



## Full wwPDB EM Validation Report ⓘ

Aug 4, 2025 – 10:43 AM EDT

PDB ID : 9BI5 / pdb\_00009bi5  
EMDB ID : EMD-44559  
Title : Apo form Mre11-Rad50 complex  
Authors : Yu, Y.; Patel, D.J.  
Deposited on : 2024-04-22  
Resolution : 3.50 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](mailto: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.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

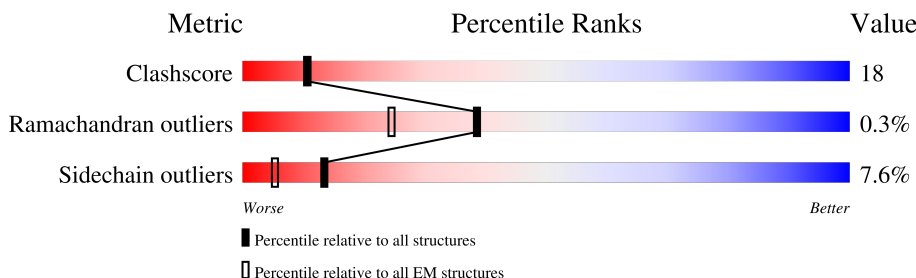
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	C	1312	
1	D	1312	
2	A	706	
2	B	706	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12413 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA repair protein RAD50.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	408	Total	C	N	O	S	0	0
			3217	2032	556	614	15		
1	C	334	Total	C	N	O	S	0	0
			2631	1661	459	499	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1235	GLN	GLU	engineered mutation	UNP P12753
C	1235	GLN	GLU	engineered mutation	UNP P12753

- Molecule 2 is a protein called Double-strand break repair protein MRE11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	411	Total	C	N	O	S	0	0
			3237	2048	553	618	18		
2	B	412	Total	C	N	O	S	0	0
			3262	2066	555	622	19		

There are 28 discrepancies between the modelled and reference sequences:

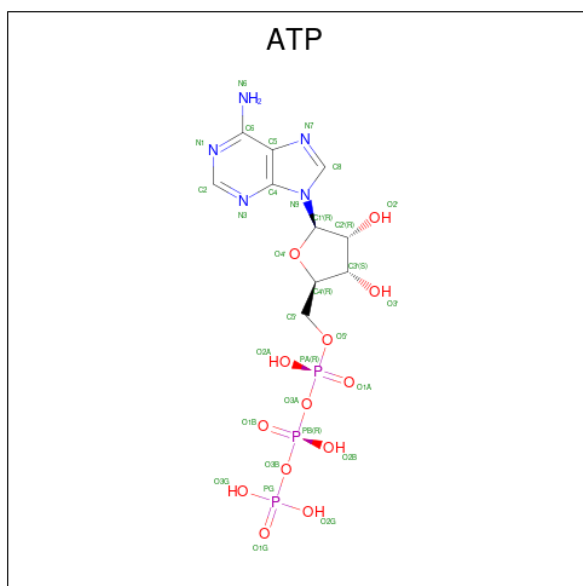
Chain	Residue	Modelled	Actual	Comment	Reference
A	693	TYR	-	expression tag	UNP P32829
A	694	ASP	-	expression tag	UNP P32829
A	695	TYR	-	expression tag	UNP P32829
A	696	LYS	-	expression tag	UNP P32829
A	697	ASP	-	expression tag	UNP P32829
A	698	ASP	-	expression tag	UNP P32829
A	699	ASP	-	expression tag	UNP P32829
A	700	ASP	-	expression tag	UNP P32829
A	701	LYS	-	expression tag	UNP P32829
A	702	HIS	-	expression tag	UNP P32829
A	703	HIS	-	expression tag	UNP P32829

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	704	HIS	-	expression tag	UNP P32829
A	705	HIS	-	expression tag	UNP P32829
A	706	HIS	-	expression tag	UNP P32829
B	693	TYR	-	expression tag	UNP P32829
B	694	ASP	-	expression tag	UNP P32829
B	695	TYR	-	expression tag	UNP P32829
B	696	LYS	-	expression tag	UNP P32829
B	697	ASP	-	expression tag	UNP P32829
B	698	ASP	-	expression tag	UNP P32829
B	699	ASP	-	expression tag	UNP P32829
B	700	ASP	-	expression tag	UNP P32829
B	701	LYS	-	expression tag	UNP P32829
B	702	HIS	-	expression tag	UNP P32829
B	703	HIS	-	expression tag	UNP P32829
B	704	HIS	-	expression tag	UNP P32829
B	705	HIS	-	expression tag	UNP P32829
B	706	HIS	-	expression tag	UNP P32829

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).

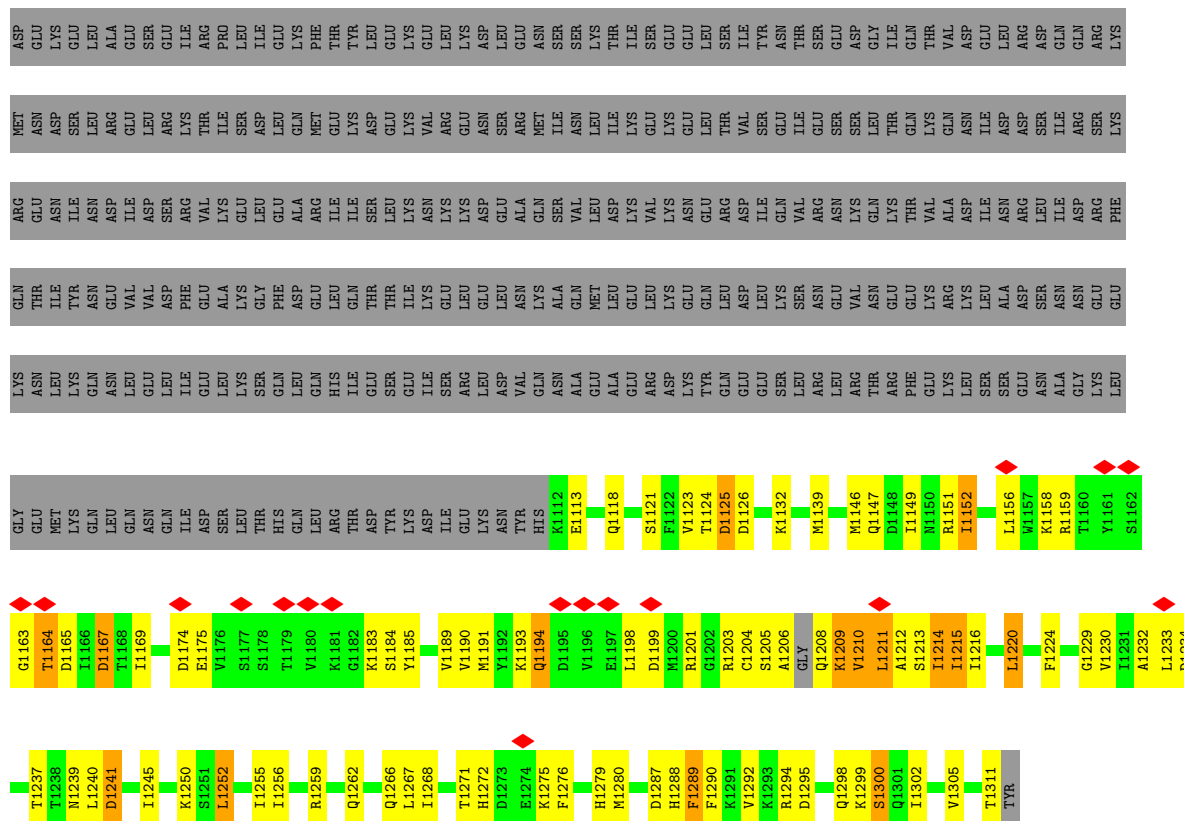


Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

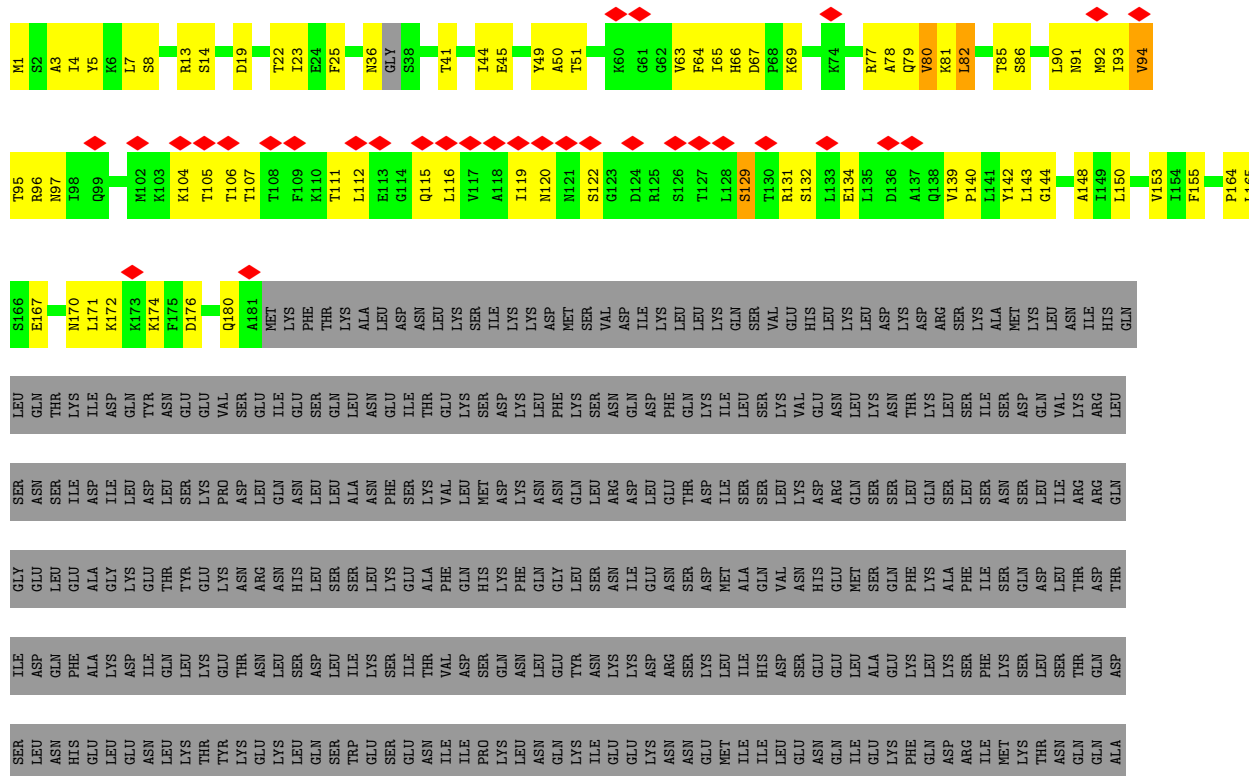
- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total 2	Mn 2	0
4	B	2	Total 2	Mn 2	0





### • Molecule 1: DNA repair protein RAD50





L174	L175	G176	L177	A178	A179	V180	R181	D182	E183	R184	L185	F189	V194	T195	F196	M201	R202	E205	W206	F207	M208	L209	M210	H213	Q214	T220	N221	T222	L225	P226	E227	G228	F229	L234	V237	L238	W239	E242	M248	M252	V259	L260	Q261	L174	L175	G176	L177	A178	A179	V180	R181	D182	E183	R184	L185	F189	V194	T195	F196	M201	R202	E205	W206	F207	M208	L209	M210	H213	Q214	T220	N221	T222	L225	P226	E227	G228	F229	L234	V237	L238	W239	E242	M248	M252	V259	L260	Q261	E688	L89	L90	S91	D92	Q95	V96	F97	H98	V99	D100	E101	F102	D109	P110	N111	F112	N113	I114	S115	I116	P117	V118	F119	G120	G123	D126	S129	G135	P136	T143	G144	N147	H148	F149	G150	K151	V152	K157	I158	K159	V160	V161	P162	L163	L164	F165	Q166	K167	T170	E688	L89	L90	S91	D92	Q95	V96	F97	H98	V99	D100	E101	F102	D109	P110	N111	F112	N113	I114	S115	I116	P117	V118	F119	G120	G123	D126	S129	G135	P136	T143	G144	N147	H148	F149	G150	K151	V152	K157	I158	K159	V160	V161	P162	L163	L164	F165	Q166	K167	T170	E688	L89	L90	S91	D92	Q95	V96	F97	H98	V99	D100	E101	F102	D109	P110	N111	F112	N113	I114	S115	I116	P117	V118	F119	G120	G123	D126	S129	G135	P136	T143	G144	N147	H148	F149	G150	K151	V152	K157	I158	K159	V160	V161	P162	L163	L164	F165	Q166	K167	T170	E688	L89	L90	S91	D92	Q95	V96	F97	H98	V99	D100	E101	F102	D109	P110	N111	F112	N113	I114	S115	I116	P117	V118	F119	G120	G123	D126	S129	G135	P136	T143	G144	N147	H148	F149	G150	K151	V152	K157	I158	K159	V160	V161	P162	L163	L164	F165	Q166	K167	T170	E688	L89	L90	S91	D92	Q95	V96	F97	H98	V99	D100	E101	F102	D109	P110	N111	F112	N113	I114	S115	I116	P117	V118	F119	G120	G123	D126	S129	G135	P136	T143	G144	N147	H148	F149	G150	K151	V152	K157	I158	K159	V160	V161	P162	L163	L164	F165	Q166	K167	T170	E688	L89	L90	S91	D92	Q95	V96	F97	H98	V99	D100	E101	F102	D109	P110	N111	F112	N113	I114	S115	I116	P117	V118	F119	G120	G123	D126	S129	G135	P136	T143	G144	N147	H148	F149	G150	K151	V152	K157	I158	K159	V160	V161	P162	L163	L164	F165	Q166	K167	T170	E688	L89	L90	S91	D92	Q95	V96	F97	H98	V99	D100	E101	F102	D109	P110	N111	F112	N113	I114	S115	I116	P117	V118	F119	G120	G123	D126	S129	G135	P136	T143	G144	N147	H148	F149	G150	K151	V152	K157	I158	K159	V160	V161	P162	L163	L164	F165	Q166	K167	T170	E688	L89	L90	S91	D92	Q95	V96	F97	H98	V99	D100	E101	F102	D109	P110	N111	F112	N113	I114	S115	I116	P117	V118	F119	G120	G123	D126	S129	G135	P136	T143	G144	N147	H148	F149	G150	K151	V152	K157	I158	K159	V160	V161	P162	L163	L164	F165	Q166	K167	T170	E688	L89	L90	S91	D92	Q95	V96	F97	H98	V99	D100	E101	F102	D109	P110	N111	F112	N113	I114	S115	I116	P117	V118	F119	G120	G123	D126	S129	G135	P136	T14
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	232521	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 ( $e^-/\text{\AA}^2$ )	51.22	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.547	Depositor
Minimum map value	-1.463	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.25	Depositor
Map size ( $\text{\AA}$ )	303.24, 303.24, 303.24	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.083, 1.083, 1.083	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: ATP, MN

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	C	0.22	0/2669	0.48	0/3596
1	D	0.22	0/3263	0.52	2/4393 (0.0%)
2	A	0.25	0/3316	0.43	0/4508
2	B	0.22	0/3342	0.41	0/4541
All	All	0.23	0/12590	0.46	2/17038 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1204	CYS	N-CA-C	7.39	119.28	108.86
1	D	64	PHE	N-CA-C	-6.75	105.67	114.04

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2631	0	2639	110	0
1	D	3217	0	3260	162	0
2	A	3237	0	3108	126	0
2	B	3262	0	3149	86	0
3	D	62	0	24	13	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	12413	0	12180	452	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 18.

All (452) 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)
2:A:412:ARG:HB3	2:A:412:ARG:HH11	1.13	1.12
1:D:115:GLN:HE21	1:D:127:THR:CG2	1.64	1.09
2:B:119:PHE:HB3	2:B:149:PHE:HE2	1.17	1.05
1:D:44:ILE:HD11	1:D:1268:ILE:HD13	1.38	1.03
2:B:119:PHE:HB3	2:B:149:PHE:CE2	1.96	1.00
1:D:165:LEU:HD11	1:D:1212:ALA:HB3	1.41	0.98
1:D:25:PHE:HD1	1:D:30:THR:HG21	1.25	0.98
1:D:115:GLN:HE21	1:D:127:THR:HG22	1.27	0.97
1:D:44:ILE:HD11	1:D:1268:ILE:CD1	1.95	0.95
1:D:1212:ALA:HA	1:D:1215:ILE:HG23	1.51	0.92
1:D:25:PHE:CD1	1:D:30:THR:HG21	2.05	0.91
2:A:412:ARG:HB3	2:A:412:ARG:NH1	1.88	0.87
1:C:50:ALA:HA	1:C:96:ARG:HE	1.41	0.85
1:C:80:VAL:O	1:C:95:THR:HA	1.76	0.85
2:B:119:PHE:CB	2:B:149:PHE:HE2	1.89	0.84
1:C:139:VAL:O	1:C:143:LEU:HB2	1.79	0.82
1:C:144:GLY:HA3	1:C:1227:ASN:HB3	1.61	0.82
1:D:115:GLN:NE2	1:D:127:THR:CG2	2.42	0.81
1:D:115:GLN:NE2	1:D:127:THR:HG22	1.96	0.81
1:D:1146:MET:O	1:D:1149:ILE:HG12	1.80	0.80
1:D:1289:PHE:CE2	1:D:1305:VAL:HG13	2.16	0.80
2:A:96:VAL:HG13	2:A:161:VAL:HG23	1.65	0.78
1:C:105:THR:HG22	1:C:105:THR:O	1.82	0.78
1:D:115:GLN:CG	1:D:127:THR:HG22	2.14	0.77
2:A:158:ILE:HB	2:A:194:VAL:HG12	1.69	0.74
1:D:45:GLU:HG3	1:D:56:PRO:HG2	1.70	0.73
1:C:165:LEU:HG	1:C:1189:VAL:HG11	1.71	0.73
2:B:210:MET:HB3	2:B:237:VAL:HG12	1.70	0.73
1:D:150:LEU:HA	1:D:154:ILE:HB	1.71	0.72
2:A:364:LEU:HD22	2:A:401:ASN:HB3	1.71	0.72
1:D:16:ASP:CG	1:D:1299:LYS:HD3	2.15	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ILE:CD1	1:D:1268:ILE:HD13	2.19	0.71
1:D:117:VAL:HG21	1:D:125:ARG:HG3	1.71	0.70
2:B:213:HIS:HD2	2:B:241:HIS:HB2	1.56	0.70
1:D:115:GLN:HE21	1:D:127:THR:HG23	1.55	0.70
1:D:168:PRO:HA	1:D:172:LYS:HB3	1.72	0.69
1:C:1297:ARG:HG3	1:C:1299:LYS:HG2	1.75	0.69
1:D:1165:ASP:O	2:A:387:ASN:ND2	2.25	0.69
1:C:165:LEU:HD13	1:C:1209:LYS:HG3	1.75	0.69
2:A:119:PHE:HB3	2:A:147:ASN:HB2	1.75	0.69
1:D:131:ARG:HB3	1:D:134:GLU:HB3	1.75	0.68
1:C:120:ASN:ND2	1:C:122:SER:OG	2.26	0.68
2:A:227:GLU:OE1	2:A:252:ASN:ND2	2.26	0.68
3:D:1402:ATP:O1B	1:C:36:ASN:C	2.37	0.68
2:A:345:LYS:HG3	2:A:360:LEU:HD11	1.74	0.68
1:C:1222:GLU:OE1	1:C:1259:ARG:NH1	2.27	0.68
2:B:51:VAL:O	2:B:118:VAL:HA	1.94	0.68
2:A:42:LEU:O	2:A:46:ASN:ND2	2.27	0.67
2:A:86:GLU:C	2:A:167:LYS:HD3	2.19	0.67
1:C:7:LEU:HA	1:C:82:LEU:HA	1.76	0.67
2:A:49:ASP:OD2	2:A:167:LYS:HE2	1.94	0.67
1:D:168:PRO:HD3	1:D:1201:ARG:HD3	1.75	0.66
1:C:1241:ASP:O	1:C:1245:ILE:N	2.29	0.66
2:A:27:ILE:HG23	2:A:28:THR:HG22	1.78	0.66
2:B:4:PRO:HG3	2:B:10:ARG:HE	1.60	0.66
1:D:11:GLY:O	1:D:66:HIS:N	2.29	0.65
2:A:87:LEU:HD23	2:A:167:LYS:HG3	1.78	0.65
1:D:30:THR:HG23	1:D:30:THR:O	1.96	0.65
2:A:41:MET:O	2:A:45:ASN:ND2	2.29	0.65
2:A:49:ASP:OD2	2:A:167:LYS:NZ	2.30	0.65
2:A:109:ASP:OD2	2:B:76:ARG:NH2	2.29	0.65
1:D:1208:GLN:N	3:D:1402:ATP:HO3'	1.95	0.65
1:D:1298:GLN:NE2	1:C:1165:ASP:O	2.29	0.65
2:A:36:PHE:HE2	2:A:71:VAL:HG13	1.60	0.65
2:B:106:ASN:OD1	2:B:147:ASN:ND2	2.30	0.64
2:A:362:LYS:HB2	2:A:400:ALA:HB2	1.80	0.64
1:D:44:ILE:CD1	1:D:1268:ILE:HG21	2.28	0.64
1:C:93:ILE:HG13	1:C:119:ILE:HD11	1.79	0.64
2:A:214:GLN:O	2:A:239:TRP:NE1	2.29	0.63
3:D:1401:ATP:N7	1:C:1203:ARG:CB	2.62	0.63
1:D:179:PHE:O	1:D:181:ALA:N	2.31	0.63
2:A:79:CYS:HA	2:A:116:ILE:HG12	1.81	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:159:LYS:NZ	2:A:160:VAL:O	2.31	0.62
2:A:95:GLN:O	2:A:98:HIS:ND1	2.31	0.62
2:B:367:LEU:HB2	2:B:406:VAL:HG12	1.81	0.62
2:A:111:ASN:HB2	2:B:80:MET:HE2	1.80	0.62
1:D:1212:ALA:HA	1:D:1215:ILE:CG2	2.29	0.62
1:D:1289:PHE:CE2	1:D:1305:VAL:CG1	2.82	0.61
2:A:336:MET:HE1	2:A:367:LEU:HB2	1.82	0.61
1:C:1271:THR:HG22	1:C:1273:ASP:H	1.65	0.61
1:D:25:PHE:CE1	1:D:1268:ILE:HD11	2.36	0.61
1:C:139:VAL:O	1:C:143:LEU:CB	2.48	0.61
1:D:1229:GLY:O	1:D:1266:GLN:N	2.28	0.60
2:B:118:VAL:O	2:B:118:VAL:HG22	2.01	0.60
2:A:368:ARG:HA	2:A:407:GLN:HB3	1.84	0.60
1:D:155:PHE:HD1	1:D:1232:ALA:HB2	1.66	0.60
2:A:61:ASN:HA	2:A:126:ASP:HA	1.84	0.60
2:B:61:ASN:HA	2:B:126:ASP:HA	1.84	0.60
1:D:1193:LYS:O	1:C:69:LYS:NZ	2.34	0.60
2:A:49:ASP:OD2	2:A:167:LYS:CE	2.49	0.60
1:D:165:LEU:HD11	1:D:1212:ALA:CB	2.23	0.59
1:D:1209:LYS:O	1:D:1211:LEU:N	2.35	0.59
2:A:119:PHE:HD2	2:A:147:ASN:HD22	1.49	0.59
2:B:213:HIS:CD2	2:B:241:HIS:HB2	2.37	0.59
1:D:1203:ARG:HH22	1:C:13:ARG:HA	1.68	0.59
1:D:1205:SER:CB	3:D:1402:ATP:H5'1	2.33	0.59
1:D:208:SER:HB3	1:D:1113:GLU:HB2	1.83	0.59
2:A:56:ASP:H	2:A:123:GLY:HA3	1.68	0.59
1:C:44:ILE:HG13	1:C:155:PHE:HB3	1.85	0.59
1:D:202:ILE:HD12	1:D:205:LEU:HD12	1.86	0.58
2:A:412:ARG:HH11	2:A:412:ARG:CB	2.03	0.58
3:D:1402:ATP:O2B	1:C:41:THR:CB	2.51	0.58
1:D:1214:ILE:HG13	1:D:1233:LEU:HD11	1.85	0.58
1:D:1209:LYS:O	1:D:1210:VAL:C	2.46	0.58
1:D:1241:ASP:OD1	1:D:1241:ASP:N	2.36	0.57
1:D:1287:ASP:HA	2:A:184:ARG:HH21	1.69	0.57
1:C:1164:THR:CG2	2:B:389:ARG:HD3	2.34	0.57
2:B:106:ASN:HB2	2:B:114:ILE:HD12	1.86	0.57
1:D:4:ILE:HG23	1:D:82:LEU:HD21	1.87	0.57
2:A:312:GLN:OE1	2:A:372:SER:OG	2.21	0.57
2:B:94:SER:HA	2:B:103:THR:HB	1.86	0.57
1:C:14:SER:OG	1:C:1294:ARG:NH2	2.37	0.57
1:C:50:ALA:CB	1:C:80:VAL:HG11	2.34	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1153:ILE:HD11	1:C:1216:ILE:HA	1.87	0.57
2:B:315:PRO:O	2:B:316:HIS:ND1	2.37	0.57
2:B:365:ILE:H	2:B:401:ASN:HD21	1.53	0.57
1:D:94:VAL:HG12	1:D:116:LEU:HG	1.86	0.57
1:C:1:MET:HG2	1:C:1226:ALA:HB1	1.86	0.56
2:A:344:THR:HG22	2:A:360:LEU:HD22	1.86	0.56
1:C:1193:LYS:HG3	1:C:1198:LEU:HD22	1.88	0.56
2:B:41:MET:O	2:B:45:ASN:ND2	2.38	0.56
1:D:10:GLN:HE21	1:D:20:ARG:HB3	1.70	0.56
2:A:102:PHE:HZ	2:B:73:LYS:HA	1.69	0.56
2:B:171:LYS:HB2	2:B:206:TRP:HA	1.86	0.56
1:D:30:THR:OG1	1:D:1290:PHE:HE2	1.88	0.56
2:A:306:MET:HG3	2:A:366:ARG:HB3	1.87	0.56
2:B:121:ILE:HD11	2:B:213:HIS:HB2	1.88	0.56
2:A:80:MET:HE1	2:B:112:PHE:CE1	2.40	0.56
1:D:1183:LYS:NZ	1:D:1184:SER:O	2.39	0.56
2:A:17:ASN:HB2	2:A:57:LEU:HD12	1.88	0.56
1:D:44:ILE:HD11	1:D:1268:ILE:HG21	1.88	0.55
1:C:50:ALA:HB2	1:C:80:VAL:HG11	1.88	0.55
1:D:50:ALA:HB3	1:D:82:LEU:HD12	1.88	0.55
2:B:106:ASN:H	2:B:147:ASN:HD21	1.54	0.55
1:C:1209:LYS:O	1:C:1213:SER:OG	2.25	0.55
1:C:1237:THR:O	1:C:1237:THR:OG1	2.19	0.55
1:D:1125:ASP:OD1	1:D:1125:ASP:N	2.34	0.55
2:A:86:GLU:HB2	2:A:167:LYS:NZ	2.22	0.55
2:A:412:ARG:HD2	2:A:412:ARG:C	2.32	0.55
1:C:105:THR:O	1:C:105:THR:CG2	2.52	0.55
1:D:1276:PHE:HA	1:D:1279:HIS:HB2	1.88	0.55
2:A:185:LEU:HD22	2:A:225:LEU:HD11	1.88	0.55
2:B:285:ILE:HA	2:B:291:PRO:HB3	1.89	0.55
1:D:1184:SER:OG	1:D:1185:TYR:N	2.38	0.55
1:D:1191:MET:HG3	1:D:1198:LEU:HB3	1.87	0.55
3:D:1401:ATP:H5'2	3:D:1401:ATP:H8	1.72	0.55
2:A:86:GLU:HB2	2:A:167:LYS:CD	2.37	0.55
1:D:131:ARG:HG2	1:D:134:GLU:HB2	1.89	0.54
1:C:66:HIS:NE2	1:C:1299:LYS:HE2	2.23	0.54
1:D:1233:LEU:HB3	1:D:1267:LEU:HD11	1.89	0.54
2:A:27:ILE:O	2:A:302:ARG:NH2	2.41	0.54
1:D:21:GLU:OE2	1:D:1299:LYS:NZ	2.41	0.54
2:A:322:LYS:HE2	2:A:384:GLN:HB3	1.90	0.54
1:C:1255:ILE:HG23	1:C:1259:ARG:HD3	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:164:LEU:HB3	2:A:206:TRP:HH2	1.73	0.53
2:B:357:VAL:HG23	2:B:357:VAL:O	2.09	0.53
1:C:3:ALA:HA	1:C:1266:GLN:HE22	1.73	0.53
2:B:334:GLU:OE2	2:B:398:ARG:NH1	2.31	0.53
1:D:198:MET:HG3	1:D:1124:THR:HA	1.91	0.53
1:D:31:LEU:HG	1:D:1289:PHE:HB2	1.91	0.53
1:D:1159:ARG:NH1	2:A:407:GLN:OE1	2.42	0.53
2:A:96:VAL:HA	2:A:161:VAL:HG21	1.91	0.53
1:C:1170:LYS:NZ	1:C:1192:TYR:OH	2.32	0.53
1:D:164:PRO:HB2	1:D:1213:SER:HA	1.90	0.53
1:C:97:ASN:HB2	1:C:112:LEU:HB2	1.90	0.53
1:D:1230:VAL:HA	1:D:1266:GLN:HB2	1.91	0.53
1:D:74:LYS:NZ	1:D:103:LYS:O	2.36	0.52
1:D:155:PHE:HA	1:D:1232:ALA:HB3	1.91	0.52
1:D:1147:GLN:HE21	2:A:378:GLN:HE21	1.58	0.52
2:B:106:ASN:OD1	2:B:106:ASN:N	2.42	0.52
1:C:140:PRO:HA	1:C:143:LEU:HB3	1.91	0.52
1:D:1174:ASP:OD1	1:D:1174:ASP:N	2.43	0.52
2:A:40:MET:HE1	2:A:51:VAL:HG11	1.92	0.52
2:A:152:VAL:HG22	2:A:178:ALA:HB3	1.91	0.52
2:A:293:MET:HG3	2:A:295:PRO:HD3	1.91	0.52
1:C:1190:VAL:HG12	1:C:1199:ASP:OD1	2.10	0.52
1:D:44:ILE:HD13	1:D:1268:ILE:HG21	1.92	0.52
1:D:120:ASN:HD21	1:D:124:ASP:HB2	1.75	0.52
2:A:181:ARG:HB3	2:A:184:ARG:HG3	1.91	0.52
1:C:1159:ARG:HH11	1:C:1251:SER:HA	1.74	0.52
1:C:1235:GLN:HE21	1:C:1272:HIS:CE1	2.27	0.52
1:D:25:PHE:CE1	1:D:1268:ILE:CD1	2.93	0.51
1:D:1158:LYS:HA	1:D:1164:THR:HG23	1.91	0.51
1:C:1:MET:HA	1:C:1227:ASN:HA	1.91	0.51
2:A:86:GLU:HB2	2:A:167:LYS:HD3	1.92	0.51
2:A:196:PHE:CE2	2:A:210:MET:HE1	2.45	0.51
1:D:50:ALA:O	1:D:96:ARG:NH2	2.43	0.51
1:D:199:SER:O	1:D:203:LYS:NZ	2.44	0.51
1:D:31:LEU:HD23	1:D:31:LEU:H	1.76	0.51
2:A:394:ARG:HG3	2:A:395:PHE:HD1	1.76	0.51
2:B:119:PHE:CD1	2:B:119:PHE:N	2.78	0.51
1:D:149:ILE:HG12	1:D:154:ILE:HG12	1.91	0.51
1:C:1156:LEU:O	1:C:1160:THR:OG1	2.28	0.51
1:C:172:LYS:HE3	1:C:1187:TYR:H	1.76	0.51
1:D:40:LYS:HE3	1:D:1272:HIS:CE1	2.45	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:207:PHE:HE2	2:A:209:LEU:HD12	1.76	0.50
1:C:167:GLU:OE1	1:C:170:ASN:N	2.36	0.50
1:D:1194:GLN:NE2	1:C:69:LYS:O	2.43	0.50
2:B:8:THR:O	2:B:167:LYS:NZ	2.33	0.50
2:B:329:LEU:HB2	2:B:391:PHE:HZ	1.77	0.50
1:D:30:THR:OG1	1:D:1290:PHE:CE2	2.65	0.50
1:D:195:LYS:O	1:D:199:SER:N	2.44	0.50
2:B:17:ASN:HB2	2:B:57:LEU:HD12	1.93	0.50
1:D:1146:MET:O	1:D:1149:ILE:CG1	2.57	0.50
1:D:1289:PHE:CD2	1:D:1305:VAL:HG13	2.47	0.50
2:A:44:LYS:HD3	2:A:78:CYS:HA	1.93	0.50
1:C:1271:THR:HG21	1:C:1276:PHE:HD2	1.76	0.50
2:B:317:LEU:HD12	2:B:325:THR:HG22	1.93	0.50
1:D:1175:GLU:HG2	1:D:1183:LYS:HE2	1.94	0.50
1:D:115:GLN:HG3	1:D:127:THR:HG22	1.89	0.50
1:D:1275:LYS:HZ2	1:C:1275:LYS:HE2	1.75	0.50
2:A:367:LEU:O	2:A:407:GLN:N	2.43	0.50
1:D:1240:LEU:HG	1:D:1245:ILE:HB	1.93	0.49
2:A:367:LEU:HB3	2:A:406:VAL:HG23	1.92	0.49
2:B:389:ARG:HG3	2:B:403:ASN:HB3	1.94	0.49
2:A:279:TYR:HD2	2:A:295:PRO:HB2	1.77	0.49
2:B:126:ASP:HB2	2:B:136:PRO:HG2	1.94	0.49
1:D:173:LYS:HZ3	1:D:1185:TYR:HB3	1.76	0.49
1:D:1241:ASP:HA	1:C:1272:HIS:CD2	2.48	0.49
1:C:5:TYR:HA	1:C:25:PHE:CE1	2.48	0.49
1:C:1190:VAL:HG23	1:C:1190:VAL:O	2.12	0.49
2:A:69:TYR:HB3	2:B:134:LEU:HD21	1.95	0.49
2:A:412:ARG:C	2:A:412:ARG:CD	2.85	0.49
1:C:104:LYS:HG3	1:C:105:THR:N	2.28	0.49
1:C:1156:LEU:H	1:C:1156:LEU:HD12	1.76	0.49
1:C:1200:MET:HB2	1:C:1204:CYS:HB3	1.94	0.49
1:D:93:ILE:HG12	1:D:119:ILE:HD13	1.94	0.49
1:D:1271:THR:HG21	1:D:1276:PHE:HD2	1.77	0.49
2:A:87:LEU:HA	2:A:167:LYS:HG2	1.95	0.49
1:C:50:ALA:CB	1:C:80:VAL:CG1	2.89	0.49
1:C:1308:ASN:HB3	1:C:1309:ARG:HH11	1.77	0.49
1:D:167:GLU:HG3	1:D:171:LEU:HB2	1.95	0.49
1:C:94:VAL:HA	1:C:115:GLN:HG2	1.94	0.49
1:C:148:ALA:HB1	1:C:174:LYS:HE2	1.95	0.49
2:B:270:LEU:HB2	2:B:366:ARG:HE	1.78	0.49
1:C:1189:VAL:CG2	1:C:1200:MET:HG3	2.43	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:GLU:O	1:C:49:TYR:HB2	2.13	0.48
1:C:77:ARG:NH2	1:C:79:GLN:OE1	2.29	0.48
2:B:12:LEU:HB2	2:B:48:VAL:HG11	1.94	0.48
1:C:1245:ILE:HD12	1:C:1248:LEU:HD22	1.93	0.48
1:D:116:LEU:O	1:D:128:LEU:N	2.44	0.48
2:A:56:ASP:HB2	2:A:213:HIS:CE1	2.48	0.48
2:A:388:PRO:HB3	2:A:403:ASN:O	2.13	0.48
1:C:1189:VAL:HG23	1:C:1200:MET:CG	2.43	0.48
1:D:68:PRO:O	1:D:72:GLY:N	2.34	0.48
1:D:1292:VAL:HG12	1:D:1302:ILE:HG12	1.96	0.48
1:D:1203:ARG:NH1	1:C:64:PHE:HA	2.29	0.48
1:D:1123:VAL:HA	1:D:1126:ASP:HB2	1.95	0.48
2:A:90:LEU:HG	2:A:166:GLN:HB2	1.95	0.48
2:A:87:LEU:HD23	2:A:167:LYS:CG	2.43	0.48
3:D:1401:ATP:H5'2	3:D:1401:ATP:C8	2.49	0.47
1:D:1152:ILE:O	1:D:1156:LEU:N	2.32	0.47
2:A:10:ARG:HG2	2:A:48:VAL:HG12	1.96	0.47
2:A:49:ASP:O	2:A:117:PRO:HD2	2.14	0.47
2:A:242:GLU:HB2	2:A:261:GLN:NE2	2.29	0.47
1:C:8:SER:OG	1:C:81:LYS:N	2.25	0.47
2:B:390:ARG:HA	2:B:393:ASN:HB2	1.96	0.47
1:D:81:LYS:NZ	1:D:95:THR:OG1	2.46	0.47
1:D:1205:SER:O	1:D:1209:LYS:N	2.37	0.47
2:A:189:PHE:HE1	2:A:194:VAL:HG11	1.80	0.47
1:C:50:ALA:HA	1:C:96:ARG:NE	2.20	0.47
2:B:170:THR:HG22	2:B:287:TYR:H	1.80	0.47
1:D:1163:GLY:HA3	2:A:388:PRO:HG3	1.95	0.47
2:A:76:ARG:HG3	2:A:80:MET:HE2	1.97	0.47
2:B:293:MET:HG3	2:B:295:PRO:HD3	1.95	0.47
2:B:49:ASP:O	2:B:117:PRO:HD2	2.15	0.47
2:B:88:GLU:O	2:B:166:GLN:N	2.47	0.47
1:D:115:GLN:CD	1:D:127:THR:HG22	2.39	0.47
1:D:1211:LEU:O	1:D:1215:ILE:HG23	2.15	0.47
1:D:1311:THR:HA	2:A:129:SER:HB2	1.96	0.47
2:A:112:PHE:HE2	2:A:144:GLY:HA3	1.79	0.47
2:A:210:MET:HE3	2:A:210:MET:HB2	1.73	0.47
1:C:50:ALA:HB2	1:C:80:VAL:CG1	2.44	0.47
1:C:104:LYS:HG3	1:C:105:THR:H	1.79	0.47
2:B:270:LEU:HD22	2:B:304:PHE:HE2	1.79	0.47
1:C:150:LEU:H	1:C:150:LEU:HD23	1.79	0.47
1:D:168:PRO:O	1:D:169:SER:C	2.58	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1240:LEU:HD21	1:D:1245:ILE:HD12	1.96	0.47
2:A:91:SER:OG	2:A:92:ASP:N	2.47	0.47
2:B:19:VAL:HA	2:B:32:SER:HB3	1.97	0.47
1:C:19:ASP:OD1	1:C:19:ASP:N	2.45	0.46
1:C:65:ILE:HG23	1:C:78:ALA:HB2	1.97	0.46
1:C:1242:GLU:HA	1:C:1245:ILE:HG22	1.96	0.46
2:B:7:ASP:OD1	2:B:286:LYS:NZ	2.48	0.46
1:D:168:PRO:O	1:D:172:LYS:N	2.46	0.46
2:A:37:HIS:NE2	2:A:41:MET:HE2	2.30	0.46
2:A:196:PHE:HE2	2:A:210:MET:HE1	1.80	0.46
2:B:50:MET:CB	2:B:117:PRO:HG2	2.46	0.46
1:D:1205:SER:O	1:D:1206:ALA:C	2.57	0.46
2:A:101:GLU:OE2	2:B:73:LYS:NZ	2.36	0.46
2:B:30:ASP:OD2	2:B:33:TRP:NE1	2.47	0.46
2:B:28:THR:HG22	2:B:400:ALA:HB1	1.97	0.46
2:B:50:MET:HB2	2:B:117:PRO:HG2	1.98	0.46
1:C:44:ILE:HD12	1:C:44:ILE:HA	1.85	0.46
1:C:129:SER:OG	1:C:134:GLU:OE2	2.33	0.46
2:A:157:LYS:NZ	2:A:195:THR:OG1	2.48	0.46
2:A:201:MET:SD	2:A:201:MET:N	2.87	0.46
1:C:91:ASN:O	1:C:119:ILE:N	2.42	0.46
1:D:1190:VAL:HG12	1:D:1199:ASP:HA	1.98	0.46
2:A:164:LEU:HD22	2:A:206:TRP:CZ3	2.51	0.46
2:B:149:PHE:CE1	2:B:176:GLY:HA3	2.50	0.46
1:D:40:LYS:NZ	3:D:1401:ATP:O1G	2.42	0.46
1:D:171:LEU:O	1:D:174:LYS:HB2	2.16	0.46
2:A:11:ILE:HD11	2:A:52:VAL:HB	1.98	0.46
2:A:25:ASP:HB2	2:A:28:THR:O	2.16	0.46
2:A:53:GLN:HB2	2:A:120:GLY:HA3	1.98	0.46
2:A:149:PHE:CE2	2:A:174:LEU:HG	2.51	0.46
1:D:1234:ASP:OD1	1:D:1234:ASP:N	2.48	0.45
3:D:1402:ATP:N6	1:C:67:ASP:OD1	2.49	0.45
1:C:1189:VAL:HG23	1:C:1200:MET:HG2	1.98	0.45
1:C:1256:ILE:HG12	1:C:1265:PHE:CE2	2.51	0.45
1:D:15:PHE:HD1	1:D:1300:SER:HG	1.61	0.45
1:D:1139:MET:SD	1:D:1183:LYS:HE3	2.56	0.45
2:A:260:LEU:HD23	2:A:260:LEU:HA	1.81	0.45
1:D:30:THR:O	1:D:30:THR:CG2	2.62	0.45
2:B:371:TYR:CE1	2:B:408:PHE:HB3	2.51	0.45
1:D:36:ASN:ND2	1:C:1207:GLY:HA3	2.31	0.45
3:D:1401:ATP:C5	1:C:1203:ARG:CB	3.00	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:150:GLY:HA3	2:A:176:GLY:HA3	1.99	0.45
1:C:1154:ASP:OD1	1:C:1154:ASP:N	2.50	0.45
1:C:1249:ALA:HB2	1:C:1276:PHE:CE1	2.51	0.45
1:C:1297:ARG:O	1:C:1299:LYS:HE3	2.16	0.45
1:D:171:LEU:HA	1:D:174:LYS:HG3	1.99	0.45
1:D:173:LYS:O	1:D:174:LYS:C	2.60	0.45
2:A:214:GLN:HG3	2:A:225:LEU:HD13	1.97	0.45
1:D:1167:ASP:CG	1:D:1193:LYS:HA	2.42	0.45
2:A:180:VAL:O	2:A:214:GLN:NE2	2.50	0.45
1:C:131:ARG:HH11	1:C:132:SER:H	1.65	0.45
1:C:1265:PHE:CE2	1:C:1267:LEU:HB2	2.51	0.45
2:B:214:GLN:O	2:B:239:TRP:NE1	2.50	0.45
1:D:1164:THR:HG22	1:D:1165:ASP:H	1.82	0.45
1:C:1146:MET:HG2	1:C:1149:ILE:HD13	1.98	0.45
1:C:1164:THR:HG22	2:B:389:ARG:HD3	1.98	0.45
1:C:1253:HIS:NE2	1:C:1280:MET:O	2.30	0.45
2:B:278:LYS:HG2	2:B:301:ILE:HD12	1.98	0.45
2:B:1:MET:O	2:B:47:ASN:ND2	2.50	0.44
2:B:234:LEU:HD12	2:B:234:LEU:HA	1.78	0.44
1:D:49:TYR:HE2	1:D:55:LEU:HD12	1.82	0.44
3:D:1401:ATP:N3	1:C:1198:LEU:HD21	2.33	0.44
2:A:79:CYS:O	2:A:115:SER:OG	2.25	0.44
2:A:248:ASN:OD1	2:A:248:ASN:N	2.50	0.44
2:A:210:MET:SD	2:A:234:LEU:HD11	2.57	0.44
2:B:11:ILE:HG12	2:B:283:LEU:HB3	1.99	0.44
1:D:44:ILE:HD11	1:D:1268:ILE:HD12	1.89	0.44
1:D:1259:ARG:HD3	1:D:1262:GLN:HG3	1.99	0.44
1:D:164:PRO:HB3	1:D:1216:ILE:HB	1.98	0.44
2:A:226:PRO:HG2	2:A:229:PHE:CG	2.52	0.44
1:D:145:VAL:HB	1:D:149:ILE:HG21	2.00	0.44
1:D:1212:ALA:HB1	1:D:1215:ILE:HG12	1.99	0.44
2:B:247:PRO:HA	2:B:281:PHE:CE2	2.52	0.44
1:D:8:SER:O	1:D:8:SER:OG	2.34	0.44
2:A:12:LEU:HD12	2:A:282:ILE:HD11	2.00	0.44
2:B:117:PRO:HB2	2:B:119:PHE:CE1	2.53	0.44
2:A:264:SER:OG	2:A:265:SER:N	2.51	0.44
1:D:167:GLU:HG2	1:D:171:LEU:HD23	2.00	0.44
2:A:377:THR:OG1	2:A:378:GLN:N	2.51	0.44
2:B:306:MET:SD	2:B:307:LYS:N	2.91	0.44
1:C:1154:ASP:HB2	1:C:1168:THR:HG22	1.99	0.43
2:B:329:LEU:O	2:B:333:VAL:HG23	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:283:LEU:HG	2:A:293:MET:HE2	1.99	0.43
1:C:1255:ILE:O	1:C:1259:ARG:HB2	2.18	0.43
1:C:1248:LEU:HD12	1:C:1248:LEU:HA	1.77	0.43
1:C:164:PRO:HA	1:C:171:LEU:HD21	2.00	0.43
1:D:173:LYS:O	1:D:176:ASP:N	2.52	0.43
2:A:64:SER:HA	2:B:62:LYS:NZ	2.33	0.43
1:D:168:PRO:HA	1:D:172:LYS:CB	2.46	0.43
1:D:1294:ARG:NH1	1:C:1165:ASP:OD2	2.37	0.43
2:A:22:ASN:O	2:A:29:GLY:HA2	2.19	0.43
2:A:189:PHE:CE1	2:A:194:VAL:HG11	2.54	0.43
2:A:365:ILE:O	2:A:401:ASN:ND2	2.33	0.43
1:C:8:SER:HA	1:C:22:THR:OG1	2.19	0.43
1:D:174:LYS:HB3	1:D:174:LYS:HE3	1.58	0.43
2:A:76:ARG:NH1	2:B:141:HIS:O	2.51	0.43
1:D:1220:LEU:HD12	1:D:1224:PHE:HD2	1.84	0.43
1:D:1203:ARG:HD3	1:C:63:VAL:HB	2.01	0.43
2:A:237:VAL:HG13	2:A:259:VAL:HG13	2.00	0.43
2:B:15:THR:OG1	2:B:16:ASP:OD2	2.22	0.43
1:D:1151:ARG:NH1	2:A:378:GLN:OE1	2.52	0.42
1:D:1233:LEU:HB3	1:D:1267:LEU:CD1	2.49	0.42
2:B:247:PRO:HA	2:B:281:PHE:HE2	1.83	0.42
1:D:1295:ASP:OD1	1:D:1299:LYS:N	2.32	0.42
1:C:1160:THR:HG22	1:C:1247:SER:O	2.18	0.42
1:D:1272:HIS:HE2	1:C:1239:ASN:C	2.23	0.42
1:C:23:ILE:HD12	1:C:23:ILE:HA	1.79	0.42
1:C:1230:VAL:HG22	1:C:1266:GLN:H	1.83	0.42
2:B:187:ARG:HH21	2:B:190:LYS:HG3	1.84	0.42
1:D:16:ASP:OD2	1:D:1299:LYS:HD3	2.19	0.42
1:D:135:LEU:O	1:D:139:VAL:HG23	2.20	0.42
1:D:1118:GLN:OE1	1:D:1121:SER:OG	2.27	0.42
1:D:1250:LYS:HA	1:D:1250:LYS:HD3	1.80	0.42
2:A:180:VAL:H	2:A:214:GLN:HE22	1.66	0.42
2:A:205:GLU:HA	2:A:287:TYR:CZ	2.54	0.42
1:D:1132:LYS:HA	1:D:1132:LYS:HD3	1.92	0.42
2:A:112:PHE:HB3	2:A:114:ILE:HG12	2.00	0.42
2:B:89:LEU:HD11	2:B:163:LEU:HD11	2.01	0.42
2:B:207:PHE:HD2	2:B:285:ILE:HD12	1.83	0.42
1:D:39:GLY:HA2	3:D:1401:ATP:O2A	2.19	0.42
1:D:1280:MET:HE2	1:D:1280:MET:HB2	1.94	0.42
1:C:1144:LEU:HG	1:C:1145:LYS:HD2	2.02	0.42
1:D:1146:MET:HE3	1:D:1146:MET:HB3	1.79	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1189:VAL:O	1:C:1200:MET:HG2	2.20	0.42
1:C:153:VAL:O	1:C:1217:ARG:NE	2.51	0.42
2:B:317:LEU:HD13	2:B:317:LEU:HA	1.84	0.42
1:D:25:PHE:HD1	1:D:30:THR:CG2	2.14	0.41
1:D:1212:ALA:CA	1:D:1215:ILE:HG12	2.50	0.41
2:A:111:ASN:ND2	2:B:80:MET:HB2	2.35	0.41
2:A:279:TYR:CD2	2:A:295:PRO:HB2	2.55	0.41
2:B:30:ASP:HB3	2:B:33:TRP:HE1	1.85	0.41
1:D:171:LEU:HA	1:D:171:LEU:HD13	1.80	0.41
1:D:1156:LEU:HD11	1:D:1255:ILE:HD11	2.02	0.41
1:D:1237:THR:HG21	1:D:1276:PHE:HB2	2.01	0.41
2:A:126:ASP:HB2	2:A:136:PRO:HG2	2.01	0.41
2:A:181:ARG:HG2	2:A:183:GLU:OE2	2.20	0.41
1:D:16:ASP:OD1	1:D:16:ASP:C	2.63	0.41
1:D:17:SER:OG	1:D:77:ARG:O	2.29	0.41
1:D:196:LYS:HD2	1:D:196:LYS:HA	1.89	0.41
2:A:97:PHE:HZ	2:A:163:LEU:HD21	1.85	0.41
2:A:135:CYS:SG	2:A:148:HIS:HE1	2.43	0.41
1:D:166:SER:O	1:D:167:GLU:C	2.62	0.41
1:D:1252:LEU:O	1:D:1256:ILE:HG13	2.21	0.41
2:A:365:ILE:HD13	2:A:365:ILE:HA	1.80	0.41
2:A:371:TYR:H	2:A:371:TYR:HD1	1.67	0.41
1:D:91:ASN:OD1	1:D:91:ASN:N	2.54	0.41
2:A:113:ASN:HD21	2:B:111:ASN:HA	1.84	0.41
2:B:164:LEU:HD22	2:B:206:TRP:CZ3	2.55	0.41
1:D:115:GLN:HG2	1:D:127:THR:HG22	1.97	0.41
2:A:189:PHE:HD2	2:A:229:PHE:HD2	1.68	0.41
2:B:182:ASP:OD1	2:B:214:GLN:NE2	2.54	0.41
2:A:136:PRO:HD3	2:B:65:LYS:NZ	2.35	0.41
2:A:281:PHE:CD2	2:A:295:PRO:HB3	2.55	0.41
1:D:37:GLY:N	3:D:1401:ATP:O1B	2.53	0.41
1:C:1186:ASN:OD1	1:C:1188:ARG:NH1	2.53	0.41
1:C:1189:VAL:HG21	1:C:1200:MET:HG3	2.03	0.41
1:C:111:THR:OG1	1:C:112:LEU:N	2.54	0.41
1:C:1294:ARG:HA	1:C:1300:SER:HA	2.03	0.41
2:B:189:PHE:CD2	2:B:229:PHE:HB3	2.56	0.41
2:B:412:ARG:H	2:B:412:ARG:HG3	1.72	0.41
1:C:1:MET:HE3	1:C:1230:VAL:HG12	2.02	0.41
2:B:316:HIS:HA	2:B:318:ARG:HH12	1.86	0.41
1:D:43:ILE:HD12	1:D:43:ILE:H	1.85	0.40
2:A:112:PHE:CE1	2:B:80:MET:HE1	2.56	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:PHE:HB3	2:B:149:PHE:CD2	2.52	0.40
1:D:117:VAL:HG11	1:D:125:ARG:HE	1.86	0.40
2:A:4:PRO:HB2	2:A:8:THR:HB	2.03	0.40
2:A:97:PHE:CZ	2:A:163:LEU:HD21	2.56	0.40
1:C:86:SER:HB2	1:C:92:MET:HE2	2.03	0.40
1:C:1230:VAL:CG2	1:C:1266:GLN:H	2.35	0.40
1:D:70:ILE:HD12	1:D:70:ILE:HA	1.81	0.40
2:A:65:LYS:HG2	2:B:139:ILE:HD11	2.03	0.40
1:D:194:ILE:HD12	1:D:194:ILE:HA	1.99	0.40
2:A:143:THR:HA	2:B:72:LEU:HD22	2.04	0.40
2:B:392:SER:HB2	2:B:405:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	C	324/1312 (25%)	280 (86%)	44 (14%)	0	100	100
1	D	402/1312 (31%)	355 (88%)	43 (11%)	4 (1%)	13	46
2	A	409/706 (58%)	382 (93%)	27 (7%)	0	100	100
2	B	410/706 (58%)	384 (94%)	25 (6%)	1 (0%)	44	75
All	All	1545/4036 (38%)	1401 (91%)	139 (9%)	5 (0%)	38	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	168	PRO
1	D	1167	ASP
1	D	1210	VAL
1	D	180	GLN

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	118	VAL

### 5.3.2 Protein sidechains ⓘ

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	C	289/1234 (23%)	263 (91%)	26 (9%)	8	30
1	D	358/1234 (29%)	324 (90%)	34 (10%)	7	28
2	A	359/635 (56%)	337 (94%)	22 (6%)	15	43
2	B	364/635 (57%)	342 (94%)	22 (6%)	16	43
All	All	1370/3738 (37%)	1266 (92%)	104 (8%)	13	35

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	23	ILE
1	D	29	LEU
1	D	31	LEU
1	D	40	LYS
1	D	45	GLU
1	D	70	ILE
1	D	79	GLN
1	D	90	LEU
1	D	91	ASN
1	D	117	VAL
1	D	119	ILE
1	D	128	LEU
1	D	157	HIS
1	D	171	LEU
1	D	172	LYS
1	D	174	LYS
1	D	176	ASP
1	D	1125	ASP
1	D	1152	ILE
1	D	1164	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	1169	ILE
1	D	1189	VAL
1	D	1194	GLN
1	D	1209	LYS
1	D	1211	LEU
1	D	1214	ILE
1	D	1215	ILE
1	D	1220	LEU
1	D	1239	ASN
1	D	1241	ASP
1	D	1252	LEU
1	D	1288	HIS
1	D	1289	PHE
1	D	1300	SER
2	A	28	THR
2	A	60	VAL
2	A	89	LEU
2	A	98	HIS
2	A	100	ASP
2	A	118	VAL
2	A	119	PHE
2	A	166	GLN
2	A	170	THR
2	A	180	VAL
2	A	208	ASN
2	A	220	THR
2	A	225	LEU
2	A	248	ASN
2	A	280	VAL
2	A	283	LEU
2	A	301	ILE
2	A	303	THR
2	A	309	ILE
2	A	323	ASP
2	A	399	VAL
2	A	412	ARG
1	C	4	ILE
1	C	51	THR
1	C	80	VAL
1	C	82	LEU
1	C	85	THR
1	C	90	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	94	VAL
1	C	106	THR
1	C	107	THR
1	C	116	LEU
1	C	129	SER
1	C	142	TYR
1	C	176	ASP
1	C	180	GLN
1	C	1152	ILE
1	C	1165	ASP
1	C	1213	SER
1	C	1222	GLU
1	C	1231	ILE
1	C	1234	ASP
1	C	1237	THR
1	C	1238	THR
1	C	1266	GLN
1	C	1269	VAL
1	C	1304	TRP
1	C	1305	VAL
2	B	11	ILE
2	B	19	VAL
2	B	28	THR
2	B	52	VAL
2	B	64	SER
2	B	79	CYS
2	B	101	GLU
2	B	104	ASN
2	B	116	ILE
2	B	118	VAL
2	B	121	ILE
2	B	133	LEU
2	B	146	ILE
2	B	180	VAL
2	B	212	VAL
2	B	234	LEU
2	B	249	LEU
2	B	266	VAL
2	B	294	THR
2	B	301	ILE
2	B	317	LEU
2	B	343	GLU

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

Mol	Chain	Res	Type
1	D	10	GLN
1	D	36	ASN
1	D	115	GLN
1	D	121	ASN
1	D	1147	GLN
1	D	1194	GLN
2	A	22	ASN
2	A	45	ASN
2	A	95	GLN
2	A	148	HIS
2	A	228	GLN
2	A	320	HIS
2	A	341	ASN
2	A	393	ASN
1	C	120	ASN
1	C	1235	GLN
1	C	1244	ASN
1	C	1266	GLN
2	B	45	ASN
2	B	46	ASN
2	B	47	ASN
2	B	98	HIS
2	B	214	GLN
2	B	252	ASN
2	B	261	GLN
2	B	312	GLN
2	B	393	ASN
2	B	401	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z  > 2$
3	ATP	D	1401	-	28,33,33	0.72	0	34,52,52	0.66	1 (2%)
3	ATP	D	1402	-	28,33,33	0.73	0	34,52,52	0.83	2 (5%)

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
3	ATP	D	1401	-	-	4/18/38/38	0/3/3/3
3	ATP	D	1402	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1402	ATP	C5-C6-N6	2.41	123.98	120.31
3	D	1402	ATP	O4'-C1'-N9	2.26	111.74	108.75
3	D	1401	ATP	C5-C6-N6	2.08	123.48	120.31

There are no chirality outliers.

All (9) torsion outliers are listed below:

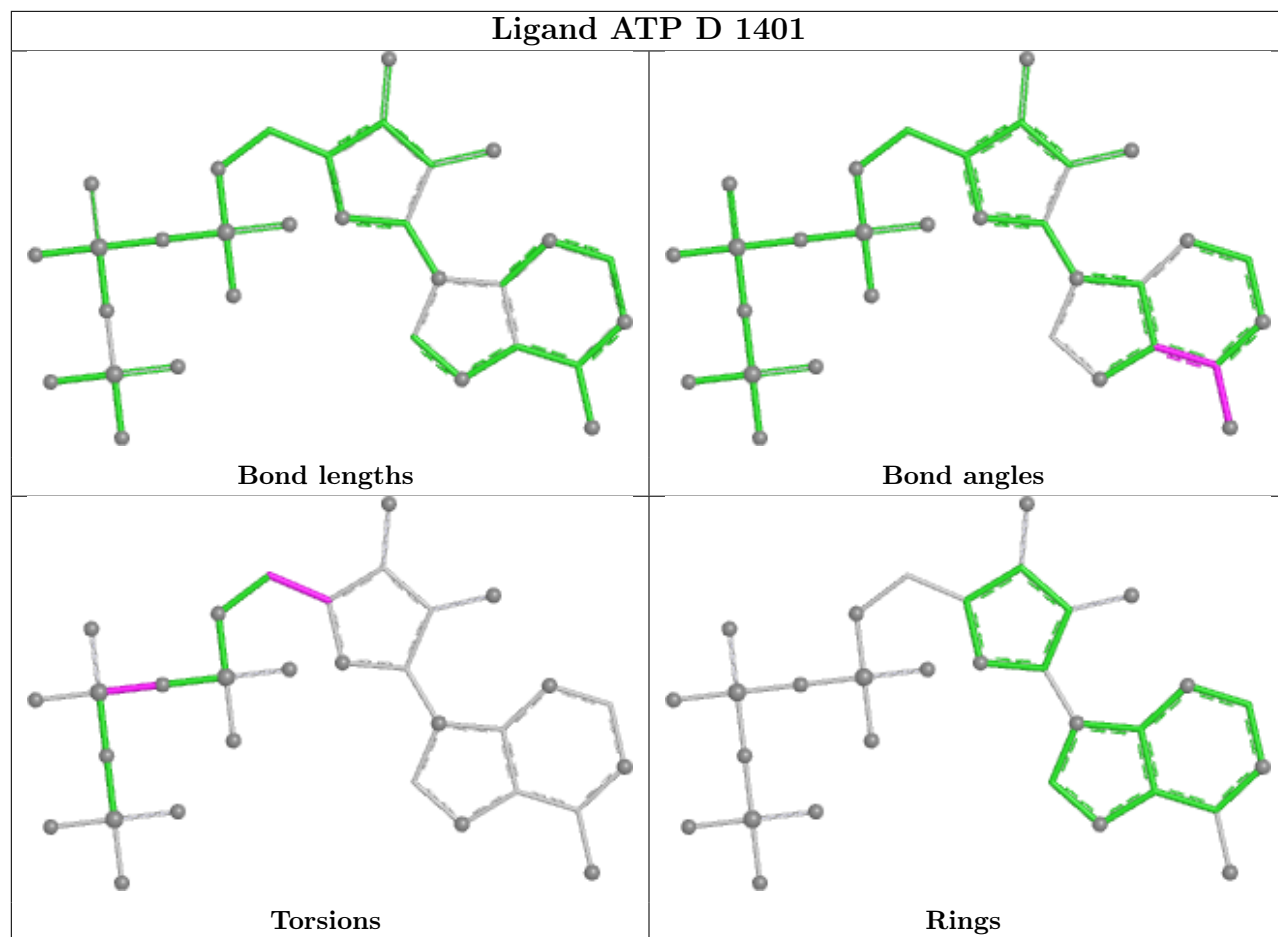
Mol	Chain	Res	Type	Atoms
3	D	1401	ATP	C3'-C4'-C5'-O5'
3	D	1401	ATP	O4'-C4'-C5'-O5'
3	D	1402	ATP	PG-O3B-PB-O1B
3	D	1402	ATP	PG-O3B-PB-O2B
3	D	1401	ATP	PA-O3A-PB-O1B
3	D	1401	ATP	PA-O3A-PB-O2B
3	D	1402	ATP	PA-O3A-PB-O1B
3	D	1402	ATP	PB-O3A-PA-O1A
3	D	1402	ATP	PB-O3A-PA-O2A

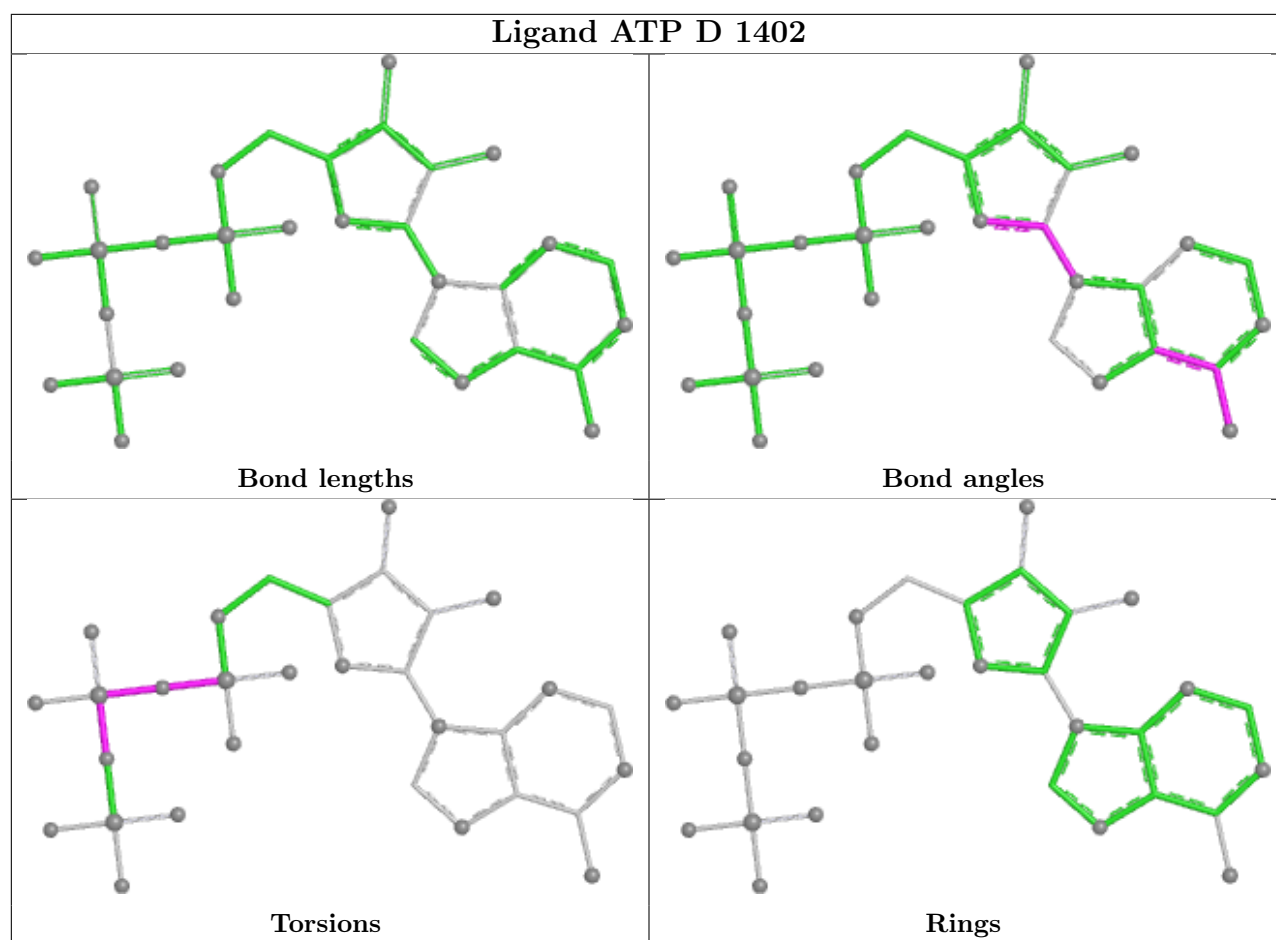
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1401	ATP	8	0
3	D	1402	ATP	5	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 [i](#)

There are no chain breaks in this entry.

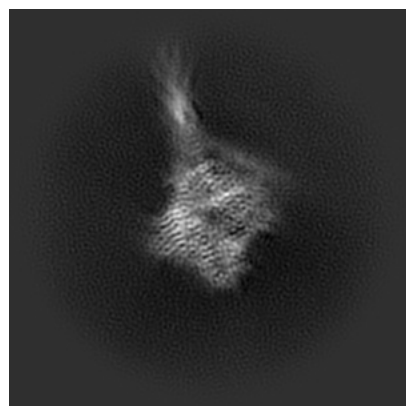
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44559. These allow visual inspection of the internal detail of the map and identification of artifacts.

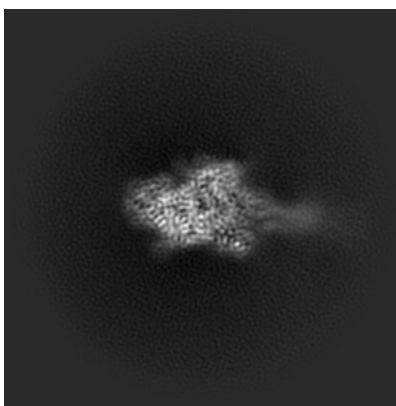
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

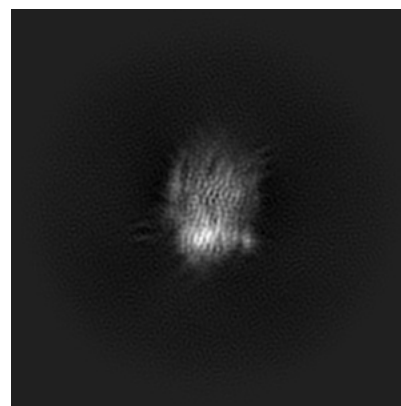
#### 6.1.1 Primary map



X

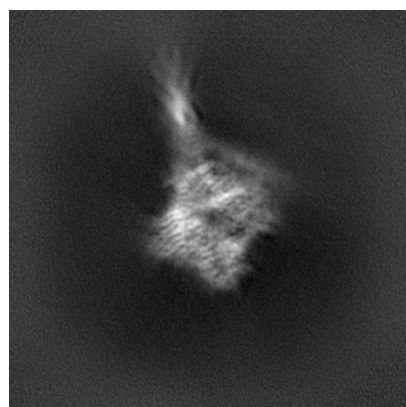


Y

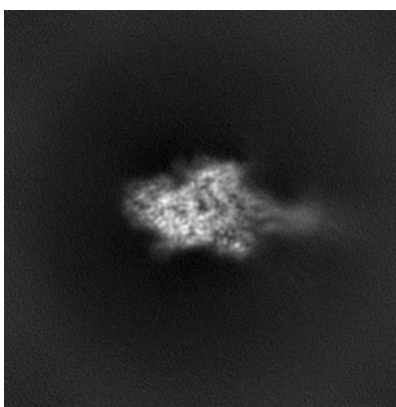


Z

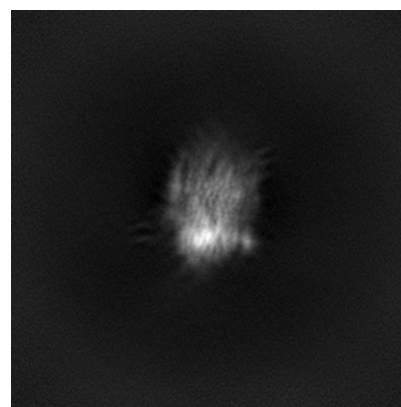
#### 6.1.2 Raw map



X



Y

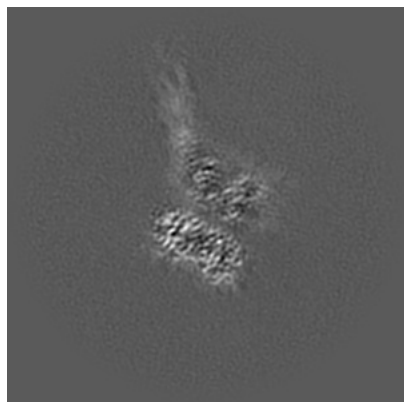


Z

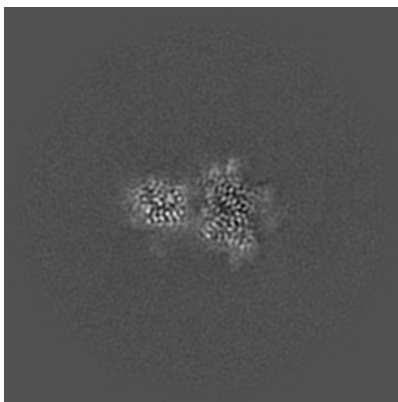
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

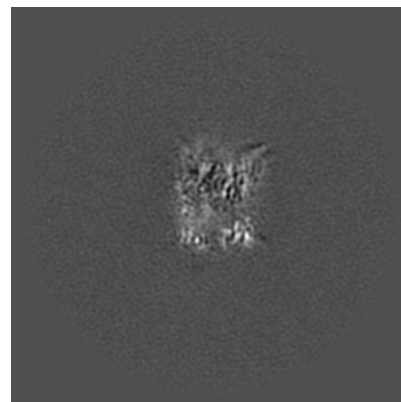
### 6.2.1 Primary map



X Index: 140

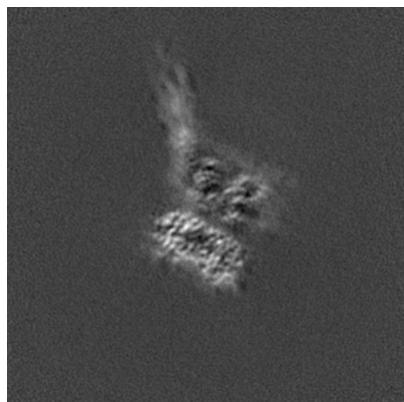


Y Index: 140

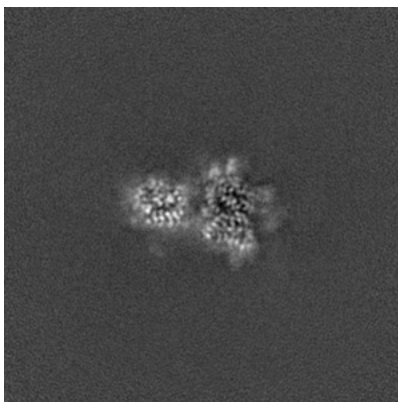


Z Index: 140

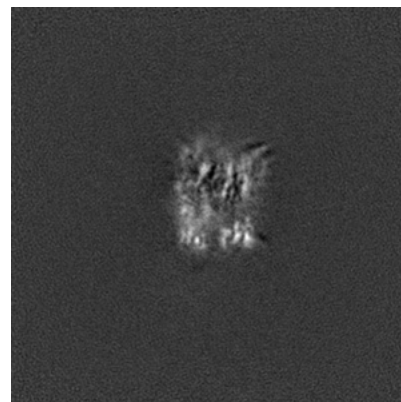
### 6.2.2 Raw map



X Index: 140



Y Index: 140

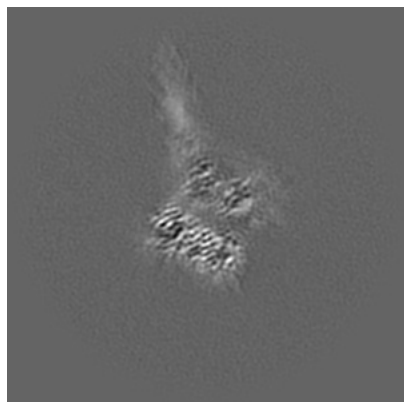


Z Index: 140

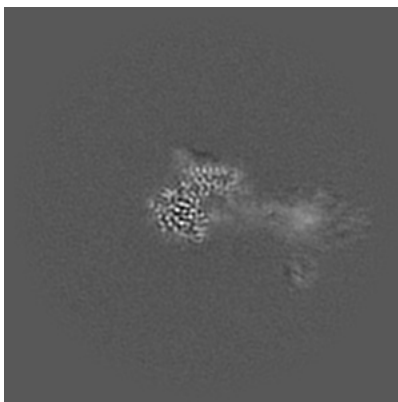
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

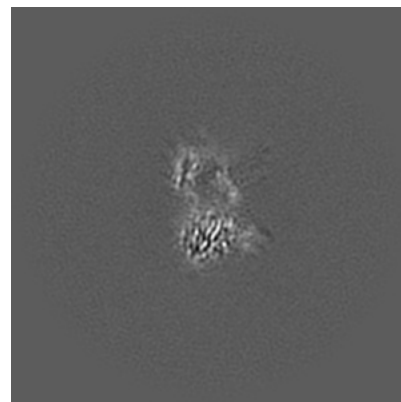
### 6.3.1 Primary map



X Index: 135

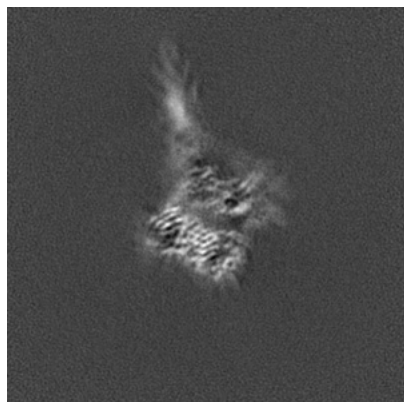


Y Index: 118

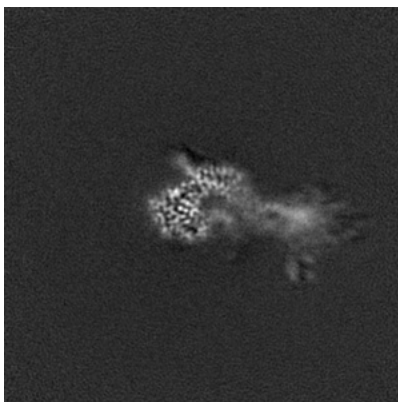


Z Index: 128

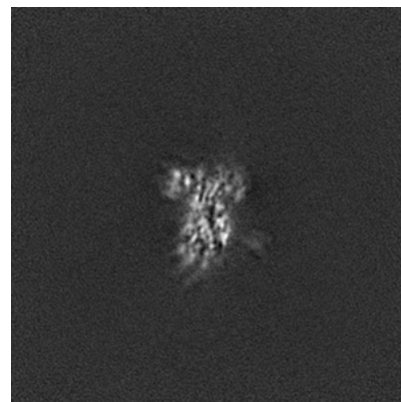
### 6.3.2 Raw map



X Index: 134



Y Index: 121

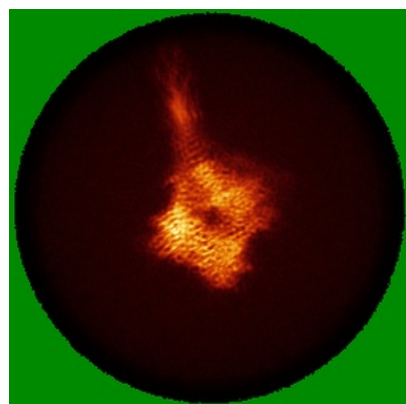


Z Index: 116

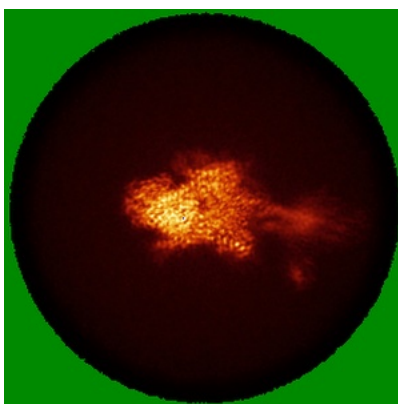
The images above show the largest variance slices of the map in three orthogonal directions.

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

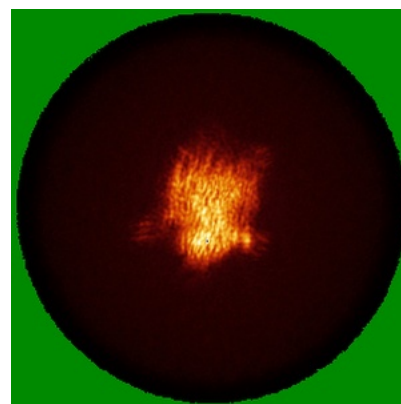
### 6.4.1 Primary map



X

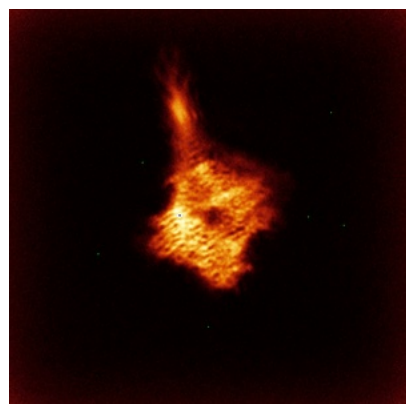


Y



Z

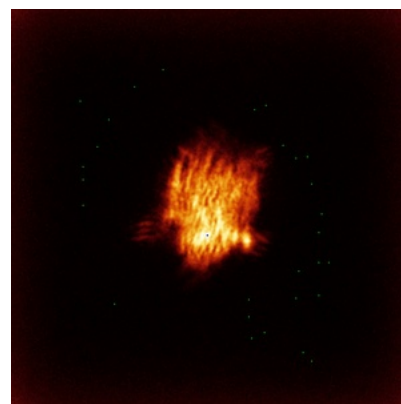
### 6.4.2 Raw map



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.

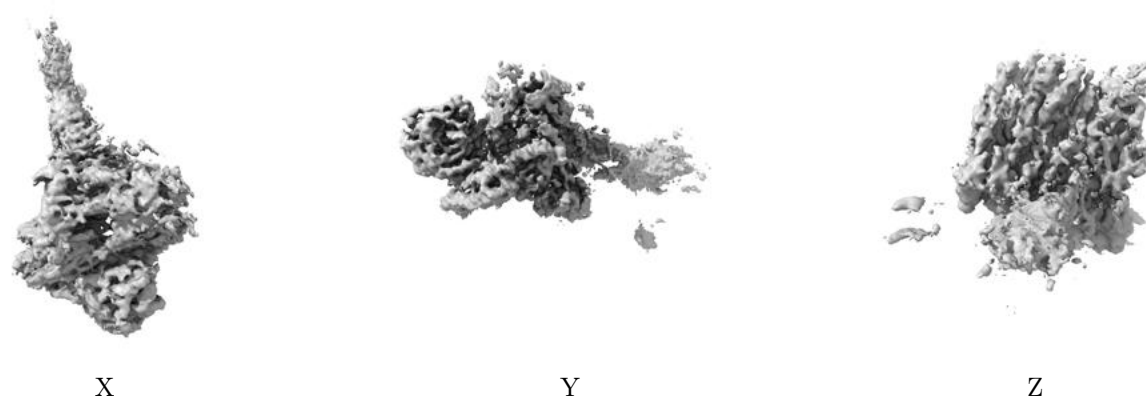
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

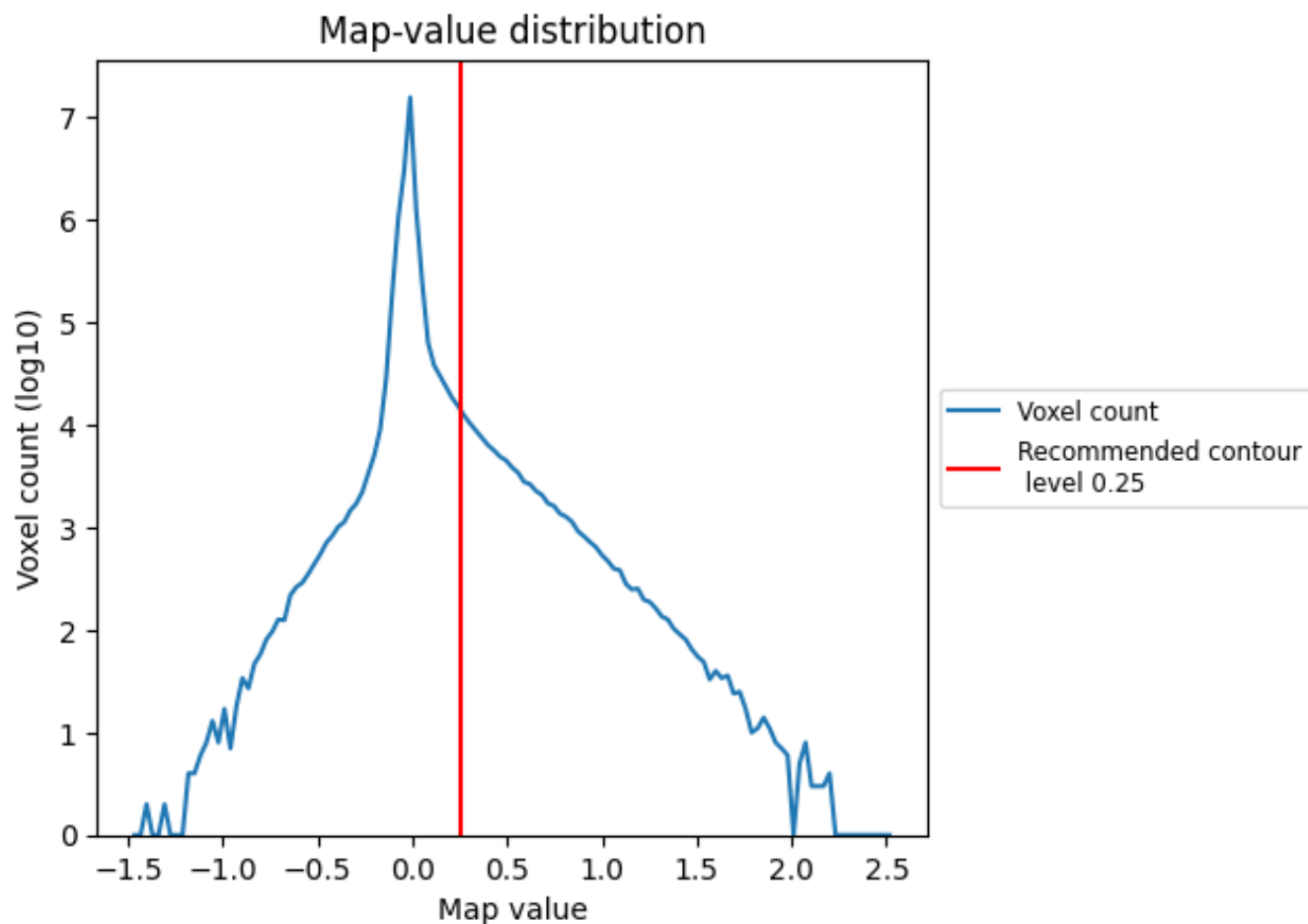
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

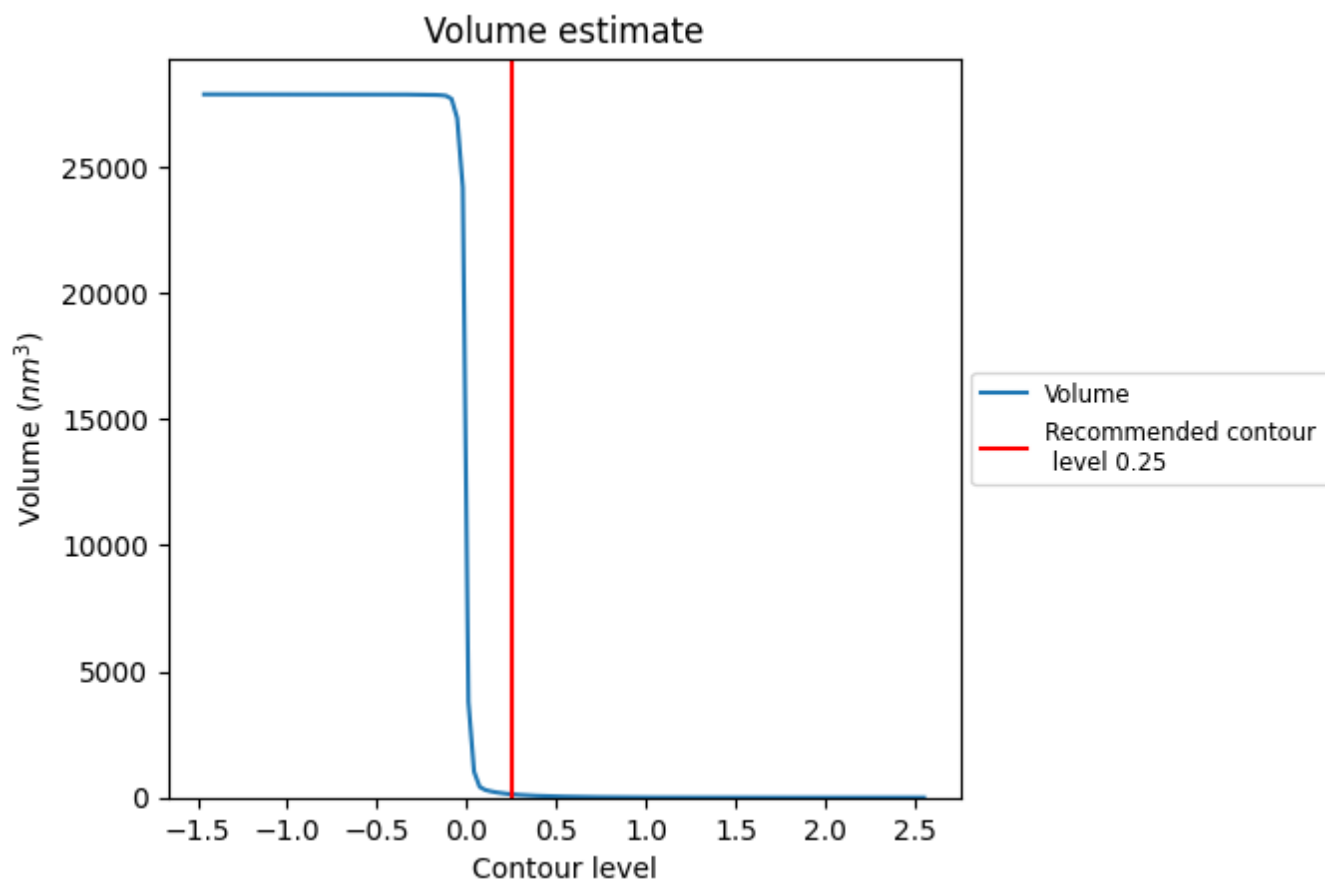
This section contains the results of statistical analysis of the map.

### 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.

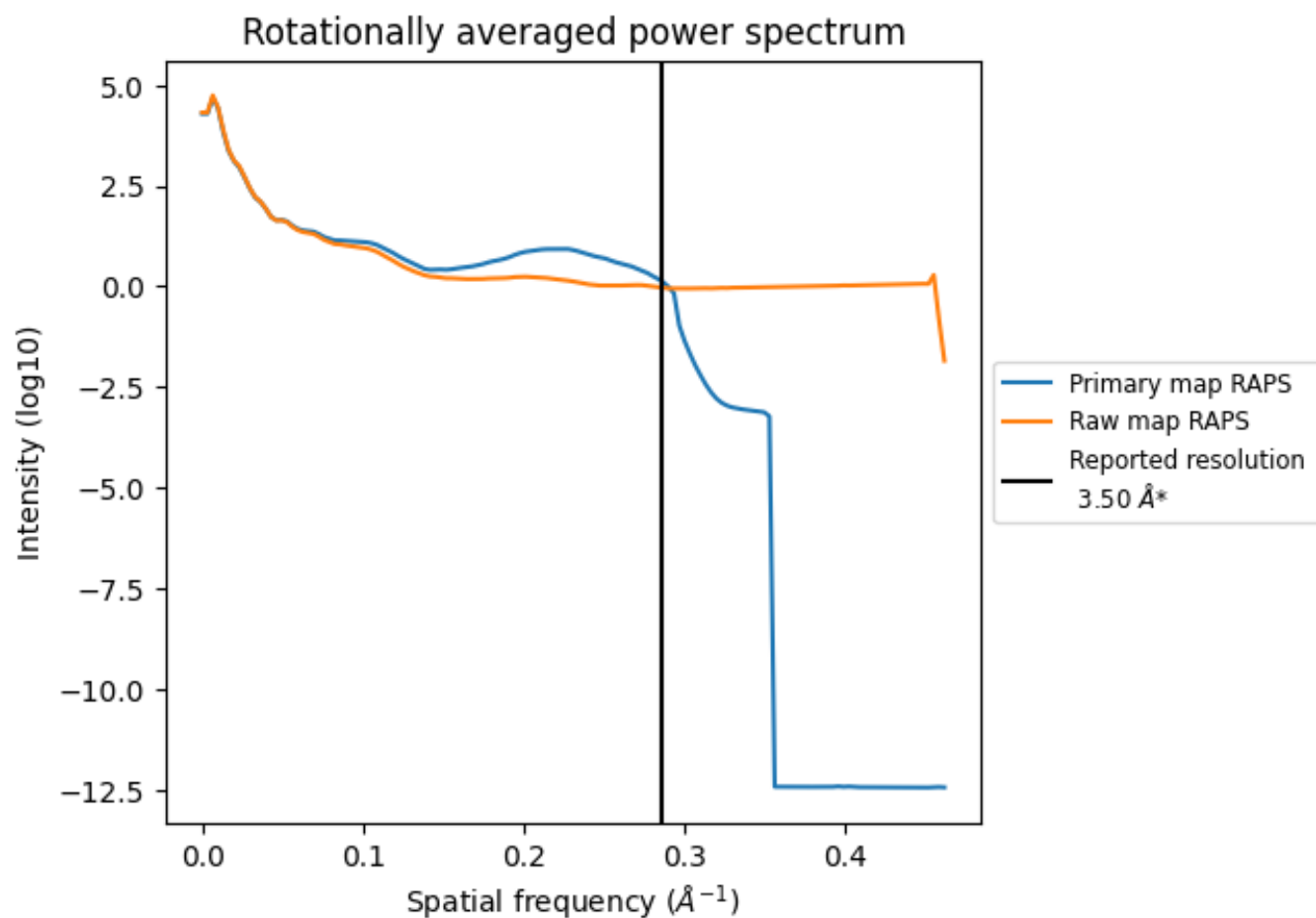
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132  $\text{nm}^3$ ; this corresponds to an approximate mass of 119 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

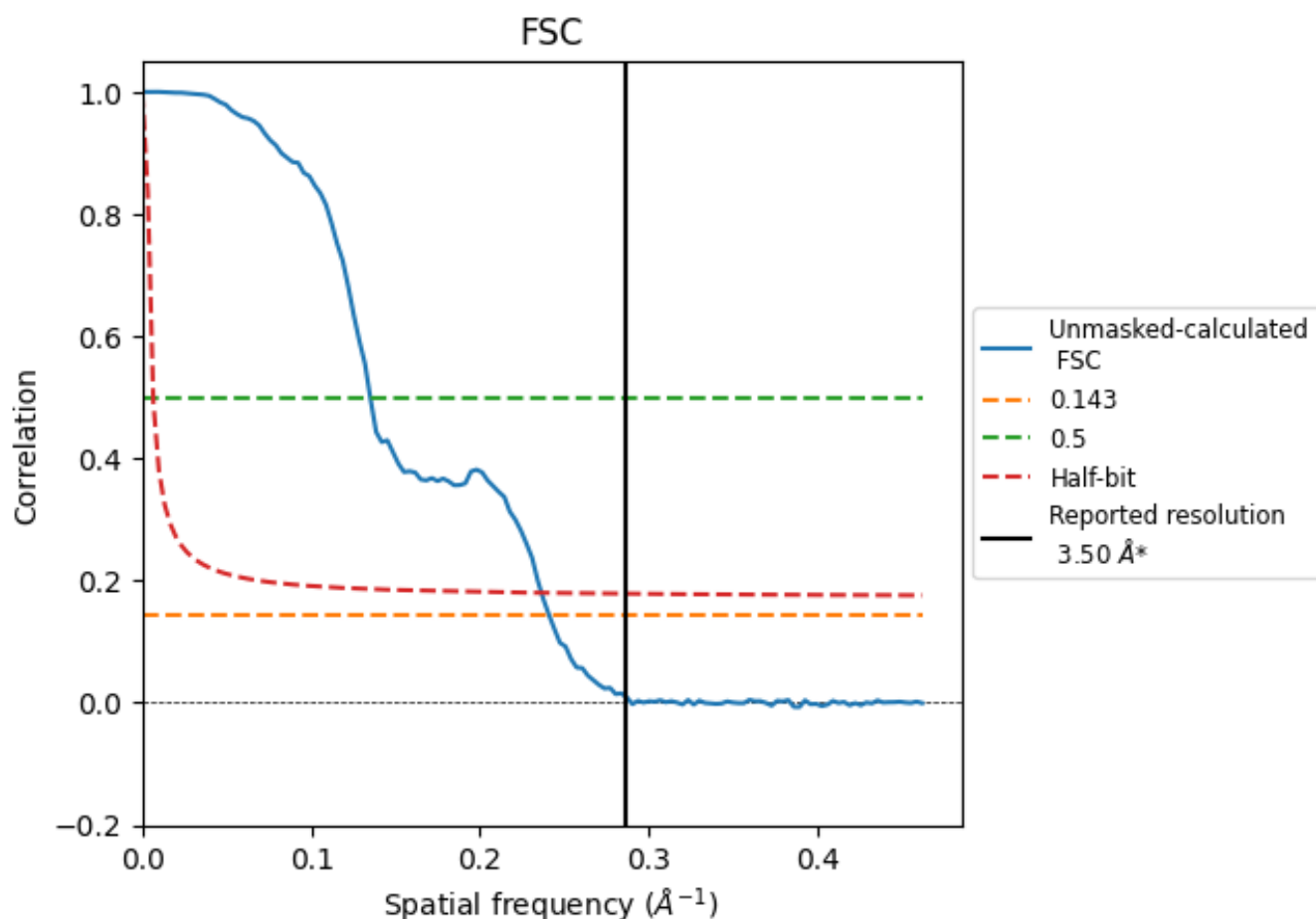


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 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 0.286 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

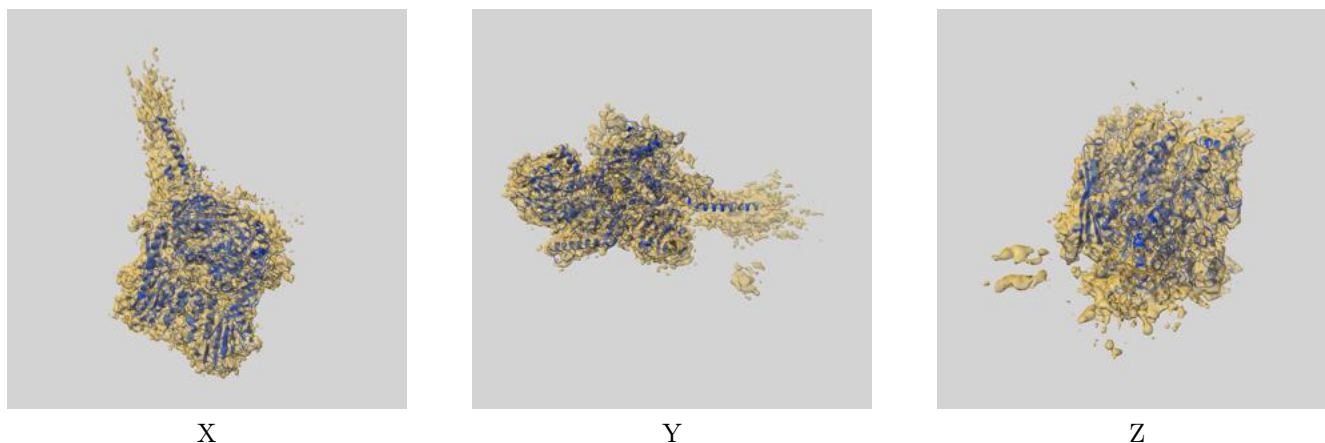
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.15	7.41	4.23

\*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 4.15 differs from the reported value 3.5 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44559 and PDB model 9BI5. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



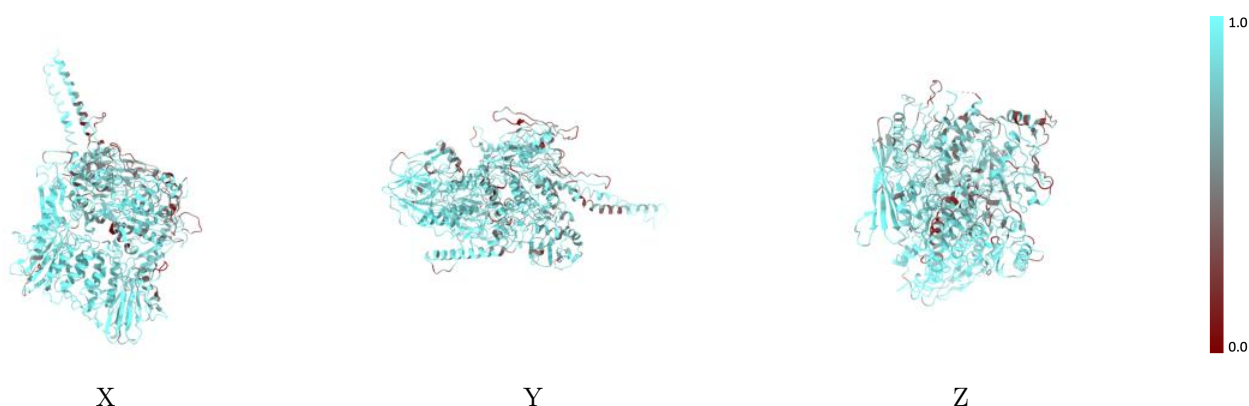
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



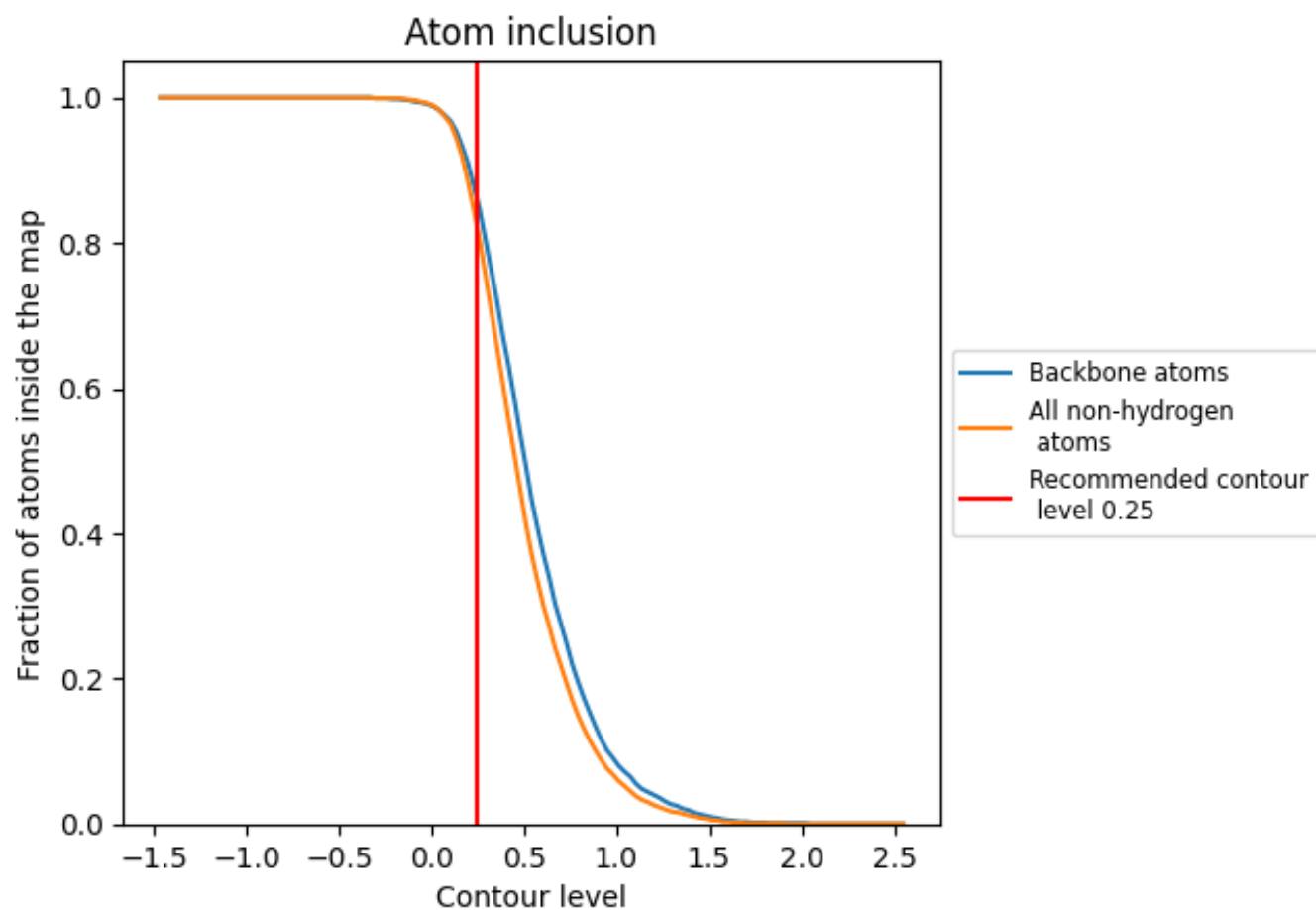
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8190	<div></div> 0.3970
A	<div></div> 0.8950	<div></div> 0.4270
B	<div></div> 0.8480	<div></div> 0.4150
C	<div></div> 0.7370	<div></div> 0.3610
D	<div></div> 0.7810	<div></div> 0.3790

