



Full wwPDB EM Validation Report ⓘ

Aug 8, 2026 – 02:06 PM EDT

PDB ID : 9Z3Z / pdb_00009z3z
EMDB ID : EMD-73796
Title : Cryo-EM structure of human nonmuscle myosin-2B, Class 2
Authors : Heissler, S.M.; Chinthalapudi, K.
Deposited on : 2025-11-07
Resolution : 5.24 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

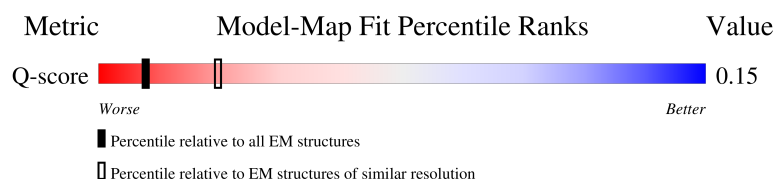
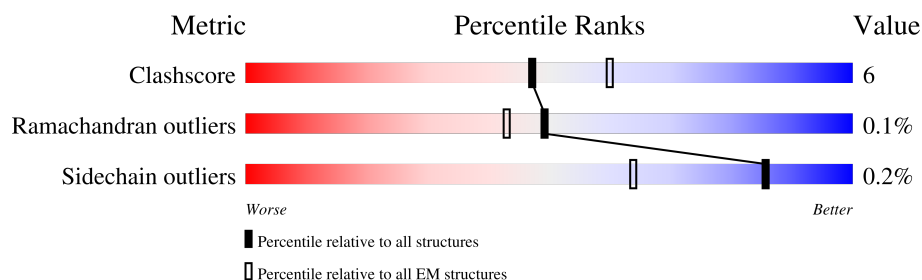
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

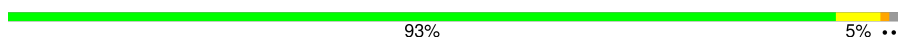
The reported resolution of this entry is 5.24 Å.

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	600 (4.74 - 5.72)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1976	
1	B	1976	
2	C	151	
2	F	151	

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Mol	Chain	Length	Quality of chain
3	D	171	 91% 8% ..
3	E	171	 82% 11% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	B	2002	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28278 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 Myosin-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1416	Total	C	N	O	S	0	0
			11563	7225	2050	2239	49		
1	B	1428	Total	C	N	O	S	0	0
			11657	7284	2067	2256	50		

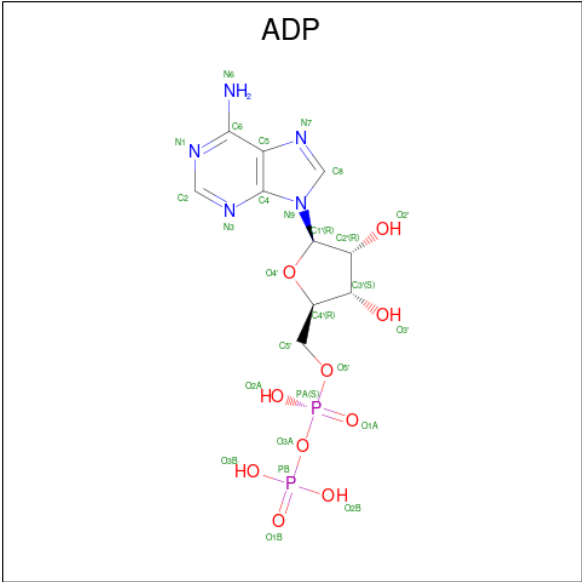
- Molecule 2 is a protein called Myosin light polypeptide 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	149	Total	C	N	O	S	0	0
			1170	730	195	237	8		
2	F	149	Total	C	N	O	S	0	0
			1170	730	195	237	8		

- Molecule 3 is a protein called Myosin regulatory light chain 12B.

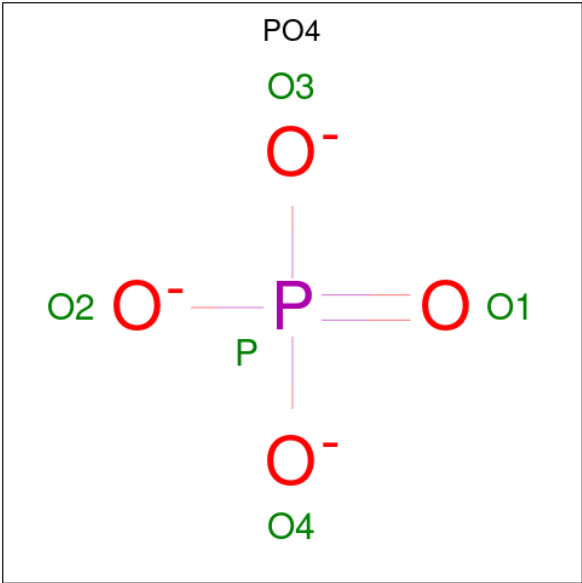
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	169	Total	C	N	O	S	0	0
			1366	854	228	275	9		
3	E	159	Total	C	N	O	S	0	0
			1286	803	212	262	9		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



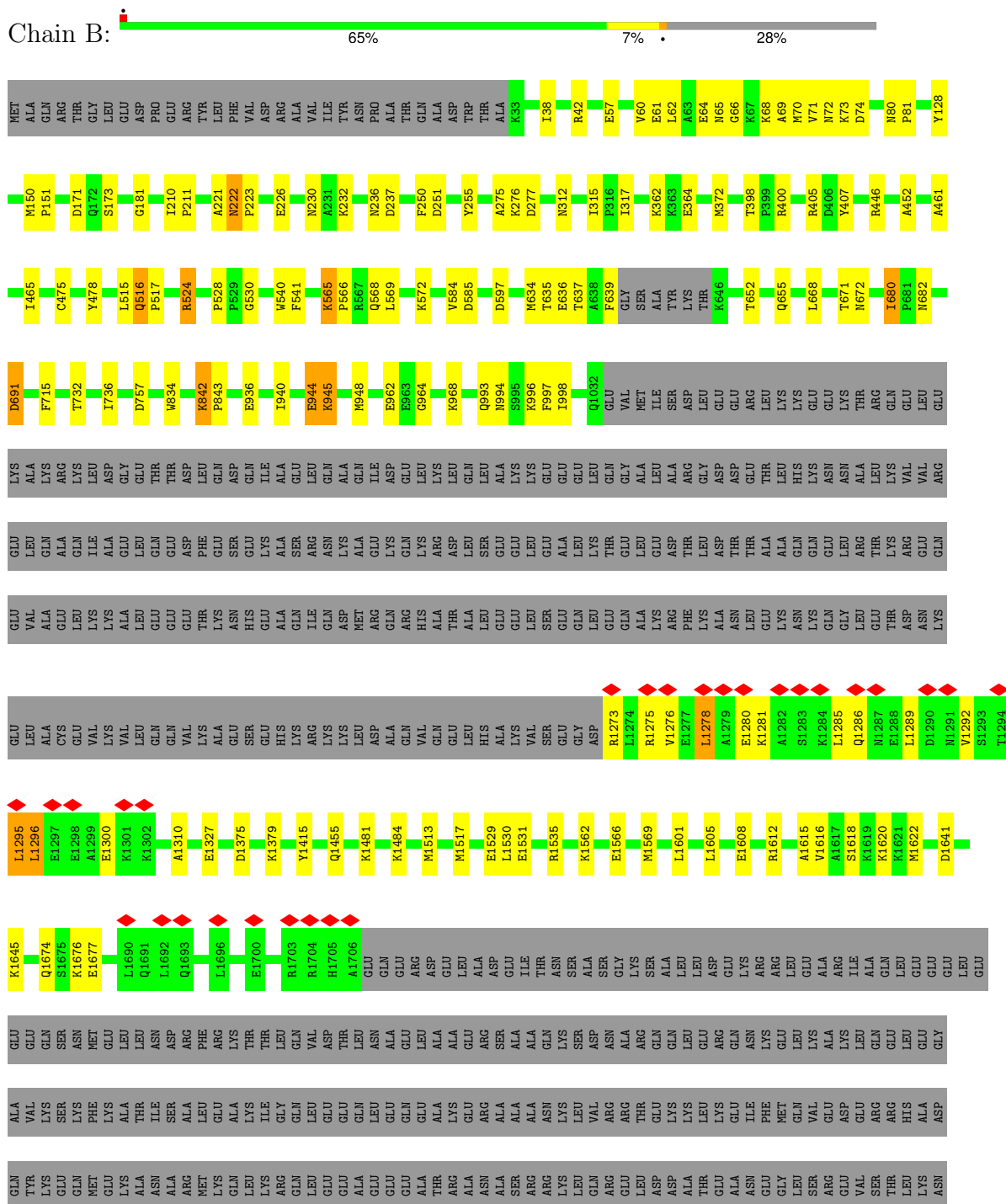
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	O	P	0
			5	4	1	
5	B	1	Total	O	P	0
			5	4	1	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total 1	Mg 1	0
6	B	1	Total 1	Mg 1	0

ASN	ARG	LEU	ARG	ARG	GLY	GLY	PRO	ILE	SER	PHE	SER	SER	SER	SER	ARG	GLY	ARG	ARG	GLN	LEU	HIS	LEU	LEU	GLY	GLY	ALA	SER	LEU	LEU	GLU	ASP	ASP	THR	THR	GLU	SER	SER	LYS	THR	THR	ASP	ASP	VAL	ASN	GLU	THR	GLN	PRO	PRO	GLN	SER	GLU
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- Molecule 1: Myosin-10



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

• Molecule 2: Myosin light polypeptide 6

Chain C: 91% 7% ..

MET
CYS
D3
T22
G23
D24
M42
N54
P55
D58
D66
F67
E68
L71
P72
D134
G151

• Molecule 2: Myosin light polypeptide 6

Chain F: 93% 5% ..

MET
CYS
D3
K26
M42
P43
N54
D66
L71
P72
D97
G100
G151

• Molecule 3: Myosin regulatory light chain 12B

Chain D: 91% 8% ..

SER
SER
K3
K4
R13
P14
N63
A76
P77
G78
R88
K92
D97
D148
R160
I161
H164
G165
D171

• Molecule 3: Myosin regulatory light chain 12B

Chain E: 82% 11% 7%

SER
SER
LYS
LYS
ALA
THR
LYS
THR
THR
LYS
LYS
R13
N63
D70
N74
E75
A76
P77
G78
N81
F82
T83
K92
D97
R103
F106
A113
T114
G115
T116
E124
T128
F153
I161
G165
D171

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57849	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 ($e^-/\text{\AA}^2$)	72	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	8.674	Depositor
Minimum map value	-0.084	Depositor
Average map value	-0.011	Depositor
Map value standard deviation	0.212	Depositor
Recommended contour level	0.214	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, PO4

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	0.69	0/11711	0.78	49/15686 (0.3%)
1	B	0.68	0/11807	0.79	49/15814 (0.3%)
2	C	0.67	0/1188	0.78	6/1598 (0.4%)
2	F	0.68	0/1188	0.80	6/1598 (0.4%)
3	D	0.68	0/1390	0.86	10/1865 (0.5%)
3	E	0.70	0/1310	0.89	8/1762 (0.5%)
All	All	0.69	0/28594	0.79	128/38323 (0.3%)

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	A	0	4
1	B	0	2
All	All	0	6

There are no bond length outliers.

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ASN	CA-C-N	9.90	126.79	119.66
1	A	80	ASN	C-N-CA	9.90	126.79	119.66
1	B	80	ASN	CA-C-N	9.28	126.43	119.66
1	B	80	ASN	C-N-CA	9.28	126.43	119.66
1	B	715	PHE	CA-C-N	7.97	127.69	119.56
1	B	715	PHE	C-N-CA	7.97	127.69	119.56
2	C	54	ASN	CA-C-N	7.88	127.77	120.21
2	C	54	ASN	C-N-CA	7.88	127.77	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	736	ILE	CA-C-N	7.84	127.85	119.78
1	B	736	ILE	C-N-CA	7.84	127.85	119.78
3	E	78	GLY	CA-C-N	7.80	127.82	119.78
3	E	78	GLY	C-N-CA	7.80	127.82	119.78
1	B	81	PRO	CA-C-N	7.74	127.92	119.87
1	B	81	PRO	C-N-CA	7.74	127.92	119.87
3	E	97	ASP	CA-C-N	7.60	128.05	119.92
3	E	97	ASP	C-N-CA	7.60	128.05	119.92
1	B	757	ASP	CA-C-N	7.34	127.05	119.56
1	B	757	ASP	C-N-CA	7.34	127.05	119.56
1	A	691	ASP	CA-C-N	7.30	126.93	119.56
1	A	691	ASP	C-N-CA	7.30	126.93	119.56
1	A	757	ASP	CA-C-N	7.26	127.42	119.87
1	A	757	ASP	C-N-CA	7.26	127.42	119.87
1	A	680	ILE	CA-C-N	7.14	127.75	119.47
1	A	680	ILE	C-N-CA	7.14	127.75	119.47
1	A	715	PHE	CA-C-N	7.14	127.30	119.87
1	A	715	PHE	C-N-CA	7.14	127.30	119.87
1	A	38	ILE	CA-C-N	7.12	127.04	119.85
1	A	38	ILE	C-N-CA	7.12	127.04	119.85
2	F	42	ASN	CA-C-N	7.09	127.05	120.03
2	F	42	ASN	C-N-CA	7.09	127.05	120.03
2	F	54	ASN	CA-C-N	7.09	127.01	119.85
2	F	54	ASN	C-N-CA	7.09	127.01	119.85
3	E	63	ASN	CA-C-N	7.07	126.99	119.85
3	E	63	ASN	C-N-CA	7.07	126.99	119.85
3	D	97	ASP	CA-C-N	7.07	127.06	119.78
3	D	97	ASP	C-N-CA	7.07	127.06	119.78
1	A	398	THR	CA-C-N	7.02	127.01	119.78
1	A	398	THR	C-N-CA	7.02	127.01	119.78
2	C	42	ASN	CA-C-N	7.00	127.17	120.31
2	C	42	ASN	C-N-CA	7.00	127.17	120.31
3	D	76	ALA	CA-C-N	6.93	126.63	119.56
3	D	76	ALA	C-N-CA	6.93	126.63	119.56
1	A	317	ILE	CA-C-N	6.88	126.51	119.56
1	A	317	ILE	C-N-CA	6.88	126.51	119.56
3	D	63	ASN	CA-C-N	6.84	126.76	119.85
3	D	63	ASN	C-N-CA	6.84	126.76	119.85
1	A	151	PRO	CA-C-N	6.81	126.77	119.76
1	A	151	PRO	C-N-CA	6.81	126.77	119.76
3	D	13	ARG	CA-C-N	6.77	126.79	119.89
3	D	13	ARG	C-N-CA	6.77	126.79	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	PRO	CA-C-N	6.71	126.67	119.76
1	B	151	PRO	C-N-CA	6.71	126.67	119.76
1	A	1528	HIS	CB-CA-C	-6.64	108.91	116.54
1	A	150	MET	CA-C-N	6.63	127.20	120.38
1	A	150	MET	C-N-CA	6.63	127.20	120.38
3	E	76	ALA	CA-C-N	6.62	126.76	119.87
3	E	76	ALA	C-N-CA	6.62	126.76	119.87
1	A	372	MET	CA-C-N	6.62	126.53	119.85
1	A	372	MET	C-N-CA	6.62	126.53	119.85
1	B	691	ASP	CA-C-N	6.60	126.23	119.56
1	B	691	ASP	C-N-CA	6.60	126.23	119.56
1	B	541	PHE	CA-C-N	6.60	126.22	119.56
1	B	541	PHE	C-N-CA	6.60	126.22	119.56
1	B	597	ASP	CA-C-N	6.56	126.54	119.78
1	B	597	ASP	C-N-CA	6.56	126.54	119.78
1	B	150	MET	CA-C-N	6.56	127.13	120.38
1	B	150	MET	C-N-CA	6.56	127.13	120.38
1	B	398	THR	CA-C-N	6.54	126.45	119.85
1	B	398	THR	C-N-CA	6.54	126.45	119.85
1	A	524	ARG	CA-C-N	6.52	127.08	120.04
1	A	524	ARG	C-N-CA	6.52	127.08	120.04
1	A	597	ASP	CA-C-N	6.51	126.42	119.85
1	A	597	ASP	C-N-CA	6.51	126.42	119.85
1	B	372	MET	CA-C-N	6.50	126.13	119.56
1	B	372	MET	C-N-CA	6.50	126.13	119.56
1	A	315	ILE	CA-C-N	6.46	126.64	120.31
1	A	315	ILE	C-N-CA	6.46	126.64	120.31
1	A	672	ASN	CA-C-N	6.44	126.35	119.85
1	A	672	ASN	C-N-CA	6.44	126.35	119.85
1	B	317	ILE	CA-C-N	6.42	126.33	119.85
1	B	317	ILE	C-N-CA	6.42	126.33	119.85
1	B	524	ARG	CA-C-N	6.35	125.97	119.56
1	B	524	ARG	C-N-CA	6.35	125.97	119.56
1	B	528	PRO	CA-C-N	6.27	126.18	119.85
1	B	528	PRO	C-N-CA	6.27	126.18	119.85
1	A	126	ASN	CA-C-N	6.26	125.96	119.64
1	A	126	ASN	C-N-CA	6.26	125.96	119.64
1	B	315	ILE	CA-C-N	6.25	126.20	119.76
1	B	315	ILE	C-N-CA	6.25	126.20	119.76
1	B	732	THR	CA-C-N	6.25	126.19	119.76
1	B	732	THR	C-N-CA	6.25	126.19	119.76
3	D	78	GLY	CA-C-N	6.18	126.20	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	78	GLY	C-N-CA	6.18	126.20	119.90
1	B	222	ASN	CA-C-N	6.14	125.82	119.56
1	B	222	ASN	C-N-CA	6.14	125.82	119.56
1	B	672	ASN	CA-C-N	6.09	125.85	119.76
1	B	672	ASN	C-N-CA	6.09	125.85	119.76
1	A	736	ILE	CA-C-N	6.03	126.00	120.03
1	A	736	ILE	C-N-CA	6.03	126.00	120.03
1	A	528	PRO	CA-C-N	5.88	125.84	119.78
1	A	528	PRO	C-N-CA	5.88	125.84	119.78
1	B	565	LYS	CA-C-N	5.86	125.77	119.85
1	B	565	LYS	C-N-CA	5.86	125.77	119.85
1	A	625	ILE	N-CA-C	-5.80	104.70	110.62
1	A	936	GLU	CB-CA-C	-5.76	109.91	116.54
1	B	680	ILE	CA-C-N	5.76	125.30	119.19
1	B	680	ILE	C-N-CA	5.76	125.30	119.19
1	B	516	GLN	CA-C-N	5.73	125.40	119.56
1	B	516	GLN	C-N-CA	5.73	125.40	119.56
1	A	565	LYS	CA-C-N	5.62	125.90	119.83
1	A	565	LYS	C-N-CA	5.62	125.90	119.83
2	F	71	LEU	CA-C-N	5.61	125.97	119.47
2	F	71	LEU	C-N-CA	5.61	125.97	119.47
1	B	38	ILE	CA-C-N	5.55	125.87	119.93
1	B	38	ILE	C-N-CA	5.55	125.87	119.93
2	C	71	LEU	CA-C-N	5.40	124.92	119.19
2	C	71	LEU	C-N-CA	5.40	124.92	119.19
1	B	842	LYS	CA-C-N	5.27	124.88	119.56
1	B	842	LYS	C-N-CA	5.27	124.88	119.56
1	A	516	GLN	CA-C-N	5.27	124.93	119.56
1	A	516	GLN	C-N-CA	5.27	124.93	119.56
1	A	541	PHE	CA-C-N	5.22	125.46	119.83
1	A	541	PHE	C-N-CA	5.22	125.46	119.83
1	B	944	GLU	N-CA-C	-5.16	105.83	111.82
1	A	222	ASN	CA-C-N	5.09	124.88	119.28
1	A	222	ASN	C-N-CA	5.09	124.88	119.28
1	A	842	LYS	CA-C-N	5.05	125.13	119.87
1	A	842	LYS	C-N-CA	5.05	125.13	119.87

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1275	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1612	ARG	Sidechain
1	A	624	ARG	Sidechain
1	A	830	ARG	Sidechain
1	B	1273	ARG	Sidechain
1	B	1275	ARG	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	11563	0	11650	181	0
1	B	11657	0	11741	191	0
2	C	1170	0	1122	12	0
2	F	1170	0	1122	4	0
3	D	1366	0	1310	19	0
3	E	1286	0	1206	8	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	5	0	0	1	0
5	B	5	0	0	4	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	28278	0	28175	337	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 (337) 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)
1:A:1609:ARG:HG3	1:B:1605:LEU:CD2	1.26	1.62
1:B:994:ASN:HA	1:B:997:PHE:CE2	1.33	1.58
1:A:1609:ARG:CG	1:B:1605:LEU:HD23	1.34	1.55
1:A:1623:GLU:CG	1:B:1622:MET:CE	2.03	1.37
1:A:1605:LEU:HD22	1:B:1605:LEU:CD1	1.51	1.36
1:B:405:ARG:HD3	1:B:936:GLU:CB	1.58	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:CG2	1:A:211:PRO:HD2	1.61	1.30
1:A:1623:GLU:HG3	1:B:1622:MET:SD	1.75	1.25
1:A:1605:LEU:CD2	1:B:1605:LEU:CD1	2.18	1.22
1:A:1623:GLU:CD	1:B:1622:MET:HE1	1.66	1.21
1:B:994:ASN:CA	1:B:997:PHE:CE2	2.25	1.19
1:A:1609:ARG:CG	1:B:1605:LEU:CD2	2.04	1.18
1:A:210:ILE:CG2	1:A:211:PRO:CD	2.24	1.15
1:A:1623:GLU:OE2	1:B:1622:MET:HE1	1.45	1.15
1:A:210:ILE:HG22	1:A:211:PRO:HD2	1.30	1.11
1:A:1609:ARG:HG2	1:B:1605:LEU:HD23	1.22	1.10
1:A:1623:GLU:HG2	1:B:1622:MET:CE	1.76	1.10
1:B:569:LEU:HD13	1:B:572:LYS:HD2	1.30	1.10
1:A:210:ILE:HG23	1:A:211:PRO:CD	1.82	1.09
1:B:1616:VAL:HG13	1:B:1620:LYS:HE3	1.36	1.08
1:A:1609:ARG:HG3	1:B:1605:LEU:HD21	1.12	1.07
1:B:405:ARG:NE	1:B:936:GLU:HG2	1.68	1.07
1:B:405:ARG:HE	1:B:936:GLU:HG2	1.08	1.07
1:A:626:VAL:HG13	1:A:649:MET:HG3	1.33	1.06
1:A:1295:LEU:HD22	1:B:1296:LEU:HD23	1.37	1.06
1:B:173:SER:HB2	1:B:671:THR:HG21	1.39	1.04
1:A:832:TRP:CZ3	3:D:88:MET:HE2	1.92	1.03
1:A:832:TRP:CH2	3:D:88:MET:HE2	1.93	1.03
1:A:1623:GLU:HG2	1:B:1622:MET:HE2	1.34	1.03
1:B:405:ARG:CD	1:B:936:GLU:HB2	1.88	1.03
1:A:1572:MET:HG2	1:A:1576:PHE:CZ	1.94	1.02
1:A:1623:GLU:CG	1:B:1622:MET:HE1	1.73	1.02
1:A:210:ILE:HG23	1:A:211:PRO:HD2	1.35	1.02
1:A:1608:GLU:HG2	1:A:1612:ARG:NH1	1.74	1.01
1:A:1608:GLU:HG2	1:A:1612:ARG:HH12	1.20	1.00
1:A:829:LEU:HD13	3:D:92:LYS:HG3	1.44	0.99
1:A:593:MET:HE2	1:A:596:MET:HE3	1.44	0.99
1:A:1605:LEU:HD22	1:B:1605:LEU:HD12	1.01	0.98
1:A:1623:GLU:CG	1:B:1622:MET:SD	2.43	0.98
1:A:1623:GLU:HG3	1:B:1622:MET:CE	1.82	0.98
1:A:1612:ARG:HD3	1:B:1608:GLU:O	1.63	0.98
1:B:405:ARG:HD3	1:B:936:GLU:HB2	0.98	0.95
1:B:1616:VAL:CG1	1:B:1620:LYS:HE3	1.94	0.95
1:A:1623:GLU:OE2	1:B:1622:MET:CE	2.14	0.94
1:A:1605:LEU:CD2	1:B:1605:LEU:HD11	1.95	0.94
1:A:1605:LEU:CB	1:B:1605:LEU:HD11	1.98	0.94
1:A:1605:LEU:HB3	1:B:1605:LEU:HD11	1.45	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1284:LYS:HB3	1:B:1285:LEU:HD11	1.47	0.93
1:B:668:LEU:O	1:B:671:THR:HG22	1.67	0.93
1:A:1608:GLU:CG	1:A:1612:ARG:HH12	1.80	0.93
1:A:210:ILE:HG22	1:A:211:PRO:CD	1.91	0.92
1:A:829:LEU:HD13	3:D:92:LYS:CG	1.98	0.92
1:A:1284:LYS:CB	1:B:1285:LEU:HD11	2.01	0.91
1:A:1572:MET:HG2	1:A:1576:PHE:CE1	2.07	0.89
1:B:405:ARG:HG2	1:B:936:GLU:OE1	1.69	0.89
1:B:994:ASN:CA	1:B:997:PHE:HE2	1.70	0.89
1:A:593:MET:CE	1:A:596:MET:HE3	2.02	0.89
1:A:1612:ARG:HG2	1:B:1612:ARG:HB2	1.55	0.87
1:B:405:ARG:HD3	1:B:936:GLU:CG	2.05	0.87
1:A:1605:LEU:CD2	1:B:1605:LEU:HD12	1.92	0.85
1:B:405:ARG:HE	1:B:936:GLU:CG	1.89	0.85
1:B:994:ASN:ND2	1:B:997:PHE:HZ	1.73	0.85
1:A:1605:LEU:HD22	1:B:1605:LEU:HD11	1.56	0.85
1:A:593:MET:CE	1:A:596:MET:CE	2.57	0.82
1:B:57:GLU:HA	1:B:72:ASN:HB2	1.61	0.82
1:A:832:TRP:CH2	3:D:88:MET:CE	2.62	0.82
1:A:593:MET:HE2	1:A:596:MET:CE	2.08	0.81
1:B:994:ASN:ND2	1:B:997:PHE:CZ	2.47	0.81
1:A:419:PHE:HE2	1:A:628:LEU:HD21	1.46	0.81
1:A:1616:VAL:HA	1:A:1619:LYS:HD3	1.62	0.81
1:B:1278:LEU:HD13	1:B:1278:LEU:C	2.05	0.80
1:A:1605:LEU:O	1:B:1605:LEU:HD21	1.81	0.80
1:B:461:ALA:HB2	5:B:2002:PO4:O1	1.82	0.80
1:A:1295:LEU:HD22	1:B:1296:LEU:CD2	2.09	0.80
1:B:405:ARG:CD	1:B:936:GLU:CG	2.60	0.80
1:A:1572:MET:CG	1:A:1576:PHE:CZ	2.66	0.79
1:B:405:ARG:CD	1:B:936:GLU:CB	2.51	0.79
1:A:210:ILE:HG23	1:A:211:PRO:HD3	1.65	0.79
1:B:1295:LEU:HD13	1:B:1295:LEU:C	2.09	0.78
1:B:1296:LEU:C	1:B:1296:LEU:HD13	2.10	0.77
1:A:832:TRP:CZ3	3:D:88:MET:CE	2.67	0.77
1:A:1605:LEU:HD23	1:B:1605:LEU:CD1	2.14	0.76
1:B:1296:LEU:HD13	1:B:1296:LEU:O	1.86	0.76
1:A:1572:MET:CG	1:A:1576:PHE:CE1	2.68	0.76
1:A:1623:GLU:CD	1:B:1622:MET:CE	2.42	0.76
1:A:431:ARG:NH2	1:A:623:ASP:OD2	2.19	0.75
1:B:72:ASN:OD1	1:B:73:LYS:N	2.19	0.75
1:B:1295:LEU:HD13	1:B:1295:LEU:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:994:ASN:HA	1:B:997:PHE:CD2	2.17	0.75
1:B:569:LEU:HD13	1:B:572:LYS:CD	2.15	0.74
1:A:829:LEU:CD1	3:D:92:LYS:HG3	2.18	0.74
1:B:1278:LEU:HD13	1:B:1278:LEU:O	1.87	0.73
1:B:405:ARG:NE	1:B:936:GLU:CG	2.46	0.73
1:B:461:ALA:CB	5:B:2002:PO4:O1	2.37	0.73
1:B:1601:LEU:O	1:B:1605:LEU:HG	1.89	0.72
1:B:173:SER:CB	1:B:671:THR:HG21	2.19	0.71
1:A:1619:LYS:HD2	1:B:1615:ALA:HA	1.73	0.71
1:A:832:TRP:CZ2	3:D:88:MET:HB3	2.26	0.70
1:A:1623:GLU:CG	1:B:1622:MET:HE2	2.00	0.70
1:A:1284:LYS:CD	1:B:1285:LEU:HD13	2.22	0.69
1:B:405:ARG:CD	1:B:936:GLU:HG2	2.22	0.68
1:A:1623:GLU:HG3	1:B:1622:MET:HE1	1.56	0.68
1:A:1608:GLU:CD	1:A:1612:ARG:HH12	2.02	0.67
1:A:1609:ARG:CD	1:B:1605:LEU:HD23	2.22	0.67
1:A:626:VAL:HG23	1:A:627:GLY:H	1.60	0.66
1:B:637:THR:O	1:B:637:THR:HG22	1.96	0.66
1:B:171:ASP:OD1	1:B:671:THR:HA	1.96	0.65
1:B:461:ALA:HA	5:B:2002:PO4:O1	1.96	0.65
1:B:461:ALA:CA	5:B:2002:PO4:O1	2.45	0.64
1:B:1616:VAL:CG1	1:B:1620:LYS:CE	2.73	0.64
1:A:401:ILE:HG23	1:A:629:ASP:OD2	1.98	0.64
1:A:623:ASP:O	1:A:624:ARG:C	2.40	0.64
1:B:173:SER:HB2	1:B:671:THR:CG2	2.24	0.63
1:B:1276:VAL:HG12	1:B:1280:GLU:OE2	1.99	0.63
1:A:1612:ARG:CG	1:B:1612:ARG:HB2	2.28	0.63
1:A:210:ILE:HG22	1:A:211:PRO:N	2.11	0.62
1:A:1612:ARG:HD3	1:B:1608:GLU:C	2.24	0.62
1:A:832:TRP:CZ2	3:D:88:MET:CB	2.82	0.62
1:B:1616:VAL:O	1:B:1620:LYS:HG3	1.99	0.61
1:B:635:THR:O	1:B:635:THR:HG22	1.98	0.61
1:A:830:ARG:HA	1:A:834:TRP:CG	2.36	0.61
1:A:211:PRO:O	1:A:212:GLY:C	2.44	0.61
1:A:540:TRP:HH2	1:A:626:VAL:HG11	1.66	0.61
1:B:222:ASN:N	1:B:223:PRO:CD	2.64	0.61
1:A:1284:LYS:HB2	1:B:1285:LEU:HD11	1.82	0.60
1:B:68:LYS:HG3	1:B:70:MET:CE	2.31	0.60
1:B:171:ASP:C	1:B:671:THR:HG1	2.09	0.60
1:B:1278:LEU:C	1:B:1278:LEU:CD1	2.74	0.60
1:A:1306:PHE:CE1	1:B:1310:ALA:HB1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1623:GLU:HG2	1:B:1622:MET:SD	2.30	0.59
1:A:1572:MET:SD	1:A:1576:PHE:CZ	2.95	0.59
1:B:1641:ASP:OD2	1:B:1645:LYS:NZ	2.36	0.59
1:A:1306:PHE:CZ	1:B:1310:ALA:HB1	2.38	0.59
1:B:944:GLU:O	1:B:948:MET:HG3	2.03	0.59
3:E:81:ASN:ND2	3:E:83:THR:OG1	2.35	0.59
1:A:268:LYS:NZ	1:A:597:ASP:OD2	2.36	0.58
1:A:539:CYS:SG	1:A:596:MET:HG3	2.44	0.58
1:A:626:VAL:HG23	1:A:627:GLY:N	2.18	0.58
1:B:569:LEU:CD1	1:B:572:LYS:HD2	2.21	0.58
1:B:964:GLY:O	1:B:968:LYS:N	2.37	0.58
1:A:1284:LYS:HD2	1:B:1285:LEU:HD13	1.84	0.58
1:B:465:ILE:HG12	1:B:584:VAL:HG22	1.85	0.57
1:B:71:VAL:HG11	1:B:74:ASP:HB2	1.86	0.57
1:A:1284:LYS:HD3	1:B:1285:LEU:HD13	1.86	0.57
2:F:26:LYS:NZ	2:F:66:ASP:OD1	2.34	0.57
1:B:69:ALA:O	1:B:70:MET:HE2	2.04	0.57
1:A:1676:LYS:NZ	1:B:1677:GLU:OE1	2.37	0.57
1:B:1289:LEU:HA	1:B:1292:VAL:HG12	1.86	0.57
1:B:1295:LEU:C	1:B:1295:LEU:CD1	2.77	0.57
1:A:593:MET:HE1	1:A:596:MET:CE	2.34	0.57
1:A:997:PHE:O	1:A:1001:LYS:N	2.38	0.57
1:B:446:ARG:O	1:B:446:ARG:HG2	2.05	0.57
1:A:103:HIS:HA	1:A:106:LYS:HE2	1.86	0.57
1:B:993:GLN:O	1:B:997:PHE:CD2	2.58	0.56
1:B:62:LEU:HD12	1:B:65:ASN:ND2	2.22	0.56
1:B:516:GLN:N	1:B:517:PRO:CD	2.69	0.55
1:A:622:VAL:O	1:A:623:ASP:OD1	2.24	0.55
1:B:994:ASN:C	1:B:997:PHE:CE2	2.83	0.55
1:A:1284:LYS:CB	1:B:1285:LEU:CD1	2.79	0.55
1:B:62:LEU:HD12	1:B:65:ASN:HD22	1.72	0.55
1:A:516:GLN:N	1:A:517:PRO:CD	2.69	0.55
1:A:1605:LEU:CG	1:B:1605:LEU:HD11	2.37	0.55
1:A:565:LYS:N	1:A:566:PRO:CD	2.70	0.55
1:B:1484:LYS:NZ	2:C:3:ASP:OD2	2.39	0.55
1:A:592:LEU:HB3	1:A:596:MET:HE2	1.88	0.54
1:B:993:GLN:O	1:B:997:PHE:HD2	1.90	0.54
1:B:226:GLU:O	1:B:230:ASN:N	2.40	0.54
1:B:1296:LEU:C	1:B:1296:LEU:CD1	2.78	0.54
1:B:524:ARG:O	1:B:530:GLY:N	2.38	0.54
1:A:479:THR:OG1	1:A:657:TYR:OH	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:TRP:CG	1:A:507:ASN:N	2.75	0.53
1:A:1572:MET:SD	1:B:1569:MET:CE	2.97	0.53
1:A:593:MET:HE1	1:A:596:MET:HE3	1.90	0.53
1:B:68:LYS:HE3	1:B:70:MET:HE1	1.89	0.53
1:A:626:VAL:CG1	1:A:649:MET:HG3	2.22	0.53
1:B:405:ARG:HG2	1:B:936:GLU:CD	2.33	0.53
1:A:842:LYS:N	1:A:843:PRO:HD2	2.23	0.53
1:B:42:ARG:HH22	1:B:64:GLU:CD	2.18	0.52
1:B:173:SER:CB	1:B:671:THR:CG2	2.86	0.51
1:A:217:GLN:N	1:A:217:GLN:OE1	2.41	0.51
1:A:249:ASN:OD1	1:A:258:GLY:N	2.43	0.51
1:A:593:MET:CE	1:A:596:MET:HE1	2.40	0.51
1:A:1562:LYS:NZ	1:A:1566:GLU:OE2	2.43	0.51
1:A:1572:MET:SD	1:A:1576:PHE:HZ	2.33	0.51
1:A:1609:ARG:CD	1:B:1605:LEU:CD2	2.83	0.51
1:B:128:TYR:OH	1:B:682:ASN:O	2.23	0.50
1:A:529:PRO:O	1:A:557:GLN:NE2	2.44	0.50
2:C:68:GLU:OE1	3:D:4:LYS:NZ	2.44	0.50
1:A:540:TRP:CH2	1:A:626:VAL:HG11	2.46	0.50
1:A:543:LYS:H	1:A:632:THR:HG23	1.77	0.50
1:A:1670:GLU:OE1	1:B:1676:LYS:NZ	2.41	0.50
1:B:994:ASN:CG	1:B:997:PHE:CZ	2.89	0.50
1:B:68:LYS:HG3	1:B:70:MET:HE1	1.94	0.50
1:B:994:ASN:O	1:B:997:PHE:CE2	2.65	0.50
1:B:250:PHE:O	1:B:452:ALA:N	2.45	0.50
1:B:1375:ASP:OD2	1:B:1379:LYS:NZ	2.45	0.49
1:B:275:ALA:O	1:B:312:ASN:ND2	2.46	0.49
1:A:231:ALA:HA	1:A:279:ARG:CZ	2.43	0.49
1:A:450:GLN:N	1:A:450:GLN:CD	2.71	0.49
1:A:539:CYS:HB3	1:A:596:MET:SD	2.53	0.49
1:A:832:TRP:CH2	3:D:88:MET:SD	3.05	0.49
3:E:124:GLU:O	3:E:128:THR:OG1	2.29	0.49
1:A:419:PHE:CE2	1:A:628:LEU:HD21	2.37	0.49
2:C:71:LEU:HB3	2:C:72:PRO:HD3	1.95	0.49
3:D:161:ILE:O	3:D:165:GLY:N	2.46	0.48
1:A:173:SER:O	1:A:674:ASN:N	2.46	0.48
1:A:1331:LYS:NZ	1:B:1327:GLU:OE1	2.46	0.48
1:B:61:GLU:HB3	1:B:66:GLY:HA2	1.95	0.48
2:F:71:LEU:HB2	2:F:72:PRO:HD3	1.95	0.48
1:A:1609:ARG:CG	1:B:1605:LEU:HD21	2.05	0.48
1:B:1513:MET:O	1:B:1517:MET:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LEU:HD12	1:B:65:ASN:HB2	1.95	0.48
1:B:962:GLU:C	1:B:964:GLY:H	2.21	0.48
1:A:322:ASP:N	1:A:322:ASP:OD1	2.44	0.48
1:A:808:LYS:NZ	1:A:1577:GLU:OE1	2.46	0.48
1:B:997:PHE:CE1	1:B:998:ILE:HG13	2.49	0.48
1:A:1375:ASP:OD2	1:A:1379:LYS:NZ	2.47	0.47
1:B:565:LYS:N	1:B:566:PRO:HD2	2.28	0.47
1:B:210:ILE:N	1:B:211:PRO:HD2	2.29	0.47
1:A:1284:LYS:HB2	1:B:1285:LEU:CD1	2.44	0.47
1:A:832:TRP:HH2	3:D:88:MET:SD	2.37	0.47
1:A:1477:GLU:OE2	1:A:1481:LYS:NZ	2.45	0.47
1:A:1605:LEU:HD23	1:B:1605:LEU:HD13	1.94	0.47
1:A:1608:GLU:CG	1:A:1612:ARG:NH1	2.53	0.47
1:B:221:ALA:C	1:B:223:PRO:HD2	2.39	0.47
1:B:634:MET:HB2	1:B:637:THR:HA	1.96	0.47
1:A:761:TYR:CZ	1:A:774:VAL:HG13	2.50	0.47
1:B:362:LYS:NZ	1:B:364:GLU:OE2	2.48	0.47
3:D:13:ARG:HB3	3:D:14:PRO:HD2	1.97	0.47
1:A:1518:SER:O	1:A:1522:ASP:N	2.48	0.46
1:B:540:TRP:CG	1:B:540:TRP:O	2.68	0.46
1:B:842:LYS:N	1:B:843:PRO:HD2	2.30	0.46
3:E:70:ASP:O	3:E:74:ASN:N	2.48	0.46
1:A:832:TRP:CZ2	3:D:88:MET:HB2	2.49	0.46
2:C:66:ASP:OD1	2:C:66:ASP:C	2.59	0.46
1:B:65:ASN:HD22	1:B:68:LYS:HE2	1.80	0.46
1:A:710:ILE:O	1:A:714:GLY:N	2.48	0.46
1:A:222:ASN:HB3	1:A:223:PRO:CD	2.46	0.46
1:A:829:LEU:HD13	3:D:92:LYS:HG2	1.92	0.46
1:B:1455:GLN:OE1	1:B:1455:GLN:N	2.45	0.46
1:A:515:LEU:C	1:A:517:PRO:HD2	2.41	0.46
1:B:691:ASP:OD1	1:B:691:ASP:C	2.59	0.46
1:B:1529:GLU:O	1:B:1530:LEU:C	2.58	0.46
1:A:528:PRO:HA	1:A:529:PRO:HD3	1.83	0.46
2:F:97:ASP:OD1	2:F:100:GLY:N	2.49	0.46
1:A:1605:LEU:CA	1:B:1605:LEU:HD11	2.46	0.45
1:B:1562:LYS:NZ	1:B:1566:GLU:OE2	2.47	0.45
1:A:830:ARG:HA	1:A:834:TRP:CD1	2.51	0.45
2:C:54:ASN:N	2:C:55:PRO:CD	2.79	0.45
1:A:524:ARG:O	1:A:530:GLY:N	2.46	0.45
1:A:210:ILE:CG2	1:A:211:PRO:N	2.70	0.45
1:A:931:VAL:O	1:A:935:GLU:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:148:ASP:C	3:D:148:ASP:OD1	2.58	0.45
1:A:1612:ARG:O	1:A:1616:VAL:HG13	2.17	0.45
1:B:994:ASN:HA	1:B:997:PHE:HE2	0.76	0.45
1:A:401:ILE:HG12	1:A:629:ASP:OD1	2.17	0.44
1:A:1573:LYS:NZ	1:A:1577:GLU:OE2	2.50	0.44
1:B:276:LYS:NZ	1:B:277:ASP:OD1	2.50	0.44
1:B:994:ASN:ND2	1:B:997:PHE:CE2	2.85	0.44
1:A:1415:TYR:OH	1:B:1415:TYR:N	2.51	0.44
1:B:842:LYS:HB2	1:B:843:PRO:HD3	1.99	0.44
1:A:179:GLU:OE2	1:A:235:LYS:NZ	2.51	0.44
1:A:761:TYR:HA	1:A:770:PHE:CD1	2.53	0.44
1:B:515:LEU:C	1:B:517:PRO:HD2	2.43	0.44
1:A:855:GLN:OE1	1:A:855:GLN:N	2.46	0.44
1:A:960:ASP:O	1:B:1674:GLN:NE2	2.50	0.44
1:A:184:LYS:NZ	5:A:2002:PO4:O2	2.51	0.44
1:B:565:LYS:HB2	1:B:566:PRO:HD3	1.99	0.44
1:A:232:LYS:NZ	1:A:237:ASP:OD1	2.50	0.44
1:B:171:ASP:C	1:B:671:THR:OG1	2.61	0.44
1:B:405:ARG:CG	1:B:936:GLU:OE1	2.54	0.44
1:A:768:ILE:CG2	1:A:770:PHE:CE1	3.00	0.43
3:D:13:ARG:HB3	3:D:14:PRO:CD	2.48	0.43
1:A:506:TRP:CG	1:A:507:ASN:H	2.35	0.43
1:A:691:ASP:OD1	1:A:691:ASP:C	2.61	0.43
1:B:232:LYS:NZ	1:B:237:ASP:OD1	2.43	0.43
1:A:593:MET:HE1	1:A:596:MET:HE1	2.00	0.43
1:A:597:ASP:N	1:A:598:PRO:CD	2.81	0.43
1:A:987:ILE:O	1:A:991:GLU:N	2.52	0.43
2:C:54:ASN:N	2:C:55:PRO:HD3	2.34	0.43
2:C:71:LEU:HB3	2:C:72:PRO:CD	2.49	0.43
1:A:203:LYS:HE2	1:A:208:HIS:CE1	2.54	0.43
1:A:626:VAL:HB	1:A:630:GLN:HB2	1.99	0.43
1:A:250:PHE:O	1:A:452:ALA:N	2.52	0.43
1:B:226:GLU:O	1:B:230:ASN:CB	2.67	0.43
3:E:103:ARG:O	3:E:106:PHE:HB3	2.19	0.43
1:A:892:LEU:O	1:A:896:LEU:N	2.50	0.42
1:A:1613:ALA:O	1:A:1616:VAL:HG22	2.19	0.42
1:A:1302:LYS:NZ	1:B:1300:GLU:HG3	2.34	0.42
1:A:565:LYS:N	1:A:566:PRO:HD3	2.33	0.42
1:A:1575:GLN:O	1:A:1579:ASP:N	2.47	0.42
1:A:624:ARG:HD3	1:A:651:ARG:HB2	2.01	0.42
1:B:222:ASN:N	1:B:223:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:GLY:N	1:B:236:ASN:HD21	2.17	0.42
2:F:42:ASN:N	2:F:43:PRO:CD	2.82	0.42
1:A:1276:VAL:O	1:A:1280:GLU:HG3	2.20	0.42
1:A:565:LYS:NZ	1:A:570:LYS:O	2.53	0.41
1:B:1281:LYS:HD2	1:B:1281:LYS:HA	1.80	0.41
1:B:634:MET:HG3	1:B:639:PHE:HB3	2.01	0.41
2:C:71:LEU:N	2:C:72:PRO:HD2	2.35	0.41
3:D:160:ARG:O	3:D:164:HIS:CD2	2.72	0.41
1:A:624:ARG:CD	1:A:651:ARG:HB2	2.51	0.41
1:B:834:TRP:CH2	3:E:92:LYS:HB3	2.55	0.41
1:A:1522:ASP:O	1:A:1526:ASN:N	2.54	0.41
1:B:255:TYR:N	1:B:255:TYR:CD1	2.88	0.41
1:B:475:CYS:HA	1:B:478:TYR:CE2	2.55	0.41
1:B:945:LYS:O	1:B:948:MET:HB2	2.21	0.41
1:A:401:ILE:HD13	1:A:410:LYS:HD2	2.03	0.41
1:B:565:LYS:HB2	1:B:566:PRO:CD	2.50	0.41
1:B:940:ILE:O	1:B:944:GLU:HG3	2.20	0.41
1:B:1531:GLU:O	1:B:1535:ARG:HB2	2.19	0.41
3:E:116:THR:HA	3:E:153:PHE:O	2.20	0.41
1:B:69:ALA:C	1:B:70:MET:HE2	2.46	0.41
2:C:22:THR:OG1	2:C:24:ASP:OD1	2.38	0.41
2:C:134:ASP:OD1	2:C:134:ASP:C	2.63	0.41
1:A:1282:ALA:O	1:A:1286:GLN:N	2.46	0.41
1:B:60:VAL:O	1:B:70:MET:HG3	2.21	0.41
1:B:400:ARG:HG3	1:B:407:TYR:HB3	2.02	0.41
1:B:568:GLN:NE2	1:B:585:ASP:OD1	2.54	0.41
1:B:652:THR:OG1	1:B:655:GLN:HG3	2.21	0.41
1:B:680:ILE:CG2	1:B:682:ASN:O	2.69	0.41
2:C:58:ASP:OD1	2:C:58:ASP:N	2.53	0.41
1:A:1619:LYS:HD2	1:B:1618:SER:HB2	2.03	0.40
1:B:1286:GLN:HA	1:B:1289:LEU:HD12	2.03	0.40
1:B:1289:LEU:O	1:B:1292:VAL:CG1	2.69	0.40
3:E:113:ALA:C	3:E:115:GLY:H	2.28	0.40
3:E:161:ILE:O	3:E:165:GLY:N	2.53	0.40
1:A:997:PHE:CD1	1:B:996:LYS:HB3	2.56	0.40
1:B:405:ARG:CG	1:B:936:GLU:HB2	2.49	0.40
1:A:626:VAL:CG2	1:A:627:GLY:H	2.31	0.40
1:A:829:LEU:HB2	1:A:833:GLN:HE22	1.86	0.40
1:B:1481:LYS:NZ	2:C:3:ASP:OD1	2.55	0.40
1:A:151:PRO:HA	1:A:152:PRO:HD3	1.89	0.40
1:A:307:TYR:HB2	1:A:310:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:HIS:HA	1:A:835:TRP:NE1	2.36	0.40
1:B:251:ASP:N	1:B:255:TYR:O	2.43	0.40
1:B:446:ARG:O	1:B:446:ARG:CG	2.69	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	1410/1976 (71%)	1393 (99%)	14 (1%)	3 (0%)	43	77
1	B	1422/1976 (72%)	1404 (99%)	17 (1%)	1 (0%)	48	82
2	C	147/151 (97%)	147 (100%)	0	0	100	100
2	F	147/151 (97%)	147 (100%)	0	0	100	100
3	D	167/171 (98%)	166 (99%)	1 (1%)	0	100	100
3	E	157/171 (92%)	154 (98%)	3 (2%)	0	100	100
All	All	3450/4596 (75%)	3411 (99%)	35 (1%)	4 (0%)	49	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	GLY
1	A	624	ARG
1	B	636	GLU
1	A	210	ILE

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1251/1733 (72%)	1250 (100%)	1 (0%)	88	88
1	B	1260/1733 (73%)	1256 (100%)	4 (0%)	86	84
2	C	127/129 (98%)	127 (100%)	0	100	100
2	F	127/129 (98%)	127 (100%)	0	100	100
3	D	147/149 (99%)	147 (100%)	0	100	100
3	E	138/149 (93%)	138 (100%)	0	100	100
All	All	3050/4022 (76%)	3045 (100%)	5 (0%)	85	86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	631	VAL
1	B	945	LYS
1	B	1278	LEU
1	B	1295	LEU
1	B	1296	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	208	HIS
1	A	286	GLN
1	A	340	HIS
1	A	485	GLN
1	A	777	HIS
1	A	812	GLN
1	A	831	HIS
1	A	938	ASN
1	A	1316	GLN
1	A	1351	GLN
1	A	1438	HIS
1	A	1450	GLN
1	A	1691	GLN
1	B	65	ASN
1	B	202	HIS

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Mol	Chain	Res	Type
1	B	208	HIS
1	B	409	GLN
1	B	450	GLN
1	B	485	GLN
1	B	489	HIS
1	B	970	GLN
1	B	994	ASN
1	B	1351	GLN
1	B	1691	GLN
2	C	17	GLN
3	E	31	GLN
2	F	54	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 6 ligands modelled in this entry, 2 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	$\# Z > 2$
4	ADP	A	2001	6	28,29,29	1.00	0	43,45,45	1.79	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	B	2001	6	28,29,29	1.04	0	43,45,45	1.82	9 (20%)
5	PO4	B	2002	6	4,4,4	1.68	1 (25%)	6,6,6	0.89	0
5	PO4	A	2002	6	4,4,4	1.81	1 (25%)	6,6,6	1.15	1 (16%)

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
4	ADP	A	2001	6	-	3/16/32/32	0/3/3/3
4	ADP	B	2001	6	-	5/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2002	PO4	P-O1	3.19	1.58	1.50
5	B	2002	PO4	P-O1	2.79	1.57	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	ADP	C5-C4-N3	-5.55	119.08	126.72
4	B	2001	ADP	C5-C4-N3	-5.51	119.12	126.72
4	B	2001	ADP	N3-C4-N9	4.69	135.14	127.17
4	A	2001	ADP	N3-C4-N9	4.63	135.05	127.17
4	A	2001	ADP	N3-C2-N1	-4.35	121.99	128.58
4	B	2001	ADP	N3-C2-N1	-4.26	122.14	128.58
4	B	2001	ADP	C5-N7-C8	3.71	109.28	103.45
4	A	2001	ADP	C2-N3-C4	3.70	120.88	111.83
4	A	2001	ADP	C5-N7-C8	3.70	109.26	103.45
4	B	2001	ADP	C2-N3-C4	3.64	120.72	111.83
4	B	2001	ADP	C4-C5-N7	-2.99	107.17	110.58
4	A	2001	ADP	C4-C5-N7	-2.92	107.24	110.58
4	A	2001	ADP	N9-C8-N7	-2.35	110.61	113.94
4	B	2001	ADP	N9-C8-N7	-2.31	110.66	113.94
5	A	2002	PO4	O2-P-O1	-2.26	102.94	110.95
4	B	2001	ADP	O3B-PB-O3A	2.14	111.80	104.64
4	B	2001	ADP	O2B-PB-O3A	2.07	111.59	104.64
4	A	2001	ADP	C3'-C2'-C1'	2.06	105.36	101.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

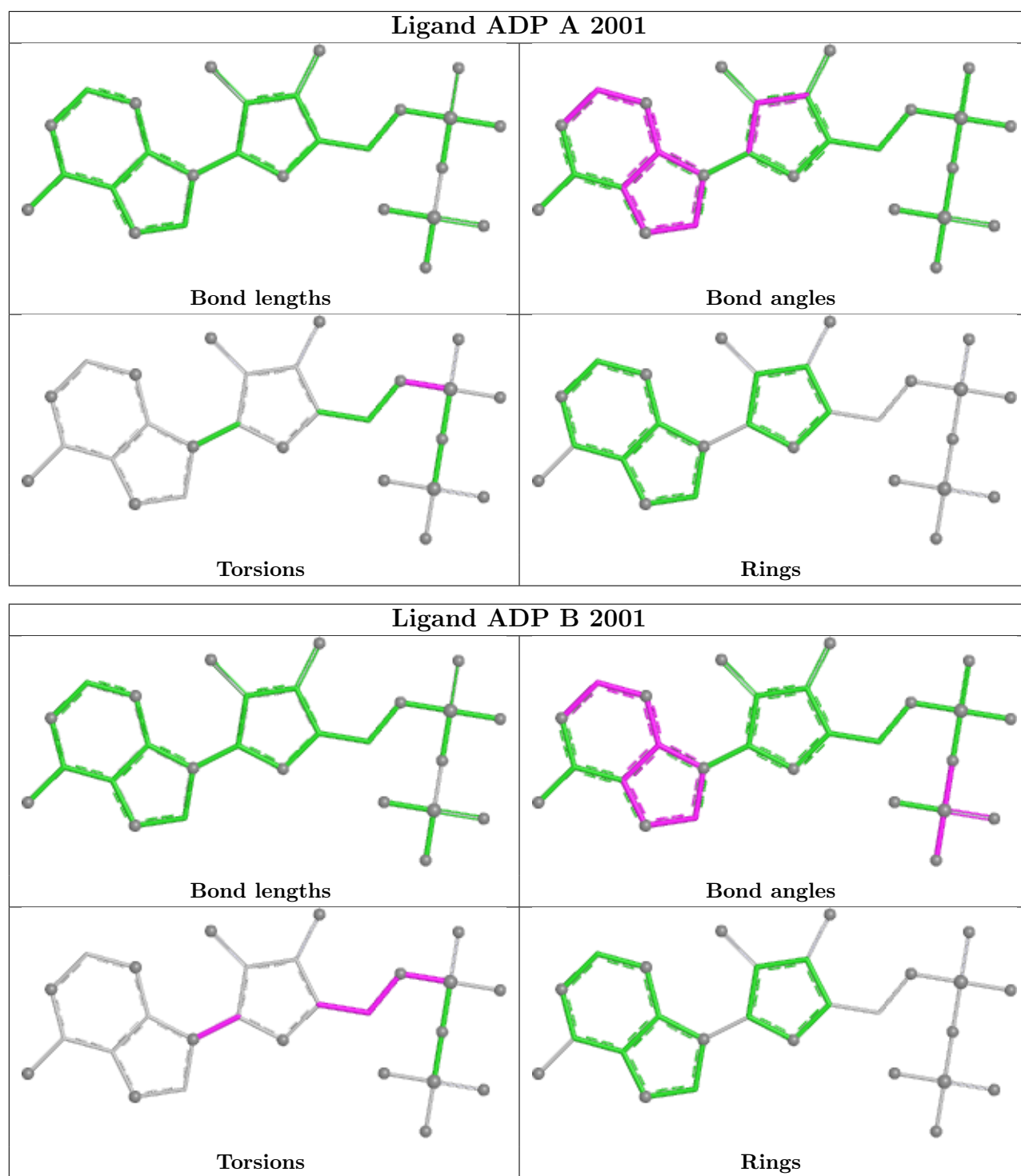
Mol	Chain	Res	Type	Atoms
4	A	2001	ADP	C5'-O5'-PA-O2A
4	A	2001	ADP	C5'-O5'-PA-O3A
4	B	2001	ADP	C5'-O5'-PA-O1A
4	B	2001	ADP	O4'-C4'-C5'-O5'
4	B	2001	ADP	C3'-C4'-C5'-O5'
4	A	2001	ADP	C5'-O5'-PA-O1A
4	B	2001	ADP	C2'-C1'-N9-C8
4	B	2001	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2002	PO4	4	0
5	A	2002	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73796. These allow visual inspection of the internal detail of the map and identification of artifacts.

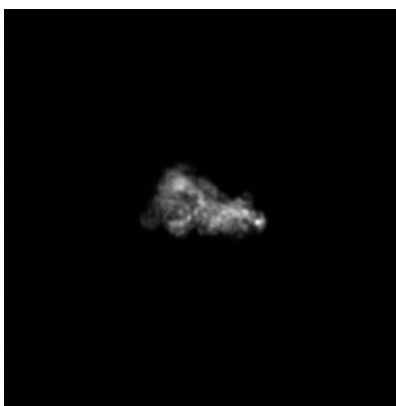
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

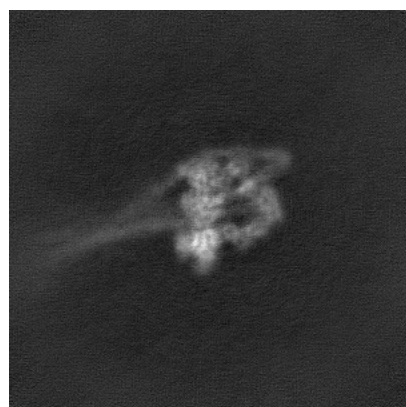


Y

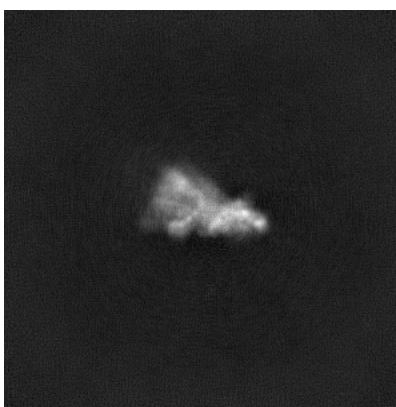


Z

6.1.2 Raw map



X



Y

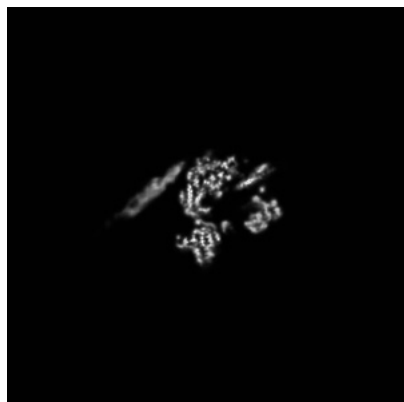


Z

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

6.2 Central slices [i](#)

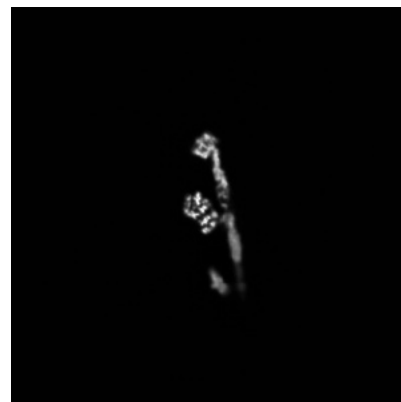
6.2.1 Primary map



X Index: 256

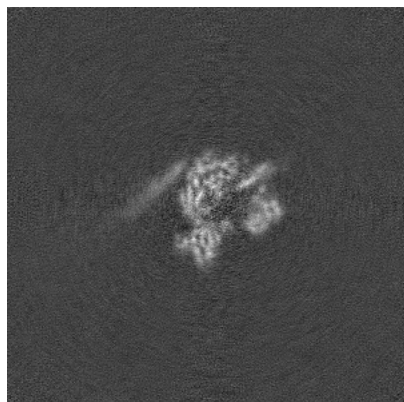


Y Index: 256

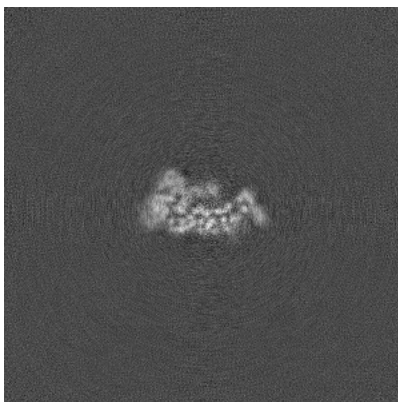


Z Index: 256

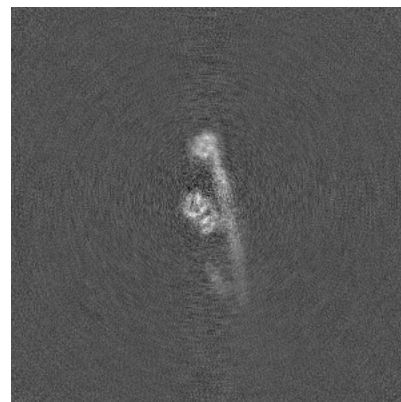
6.2.2 Raw map



X Index: 256



Y Index: 256

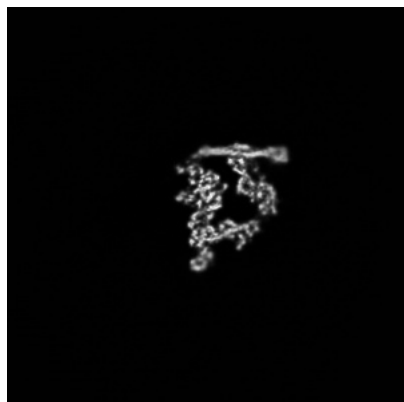


Z Index: 256

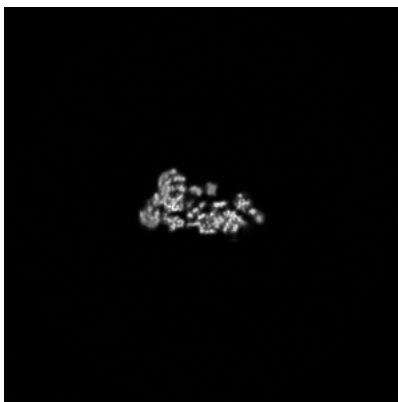
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

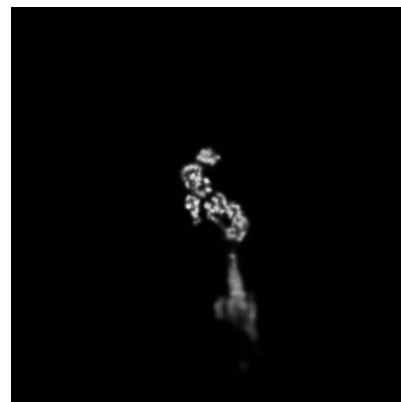
6.3.1 Primary map



X Index: 239

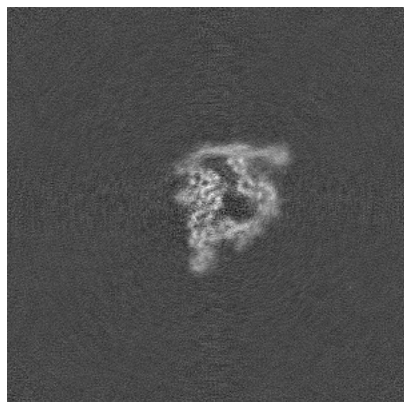


Y Index: 249

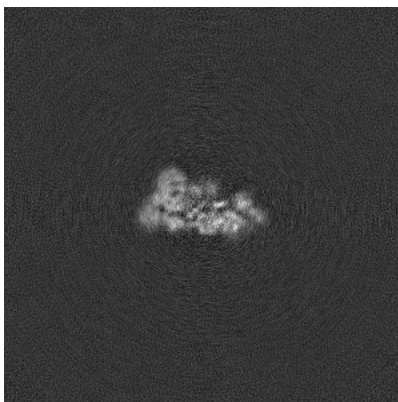


Z Index: 227

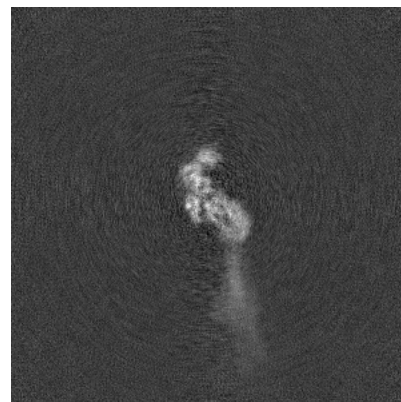
6.3.2 Raw map



X Index: 240



Y Index: 249

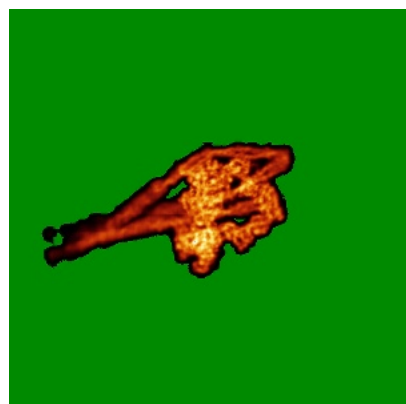


Z Index: 226

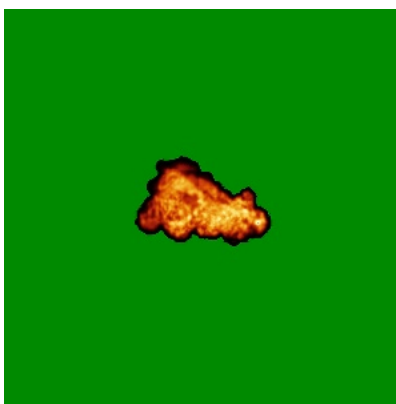
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

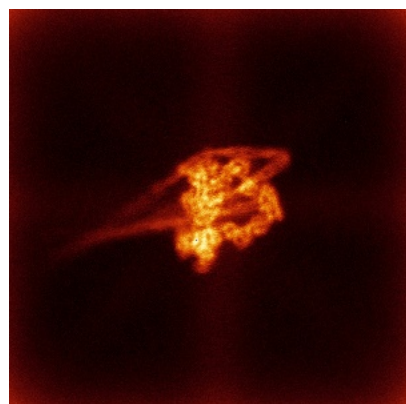


Y

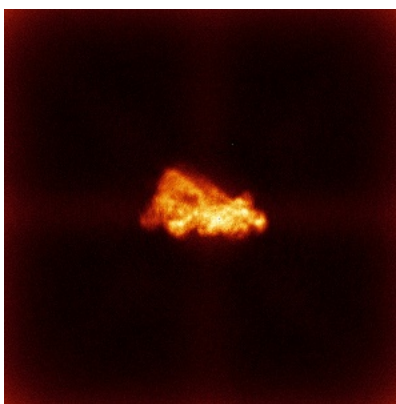


Z

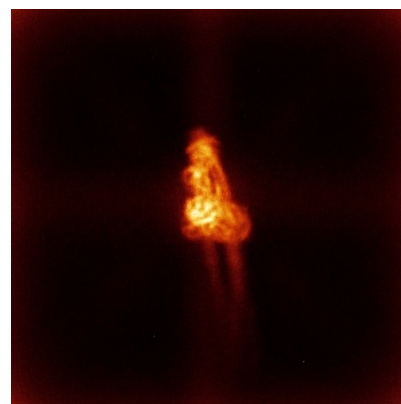
6.4.2 Raw map



X



Y

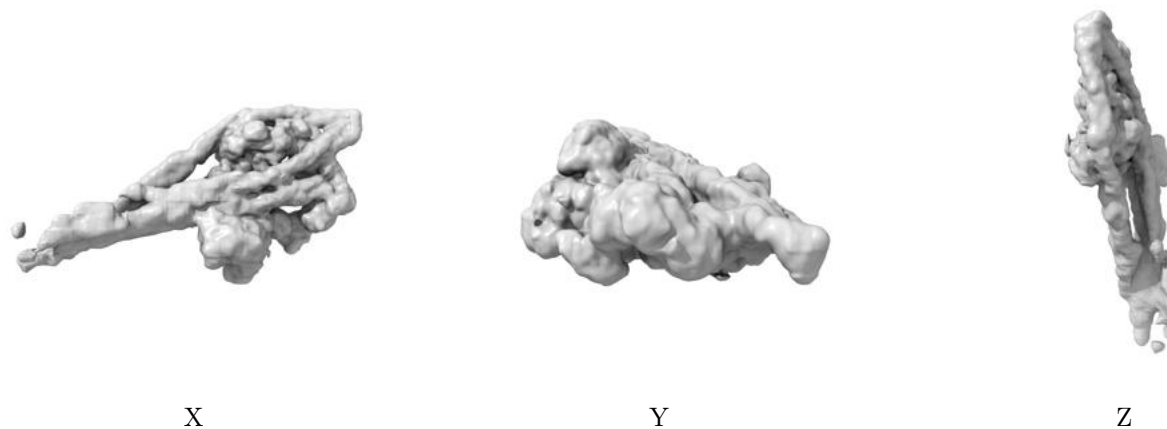


Z

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.

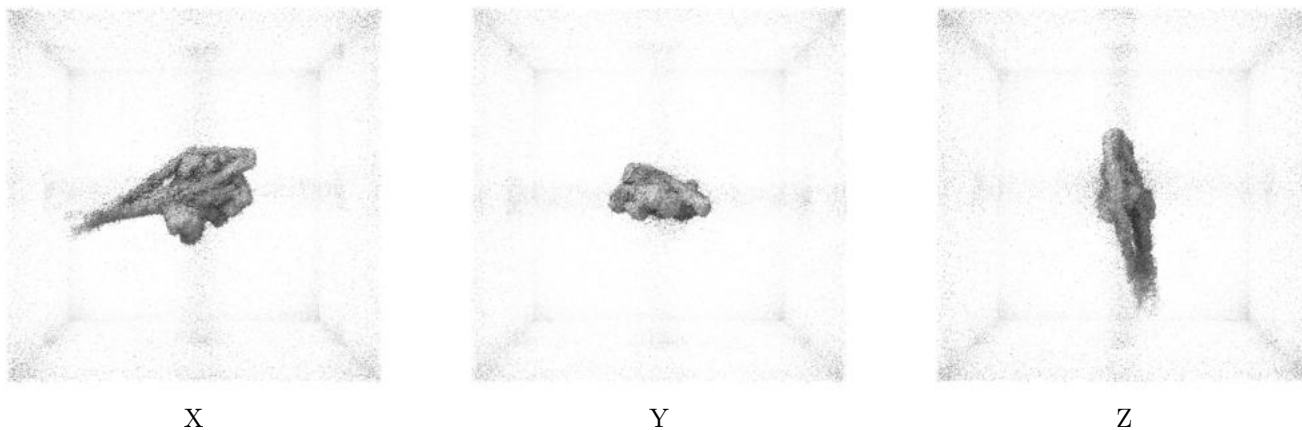
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.214. 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



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.

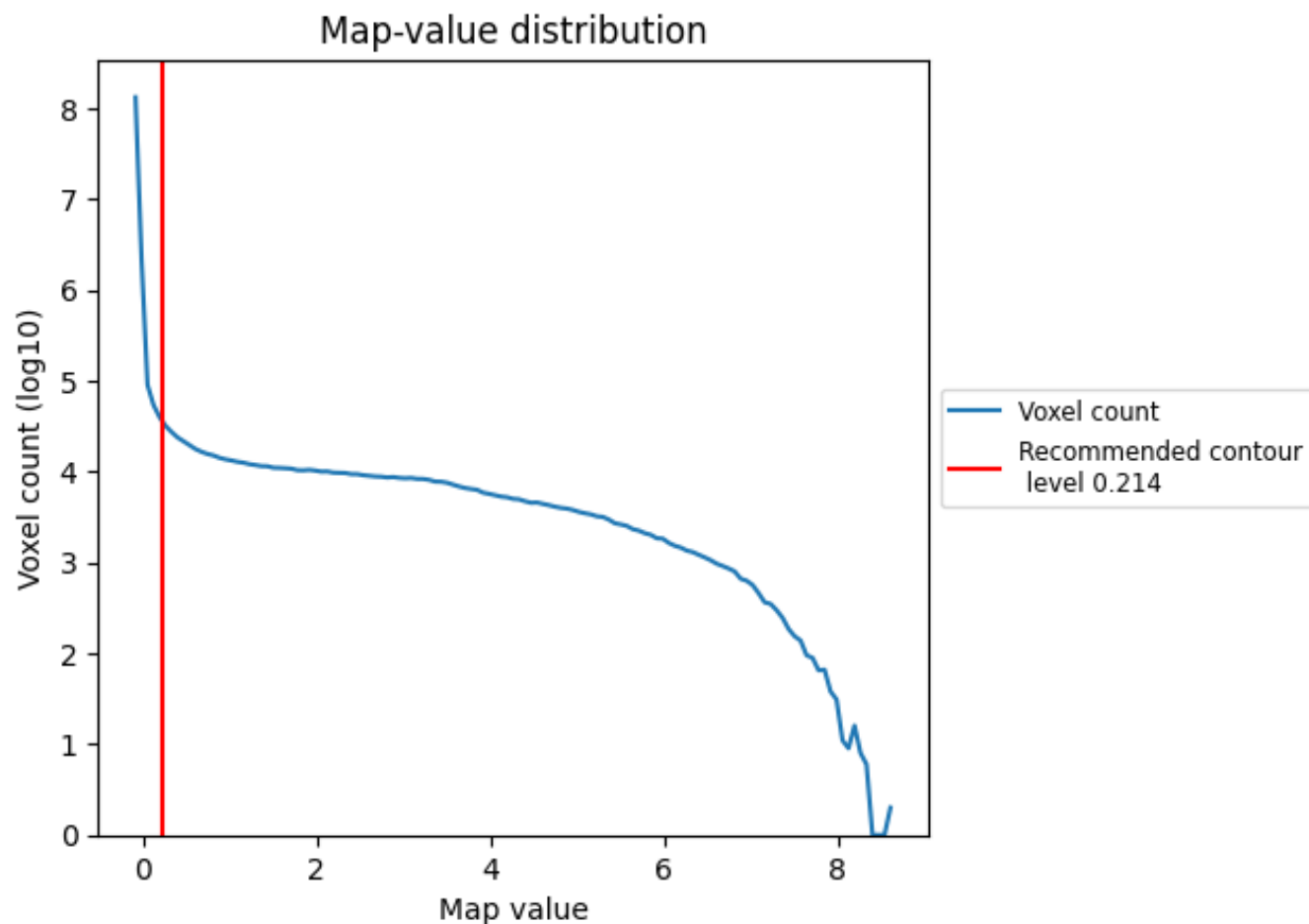
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

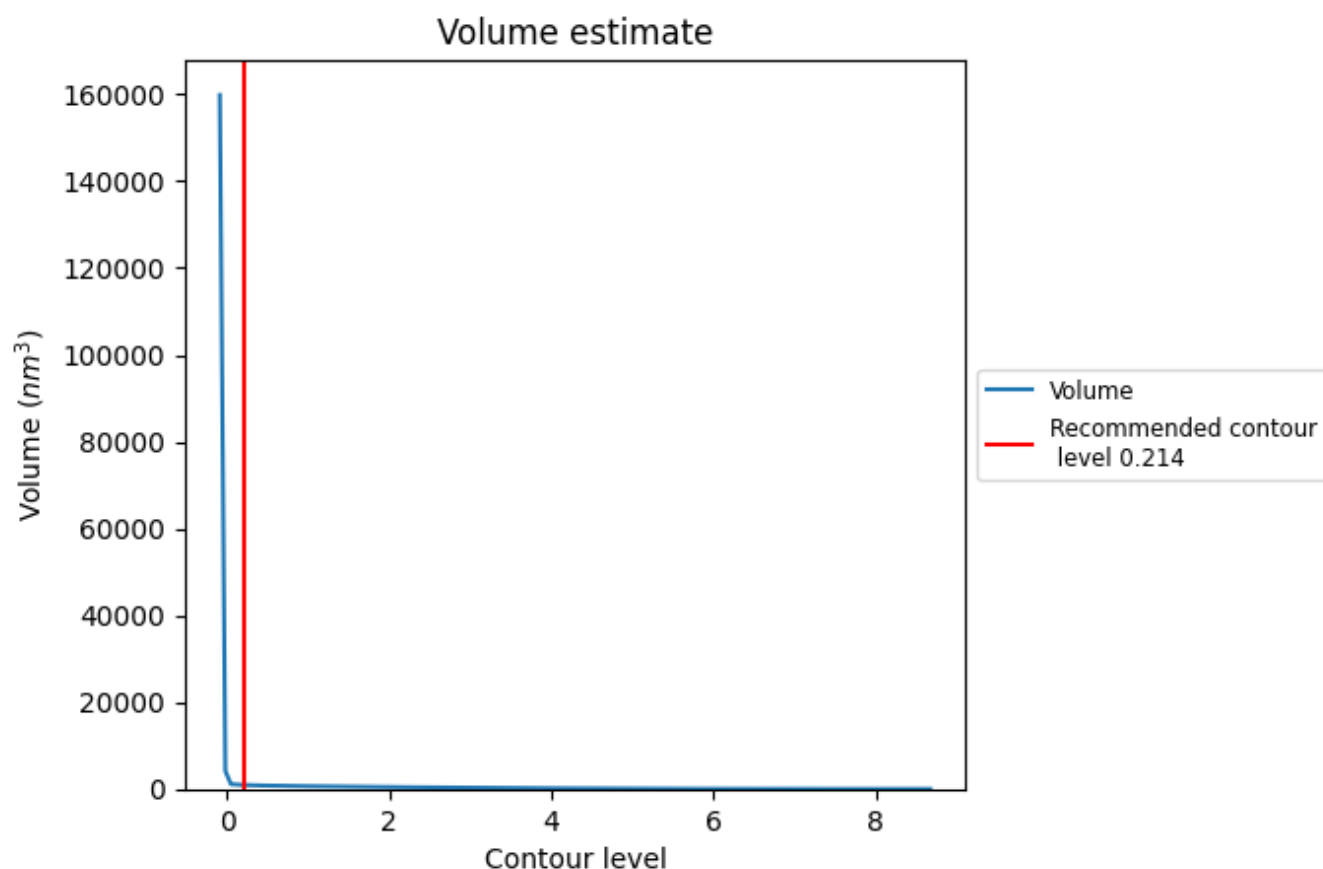
This section contains the results of statistical analysis of the map.

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.

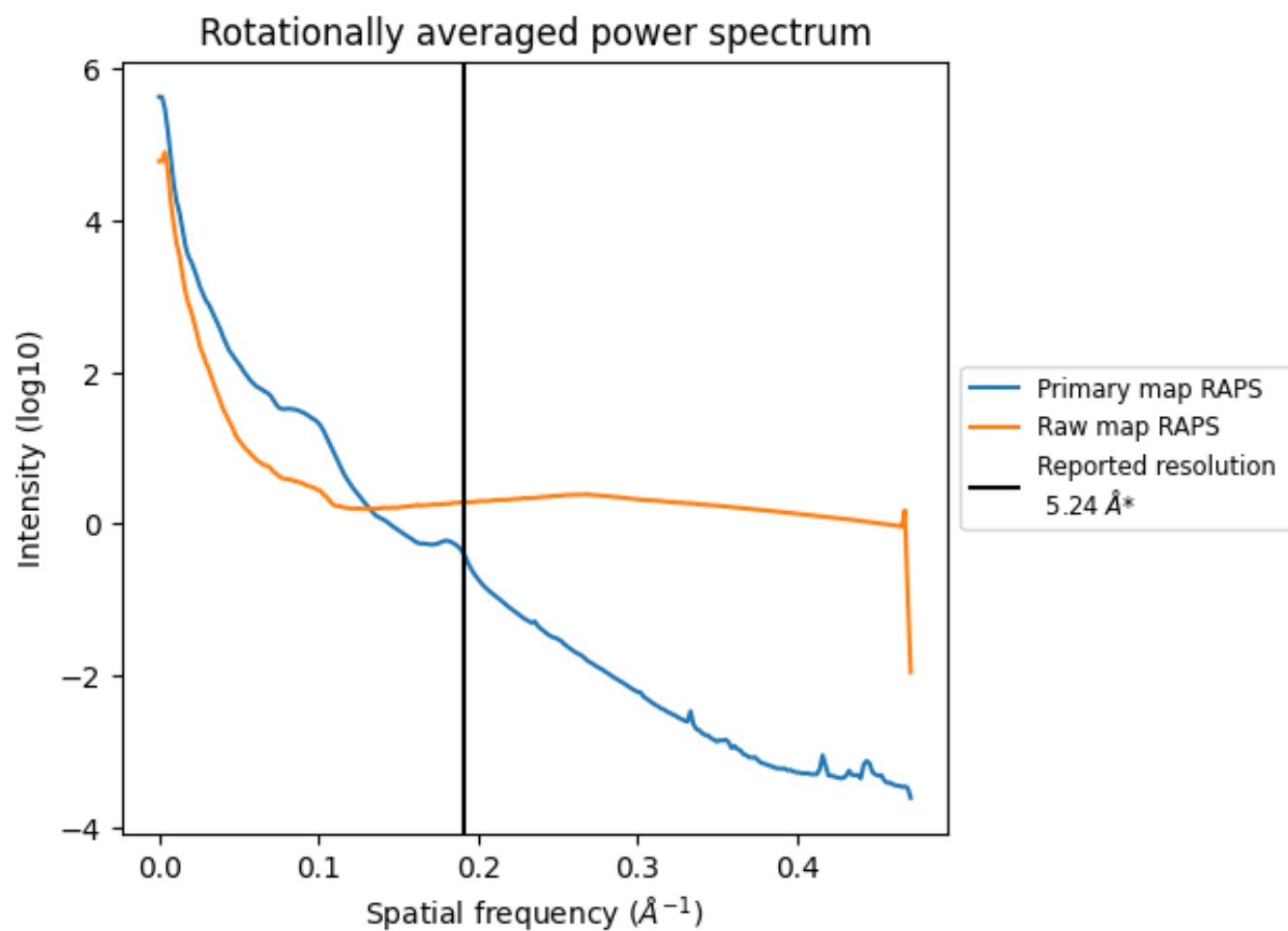
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 923 nm^3 ; this corresponds to an approximate mass of 834 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 ⓘ

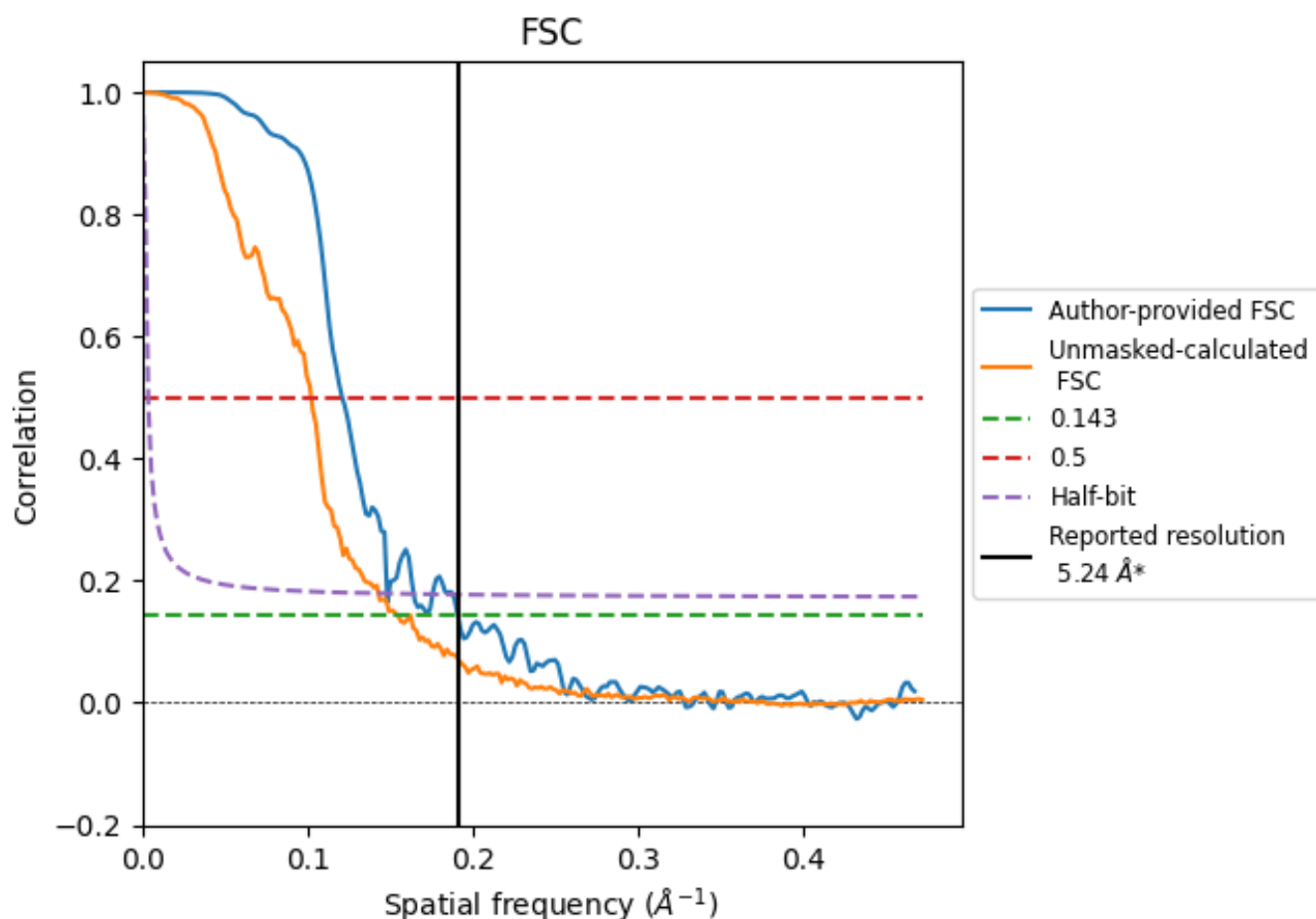


*Reported resolution corresponds to spatial frequency of 0.191 $\text{\AA}^{-1}$

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 0.191 Å⁻¹

8.2 Resolution estimates [i](#)

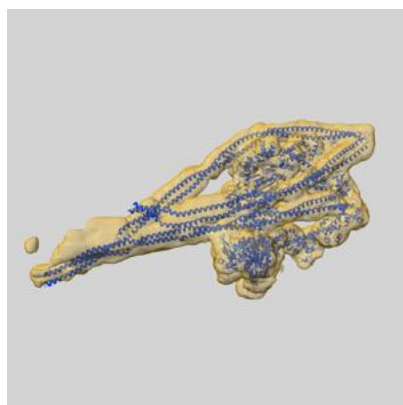
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.24	-	-
Author-provided FSC curve	5.24	8.26	6.75
Unmasked-calculated*	6.47	9.78	7.00

*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 6.47 differs from the reported value 5.24 by more than 10 %

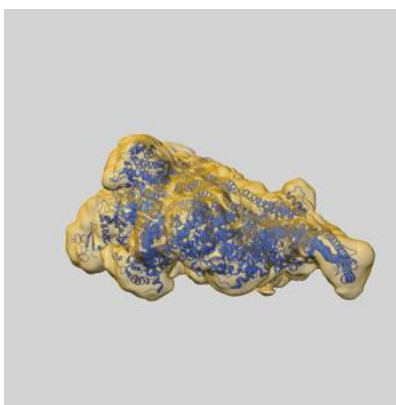
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73796 and PDB model 9Z3Z. Per-residue inclusion information can be found in section [3](#) on page [7](#).

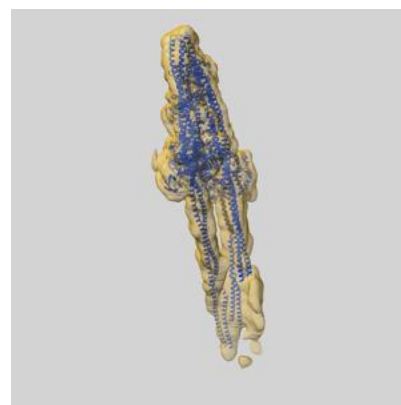
9.1 Map-model overlay [i](#)



X



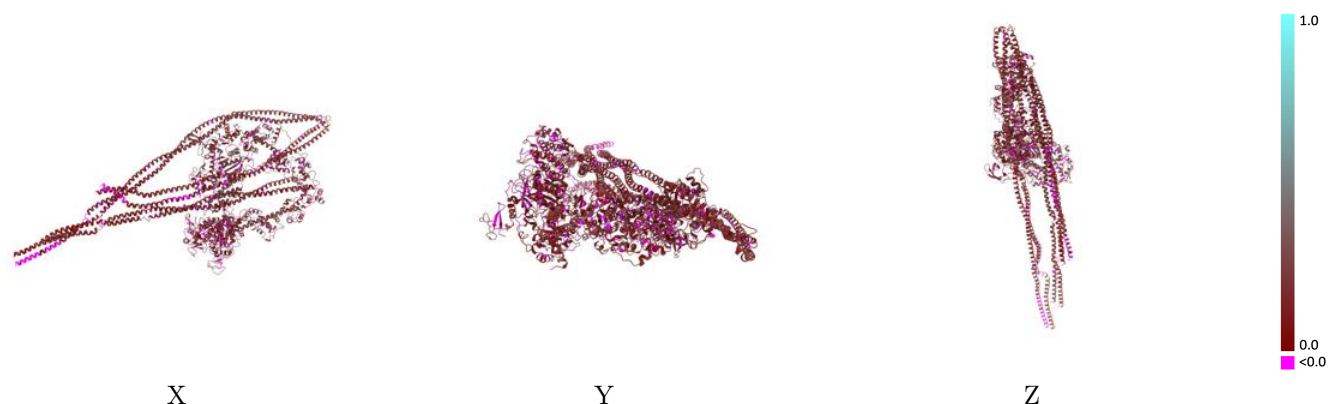
Y



Z

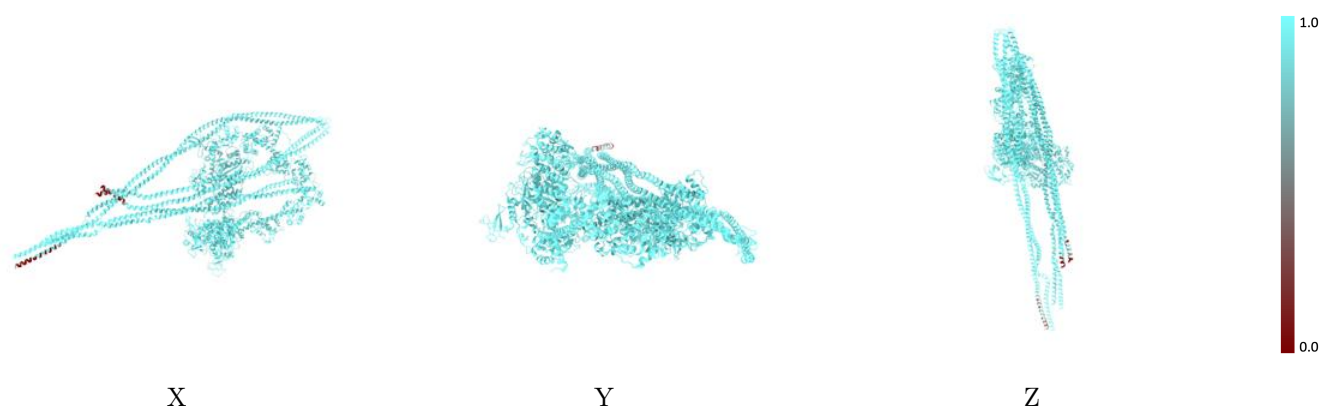
The images above show the 3D surface view of the map at the recommended contour level 0.214 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



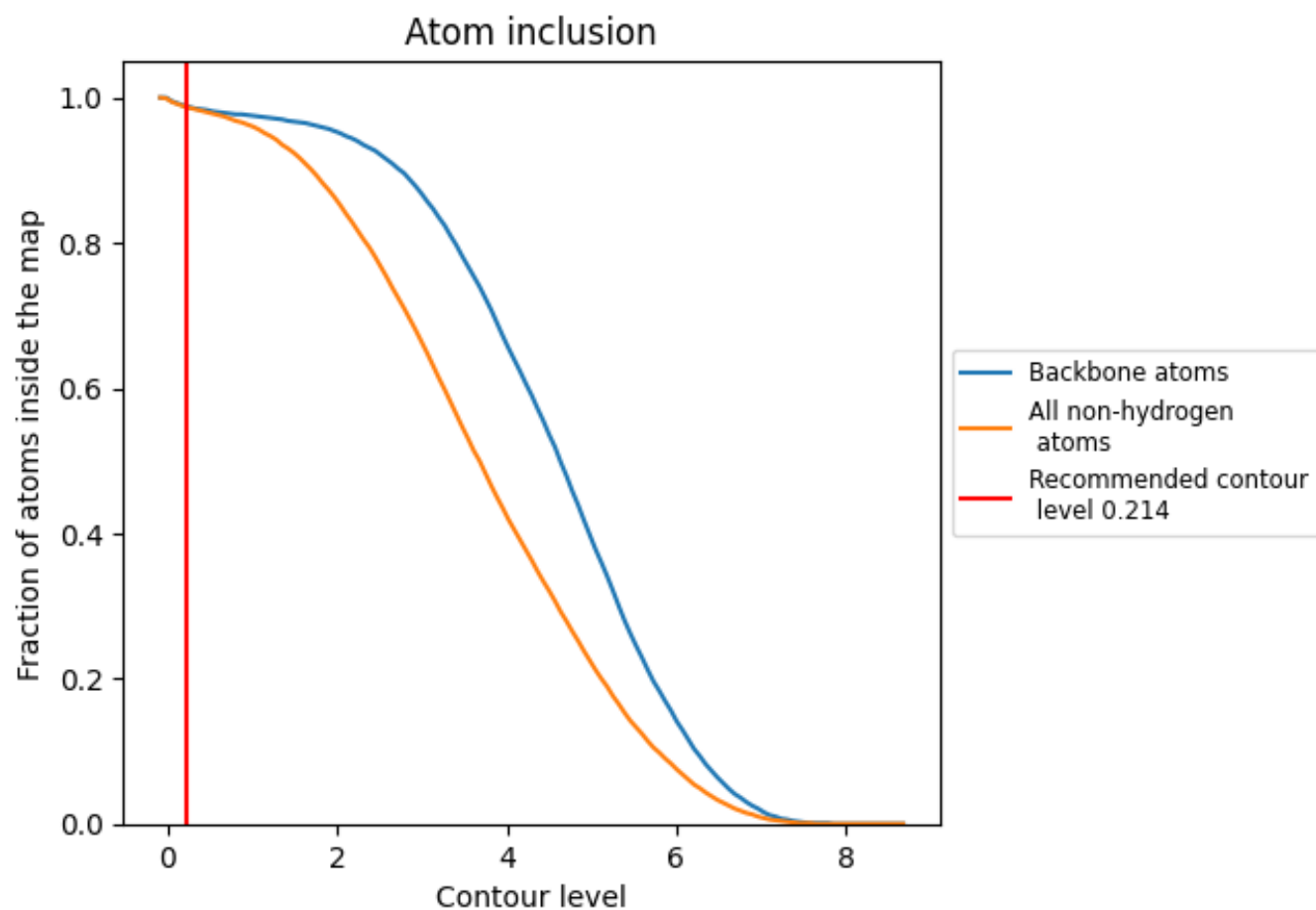
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.214).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.214) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9870	0.1500
A	0.9930	0.1580
B	0.9760	0.1360
C	1.0000	0.1830
D	0.9990	0.1680
E	0.9990	0.1470
F	0.9990	0.1560

1.0

0.0

<0.0