37	0.88
6:K:569:ILE:HG12	6:K:572:ARG:CG	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:627:ALA:HB2	6:J:639:LYS:HZ2	1.35	0.87
3:G:90:LYS:HE3	4:H:144:THR:HG21	1.59	0.85
4:H:111:GLU:OE1	5:I:244:LYS:NZ	2.11	0.83
1:C:275:HIS:CE1	1:C:316:GLU:HG2	2.15	0.82
6:K:570:LYS:HD2	6:K:570:LYS:O	1.79	0.82
2:E:105:ARG:HE	2:F:106:LEU:HD21	1.47	0.80
6:K:569:ILE:CD1	6:K:572:ARG:HD2	2.12	0.79
2:E:141:MET:SD	2:F:140:LYS:NZ	2.54	0.79
4:H:147:ARG:HG2	4:H:148:VAL:N	1.96	0.79
6:K:794:GLY:HA2	7:M:82:ARG:HB3	1.65	0.78
6:K:723:ARG:NH1	7:M:136:GLU:OE1	2.19	0.76
1:B:149:THR:HG22	1:B:167:GLU:H	1.49	0.76
7:M:159:ALA:O	7:M:164:ARG:NH2	2.18	0.75
2:E:147:GLN:O	2:E:150:GLU:HG2	1.88	0.74
6:J:627:ALA:HB2	6:J:639:LYS:HZ3	1.49	0.74
7:M:86:GLN:HG2	7:M:128:THR:HG22	1.70	0.73
1:C:275:HIS:ND1	1:C:316:GLU:HG2	2.02	0.73
3:G:71:THR:O	10:G:201:CA:CA	1.66	0.72
6:J:792:SER:HB3	7:L:173:LEU:HD13	1.72	0.72
1:B:147:ARG:NH2	6:K:371:GLU:OE2	2.22	0.72
1:B:276:GLU:O	1:B:280:ASN:ND2	2.23	0.71
1:D:111:ASN:OD1	1:D:177:ARG:NH1	2.24	0.70
7:L:71:LYS:HD2	7:L:109:MET:HB3	1.71	0.70
1:D:215:LYS:O	2:E:198:LYS:NZ	2.22	0.70
4:H:147:ARG:CG	4:H:148:VAL:H	2.04	0.70
3:G:50:GLN:CD	4:H:150:ILE:HG22	2.17	0.69
1:C:275:HIS:CG	1:C:316:GLU:HG2	2.26	0.69
6:K:730:ILE:HG13	6:K:741:GLY:HA2	1.75	0.69
7:L:48:THR:OG1	7:L:51:GLN:OE1	2.11	0.69
1:C:24:ASP:C	4:H:145:LEU:HD11	2.18	0.68
7:L:168:ASP:O	7:L:172:LYS:NZ	2.24	0.68
1:D:59:GLN:OE1	1:D:62:ARG:NH1	2.26	0.68
2:E:147:GLN:OE1	2:F:152:LYS:HE3	1.92	0.68
6:K:270:LYS:HD2	6:K:429:LYS:HB3	1.76	0.68
1:A:3:GLU:CD	1:A:3:GLU:H	2.00	0.67
3:G:157:MET:SD	4:H:51:LYS:NZ	2.60	0.67
1:B:259:GLU:OE2	1:B:312:ARG:NH2	2.16	0.67
6:K:347:ASN:OD1	6:K:351:LYS:NZ	2.27	0.66
6:J:787:ARG:NH2	7:L:127:ASP:O	2.29	0.66
1:C:24:ASP:O	4:H:145:LEU:HD11	1.96	0.66
1:D:69:TYR:OH	1:D:207:GLU:OE2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:196:GLY:O	5:I:200:THR:OG1	2.11	0.66
1:A:95:ARG:HB3	6:J:634:GLY:HA2	1.77	0.65
1:B:23:GLY:HA2	6:K:644:PHE:HZ	1.61	0.65
6:J:449:THR:O	6:J:453:ARG:NH2	2.30	0.65
6:J:708:GLY:O	6:J:766:LYS:NZ	2.30	0.65
6:K:797:SER:OG	7:M:79:ASP:O	2.13	0.64
1:A:311:ASP:HB2	2:F:90:ARG:HH12	1.62	0.64
7:M:156:HIS:O	7:M:160:THR:OG1	2.08	0.64
2:E:71:LEU:HD13	2:F:71:LEU:HA	1.80	0.64
1:B:32:PRO:HG2	1:B:59:GLN:HG3	1.80	0.63
6:J:80:ASN:OD1	6:J:80:ASN:N	2.31	0.62
6:J:196:ALA:HA	6:J:258:LEU:HD11	1.81	0.62
6:J:627:ALA:CB	6:J:639:LYS:HZ2	2.03	0.62
1:B:148:THR:HA	1:C:44:MET:HE1	1.80	0.62
1:C:23:GLY:C	4:H:145:LEU:CD1	2.72	0.62
7:M:82:ARG:O	7:M:87:ASN:ND2	2.33	0.61
1:A:5:THR:HG23	1:A:6:THR:H	1.65	0.61
1:C:5:THR:HG21	1:C:100:GLU:HB2	1.82	0.61
1:A:95:ARG:NH1	6:J:632:GLU:O	2.32	0.61
1:A:168:GLY:HA2	1:B:44:MET:HE3	1.82	0.61
4:H:95:GLN:HB3	5:I:218:ILE:HG23	1.81	0.61
7:L:94:LEU:HD12	7:L:100:PRO:HD2	1.82	0.61
6:K:569:ILE:HG12	6:K:572:ARG:HG2	1.82	0.60
1:B:110:LEU:O	1:B:177:ARG:NH1	2.34	0.60
1:D:43:VAL:HG23	1:D:44:MET:HG2	1.83	0.60
4:H:112:ARG:HD3	5:I:240:LEU:HD22	1.83	0.60
7:M:88:PRO:HD3	7:M:122:ILE:HD11	1.83	0.60
6:K:569:ILE:CG1	6:K:572:ARG:CG	2.77	0.60
3:G:73:ASP:OD2	4:H:37:LYS:NZ	2.33	0.60
2:E:147:GLN:HG3	2:E:150:GLU:OE2	2.01	0.60
1:B:157:ASP:OD1	8:B:401:ADP:O3'	2.20	0.60
6:J:54:ARG:NH1	6:J:73:GLU:OE2	2.34	0.60
1:D:95:ARG:HH12	5:I:262:ARG:HD2	1.67	0.60
2:F:212:GLU:O	2:F:216:GLN:NE2	2.35	0.60
6:K:564:GLN:CD	6:K:567:ARG:NH1	2.58	0.60
6:K:569:ILE:CG1	6:K:572:ARG:HG2	2.32	0.60
1:C:275:HIS:ND1	1:C:316:GLU:CG	2.65	0.59
1:D:241:GLU:HA	1:D:247:VAL:HG12	1.83	0.59
6:J:202:GLY:HA3	6:J:257:LYS:HE2	1.83	0.59
1:B:299:LEU:HD12	1:B:331:ALA:HB2	1.85	0.58
1:C:168:GLY:O	1:D:43:VAL:HG21	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:130:THR:HG22	7:L:132:GLU:H	1.67	0.58
4:H:147:ARG:CG	4:H:148:VAL:N	2.66	0.57
1:B:131:ALA:HB1	1:B:356:TRP:HB3	1.87	0.57
2:E:60:TYR:HB3	2:F:60:TYR:O	2.05	0.57
6:J:723:ARG:NH2	7:L:136:GLU:OE1	2.37	0.57
2:F:137:ASP:HA	2:F:140:LYS:HE3	1.86	0.57
1:D:219:VAL:HG22	1:D:258:PRO:HB2	1.85	0.57
6:J:752:ASP:OD1	6:J:752:ASP:N	2.37	0.57
6:K:587:ASP:OD1	6:K:587:ASP:N	2.34	0.57
1:A:80:ASP:OD1	1:A:84:LYS:NZ	2.37	0.57
1:B:148:THR:HG23	1:B:149:THR:HG23	1.87	0.57
6:K:720:GLN:O	7:M:139:ARG:NH1	2.38	0.57
1:C:316:GLU:OE1	1:C:316:GLU:HA	2.05	0.56
1:B:349:LEU:HD22	6:K:536:GLU:HG3	1.86	0.56
1:B:350:SER:OG	6:K:536:GLU:OE1	2.14	0.56
3:G:27:PHE:CE1	4:H:155:MET:SD	2.99	0.56
3:G:149:ASP:H	3:G:152:GLU:HB2	1.71	0.56
2:E:201:THR:HG22	2:E:205:LYS:HE3	1.88	0.55
6:K:564:GLN:OE1	6:K:567:ARG:CZ	2.52	0.55
7:L:135:VAL:HG13	7:L:186:TYR:HE1	1.70	0.55
6:K:235:THR:HG22	6:K:236:VAL:H	1.70	0.55
6:J:615:LYS:H	6:J:615:LYS:HD2	1.72	0.55
7:M:65:THR:HG22	7:M:66:PRO:HD2	1.88	0.55
6:J:602:ASN:HD21	6:J:605:VAL:HG13	1.72	0.55
6:K:186:VAL:O	6:K:190:ARG:HG2	2.06	0.55
1:B:369:ILE:HD12	1:B:372:ARG:HD2	1.87	0.55
1:B:6:THR:OG1	1:B:101:HIS:ND1	2.32	0.54
1:D:253:GLU:HA	1:D:256:ARG:HB2	1.88	0.54
3:G:27:PHE:CZ	4:H:155:MET:SD	3.00	0.54
4:H:149:ARG:O	4:H:149:ARG:HG2	2.07	0.54
6:J:41:ASP:OD2	6:J:43:LYS:NZ	2.31	0.54
6:J:785:ILE:HD11	7:L:158:LEU:HD23	1.89	0.54
3:G:136:LEU:HD11	4:H:47:LYS:HA	1.89	0.54
6:J:718:PHE:O	6:J:722:TYR:HB2	2.08	0.54
1:D:8:LEU:HD13	1:D:94:LEU:HD13	1.89	0.54
7:M:64:ARG:NH2	7:M:76:GLN:OE1	2.34	0.54
7:L:89:THR:HG23	7:L:92:GLU:H	1.73	0.54
1:D:369:ILE:HG13	1:D:372:ARG:HH21	1.72	0.54
3:G:93:SER:O	3:G:97:LEU:HG	2.08	0.54
6:J:115:TYR:HB3	6:J:152:PRO:HB2	1.89	0.54
6:J:787:ARG:NH1	7:L:129:GLY:HA3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:187:GLU:N	7:M:187:GLU:OE1	2.41	0.53
2:E:113:LEU:HD11	2:F:112:LYS:NZ	2.23	0.53
1:C:275:HIS:CE1	1:C:316:GLU:CG	2.90	0.53
1:D:214:GLU:HA	8:D:401:ADP:N1	2.23	0.53
1:B:117:GLU:OE2	1:B:371:HIS:NE2	2.36	0.53
1:A:62:ARG:HB2	1:A:204:ALA:HB1	1.91	0.53
6:J:32:ASP:HB3	6:J:35:LYS:HB3	1.90	0.53
6:K:189:LYS:O	6:K:193:GLN:HG2	2.09	0.53
6:J:692:GLN:O	6:J:696:ASN:ND2	2.35	0.53
6:K:540:PHE:HB3	6:K:543:ALA:HB2	1.90	0.53
3:G:51:ASN:OD1	3:G:51:ASN:N	2.42	0.53
7:L:93:VAL:HG23	7:L:94:LEU:HD22	1.89	0.53
7:M:132:GLU:HA	7:M:135:VAL:HB	1.90	0.53
3:G:50:GLN:OE1	4:H:150:ILE:HG22	2.08	0.53
7:L:189:PHE:O	7:L:193:ILE:HG12	2.09	0.53
1:C:4:GLU:O	1:C:5:THR:HG22	2.08	0.52
6:K:570:LYS:O	6:K:570:LYS:CD	2.55	0.52
6:J:700:GLU:OE2	6:J:703:ARG:NH2	2.39	0.52
1:A:146:GLY:C	6:J:541:PRO:HB3	2.34	0.52
6:K:700:GLU:OE1	6:K:703:ARG:NH2	2.38	0.52
1:B:212:ILE:HG12	1:B:240:TYR:CE2	2.44	0.52
6:K:55:GLU:N	6:K:55:GLU:OE1	2.43	0.52
4:H:109:ASP:OD2	5:I:212:ARG:HG3	2.10	0.52
5:I:257:GLU:O	5:I:261:LEU:HG	2.09	0.52
6:J:237:ARG:HH22	6:J:691:HIS:CE1	2.27	0.52
1:A:288:ASP:OD2	1:B:62:ARG:NE	2.41	0.52
1:D:7:ALA:HA	1:D:102:PRO:HD2	1.92	0.52
1:D:119:MET:O	1:D:123:MET:HG2	2.09	0.52
2:F:135:GLN:HE22	6:K:368:GLN:HB3	1.75	0.52
2:E:92:ILE:HD13	2:F:91:ARG:HH21	1.74	0.51
6:J:243:ARG:NH2	6:J:466:GLU:OE2	2.41	0.51
3:G:74:PHE:O	3:G:78:LEU:HG	2.10	0.51
4:H:129:LEU:HD13	5:I:261:LEU:HB2	1.93	0.51
6:K:46:PHE:HB3	6:K:99:PRO:HB3	1.92	0.51
1:A:311:ASP:CG	2:F:90:ARG:HH22	2.18	0.51
1:B:337:TYR:CZ	6:K:406:VAL:HG21	2.46	0.51
1:C:168:GLY:C	1:D:43:VAL:HG21	2.35	0.51
1:D:53:TYR:HD2	1:D:65:LEU:HD11	1.74	0.51
7:M:81:LEU:HD13	7:M:122:ILE:HD12	1.92	0.51
2:E:85:VAL:HA	2:E:88:LEU:HD23	1.92	0.51
6:K:143:ARG:NH1	6:K:159:ASP:OD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:174:MET:O	7:L:178:GLU:HG2	2.10	0.51
1:B:180:LEU:HD11	1:B:260:THR:HG22	1.93	0.51
7:L:60:MET:HE2	7:L:70:MET:HE1	1.92	0.51
3:G:52:PRO:HB2	3:G:57:LEU:HD22	1.93	0.51
3:G:95:GLU:O	3:G:98:SER:OG	2.24	0.51
3:G:149:ASP:OD1	3:G:150:TYR:N	2.36	0.51
4:H:81:CYS:HB3	5:I:238:TYR:HE1	1.76	0.51
7:M:45:ILE:HA	7:M:120:GLN:HE21	1.75	0.51
3:G:56:GLU:O	3:G:59:GLU:HG2	2.11	0.50
1:C:322:PRO:HG2	1:D:244:ASP:O	2.12	0.50
6:J:301:LEU:HD21	6:J:351:LYS:HA	1.93	0.50
6:K:500:GLU:HA	6:K:503:LYS:HE3	1.93	0.50
1:B:221:LEU:HD22	2:E:129:VAL:HG22	1.93	0.50
3:G:161:GLU:OXT	4:H:55:LEU:HD13	2.11	0.50
6:K:570:LYS:HD2	6:K:570:LYS:C	2.36	0.50
1:C:149:THR:HG22	1:C:167:GLU:H	1.76	0.50
1:D:182:GLY:HA2	1:D:185:LEU:HD12	1.93	0.50
1:A:95:ARG:O	6:J:635:LYS:N	2.44	0.50
3:G:82:VAL:O	3:G:86:LYS:N	2.45	0.49
1:A:154:ASP:HB3	1:A:161:HIS:CD2	2.47	0.49
5:I:216:LEU:HD23	5:I:216:LEU:H	1.77	0.49
6:J:46:PHE:HB3	6:J:99:PRO:HB3	1.94	0.49
6:J:483:GLU:HB3	6:J:521:ILE:HD11	1.93	0.49
1:C:169:TYR:HA	1:D:43:VAL:HG21	1.93	0.49
2:E:150:GLU:HG3	2:E:151:ALA:N	2.27	0.49
6:K:566:PRO:HD3	6:K:577:PHE:HA	1.95	0.49
7:L:191:LYS:HA	7:L:194:MET:HB2	1.95	0.49
4:H:126:ILE:HD11	5:I:254:GLN:HB3	1.93	0.49
1:B:286:ASP:OD2	1:C:39:ARG:NH2	2.46	0.49
2:E:113:LEU:HD11	2:F:112:LYS:HZ2	1.78	0.49
7:L:104:GLU:HA	7:L:108:LYS:HB2	1.95	0.49
1:B:244:ASP:CG	1:B:246:GLN:HE21	2.20	0.49
2:E:91:ARG:HH22	2:E:95:VAL:HG11	1.78	0.49
4:H:77:LEU:HD12	5:I:238:TYR:CD1	2.47	0.49
1:C:219:VAL:O	2:F:167:ARG:NH1	2.46	0.49
7:M:89:THR:HG22	7:M:92:GLU:HG2	1.95	0.49
1:B:156:GLY:O	1:B:181:ALA:HB1	2.11	0.48
1:D:80:ASP:OD1	1:D:80:ASP:N	2.45	0.48
1:D:288:ASP:N	1:D:288:ASP:OD1	2.45	0.48
3:G:120:MET:HB3	4:H:54:MET:HE1	1.93	0.48
5:I:229:LYS:O	5:I:233:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:81:CYS:HB3	5:I:238:TYR:CE1	2.48	0.48
6:K:481:THR:HG22	6:K:655:LEU:HD13	1.95	0.48
1:A:24:ASP:OD2	1:A:28:ARG:NH2	2.47	0.48
1:B:290:ARG:HD2	1:C:244:ASP:HB3	1.95	0.48
1:B:11:ASP:OD1	1:B:106:THR:OG1	2.30	0.48
1:D:178:LEU:HG	1:D:180:LEU:H	1.78	0.48
4:H:77:LEU:HD11	5:I:241:GLU:HB2	1.95	0.48
6:K:234:LYS:HB3	6:K:281:ARG:HB2	1.95	0.48
7:L:65:THR:HG22	7:L:67:LYS:H	1.78	0.48
1:D:304:THR:O	1:D:335:ARG:NH1	2.43	0.48
1:D:357:ILE:HD11	1:D:374:CYS:HB2	1.96	0.48
3:G:6:LYS:HA	3:G:9:VAL:HG12	1.95	0.48
1:B:267:ILE:HG13	1:B:269:MET:HG3	1.95	0.48
1:B:304:THR:O	1:B:335:ARG:NH1	2.47	0.48
6:K:262:ASP:OD1	6:K:262:ASP:N	2.45	0.47
1:C:23:GLY:O	4:H:145:LEU:CD1	2.61	0.47
1:D:301:GLY:O	1:D:304:THR:OG1	2.31	0.47
2:F:185:LEU:O	2:F:189:LYS:HE2	2.14	0.47
1:D:279:TYR:O	1:D:283:MET:HG2	2.14	0.47
2:E:157:ASP:O	2:E:161:LYS:HG2	2.15	0.47
6:J:711:ASN:HB2	6:J:765:PHE:HB2	1.96	0.47
6:K:128:TYR:CZ	6:K:679:LYS:HG2	2.49	0.47
1:D:222:ASP:OD1	1:D:223:PHE:N	2.46	0.47
3:G:136:LEU:HG	4:H:47:LYS:HG2	1.95	0.47
6:K:45:GLU:HG2	6:K:690:MET:HE1	1.96	0.47
7:L:112:PHE:HA	7:L:115:PHE:HB3	1.95	0.47
1:D:154:ASP:HA	1:D:300:SER:O	2.15	0.47
1:D:346:LEU:HD12	1:D:349:LEU:HD12	1.97	0.47
7:L:160:THR:HG23	7:L:161:LEU:HG	1.95	0.47
7:M:116:LEU:HB3	7:M:117:PRO:HD3	1.96	0.47
3:G:149:ASP:N	3:G:152:GLU:OE1	2.48	0.47
4:H:77:LEU:HD12	5:I:238:TYR:HA	1.96	0.47
5:I:241:GLU:HA	5:I:244:LYS:HE2	1.95	0.47
6:K:288:GLN:HB3	6:K:329:LEU:HB2	1.97	0.47
6:K:484:LYS:NZ	6:K:525:GLU:OE1	2.44	0.47
1:B:120:THR:HB	1:B:132:MET:HE3	1.97	0.46
5:I:219:ASP:OD1	5:I:219:ASP:N	2.46	0.46
6:J:379:GLU:CD	6:J:379:GLU:H	2.23	0.46
7:L:148:THR:HB	7:L:185:ASN:OD1	2.15	0.46
1:D:369:ILE:HG13	1:D:372:ARG:NH2	2.30	0.46
2:E:147:GLN:OE1	2:F:152:LYS:CE	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:83:ARG:NH2	4:H:146:ARG:HE	2.14	0.46
6:J:217:GLU:OE1	6:J:217:GLU:N	2.40	0.46
6:J:318:THR:HG22	6:J:319:THR:H	1.81	0.46
1:D:123:MET:SD	1:D:123:MET:N	2.89	0.46
6:K:96:LEU:HB2	6:K:706:ARG:HD3	1.96	0.46
1:A:282:ILE:HG12	1:A:293:LEU:HD23	1.98	0.46
6:J:627:ALA:CB	6:J:639:LYS:HZ3	2.14	0.46
6:K:338:VAL:HG23	6:K:339:LEU:HD22	1.97	0.46
6:K:415:GLN:HG3	6:K:419:GLN:HB2	1.96	0.46
1:A:17:VAL:HG23	1:A:33:SER:HB3	1.98	0.46
3:G:74:PHE:CE1	3:G:78:LEU:HD21	2.50	0.46
2:E:66:ASP:OD1	2:E:66:ASP:N	2.48	0.46
1:B:208:ILE:O	1:B:212:ILE:HG13	2.15	0.46
1:D:207:GLU:OE1	1:D:210:ARG:NH2	2.46	0.46
6:K:569:ILE:HD11	6:K:572:ARG:HD2	1.96	0.46
1:B:7:ALA:HB3	1:B:347:ALA:HB1	1.98	0.46
7:L:130:THR:HB	7:L:133:ASP:H	1.80	0.46
1:A:208:ILE:O	1:A:212:ILE:HG13	2.16	0.45
2:E:224:GLU:HA	2:E:227:VAL:HG12	1.98	0.45
7:L:74:TYR:HA	7:L:77:CYS:HB3	1.99	0.45
3:G:57:LEU:HD13	3:G:57:LEU:HA	1.84	0.45
5:I:257:GLU:HA	5:I:260:VAL:HG22	1.98	0.45
6:K:77:LEU:HD11	6:K:97:HIS:HD2	1.81	0.45
6:K:88:GLU:HG3	6:K:108:ARG:HH22	1.82	0.45
1:A:202:THR:HG22	1:A:204:ALA:H	1.81	0.45
1:A:221:LEU:HD22	2:F:90:ARG:HD2	1.96	0.45
3:G:38:THR:HA	3:G:57:LEU:HG	1.99	0.45
6:J:36:ASP:OD1	6:J:50:LYS:NZ	2.41	0.45
6:J:300:MET:SD	6:J:351:LYS:HE2	2.57	0.45
1:A:324:THR:HG21	1:B:241:GLU:OE2	2.17	0.45
1:D:126:THR:HG23	5:I:201:GLU:HG3	1.99	0.45
1:B:324:THR:HG21	1:C:241:GLU:OE1	2.16	0.45
6:K:139:VAL:HG13	6:K:194:TYR:CD2	2.51	0.45
6:K:379:GLU:CD	6:K:379:GLU:H	2.23	0.45
1:D:114:ALA:O	1:D:118:LYS:HG2	2.16	0.45
3:G:36:ILE:HD11	3:G:72:VAL:HB	1.99	0.45
3:G:109:ASP:OD1	3:G:109:ASP:N	2.49	0.45
3:G:100:LEU:HD22	4:H:58:ALA:HB1	1.99	0.45
6:J:504:GLU:OE1	6:J:762:LYS:NZ	2.43	0.45
6:K:102:LEU:O	6:K:105:LEU:HG	2.16	0.44
6:K:403:ARG:NH2	6:K:410:TYR:HB3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:PHE:HD1	1:A:375:PHE:HA	1.72	0.44
2:F:157:ASP:O	2:F:161:LYS:HG3	2.17	0.44
4:H:95:GLN:HB3	5:I:218:ILE:CG2	2.47	0.44
6:K:739:ARG:NH1	6:K:743:GLU:OE2	2.51	0.44
2:F:143:ILE:O	2:F:147:GLN:HG2	2.17	0.44
1:C:23:GLY:O	4:H:145:LEU:HD12	2.18	0.44
3:G:45:MET:HB3	3:G:50:GLN:HB2	2.00	0.44
6:J:796:LEU:HB2	7:L:173:LEU:HD21	1.99	0.44
4:H:122:ASN:HD21	5:I:251:PHE:HD1	1.62	0.44
5:I:261:LEU:HD22	5:I:264:ARG:HH11	1.83	0.44
6:K:351:LYS:HG2	6:K:387:LEU:HD22	1.99	0.44
7:M:150:MET:HG2	7:M:182:GLY:O	2.18	0.44
1:B:122:ILE:HD13	1:B:122:ILE:HA	1.85	0.44
6:K:676:ASN:HA	6:K:688:LEU:HD23	1.99	0.44
1:D:35:VAL:HG21	1:D:81:ASP:HB3	1.99	0.44
3:G:136:LEU:CG	4:H:47:LYS:HG2	2.47	0.44
1:B:311:ASP:CG	2:E:129:VAL:HG11	2.43	0.44
6:J:223:ALA:HB2	6:J:339:LEU:HD21	2.00	0.44
1:B:279:TYR:O	1:B:283:MET:HG2	2.18	0.43
6:J:204:ARG:NH2	6:J:208:GLU:OE1	2.51	0.43
1:A:286:ASP:OD2	1:B:39:ARG:NH2	2.49	0.43
6:K:479:ASN:O	6:K:483:GLU:HG2	2.18	0.43
6:K:724:ILE:HD12	6:K:724:ILE:H	1.83	0.43
6:K:791:GLN:OE1	6:K:798:ARG:NH2	2.42	0.43
3:G:72:VAL:HG13	3:G:76:GLU:HB3	2.00	0.43
6:K:45:GLU:HG3	6:K:46:PHE:CD2	2.53	0.43
7:L:164:ARG:HD3	7:L:164:ARG:HA	1.67	0.43
1:A:237:GLU:HG2	1:A:251:GLY:HA2	2.01	0.43
6:J:239:ASP:N	6:J:239:ASP:OD1	2.49	0.43
1:A:149:THR:HG22	1:A:167:GLU:H	1.84	0.43
1:A:162:ASN:ND2	1:A:278:THR:OG1	2.51	0.43
6:J:93:LEU:HD21	6:J:100:ALA:HB1	2.00	0.43
1:A:23:GLY:O	6:J:644:PHE:HE1	2.01	0.43
3:G:74:PHE:CE2	3:G:78:LEU:HD11	2.54	0.43
6:K:725:LEU:HD11	6:K:776:MET:HB3	1.99	0.43
1:A:244:ASP:OD1	1:A:244:ASP:N	2.51	0.43
1:B:5:THR:O	1:B:102:PRO:HD2	2.19	0.43
2:E:182:ARG:O	2:E:185:LEU:HG	2.18	0.43
6:J:189:LYS:O	6:J:193:GLN:HG3	2.18	0.43
6:J:240:ASN:OD1	6:J:284:HIS:HE1	2.01	0.43
2:E:160:ARG:HA	2:E:160:ARG:NE	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:194:TYR:CZ	6:J:198:ILE:HG21	2.53	0.43
6:J:210:THR:HG21	6:J:215:THR:HA	2.01	0.43
6:J:808:ARG:HH22	7:L:64:ARG:HD2	1.83	0.43
6:K:569:ILE:HG13	6:K:572:ARG:HG2	2.01	0.43
7:L:108:LYS:HG3	7:L:110:MET:HB2	1.99	0.43
1:D:238:LYS:HD2	1:D:254:ARG:NH2	2.34	0.43
6:J:109:TYR:CE2	6:J:684:ILE:HG13	2.53	0.43
6:K:90:MET:HE2	6:K:116:THR:HG21	2.00	0.43
6:K:194:TYR:O	6:K:198:ILE:HG23	2.19	0.43
7:M:101:LYS:HB2	7:M:101:LYS:HE2	1.85	0.43
2:E:141:MET:HB2	2:F:141:MET:HG2	2.00	0.42
6:K:255:THR:HG23	6:K:257:LYS:HG2	2.00	0.42
6:K:534:LEU:HA	6:K:548:PHE:HE2	1.84	0.42
6:K:792:SER:HB2	7:M:173:LEU:HD22	2.01	0.42
1:A:131:ALA:HB1	1:A:356:TRP:HB3	2.01	0.42
1:A:253:GLU:HA	1:A:256:ARG:HB2	2.01	0.42
1:D:5:THR:OG1	1:D:102:PRO:HD3	2.19	0.42
6:K:718:PHE:CE2	6:K:742:ALA:HA	2.54	0.42
7:L:139:ARG:HD3	7:L:186:TYR:OH	2.19	0.42
1:B:212:ILE:HG12	1:B:240:TYR:CD2	2.55	0.42
1:B:336:LYS:HB3	1:B:336:LYS:HE2	1.78	0.42
1:C:214:GLU:HG2	8:C:401:ADP:C4	2.54	0.42
2:E:93:GLN:O	2:E:97:GLU:HG3	2.19	0.42
7:L:187:GLU:OE2	7:L:191:LYS:NZ	2.47	0.42
1:A:360:GLN:H	1:A:360:GLN:HG2	1.65	0.42
1:D:160:THR:OG1	1:D:180:LEU:O	2.31	0.42
6:J:615:LYS:H	6:J:615:LYS:CD	2.32	0.42
7:M:105:LEU:HD23	7:M:105:LEU:HA	1.84	0.42
1:B:275:HIS:HB3	1:B:313:MET:SD	2.59	0.42
1:B:330:ILE:HG12	6:K:371:GLU:OE2	2.20	0.42
3:G:62:ASP:HA	3:G:65:ASP:HB2	2.01	0.42
6:J:365:LYS:HE2	6:J:376:ASP:CG	2.44	0.42
6:J:448:GLU:CD	6:J:453:ARG:HH22	2.27	0.42
6:J:508:TRP:NE1	6:J:510:PHE:O	2.50	0.42
3:G:137:MET:O	3:G:141:ASP:N	2.52	0.42
6:J:589:ASN:OD1	6:J:591:ILE:HG12	2.20	0.42
6:K:265:THR:HG23	6:K:440:VAL:HG11	2.01	0.42
7:M:94:LEU:O	7:M:99:LYS:HD3	2.19	0.42
4:H:133:ILE:HD13	5:I:264:ARG:NH1	2.35	0.42
5:I:212:ARG:NH2	5:I:240:LEU:HD11	2.34	0.42
7:M:112:PHE:HA	7:M:115:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:417:VAL:O	6:J:420:VAL:HG12	2.20	0.42
6:K:339:LEU:HD13	6:K:339:LEU:HA	1.95	0.42
1:B:255:PHE:C	1:B:258:PRO:HD2	2.44	0.42
7:L:61:LEU:HD13	7:L:61:LEU:HA	1.81	0.42
1:B:9:VAL:HG21	1:B:344:SER:HA	2.02	0.41
2:F:161:LYS:O	2:F:165:VAL:HG23	2.20	0.41
1:B:330:ILE:HG22	1:B:332:PRO:HD3	2.02	0.41
3:G:43:LYS:HD2	3:G:43:LYS:HA	1.73	0.41
5:I:221:LEU:HD23	5:I:226:LEU:HD23	2.02	0.41
6:J:304:THR:HG22	6:J:306:ASN:H	1.84	0.41
6:K:688:LEU:O	6:K:692:GLN:HG2	2.20	0.41
1:B:59:GLN:HE21	1:B:59:GLN:C	2.28	0.41
1:B:99:GLU:H	1:B:99:GLU:HG2	1.69	0.41
1:B:287:ILE:HG13	1:B:290:ARG:NH1	2.35	0.41
1:D:266:PHE:HD1	1:D:266:PHE:HA	1.73	0.41
1:A:330:ILE:HG22	1:A:332:PRO:HD3	2.02	0.41
3:G:121:LEU:O	3:G:124:THR:OG1	2.37	0.41
6:J:551:LYS:HE2	6:J:551:LYS:HB3	1.91	0.41
1:A:311:ASP:HB2	2:F:90:ARG:NH1	2.32	0.41
6:K:243:ARG:HA	6:K:243:ARG:HD3	1.79	0.41
6:K:320:VAL:HG13	6:K:322:SER:H	1.85	0.41
1:A:24:ASP:HB2	1:A:340:TRP:HH2	1.85	0.41
1:A:72:GLU:O	1:A:74:GLY:N	2.53	0.41
1:B:127:PHE:HD1	1:B:127:PHE:HA	1.75	0.41
1:B:180:LEU:HD12	1:B:267:ILE:HD11	2.03	0.41
1:D:155:SER:HB2	1:D:160:THR:HG23	2.02	0.41
2:F:168:LYS:HA	2:F:171:ILE:HG12	2.03	0.41
3:G:27:PHE:CZ	3:G:44:VAL:HG11	2.56	0.41
6:J:382:ASP:HA	6:J:392:SER:OG	2.20	0.41
6:K:420:VAL:O	6:K:424:THR:HG23	2.20	0.41
1:B:324:THR:HG21	1:C:241:GLU:CD	2.46	0.41
6:J:18:LYS:NZ	6:J:88:GLU:OE2	2.54	0.41
6:J:204:ARG:HA	6:J:204:ARG:NE	2.35	0.41
6:J:607:ASP:O	6:J:611:LYS:HG2	2.21	0.41
6:J:808:ARG:HH22	7:L:64:ARG:HH11	1.68	0.41
1:B:288:ASP:OD2	1:C:62:ARG:HG3	2.21	0.41
1:D:233:SER:OG	1:D:234:SER:N	2.53	0.41
2:F:157:ASP:OD1	2:F:160:ARG:NH2	2.52	0.41
6:J:272:ARG:NH1	6:J:280:GLU:OE2	2.41	0.41
2:F:158:ALA:HA	2:F:161:LYS:NZ	2.36	0.41
2:F:160:ARG:HA	2:F:163:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:534:LEU:HA	6:J:548:PHE:CE2	2.56	0.41
6:K:81:PRO:HA	6:K:82:PRO:HD3	1.97	0.41
6:K:220:ILE:HD13	6:K:220:ILE:HA	1.95	0.41
7:L:57:GLU:HA	7:L:60:MET:HE3	2.02	0.41
7:L:136:GLU:OE2	7:L:139:ARG:NH2	2.33	0.41
7:L:154:LEU:HA	7:L:157:VAL:HG22	2.02	0.41
1:D:4:GLU:HB3	1:D:5:THR:H	1.72	0.41
6:K:507:GLU:H	6:K:507:GLU:CD	2.29	0.41
6:K:688:LEU:HD12	6:K:688:LEU:HA	1.94	0.41
7:L:73:THR:HA	7:L:108:LYS:O	2.20	0.41
7:M:90:GLN:O	7:M:93:VAL:HG12	2.21	0.41
7:M:129:GLY:HA3	7:M:134:PHE:CZ	2.56	0.41
1:B:136:ILE:O	1:B:140:LEU:HD22	2.20	0.40
1:C:23:GLY:C	4:H:145:LEU:HD11	2.43	0.40
3:G:40:GLU:CD	3:G:40:GLU:H	2.28	0.40
5:I:206:LYS:HE3	5:I:206:LYS:HB3	1.89	0.40
6:K:145:LYS:HE2	6:K:150:ALA:HB2	2.03	0.40
7:L:113:ASP:OD1	7:L:113:ASP:N	2.52	0.40
1:B:189:LEU:HD12	1:B:192:ILE:HD11	2.03	0.40
1:D:35:VAL:HG22	1:D:85:ILE:HD11	2.02	0.40
2:E:88:LEU:HD11	2:F:88:LEU:HB3	2.03	0.40
4:H:83:PRO:HB3	5:I:234:TRP:CH2	2.56	0.40
6:J:163:GLN:O	6:J:167:THR:HG22	2.22	0.40
6:J:391:ASN:ND2	6:J:394:ASP:H	2.18	0.40
6:J:635:LYS:HB3	6:J:635:LYS:HE2	1.90	0.40
7:L:139:ARG:HG3	7:L:142:ASP:HB3	2.01	0.40
1:B:213:LYS:O	1:B:217:CYS:HB2	2.21	0.40
1:C:308:GLY:HA3	2:F:167:ARG:CZ	2.51	0.40
1:D:25:ASP:OD1	1:D:26:ALA:N	2.55	0.40
3:G:48:LEU:HD22	4:H:154:ALA:HB1	2.03	0.40
1:A:180:LEU:HD11	1:A:260:THR:HG22	2.03	0.40
1:B:210:ARG:O	1:B:214:GLU:HG3	2.21	0.40
1:C:275:HIS:CD2	1:C:316:GLU:HG2	2.56	0.40
1:D:136:ILE:O	1:D:140:LEU:HD22	2.22	0.40
2:F:168:LYS:O	2:F:172:ILE:HG12	2.22	0.40
3:G:96:GLU:O	3:G:100:LEU:HG	2.21	0.40
6:J:434:LYS:HA	6:J:434:LYS:HD3	1.79	0.40
6:J:740:LYS:HA	6:J:740:LYS:HD3	1.93	0.40
6:K:442:ARG:HA	6:K:445:THR:HG22	2.04	0.40
6:K:808:ARG:HB3	7:M:61:LEU:HD22	2.03	0.40
1:D:331:ALA:HB1	1:D:335:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:ARG:HH21	2:F:92:ILE:HG12	1.87	0.40
6:J:42:ASP:OD1	6:J:42:ASP:N	2.55	0.40
7:M:136:GLU:O	7:M:140:VAL:HG23	2.21	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%)	349 (94%)	24 (6%)	0	100	100
1	B	373/377 (99%)	353 (95%)	20 (5%)	0	100	100
1	C	373/377 (99%)	361 (97%)	11 (3%)	1 (0%)	36	71
1	D	373/377 (99%)	355 (95%)	17 (5%)	1 (0%)	36	71
2	E	184/284 (65%)	184 (100%)	0	0	100	100
2	F	184/284 (65%)	184 (100%)	0	0	100	100
3	G	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
4	H	132/211 (63%)	123 (93%)	7 (5%)	2 (2%)	8	38
5	I	72/285 (25%)	66 (92%)	6 (8%)	0	100	100
6	J	803/1935 (42%)	765 (95%)	38 (5%)	0	100	100
6	K	803/1935 (42%)	764 (95%)	39 (5%)	0	100	100
7	L	151/196 (77%)	144 (95%)	5 (3%)	2 (1%)	9	41
7	M	151/196 (77%)	144 (95%)	7 (5%)	0	100	100
All	All	4130/6995 (59%)	3945 (96%)	179 (4%)	6 (0%)	49	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	L	102	GLN
1	C	3	GLU
4	H	36	ALA
4	H	34	PRO
7	L	161	LEU
1	D	3	GLU

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%)	304 (96%)	14 (4%)	25	47
1	B	318/320 (99%)	302 (95%)	16 (5%)	22	43
1	C	318/320 (99%)	301 (95%)	17 (5%)	20	42
1	D	318/320 (99%)	299 (94%)	19 (6%)	17	39
2	E	159/245 (65%)	152 (96%)	7 (4%)	25	47
2	F	159/245 (65%)	156 (98%)	3 (2%)	50	66
3	G	141/142 (99%)	133 (94%)	8 (6%)	18	40
4	H	115/176 (65%)	111 (96%)	4 (4%)	32	53
5	I	69/249 (28%)	67 (97%)	2 (3%)	37	58
6	J	695/1697 (41%)	668 (96%)	27 (4%)	28	50
6	K	695/1697 (41%)	675 (97%)	20 (3%)	37	58
7	L	133/163 (82%)	125 (94%)	8 (6%)	17	39
7	M	133/163 (82%)	124 (93%)	9 (7%)	14	36
All	All	3571/6057 (59%)	3417 (96%)	154 (4%)	27	48

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	3	GLU
1	A	45	VAL

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Mol	Chain	Res	Type
1	A	49	GLN
1	A	82	MET
1	A	140	LEU
1	A	157	ASP
1	A	185	LEU
1	A	311	ASP
1	A	353	GLN
1	A	360	GLN
1	A	370	VAL
1	A	373	LYS
1	A	375	PHE
1	B	35	VAL
1	B	45	VAL
1	B	47	MET
1	B	59	GLN
1	B	82	MET
1	B	113	LYS
1	B	120	THR
1	B	140	LEU
1	B	152	VAL
1	B	159	VAL
1	B	187	ASP
1	B	202	THR
1	B	267	ILE
1	B	306	TYR
1	B	370	VAL
1	B	373	LYS
1	C	2	ASP
1	C	3	GLU
1	C	45	VAL
1	C	47	MET
1	C	59	GLN
1	C	82	MET
1	C	140	LEU
1	C	167	GLU
1	C	192	ILE
1	C	216	LEU
1	C	292	ASP
1	C	311	ASP
1	C	323	SER
1	C	334	GLU
1	C	370	VAL

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Mol	Chain	Res	Type
1	C	373	LYS
1	C	374	CYS
1	D	34	ILE
1	D	45	VAL
1	D	64	ILE
1	D	66	THR
1	D	82	MET
1	D	95	ARG
1	D	99	GLU
1	D	124	PHE
1	D	140	LEU
1	D	161	HIS
1	D	192	ILE
1	D	260	THR
1	D	266	PHE
1	D	270	GLU
1	D	288	ASP
1	D	303	THR
1	D	323	SER
1	D	374	CYS
1	D	375	PHE
2	E	66	ASP
2	E	88	LEU
2	E	112	LYS
2	E	113	LEU
2	E	148	LEU
2	E	153	HIS
2	E	169	LEU
2	F	95	VAL
2	F	99	LEU
2	F	197	LEU
3	G	13	THR
3	G	44	VAL
3	G	51	ASN
3	G	57	LEU
3	G	64	VAL
3	G	93	SER
3	G	105	ASP
3	G	128	ILE
4	H	115	VAL
4	H	128	ASP
4	H	153	ASP

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Mol	Chain	Res	Type
4	H	165	LYS
5	I	236	SER
5	I	238	TYR
6	J	28	THR
6	J	37	VAL
6	J	39	VAL
6	J	41	ASP
6	J	80	ASN
6	J	101	VAL
6	J	239	ASP
6	J	318	THR
6	J	344	GLU
6	J	379	GLU
6	J	380	GLU
6	J	392	SER
6	J	437	ASN
6	J	448	GLU
6	J	460	LEU
6	J	539	MET
6	J	587	ASP
6	J	599	ASP
6	J	615	LYS
6	J	635	LYS
6	J	644	PHE
6	J	645	GLN
6	J	678	THR
6	J	684	ILE
6	J	700	GLU
6	J	752	ASP
6	J	788	ILE
6	K	16	LEU
6	K	37	VAL
6	K	39	VAL
6	K	101	VAL
6	K	122	CYS
6	K	244	PHE
6	K	273	VAL
6	K	328	GLU
6	K	333	ASP
6	K	339	LEU
6	K	406	VAL
6	K	462	ILE

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Mol	Chain	Res	Type
6	K	470	PHE
6	K	509	GLU
6	K	585	THR
6	K	587	ASP
6	K	631	VAL
6	K	725	LEU
6	K	756	TYR
6	K	783	ARG
7	L	52	ILE
7	L	61	LEU
7	L	79	ASP
7	L	113	ASP
7	L	128	THR
7	L	144	GLU
7	L	163	GLU
7	L	183	CYS
7	M	65	THR
7	M	102	GLN
7	M	109	MET
7	M	114	THR
7	M	144	GLU
7	M	164	ARG
7	M	166	THR
7	M	174	MET
7	M	193	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	162	ASN
1	A	275	HIS
1	A	296	ASN
1	B	59	GLN
1	B	137	GLN
1	B	296	ASN
1	B	353	GLN
1	C	40	HIS
1	C	225	ASN
1	C	246	GLN
1	C	263	GLN
1	C	360	GLN

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Mol	Chain	Res	Type
1	D	73	HIS
1	D	275	HIS
1	D	314	GLN
1	D	371	HIS
2	E	202	ASN
2	E	210	GLN
2	F	144	GLN
2	F	203	ASN
2	F	216	GLN
3	G	16	GLN
3	G	50	GLN
3	G	122	GLN
4	H	95	GLN
5	I	266	ASN
6	J	163	GLN
6	J	193	GLN
6	J	284	HIS
6	J	288	GLN
6	J	358	HIS
6	J	391	ASN
6	J	401	HIS
6	J	498	GLN
6	J	555	ASN
6	J	597	ASN
6	J	602	ASN
6	J	645	GLN
6	J	668	HIS
6	K	97	HIS
6	K	172	GLN
6	K	187	ASN
6	K	288	GLN
6	K	418	GLN
7	L	102	GLN
7	L	146	ASN
7	M	87	ASN
7	M	102	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 7 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	$\#\|Z\| > 2$
8	ADP	D	401	9	28,29,29	1.39	4 (14%)	43,45,45	1.73	7 (16%)
8	ADP	B	401	9	28,29,29	1.35	5 (17%)	43,45,45	1.83	9 (20%)
8	ADP	C	401	9	28,29,29	1.41	4 (14%)	43,45,45	1.85	10 (23%)
8	ADP	A	401	9	28,29,29	1.35	4 (14%)	43,45,45	1.84	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	D	401	9	-	3/16/32/32	0/3/3/3
8	ADP	B	401	9	-	4/16/32/32	0/3/3/3
8	ADP	C	401	9	-	3/16/32/32	0/3/3/3
8	ADP	A	401	9	-	5/16/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	401	ADP	C5-C4	4.61	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	401	ADP	C5-C4	4.55	1.47	1.39
8	A	401	ADP	C5-C4	4.32	1.46	1.39
8	B	401	ADP	C5-C4	4.28	1.46	1.39
8	A	401	ADP	C5-C6	2.67	1.48	1.41
8	C	401	ADP	C5-C6	2.65	1.48	1.41
8	D	401	ADP	C5-C6	2.64	1.48	1.41
8	C	401	ADP	C5-N7	-2.62	1.34	1.39
8	B	401	ADP	C5-N7	-2.51	1.34	1.39
8	D	401	ADP	C5-N7	-2.48	1.34	1.39
8	B	401	ADP	C5-C6	2.45	1.47	1.41
8	A	401	ADP	C5-N7	-2.40	1.34	1.39
8	C	401	ADP	C8-N7	2.14	1.35	1.31
8	B	401	ADP	C8-N7	2.11	1.35	1.31
8	D	401	ADP	C4-N9	-2.10	1.33	1.37
8	B	401	ADP	C4-N9	-2.04	1.33	1.37
8	A	401	ADP	C8-N7	2.01	1.35	1.31

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	401	ADP	C5-C4-N3	-5.96	118.52	126.72
8	C	401	ADP	C5-C4-N3	-5.93	118.55	126.72
8	A	401	ADP	C5-C4-N3	-5.81	118.71	126.72
8	D	401	ADP	C5-C4-N3	-5.61	119.00	126.72
8	B	401	ADP	N3-C4-N9	4.75	135.24	127.17
8	A	401	ADP	N3-C4-N9	4.69	135.15	127.17
8	C	401	ADP	N3-C4-N9	4.64	135.07	127.17
8	D	401	ADP	N3-C4-N9	4.47	134.77	127.17
8	B	401	ADP	C2-N3-C4	3.70	120.87	111.83
8	A	401	ADP	C2-N3-C4	3.67	120.80	111.83
8	C	401	ADP	C2-N3-C4	3.64	120.73	111.83
8	D	401	ADP	C2-N3-C4	3.54	120.47	111.83
8	C	401	ADP	C4-C5-N7	-3.48	106.61	110.58
8	D	401	ADP	C4-C5-N7	-3.33	106.78	110.58
8	A	401	ADP	C4-C5-N7	-3.33	106.78	110.58
8	B	401	ADP	C4-C5-N7	-3.31	106.80	110.58
8	A	401	ADP	N3-C2-N1	-3.15	123.82	128.58
8	D	401	ADP	N3-C2-N1	-3.13	123.84	128.58
8	B	401	ADP	N3-C2-N1	-3.13	123.85	128.58
8	C	401	ADP	N3-C2-N1	-3.05	123.97	128.58
8	A	401	ADP	C4-N9-C8	2.68	108.55	105.74
8	B	401	ADP	C4-N9-C8	2.67	108.54	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	401	ADP	C5-N7-C8	2.55	107.47	103.45
8	A	401	ADP	C5-N7-C8	2.48	107.34	103.45
8	B	401	ADP	C5-N7-C8	2.47	107.33	103.45
8	D	401	ADP	C4-N9-C8	2.46	108.32	105.74
8	B	401	ADP	C3'-C2'-C1'	2.41	106.03	101.46
8	C	401	ADP	C4-N9-C8	2.36	108.22	105.74
8	C	401	ADP	C3'-C2'-C1'	2.36	105.92	101.46
8	D	401	ADP	C5-N7-C8	2.31	107.08	103.45
8	A	401	ADP	C3'-C2'-C1'	2.18	105.59	101.46
8	C	401	ADP	C2'-C1'-N9	-2.15	107.97	113.30
8	A	401	ADP	C2'-C3'-C4'	2.11	106.69	102.61
8	C	401	ADP	C6-C5-N7	2.07	136.08	132.09
8	B	401	ADP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

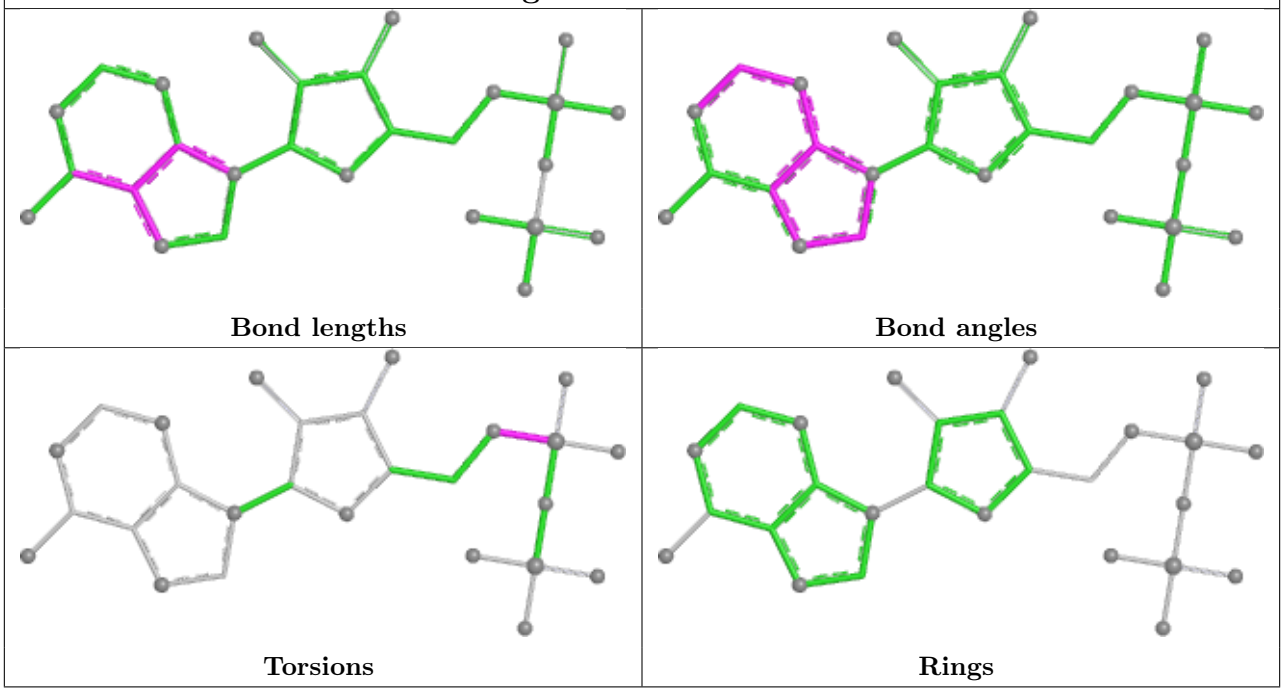
There are no ring outliers.

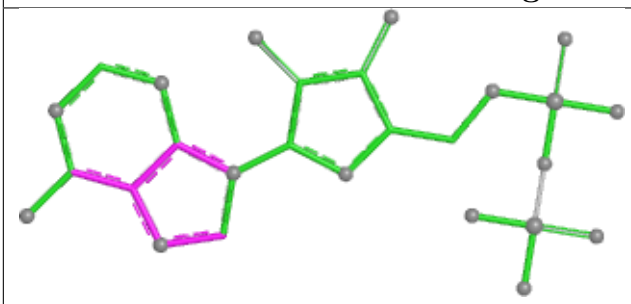
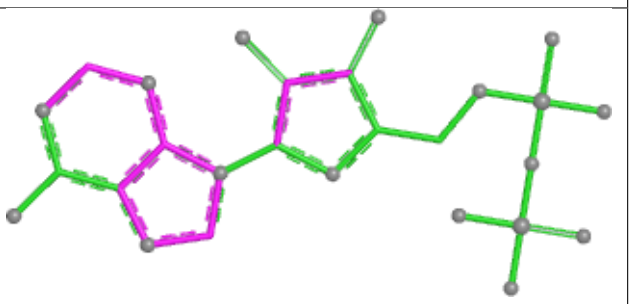
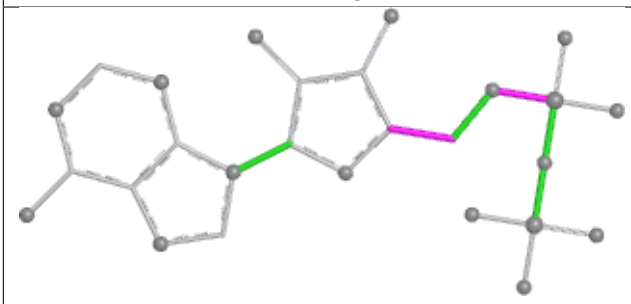
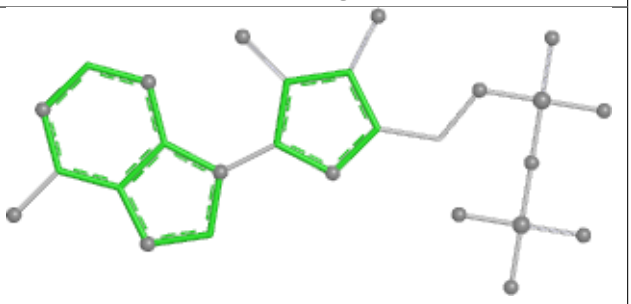
3 monomers are involved in 3 short contacts:

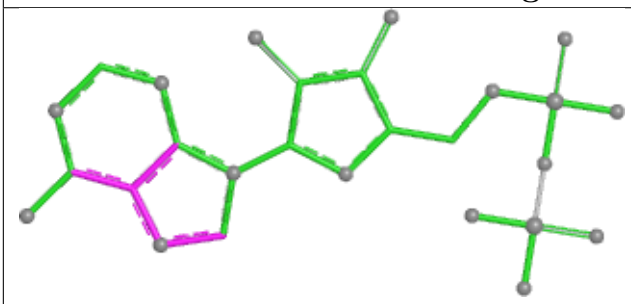
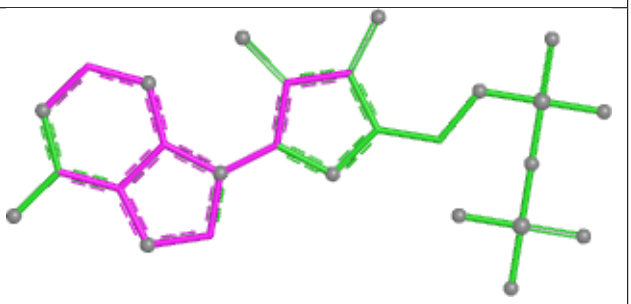
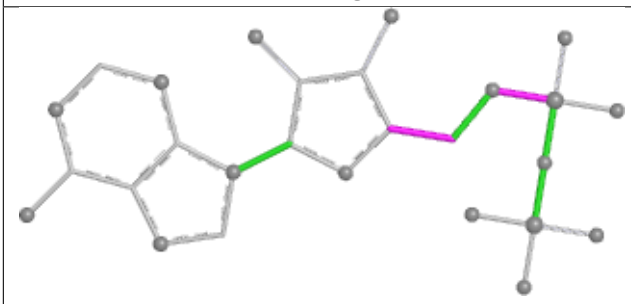
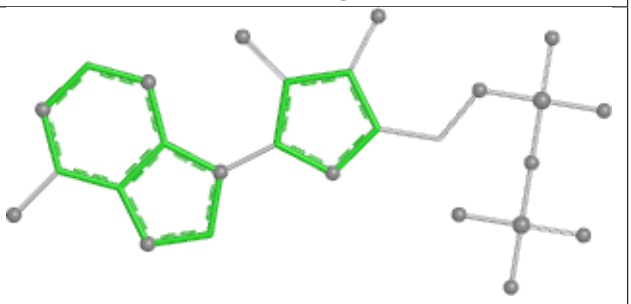
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	401	ADP	1	0
8	B	401	ADP	1	0
8	C	401	ADP	1	0

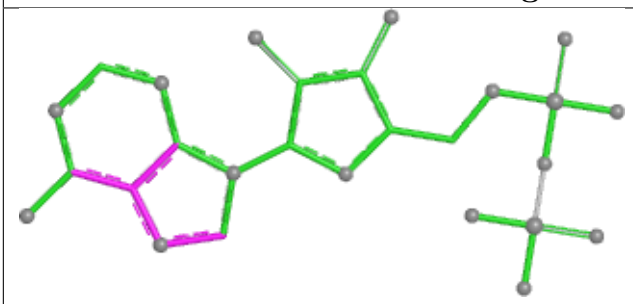
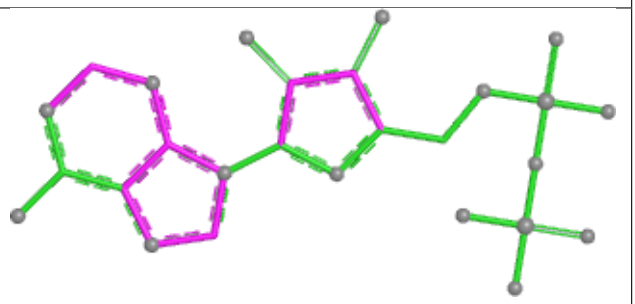
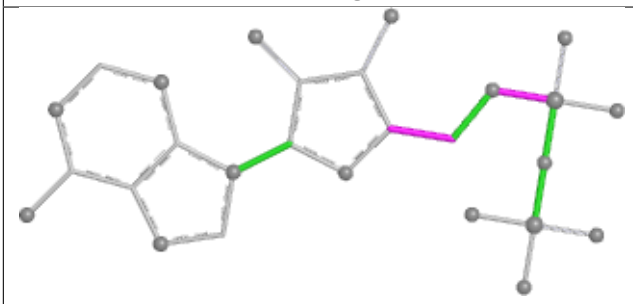
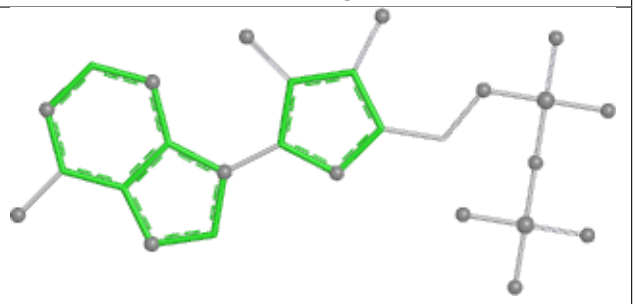
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand ADP B 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP C 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 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.

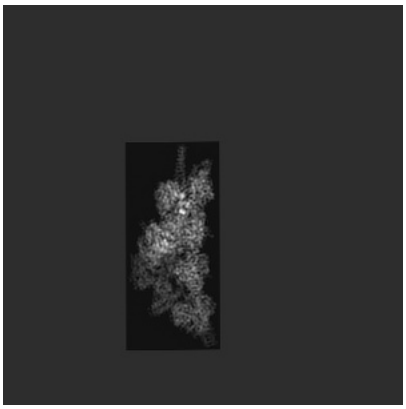
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-73030. These allow visual inspection of the internal detail of the map and identification of artifacts.

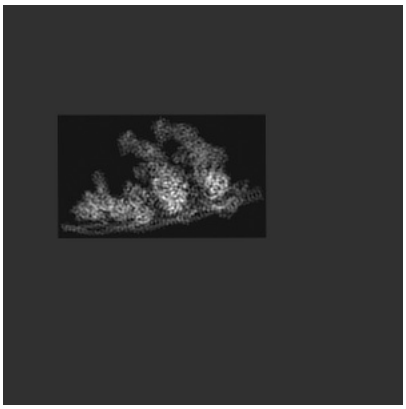
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

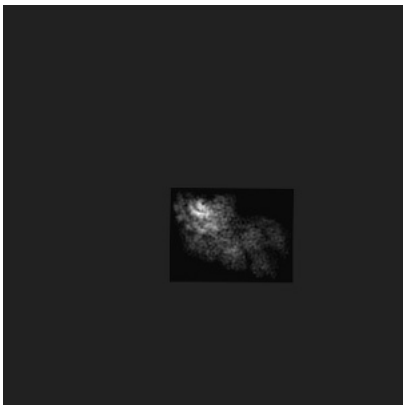
6.1.1 Primary map



X

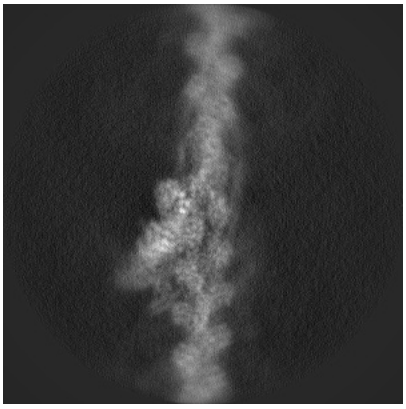


Y

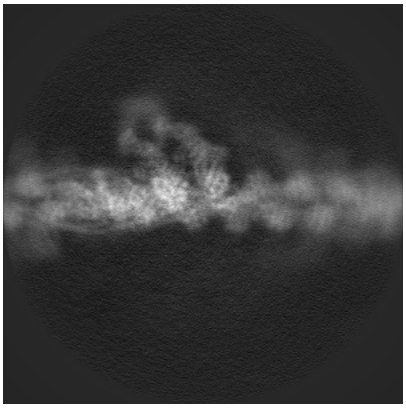


Z

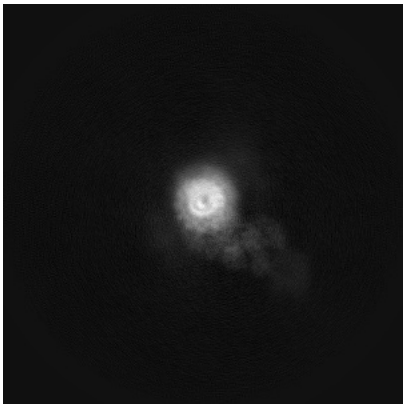
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

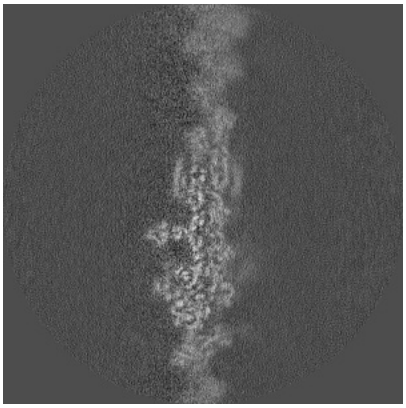
6.2.1 Primary map

X Index: 198

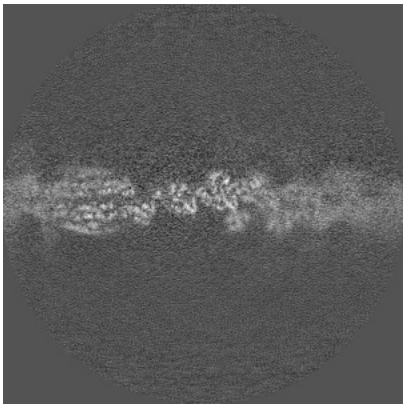
Y Index: 198

Z Index: 198

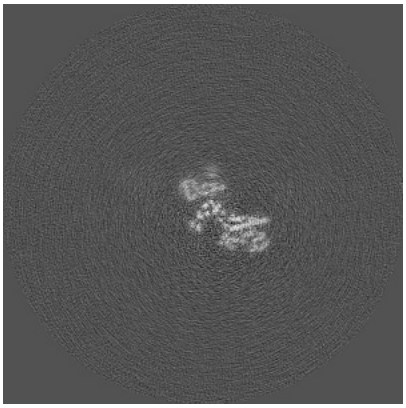
6.2.2 Raw map



X Index: 198



Y Index: 198

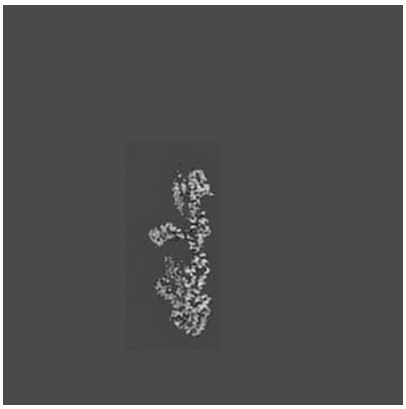


Z Index: 198

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

6.3 Largest variance slices (i)

6.3.1 Primary map

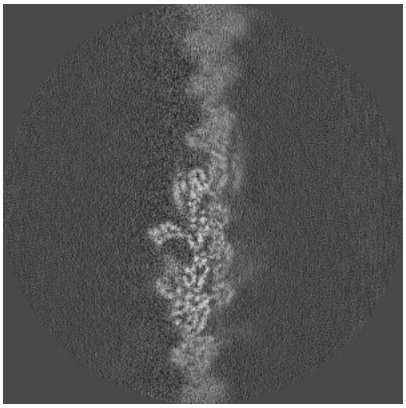


X Index: 195

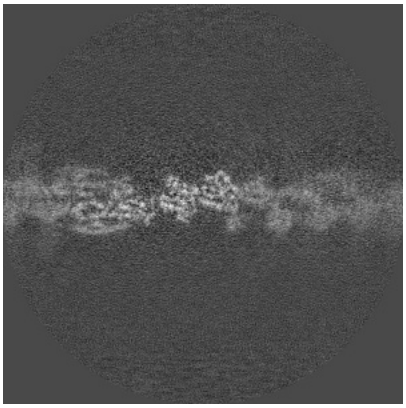
Y Index: 188

Z Index: 165

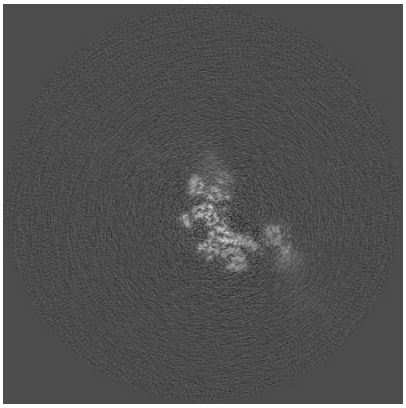
6.3.2 Raw map



X Index: 195



Y Index: 195

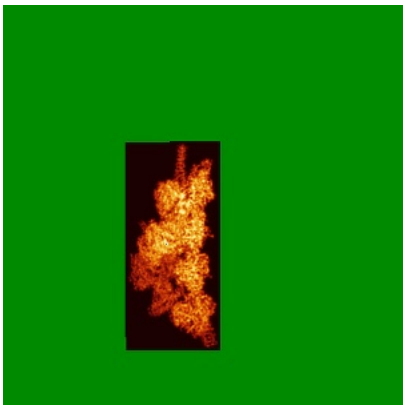


Z Index: 159

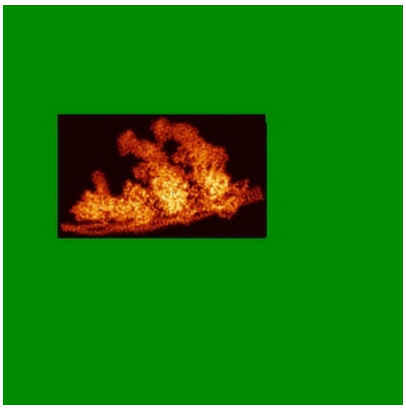
The images above show the largest variance slices of the map in three orthogonal directions.

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

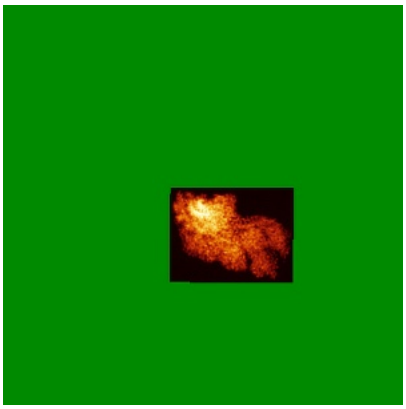
6.4.1 Primary map



X

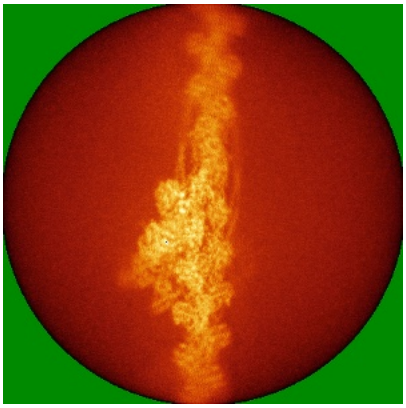


Y

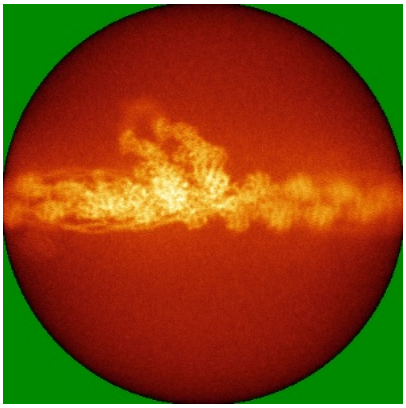


Z

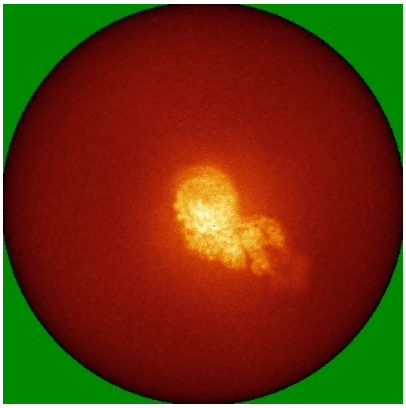
6.4.2 Raw map



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.

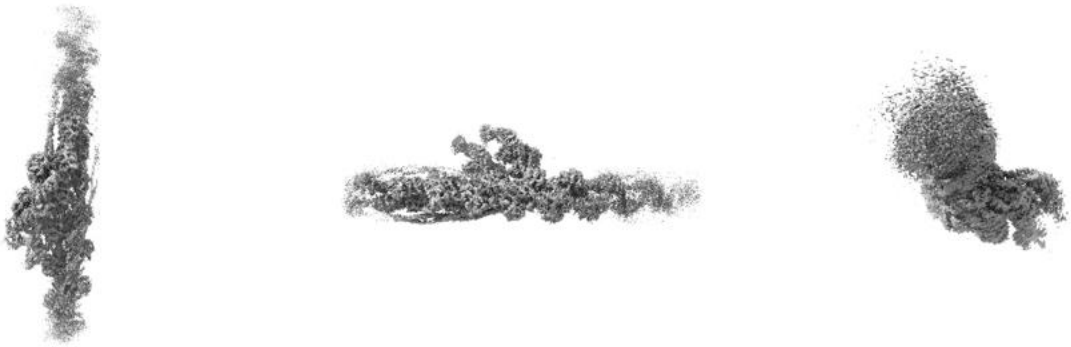
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.4. 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.

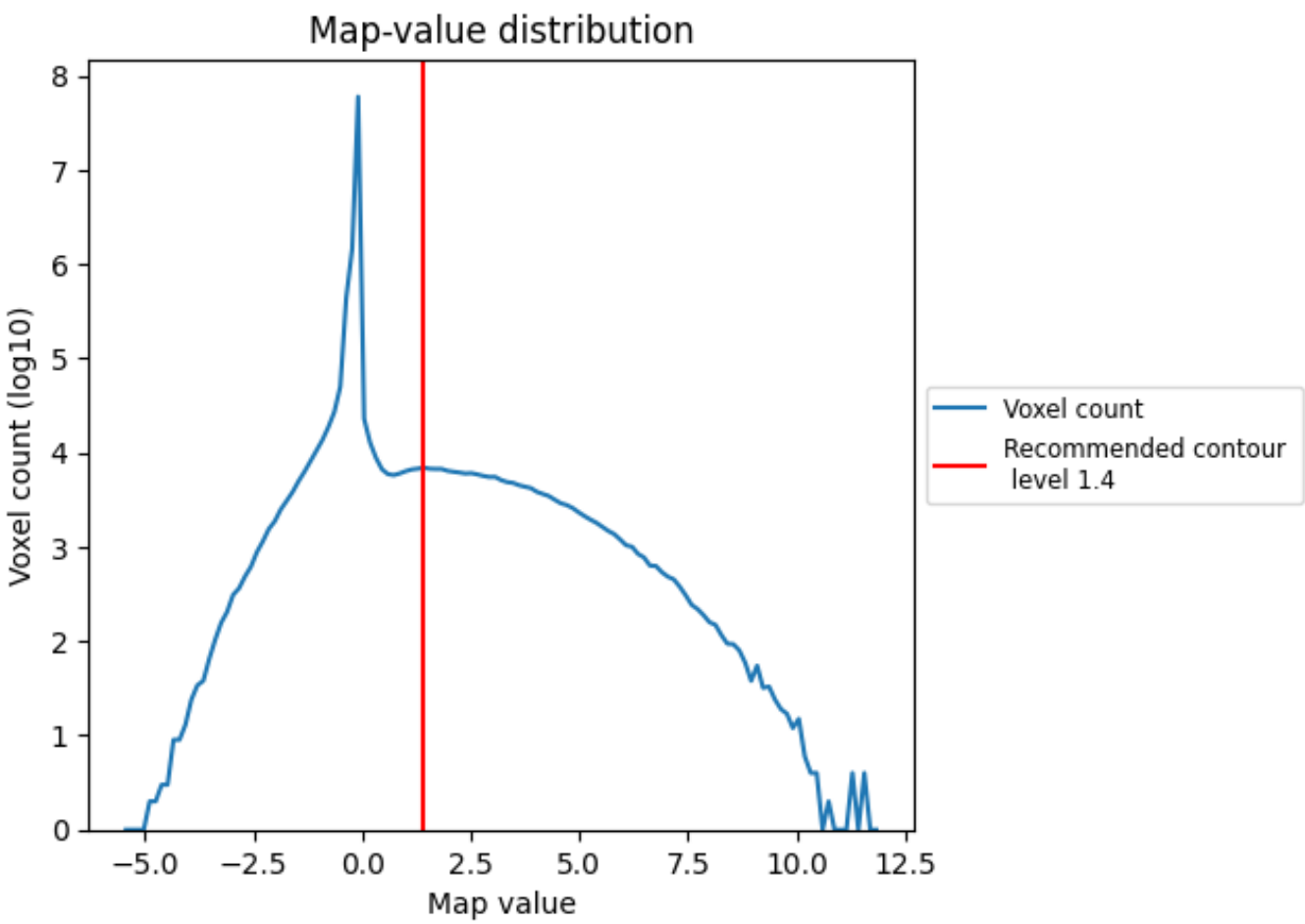
6.6 Mask visualisation (i)

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

7 Map analysis (i)

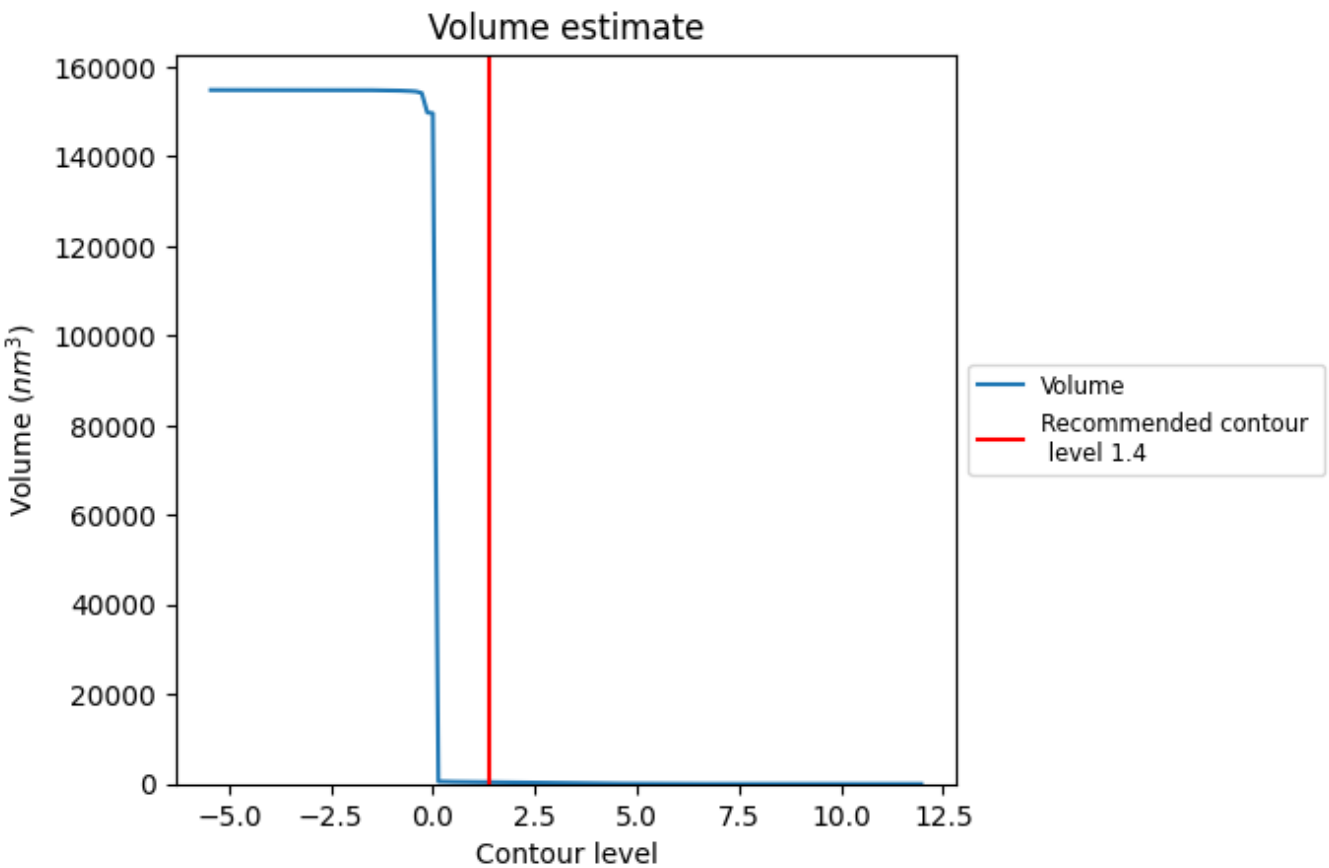
This section contains the results of statistical analysis of the map.

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.

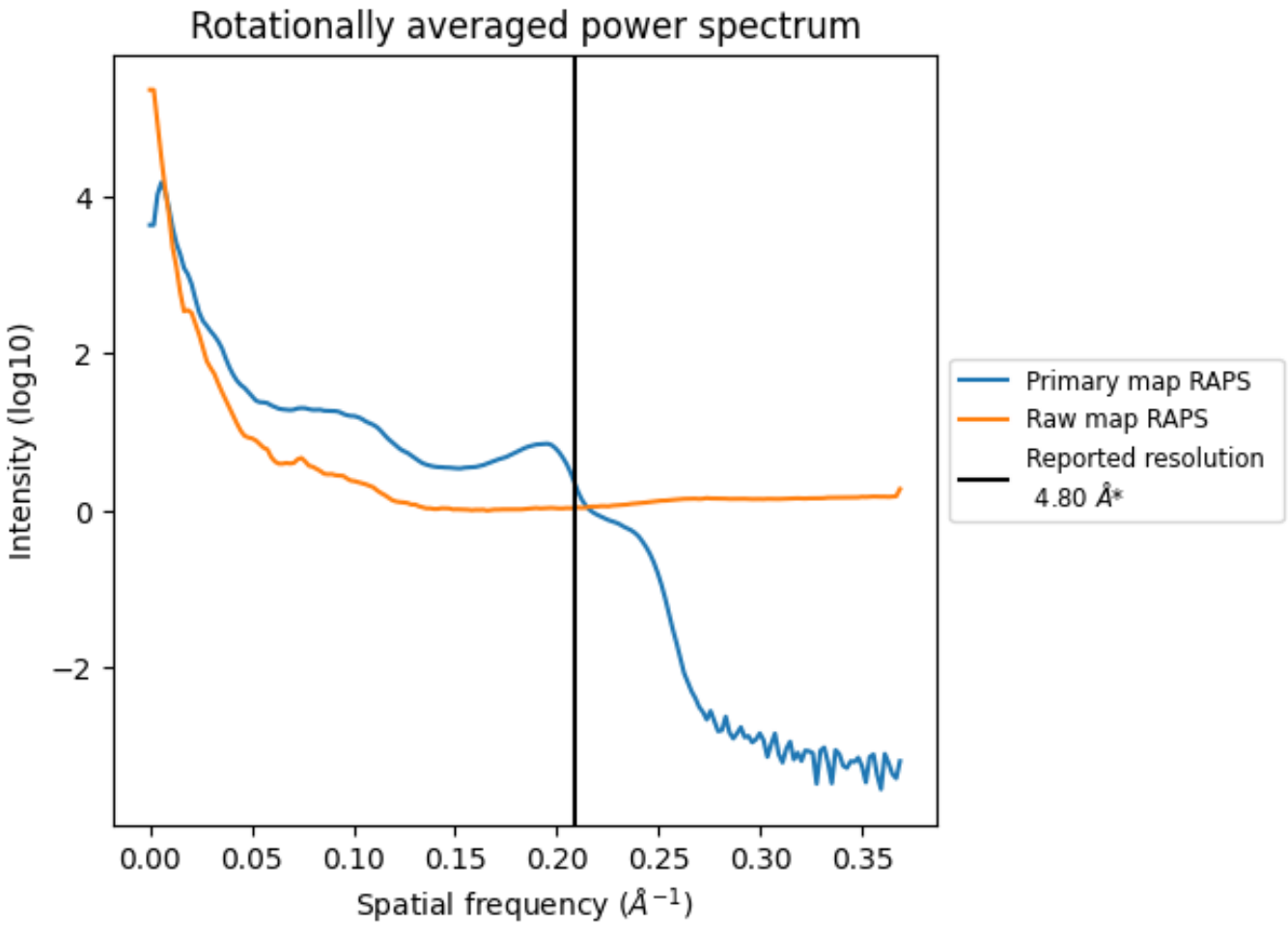
7.2 Volume estimate (i)



The volume at the recommended contour level is 385 nm^3; this corresponds to an approximate mass of 347 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)

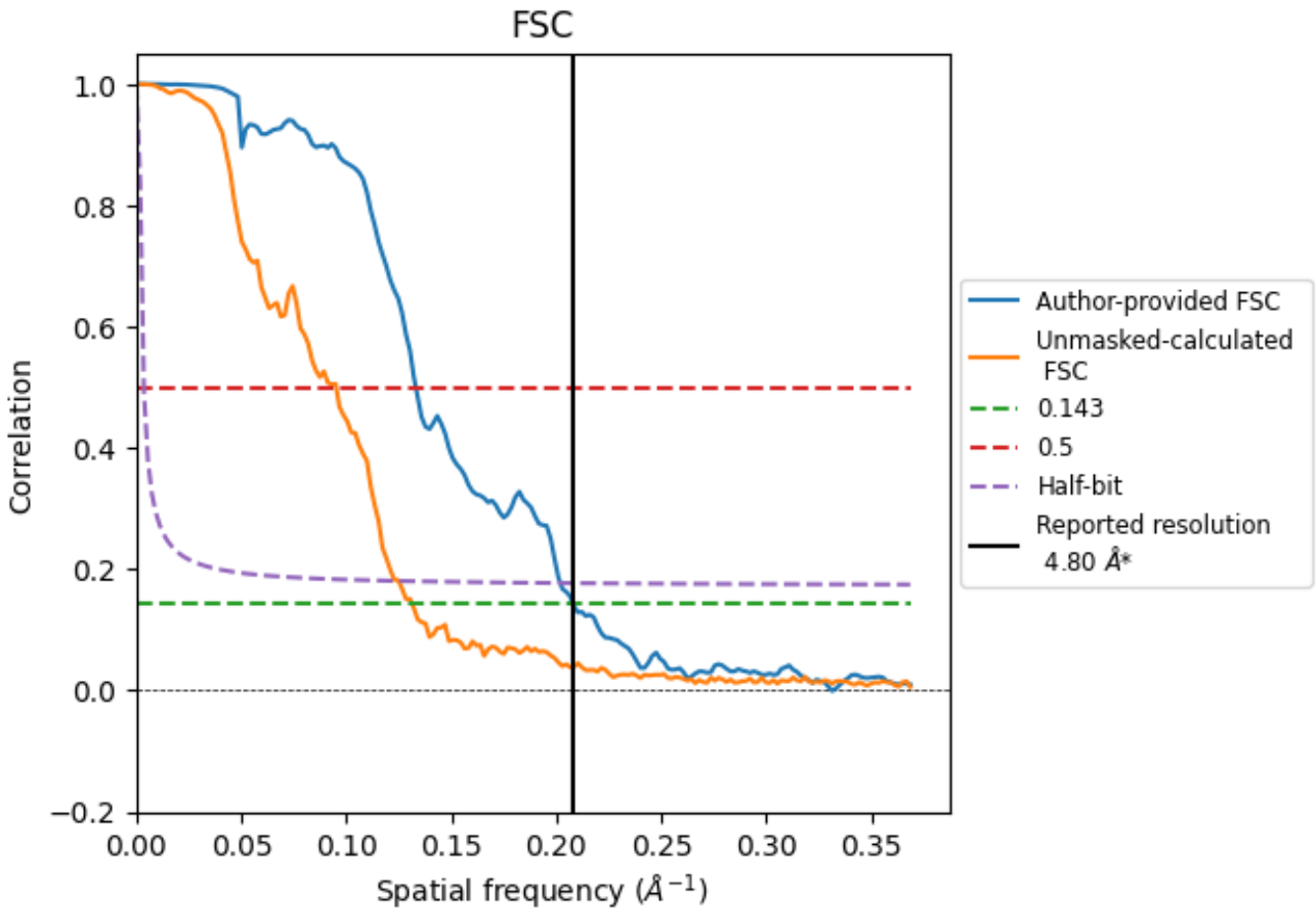


*Reported resolution corresponds to spatial frequency of 0.208 Å^{-1}

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 0.208 Å^{-1}

8.2 Resolution estimates (i)

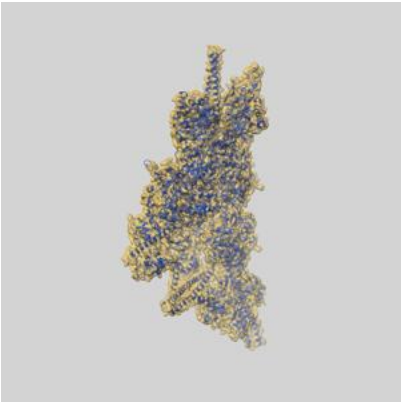
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.81	7.51	4.95
Unmasked-calculated*	7.62	10.50	8.00

*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 7.62 differs from the reported value 4.8 by more than 10 %

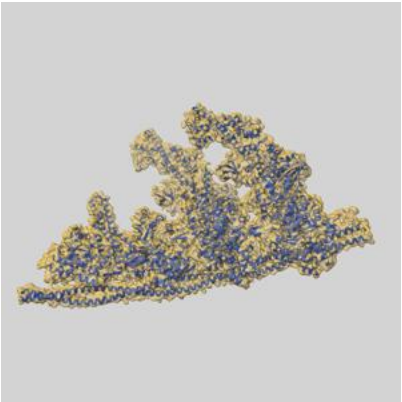
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-73030 and PDB model 9YJP. Per-residue inclusion information can be found in section 3 on page 7.

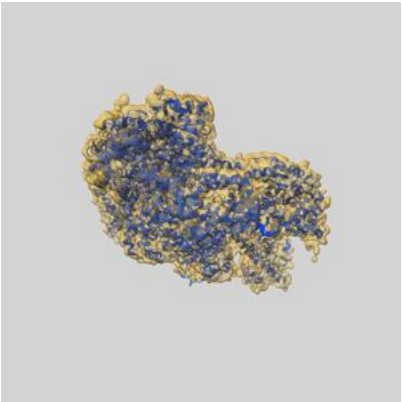
9.1 Map-model overlay (i)



X



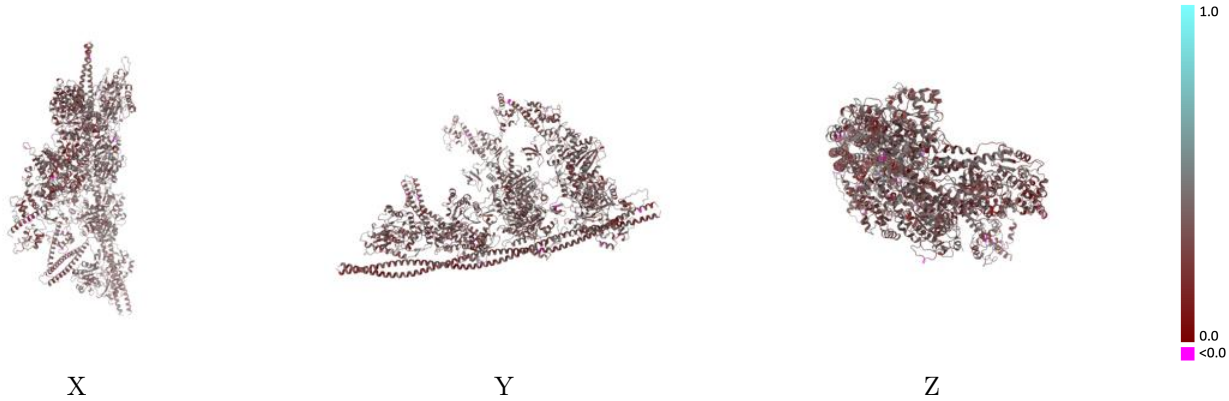
Y



Z

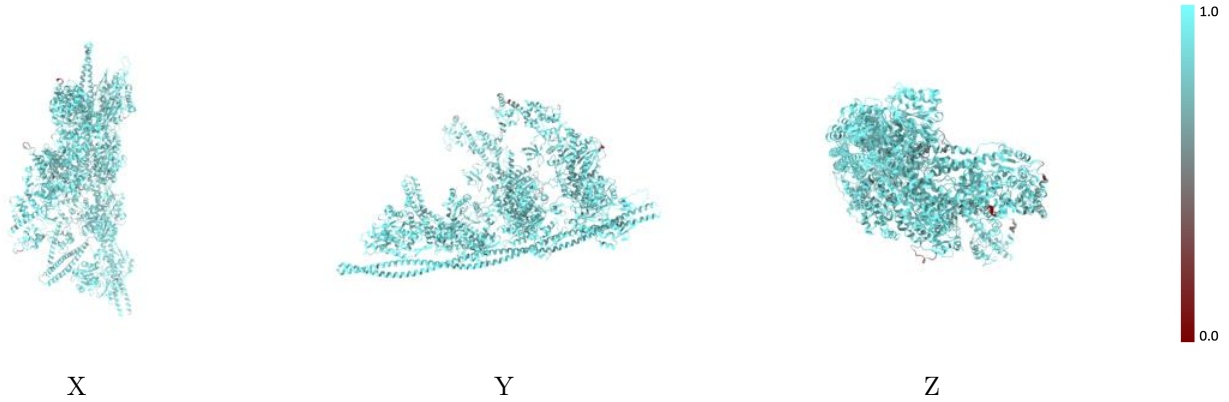
The images above show the 3D surface view of the map at the recommended contour level 1.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



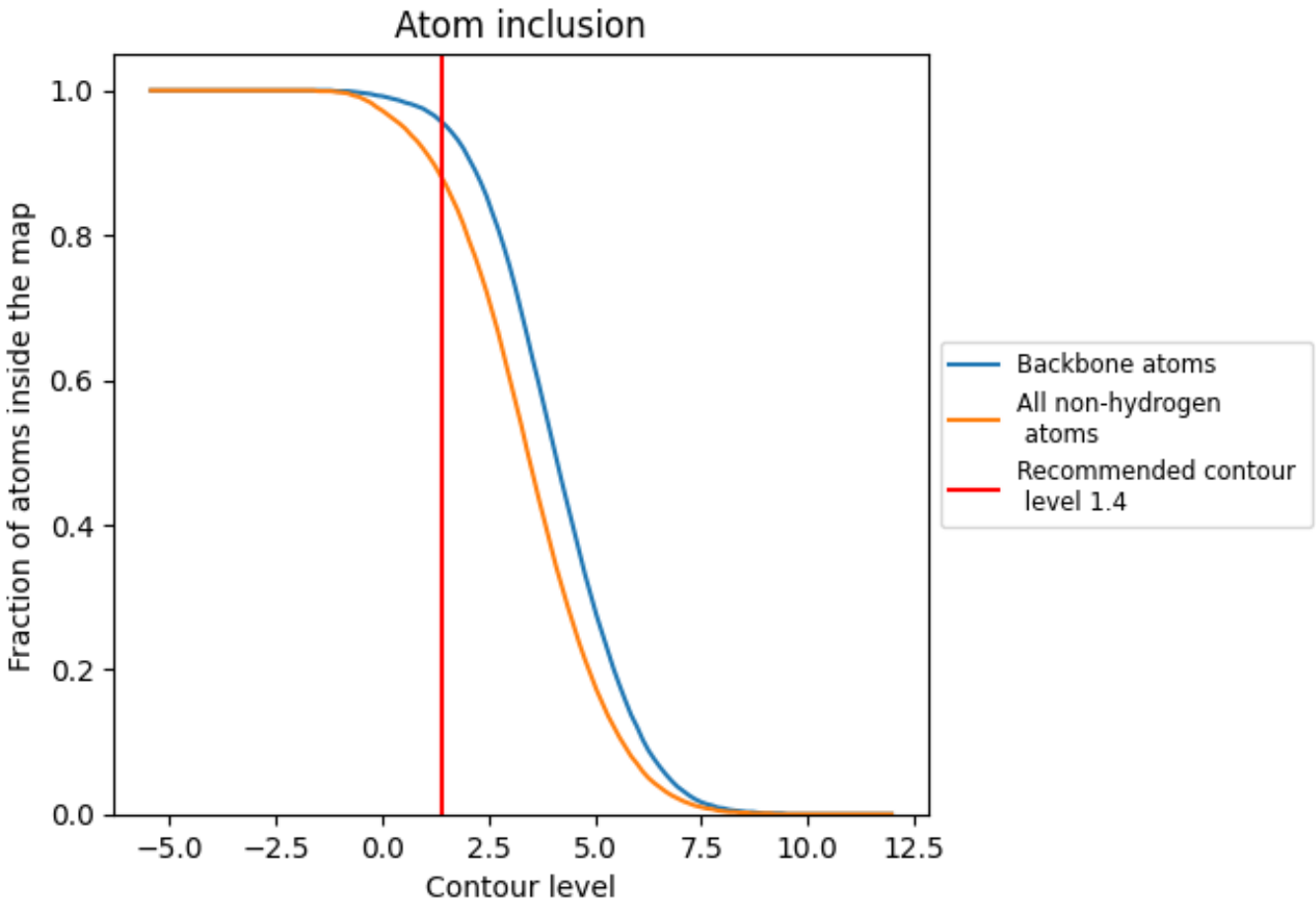
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.4).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 88% 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 (1.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8790	0.3440
A	0.8860	0.3540
B	0.8950	0.3660
C	0.8870	0.3620
D	0.9190	0.3670
E	0.8820	0.2900
F	0.8890	0.3060
G	0.8880	0.3030
H	0.8280	0.3100
I	0.8710	0.3250
J	0.8650	0.3440
K	0.8790	0.3560
L	0.8180	0.3150
M	0.8580	0.3380