



## Full wwPDB EM Validation Report ⓘ

Apr 7, 2025 – 10:24 AM EDT

PDB ID : 9D0W / pdb\_00009d0w  
EMDB ID : EMD-46464  
Title : Cryo-EM structure of CDK2/CyclinE1 in complex with CRBN/DDB1 and Cpd 4  
Authors : Kwiatkowski, N.; Liang, T.; Sha, Z.; Collier, P.N.; Yang, A.; Sathappa, M.; Paul, A.; Su, L.; Zheng, X.; Aversa, R.; Li, K.; Mehovic, R.; Breitkopf, S.B.; Chen, D.; Howarth, C.L.; Yuan, K.; Jo, H.; Growney, J.D.; Weiss, M.; Williams, J.  
Deposited on : 2024-08-07  
Resolution : 2.95 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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
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) : 2.42

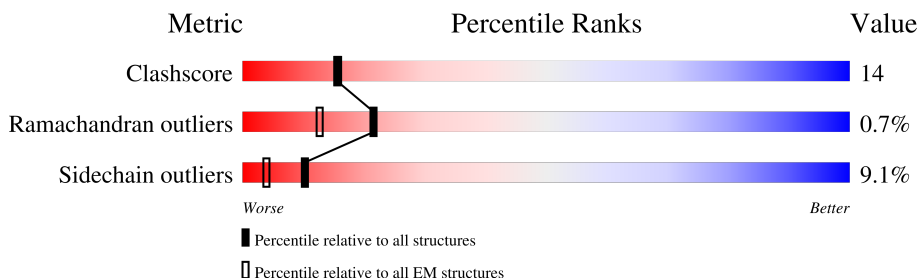
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.95 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	A	1148	
2	B	405	
3	C	298	
4	D	286	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14273 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 damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	822	6465	4098	1090	1243	34	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1141	TRP	-	expression tag	UNP Q16531
A	1142	SER	-	expression tag	UNP Q16531
A	1143	HIS	-	expression tag	UNP Q16531
A	1144	PRO	-	expression tag	UNP Q16531
A	1145	GLN	-	expression tag	UNP Q16531
A	1146	PHE	-	expression tag	UNP Q16531
A	1147	GLU	-	expression tag	UNP Q16531
A	1148	LYS	-	expression tag	UNP Q16531

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	382	3083	1964	529	566	24	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	38	GLY	-	expression tag	UNP Q96SW2
B	39	SER	-	expression tag	UNP Q96SW2

- Molecule 3 is a protein called Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
3	C	298	2401	1559	408	425	1	8	0	0

- Molecule 4 is a protein called G1/S-specific cyclin-E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	276	Total	C	N	O	S	0	0
			2260	1467	371	405	17		

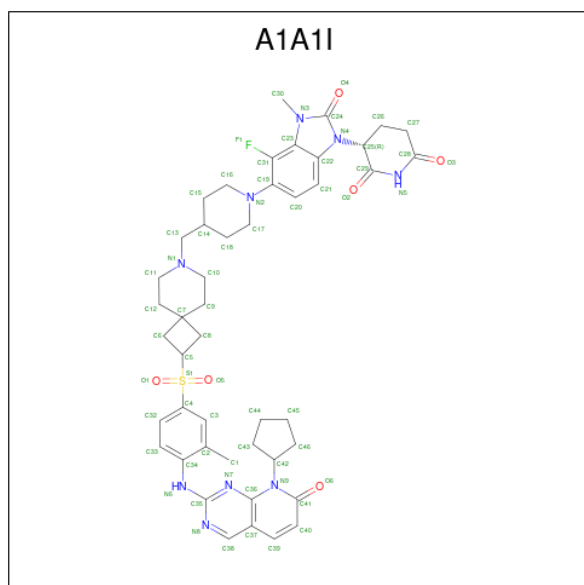
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	93	SER	-	expression tag	UNP P24864
D	94	GLY	-	expression tag	UNP P24864
D	95	SER	-	expression tag	UNP P24864

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	

- Molecule 6 is (3R)-3-(5-{4-[(2-{4-[(8-cyclopentyl-7-oxo-7,8-dihydropyrido[2,3-d]pyrimidin-2-yl)amino]-3-methylbenzene-1-sulfonyl}-7-azaspiro[3.5]nonan-7-yl)methyl]piperidin-1-yl}-4-fluoro-3-methyl-2-oxo-2,3-dihydro-1H-1,3-benzimidazol-1-yl)piperidine-2,6-dione (CCD ID: A1A1I) (formula: C<sub>46</sub>H<sub>54</sub>FN<sub>9</sub>O<sub>6</sub>S) (labeled as "Ligand of Interest" by depositor).

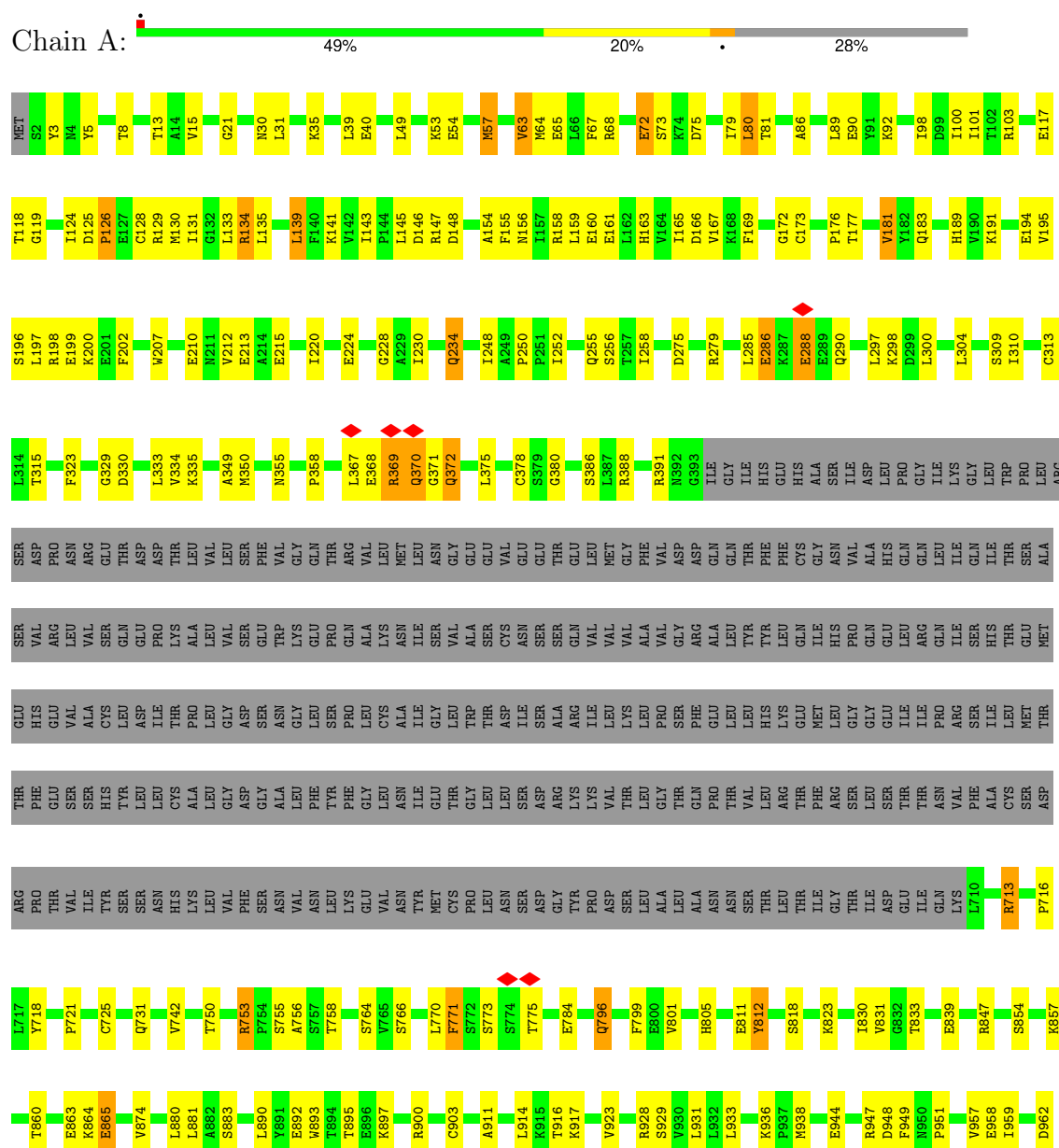


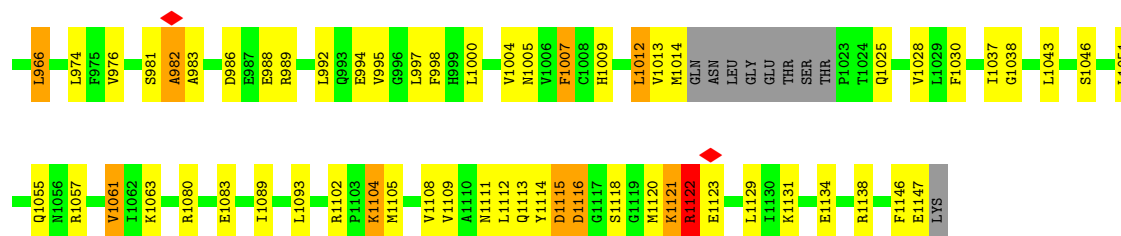
Mol	Chain	Residues	Atoms						AltConf
6	B	1	Total	C	F	N	O	S	0
			63	46	1	9	6	1	

### 3 Residue-property plots

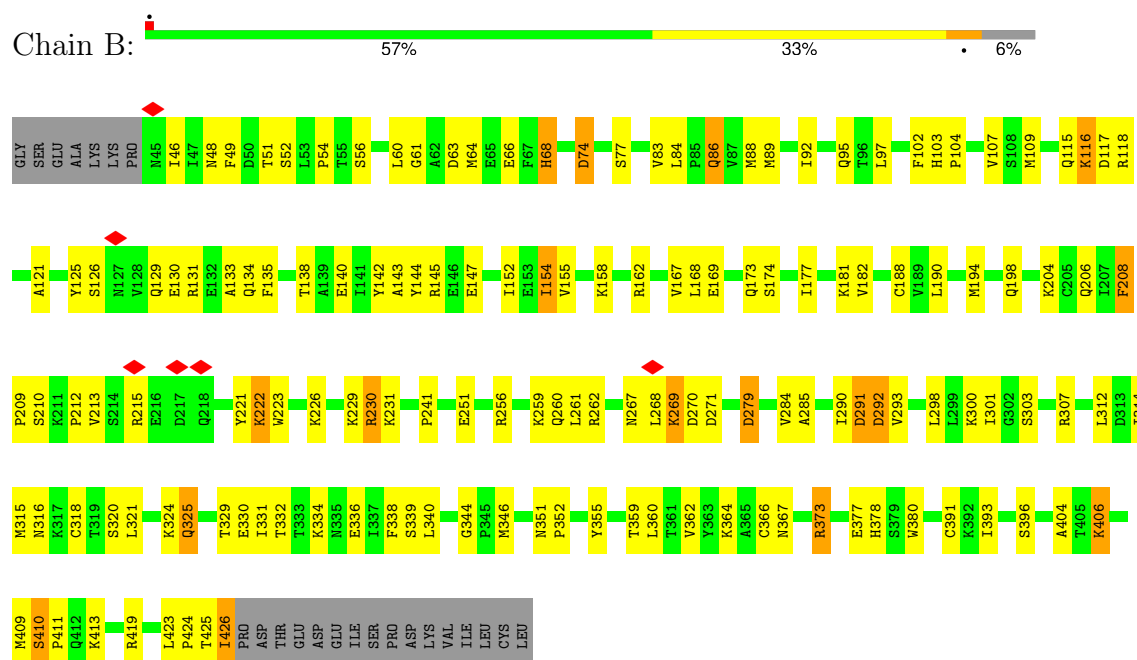
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: DNA damage-binding protein 1

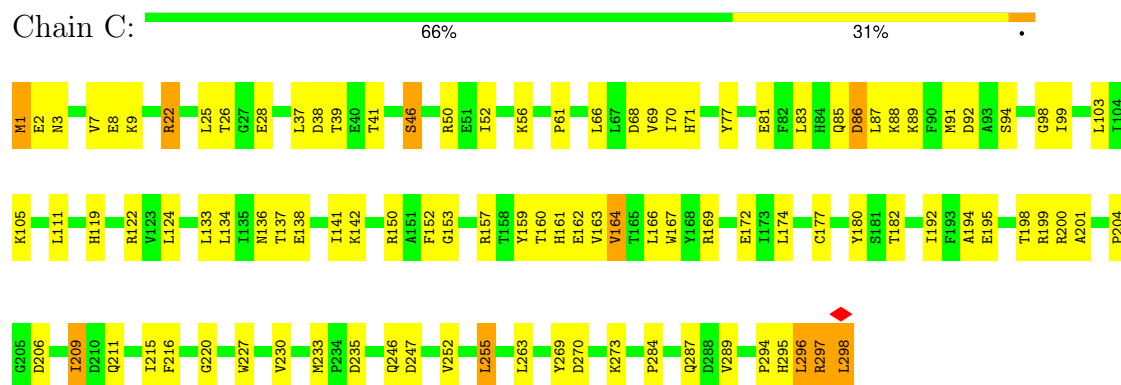




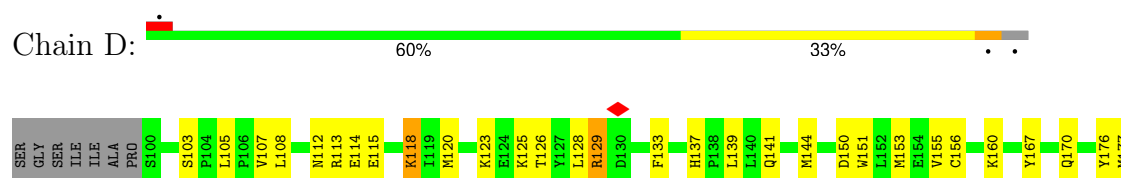
### • Molecule 2: Protein cereblon

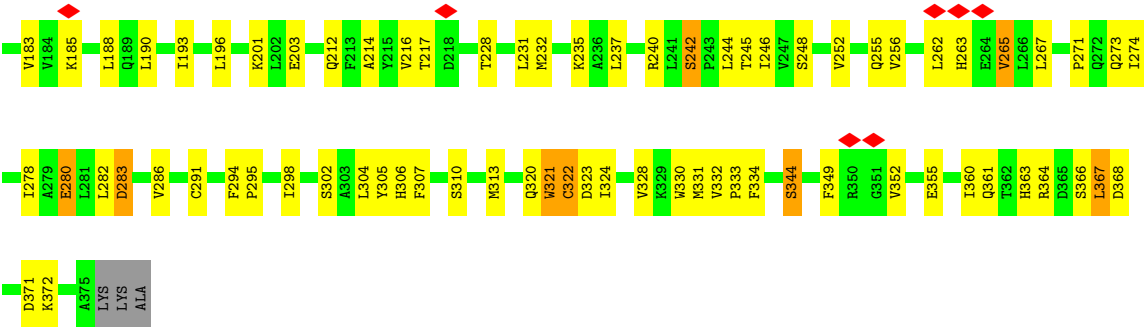


### • Molecule 3: Cyclin-dependent kinase 2



### • Molecule 4: G1/S-specific cyclin-E1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	537511	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 ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.913	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	369.152, 369.152, 369.152	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0487273, 1.0487273, 1.0487273	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: ZN, TPO, A1A1I

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	0.32	0/6586	0.57	0/8910
2	B	0.31	0/3156	0.58	0/4281
3	C	0.29	0/2451	0.56	0/3325
4	D	0.28	0/2316	0.53	0/3142
All	All	0.31	0/14509	0.56	0/19658

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	6465	0	6412	172	0
2	B	3083	0	3074	97	0
3	C	2401	0	2449	70	0
4	D	2260	0	2263	82	0
5	B	1	0	0	0	0
6	B	63	0	0	1	0
All	All	14273	0	14198	409	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 14.

All (409) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:278:ILE:HD12	4:D:304:LEU:HA	1.57	0.84
1:A:92:LYS:HD2	1:A:101:ILE:HD11	1.62	0.81
2:B:290:ILE:HA	2:B:424:PRO:HG2	1.65	0.78
2:B:126:SER:HB3	2:B:134:GLN:HE22	1.48	0.78
3:C:252:VAL:HB	3:C:255:LEU:HD21	1.67	0.76
6:B:502:A1A1I:F1	6:B:502:A1A1I:C16	2.25	0.74
4:D:352:VAL:HG11	4:D:360:ILE:HD11	1.69	0.73
4:D:320:GLN:OE1	4:D:322:CYS:N	2.20	0.73
2:B:206:GLN:NE2	2:B:231:LYS:HA	2.04	0.73
3:C:163:VAL:HG23	3:C:164:VAL:HG23	1.69	0.73
3:C:98:GLY:HA3	3:C:199:ARG:HH12	1.54	0.72
2:B:206:GLN:HE21	2:B:231:LYS:HA	1.55	0.71
2:B:134:GLN:N	2:B:134:GLN:OE1	2.22	0.71
1:A:39:LEU:HD13	1:A:64:MET:HE1	1.73	0.70
1:A:80:LEU:HD23	1:A:86:ALA:HB2	1.74	0.69
1:A:839:GLU:OE1	1:A:839:GLU:N	2.24	0.68
1:A:974:LEU:HD22	1:A:1000:LEU:HB2	1.75	0.68
1:A:252:ILE:HD11	1:A:304:LEU:HB2	1.76	0.68
1:A:931:LEU:HD21	1:A:944:GLU:HG3	1.76	0.67
4:D:114:GLU:OE1	4:D:114:GLU:N	2.23	0.66
1:A:731:GLN:OE1	1:A:796:GLN:NE2	2.28	0.66
3:C:85:GLN:HE21	3:C:89:LYS:HD3	1.61	0.66
2:B:336:GLU:N	2:B:336:GLU:OE2	2.26	0.66
4:D:313:MET:HE1	4:D:324:ILE:HG21	1.76	0.66
1:A:890:LEU:HB3	1:A:903:CYS:HB2	1.78	0.66
3:C:166:LEU:HD13	3:C:169:ARG:HH21	1.60	0.65
1:A:129:ARG:HE	1:A:176:PRO:HG3	1.61	0.65
4:D:283:ASP:OD2	4:D:361:GLN:NE2	2.29	0.65
1:A:31:LEU:HD23	1:A:49:LEU:HD21	1.79	0.65
3:C:172:GLU:OE1	3:C:172:GLU:N	2.21	0.65
3:C:137:THR:HG22	3:C:296:LEU:HD21	1.79	0.65
4:D:129:ARG:NH2	4:D:294:PHE:O	2.29	0.65
1:A:63:VAL:HG13	1:A:80:LEU:HB3	1.79	0.65
3:C:81:GLU:OE2	3:C:142:LYS:NZ	2.24	0.65
1:A:770:LEU:HD13	1:A:865:GLU:HG2	1.79	0.65
4:D:123:LYS:HD2	4:D:244:LEU:HG	1.79	0.64
2:B:107:VAL:HG22	2:B:155:VAL:HG23	1.80	0.63
4:D:313:MET:HE1	4:D:324:ILE:HD13	1.79	0.63
2:B:102:PHE:HD1	2:B:154:ILE:HG22	1.62	0.63
2:B:167:VAL:HA	2:B:182:VAL:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:294:PRO:HB2	3:C:296:LEU:HD13	1.80	0.63
1:A:161:GLU:OE2	1:A:191:LYS:NZ	2.30	0.63
2:B:208:PHE:HA	2:B:230:ARG:HH22	1.64	0.63
4:D:252:VAL:O	4:D:256:VAL:HG23	1.99	0.63
4:D:120:MET:HG2	4:D:244:LEU:HD11	1.81	0.62
1:A:983:ALA:HB1	1:A:989:ARG:HH21	1.64	0.62
4:D:232:MET:SD	4:D:232:MET:N	2.73	0.62
1:A:117:GLU:OE2	2:B:206:GLN:HB3	2.00	0.62
1:A:986:ASP:OD1	1:A:989:ARG:NH1	2.33	0.61
2:B:331:ILE:HG22	2:B:332:THR:HG23	1.81	0.61
2:B:84:LEU:HD23	2:B:109:MET:HE1	1.83	0.61
3:C:150:ARG:NH2	4:D:203:GLU:O	2.33	0.61
2:B:290:ILE:HG21	2:B:314:ILE:HD12	1.83	0.61
1:A:974:LEU:HD21	1:A:998:PHE:HD2	1.66	0.60
1:A:288:GLU:HB3	1:A:298:LYS:HD2	1.83	0.60
1:A:742:VAL:HG23	1:A:750:THR:HG23	1.83	0.60
4:D:107:VAL:HA	4:D:113:ARG:HD2	1.83	0.60
3:C:46:SER:OG	4:D:201:LYS:O	2.20	0.60
1:A:1134:GLU:OE2	1:A:1138:ARG:NH2	2.35	0.60
2:B:49:PHE:HD2	2:B:340:LEU:HD22	1.67	0.60
1:A:976:VAL:HG23	1:A:995:VAL:HG13	1.83	0.59
1:A:166:ASP:HB2	2:B:204:LYS:HD2	1.84	0.59
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	1.84	0.59
1:A:1083:GLU:N	1:A:1083:GLU:OE1	2.35	0.59
4:D:246:ILE:HG22	4:D:282:LEU:HD13	1.84	0.59
1:A:248:ILE:HD12	1:A:250:PRO:HD3	1.83	0.59
2:B:169:GLU:HB2	2:B:181:LYS:HE3	1.84	0.59
4:D:298:ILE:HG13	4:D:324:ILE:HD12	1.84	0.59
3:C:150:ARG:HH11	3:C:159:TYR:HB3	1.67	0.58
4:D:105:LEU:O	4:D:113:ARG:NH2	2.36	0.58
3:C:122:ARG:HH21	3:C:153:GLY:HA2	1.69	0.58
2:B:329:THR:HG22	2:B:393:ILE:HD13	1.86	0.57
3:C:297:ARG:HH21	3:C:298:LEU:HB3	1.69	0.57
4:D:255:GLN:NE2	4:D:267:LEU:O	2.38	0.57
4:D:242:SER:OG	4:D:242:SER:O	2.22	0.57
2:B:373:ARG:HD3	3:C:88:LYS:NZ	2.20	0.56
1:A:958:GLU:OE2	1:A:1009:HIS:NE2	2.38	0.56
2:B:154:ILE:HD12	2:B:154:ILE:O	2.06	0.56
4:D:306:HIS:HE1	4:D:328:VAL:HG13	1.70	0.56
1:A:160:GLU:CD	1:A:160:GLU:H	2.09	0.56
2:B:61:GLY:HA3	2:B:145:ARG:HH12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:153:MET:SD	4:D:361:GLN:NE2	2.79	0.56
1:A:1121:LYS:O	1:A:1123:GLU:N	2.39	0.56
4:D:129:ARG:HH22	4:D:295:PRO:HA	1.71	0.56
1:A:118:THR:HB	1:A:134:ARG:HH22	1.71	0.56
1:A:948:ASP:C	1:A:949:PHE:HD1	2.10	0.55
2:B:102:PHE:CD1	2:B:154:ILE:HG22	2.40	0.55
1:A:1061:VAL:HG13	1:A:1104:LYS:HG2	1.87	0.55
2:B:145:ARG:NE	2:B:147:GLU:OE2	2.39	0.55
2:B:425:THR:O	2:B:426:ILE:C	2.44	0.55
2:B:269:LYS:HD2	2:B:270:ASP:N	2.22	0.55
3:C:37:LEU:HD12	3:C:37:LEU:H	1.72	0.55
3:C:194:ALA:HB2	3:C:263:LEU:HD21	1.89	0.55
3:C:138:GLU:OE1	3:C:138:GLU:N	2.39	0.55
2:B:49:PHE:CD2	2:B:340:LEU:HD22	2.41	0.55
2:B:152:ILE:HG22	2:B:154:ILE:HG23	1.89	0.55
1:A:368:GLU:HB3	1:A:370:GLN:NE2	2.22	0.55
1:A:1109:VAL:HG12	1:A:1129:LEU:HD12	1.89	0.55
4:D:280:GLU:OE2	4:D:364:ARG:NH1	2.40	0.54
1:A:166:ASP:OD1	1:A:167:VAL:N	2.40	0.54
3:C:246:GLN:OE1	3:C:247:ASP:N	2.39	0.54
3:C:83:LEU:HD13	3:C:136:ASN:HB3	1.89	0.54
3:C:206:ASP:OD1	3:C:206:ASP:N	2.40	0.54
4:D:368:ASP:O	4:D:372:LYS:NZ	2.31	0.54
2:B:346:MET:HE2	2:B:360:LEU:HB2	1.88	0.54
4:D:212:GLN:O	4:D:216:VAL:HG23	2.08	0.54
4:D:103:SER:HB3	4:D:113:ARG:HH12	1.72	0.54
1:A:358:PRO:HD2	1:A:380:GLY:H	1.73	0.54
1:A:917:LYS:HB3	1:A:959:ILE:HD13	1.90	0.54
4:D:126:THR:HG21	4:D:240:ARG:HH22	1.72	0.54
1:A:119:GLY:O	1:A:134:ARG:NH2	2.33	0.54
1:A:847:ARG:NE	1:A:863:GLU:OE2	2.41	0.54
3:C:7:VAL:HG21	3:C:22:ARG:HH11	1.73	0.54
1:A:133:LEU:HB3	1:A:135:LEU:HD13	1.89	0.54
1:A:155:PHE:HZ	1:A:197:LEU:HD22	1.72	0.54
2:B:373:ARG:HD3	3:C:88:LYS:HZ1	1.73	0.54
2:B:118:ARG:HB2	2:B:118:ARG:NH1	2.23	0.53
1:A:250:PRO:HB2	1:A:252:ILE:HG22	1.89	0.53
1:A:994:GLU:OE2	1:A:997:LEU:HG	2.08	0.53
4:D:105:LEU:HD21	4:D:265:VAL:HG21	1.89	0.53
1:A:220:ILE:HG12	1:A:230:ILE:HB	1.90	0.53
2:B:116:LYS:HD2	2:B:116:LYS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:HB	1:A:181:VAL:HG22	1.91	0.53
4:D:177:MET:SD	4:D:177:MET:N	2.82	0.53
1:A:1057:ARG:NH2	1:A:1111:ASN:O	2.37	0.53
1:A:839:GLU:HB3	2:B:221:TYR:HE1	1.74	0.52
3:C:284:PRO:O	3:C:287:GLN:HB2	2.09	0.52
2:B:168:LEU:HB3	2:B:181:LYS:NZ	2.24	0.52
2:B:86:GLN:OE1	2:B:86:GLN:N	2.31	0.52
1:A:1012:LEU:HD12	1:A:1013:VAL:HG12	1.92	0.52
1:A:368:GLU:OE1	1:A:369:ARG:N	2.43	0.52
2:B:292:ASP:OD1	2:B:293:VAL:N	2.43	0.52
3:C:296:LEU:H	3:C:296:LEU:HD22	1.75	0.52
4:D:150:ASP:OD2	4:D:366:SER:HB2	2.10	0.52
3:C:38:ASP:OD1	3:C:39:THR:N	2.43	0.52
3:C:99:ILE:HG22	3:C:103:LEU:HB3	1.91	0.51
4:D:113:ARG:HG2	4:D:114:GLU:OE1	2.10	0.51
1:A:195:VAL:HG12	1:A:202:PHE:HE1	1.75	0.51
2:B:206:GLN:NE2	2:B:230:ARG:O	2.34	0.51
4:D:332:VAL:HB	4:D:333:PRO:HD3	1.90	0.51
1:A:966:LEU:HD21	1:A:1007:PHE:CZ	2.45	0.51
2:B:83:VAL:HG22	2:B:121:ALA:HB3	1.92	0.51
1:A:764:SER:OG	1:A:805:HIS:ND1	2.35	0.51
2:B:66:GLU:O	2:B:68:HIS:ND1	2.43	0.51
2:B:168:LEU:HD23	2:B:181:LYS:HE2	1.93	0.51
4:D:278:ILE:HD13	4:D:307:PHE:HD2	1.76	0.51
2:B:84:LEU:HD13	2:B:86:GLN:HE22	1.74	0.51
3:C:71:HIS:HB3	4:D:235:LYS:NZ	2.26	0.51
4:D:313:MET:CE	4:D:324:ILE:HD13	2.41	0.51
1:A:146:ASP:OD1	1:A:147:ARG:N	2.43	0.51
1:A:386:SER:OG	1:A:388:ARG:NH1	2.43	0.51
2:B:212:PRO:HG3	2:B:223:TRP:CG	2.46	0.50
2:B:215:ARG:HH21	2:B:262:ARG:HH21	1.58	0.50
2:B:315:MET:O	2:B:334:LYS:HE2	2.12	0.50
3:C:50:ARG:HH12	3:C:150:ARG:NH2	2.09	0.50
1:A:923:VAL:HG22	1:A:931:LEU:HB3	1.92	0.50
3:C:26:THR:HG23	3:C:28:GLU:HG2	1.93	0.50
3:C:68:ASP:OD1	3:C:69:VAL:N	2.44	0.50
4:D:112:ASN:HB3	4:D:115:GLU:OE1	2.10	0.50
1:A:938:MET:N	1:A:938:MET:SD	2.83	0.50
2:B:61:GLY:HA3	2:B:145:ARG:NH1	2.26	0.50
1:A:158:ARG:CZ	1:A:158:ARG:HB3	2.42	0.50
1:A:330:ASP:OD1	1:A:388:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:ALA:HB1	2:B:298:LEU:HD21	1.93	0.50
2:B:324:LYS:HZ2	2:B:325:GLN:N	2.10	0.50
4:D:231:LEU:O	4:D:235:LYS:HG2	2.12	0.50
1:A:315:THR:HG23	1:A:323:PHE:HB3	1.94	0.50
1:A:234:GLN:HE21	1:A:234:GLN:CA	2.23	0.49
4:D:344:SER:HB3	4:D:364:ARG:NH1	2.27	0.49
2:B:103:HIS:ND1	2:B:104:PRO:HD2	2.27	0.49
3:C:216:PHE:O	3:C:220:GLY:N	2.44	0.49
1:A:172:GLY:HA3	1:A:224:GLU:OE2	2.12	0.49
3:C:8:GLU:HG2	3:C:9:LYS:N	2.28	0.49
1:A:771:PHE:HE2	1:A:847:ARG:HG3	1.78	0.49
4:D:228:THR:O	4:D:232:MET:HE2	2.13	0.49
3:C:122:ARG:NH2	3:C:153:GLY:HA2	2.28	0.48
4:D:278:ILE:HD11	4:D:307:PHE:HB2	1.94	0.48
1:A:234:GLN:NE2	1:A:234:GLN:HA	2.28	0.48
2:B:115:GLN:OE1	2:B:115:GLN:N	2.33	0.48
1:A:230:ILE:HD11	1:A:285:LEU:HD21	1.94	0.48
4:D:367:LEU:H	4:D:367:LEU:HD12	1.79	0.48
1:A:933:LEU:HD23	1:A:944:GLU:HA	1.94	0.48
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.49	0.48
1:A:125:ASP:HB3	1:A:129:ARG:H	1.78	0.48
1:A:378:CYS:HB3	1:A:721:PRO:HB2	1.95	0.48
1:A:207:TRP:HZ2	1:A:228:GLY:HA2	1.79	0.47
2:B:279:ASP:OD1	2:B:279:ASP:N	2.47	0.47
2:B:410:SER:OG	2:B:411:PRO:HD3	2.14	0.47
1:A:213:GLU:HG2	1:A:215:GLU:H	1.79	0.47
1:A:830:ILE:HD13	1:A:880:LEU:HD21	1.95	0.47
2:B:129:GLN:NE2	2:B:130:GLU:OE2	2.47	0.47
4:D:115:GLU:HA	4:D:118:LYS:HE2	1.95	0.47
1:A:812:TYR:CE1	2:B:241:PRO:HB3	2.49	0.47
3:C:105:LYS:HG2	3:C:289:VAL:HG23	1.97	0.47
1:A:40:GLU:HG2	1:A:54:GLU:HG3	1.96	0.47
1:A:881:LEU:HD21	1:A:916:THR:HG21	1.96	0.47
2:B:300:LYS:HE2	2:B:300:LYS:HA	1.97	0.47
3:C:50:ARG:HH12	3:C:150:ARG:CZ	2.28	0.47
3:C:199:ARG:HD3	3:C:199:ARG:N	2.28	0.47
4:D:151:TRP:O	4:D:155:VAL:HG23	2.15	0.47
1:A:126:PRO:HD3	1:A:169:PHE:HB3	1.97	0.47
4:D:137:HIS:ND1	4:D:183:VAL:HG22	2.30	0.47
2:B:63:ASP:O	2:B:145:ARG:HD2	2.15	0.47
2:B:134:GLN:HG2	2:B:135:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:SER:HB2	2:B:330:GLU:OE2	2.14	0.47
3:C:227:TRP:CE3	3:C:269:TYR:HB3	2.49	0.47
4:D:302:SER:HB3	4:D:324:ILE:HD11	1.97	0.47
1:A:21:GLY:O	1:A:30:ASN:HB2	2.15	0.47
1:A:981:SER:O	1:A:983:ALA:N	2.47	0.47
1:A:1120:MET:C	1:A:1122:ARG:N	2.68	0.47
3:C:163:VAL:O	3:C:169:ARG:HD3	2.15	0.47
3:C:167:TRP:HA	3:C:211:GLN:HE22	1.79	0.47
1:A:234:GLN:CA	1:A:234:GLN:NE2	2.78	0.46
1:A:1121:LYS:C	1:A:1122:ARG:HG2	2.34	0.46
4:D:355:GLU:OE1	4:D:355:GLU:N	2.49	0.46
1:A:369:ARG:H	1:A:369:ARG:HG3	1.66	0.46
2:B:115:GLN:HG2	2:B:116:LYS:H	1.81	0.46
2:B:251:GLU:OE2	2:B:251:GLU:HA	2.16	0.46
2:B:256:ARG:HB3	2:B:312:LEU:HD21	1.97	0.46
3:C:133:LEU:HD11	3:C:192:ILE:HD13	1.97	0.46
4:D:306:HIS:CE1	4:D:328:VAL:HG22	2.50	0.46
1:A:173:CYS:HG	1:A:177:THR:HG1	1.59	0.46
1:A:375:LEU:HD23	1:A:1037:ILE:HD13	1.98	0.46
2:B:269:LYS:HE3	2:B:271:ASP:HB3	1.97	0.46
2:B:406:LYS:H	2:B:409:MET:HE1	1.80	0.46
4:D:295:PRO:O	4:D:298:ILE:HG22	2.15	0.46
1:A:53:LYS:HD2	1:A:98:ILE:HD12	1.97	0.46
1:A:1057:ARG:HD3	1:A:1108:VAL:O	2.16	0.46
4:D:103:SER:CB	4:D:113:ARG:HH12	2.29	0.45
4:D:331:MET:HA	4:D:334:PHE:HD2	1.81	0.45
1:A:212:VAL:HG22	1:A:213:GLU:H	1.81	0.45
1:A:215:GLU:OE1	1:A:215:GLU:HA	2.17	0.45
3:C:297:ARG:HH21	3:C:298:LEU:HD22	1.82	0.45
4:D:103:SER:HB3	4:D:113:ARG:HH22	1.82	0.45
1:A:368:GLU:HB3	1:A:370:GLN:HE21	1.82	0.45
2:B:173:GLN:HG3	2:B:174:SER:H	1.82	0.45
3:C:70:ILE:HD11	3:C:77:TYR:HD2	1.82	0.45
3:C:227:TRP:O	3:C:230:VAL:HG23	2.17	0.45
1:A:67:PHE:HB2	1:A:128:CYS:SG	2.57	0.45
2:B:339:SER:HB2	2:B:344:GLY:C	2.37	0.45
4:D:156:CYS:SG	4:D:196:LEU:HD11	2.57	0.45
1:A:892:GLU:OE2	1:A:900:ARG:NH2	2.50	0.45
3:C:169:ARG:HG2	3:C:174:LEU:HG	1.99	0.45
4:D:193:ILE:HD12	4:D:193:ILE:HA	1.82	0.45
2:B:338:PHE:CE2	2:B:340:LEU:HG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:176:TYR:HB2	4:D:237:LEU:HD11	1.99	0.45
4:D:349:PHE:CD1	4:D:360:ILE:HD12	2.52	0.45
1:A:131:ILE:HG13	1:A:145:LEU:HD11	1.99	0.45
1:A:57:MET:HE3	1:A:57:MET:HB3	1.79	0.45
1:A:1147:GLU:OE1	1:A:1147:GLU:HA	2.17	0.45
2:B:51:THR:O	2:B:54:PRO:HD2	2.16	0.45
2:B:267:ASN:OD1	2:B:268:LEU:N	2.50	0.45
4:D:123:LYS:HB2	4:D:123:LYS:HE2	1.59	0.45
1:A:196:SER:O	1:A:200:LYS:HA	2.16	0.44
2:B:359:THR:HG21	2:B:380:TRP:CZ3	2.52	0.44
3:C:297:ARG:H	3:C:297:ARG:HG3	1.54	0.44
1:A:13:THR:HB	1:A:355:ASN:HA	1.98	0.44
2:B:215:ARG:HE	2:B:262:ARG:CZ	2.31	0.44
3:C:52:ILE:O	3:C:56:LYS:HG3	2.17	0.44
3:C:70:ILE:HG13	3:C:77:TYR:HB2	1.99	0.44
1:A:15:VAL:HA	1:A:35:LYS:HA	2.00	0.44
1:A:68:ARG:HB2	1:A:75:ASP:OD1	2.18	0.44
4:D:331:MET:O	4:D:332:VAL:C	2.55	0.44
3:C:105:LYS:HD2	3:C:289:VAL:HA	1.98	0.44
3:C:209:ILE:HD13	3:C:209:ILE:HA	1.69	0.44
3:C:89:LYS:HE3	3:C:298:LEU:HG	2.00	0.44
1:A:248:ILE:HG12	1:A:300:LEU:HB3	1.98	0.44
1:A:309:SER:O	1:A:310:ILE:C	2.54	0.44
1:A:725:CYS:SG	1:A:818:SER:HB3	2.57	0.44
1:A:948:ASP:OD1	1:A:992:LEU:HB3	2.17	0.44
2:B:261:LEU:HD11	2:B:284:VAL:HG22	2.00	0.44
2:B:410:SER:H	2:B:410:SER:HG	1.53	0.44
1:A:176:PRO:HB2	1:A:195:VAL:CG2	2.47	0.44
1:A:1120:MET:O	1:A:1122:ARG:N	2.51	0.44
4:D:153:MET:HB3	4:D:363:HIS:HB2	1.99	0.44
3:C:87:LEU:O	3:C:91:MET:HG3	2.18	0.43
4:D:190:LEU:O	4:D:193:ILE:HG22	2.18	0.43
4:D:331:MET:HA	4:D:334:PHE:CD2	2.53	0.43
1:A:5:TYR:HB2	1:A:1043:LEU:HD11	2.01	0.43
1:A:285:LEU:HD23	1:A:297:LEU:HD11	1.99	0.43
1:A:1114:TYR:CE2	1:A:1116:ASP:HB3	2.53	0.43
1:A:386:SER:HB2	1:A:716:PRO:HA	2.00	0.43
2:B:352:PRO:HD3	2:B:378:HIS:ND1	2.33	0.43
2:B:168:LEU:HB3	2:B:181:LYS:HZ3	1.81	0.43
4:D:139:LEU:H	4:D:139:LEU:HD12	1.83	0.43
4:D:321:TRP:HA	4:D:321:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HB2	1:A:141:LYS:HG2	2.01	0.43
1:A:256:SER:OG	1:A:275:ASP:OD2	2.34	0.43
1:A:713:ARG:HH21	1:A:799:PHE:HD2	1.65	0.43
2:B:364:LYS:HB2	2:B:364:LYS:NZ	2.34	0.43
1:A:183:GLN:NE2	2:B:209:PRO:O	2.52	0.43
1:A:1000:LEU:HD21	1:A:1030:PHE:CE1	2.54	0.43
4:D:330:TRP:HZ3	4:D:331:MET:HE2	1.82	0.43
1:A:881:LEU:HD11	1:A:914:LEU:HD21	2.01	0.43
1:A:1007:PHE:CE1	1:A:1028:VAL:HG12	2.54	0.43
1:A:1063:LYS:HA	1:A:1063:LYS:HE2	2.00	0.43
3:C:124:LEU:HG	3:C:152:PHE:HD2	1.84	0.43
1:A:883:SER:HB3	1:A:911:ALA:HB3	2.01	0.43
2:B:74:ASP:O	2:B:77:SER:OG	2.21	0.43
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.84	0.43
1:A:196:SER:O	1:A:200:LYS:N	2.51	0.43
2:B:117:ASP:O	2:B:118:ARG:HG3	2.19	0.43
3:C:1:MET:SD	3:C:2:GLU:HG2	2.59	0.43
3:C:201:ALA:HB3	3:C:204:PRO:HG3	2.01	0.43
4:D:306:HIS:NE2	4:D:331:MET:HB3	2.34	0.43
1:A:65:GLU:N	1:A:65:GLU:OE1	2.52	0.42
1:A:823:LYS:HD3	1:A:823:LYS:HA	1.63	0.42
2:B:125:TYR:CD1	2:B:133:ALA:HB2	2.54	0.42
1:A:130:MET:HE2	1:A:130:MET:HB3	1.85	0.42
1:A:811:GLU:OE2	1:A:847:ARG:HD3	2.20	0.42
3:C:71:HIS:HB3	4:D:235:LYS:HZ3	1.83	0.42
3:C:111:LEU:HD21	3:C:141:ILE:HG12	2.00	0.42
1:A:1055:GLN:HG2	1:A:1093:LEU:HD23	2.01	0.42
3:C:3:ASN:HD21	3:C:25:LEU:HB2	1.84	0.42
1:A:982:ALA:HB3	1:A:988:GLU:HG2	2.01	0.42
1:A:1131:LYS:HB3	1:A:1131:LYS:HE2	1.77	0.42
2:B:332:THR:HG21	2:B:362:VAL:HG21	2.00	0.42
1:A:92:LYS:HB2	1:A:92:LYS:NZ	2.34	0.42
1:A:929:SER:HB2	1:A:949:PHE:CD2	2.55	0.42
1:A:948:ASP:O	1:A:949:PHE:HD1	2.02	0.42
1:A:124:ILE:O	1:A:125:ASP:C	2.57	0.42
1:A:286:GLU:HG3	1:A:288:GLU:HB2	2.02	0.42
1:A:883:SER:OG	1:A:914:LEU:HD13	2.20	0.42
3:C:119:HIS:CE1	3:C:182:THR:HB	2.55	0.42
4:D:305:TYR:CE2	4:D:321:TRP:HH2	2.37	0.42
1:A:139:LEU:HD12	1:A:156:ASN:HD22	1.85	0.42
1:A:371:GLY:C	1:A:372:GLN:HG2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:283:ASP:OD1	4:D:283:ASP:N	2.53	0.42
1:A:49:LEU:HD13	1:A:333:LEU:HD11	2.02	0.42
2:B:118:ARG:O	2:B:140:GLU:HA	2.20	0.42
2:B:194:MET:O	2:B:198:GLN:HB2	2.20	0.42
4:D:167:TYR:HB3	4:D:245:THR:HB	2.01	0.42
1:A:90:GLU:OE1	1:A:103:ARG:NE	2.53	0.42
3:C:61:PRO:O	3:C:142:LYS:HE2	2.20	0.42
4:D:214:ALA:O	4:D:217:THR:OG1	2.32	0.42
1:A:63:VAL:HG23	1:A:65:GLU:OE2	2.19	0.41
1:A:125:ASP:HB2	1:A:130:MET:H	1.84	0.41
1:A:143:ILE:HG12	1:A:154:ALA:HB2	2.02	0.41
1:A:297:LEU:HD21	1:A:300:LEU:HD13	2.02	0.41
1:A:753:ARG:HE	1:A:753:ARG:HB3	1.75	0.41
2:B:226:LYS:HB3	2:B:226:LYS:HE2	1.72	0.41
2:B:423:LEU:HD13	2:B:424:PRO:O	2.20	0.41
2:B:143:ALA:HB3	2:B:158:LYS:HB2	2.02	0.41
2:B:351:ASN:HD21	2:B:355:TYR:HD2	1.66	0.41
2:B:419:ARG:NH1	2:B:419:ARG:HG2	2.35	0.41
4:D:108:LEU:HA	4:D:108:LEU:HD23	1.84	0.41
1:A:57:MET:HE1	1:A:79:ILE:HG21	2.02	0.41
1:A:974:LEU:CD2	1:A:1000:LEU:HB2	2.47	0.41
3:C:38:ASP:OD1	3:C:39:THR:HG23	2.19	0.41
3:C:94:SER:O	3:C:98:GLY:HA2	2.20	0.41
1:A:1120:MET:C	1:A:1122:ARG:H	2.24	0.41
1:A:1121:LYS:HB3	1:A:1121:LYS:HE2	1.47	0.41
1:A:1146:PHE:O	1:A:1147:GLU:HB2	2.20	0.41
2:B:60:LEU:HD12	2:B:60:LEU:HA	1.94	0.41
3:C:66:LEU:HD11	3:C:69:VAL:CG1	2.50	0.41
1:A:811:GLU:HG2	1:A:833:THR:HB	2.02	0.41
1:A:1102:ARG:HD2	1:A:1105:MET:HE3	2.02	0.41
2:B:221:TYR:HD2	2:B:222:LYS:HZ3	1.67	0.41
2:B:301:ILE:HG21	2:B:307:ARG:N	2.36	0.41
3:C:56:LYS:HZ3	3:C:66:LEU:HD12	1.86	0.41
1:A:72:GLU:OE2	1:A:73:SER:N	2.54	0.41
2:B:173:GLN:HB3	2:B:177:ILE:HB	2.03	0.41
4:D:160:LYS:HB2	4:D:160:LYS:HE2	1.61	0.41
4:D:185:LYS:HA	4:D:188:LEU:HG	2.02	0.41
1:A:129:ARG:NE	1:A:176:PRO:HG3	2.31	0.41
1:A:165:ILE:HD13	1:A:165:ILE:HA	1.89	0.41
1:A:893:TRP:HZ2	1:A:897:LYS:HD2	1.85	0.41
3:C:86:ASP:OD1	3:C:86:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:THR:HG22	1:A:194:GLU:HG2	2.01	0.41
1:A:189:HIS:CD2	1:A:189:HIS:N	2.89	0.41
1:A:285:LEU:HB3	1:A:297:LEU:HD11	2.02	0.41
3:C:211:GLN:O	3:C:215:ILE:HG13	2.21	0.41
4:D:126:THR:O	4:D:128:LEU:HD22	2.20	0.41
4:D:271:PRO:HD2	4:D:274:ILE:HD11	2.02	0.41
1:A:207:TRP:CZ2	1:A:228:GLY:HA2	2.55	0.41
1:A:329:GLY:O	1:A:355:ASN:ND2	2.54	0.41
1:A:375:LEU:HD12	1:A:375:LEU:HA	1.83	0.41
1:A:874:VAL:HG11	1:A:916:THR:HG23	2.03	0.41
2:B:147:GLU:HB2	2:B:154:ILE:HD11	2.02	0.41
4:D:305:TYR:HB2	4:D:313:MET:SD	2.61	0.41
1:A:992:LEU:HD12	1:A:992:LEU:HA	1.94	0.41
2:B:92:ILE:O	2:B:95:GLN:HB2	2.21	0.41
3:C:194:ALA:O	3:C:198:THR:HG23	2.21	0.41
1:A:89:LEU:HB3	1:A:100:ILE:HG22	2.03	0.40
1:A:196:SER:O	1:A:200:LYS:CA	2.69	0.40
1:A:928:ARG:O	1:A:928:ARG:HG3	2.20	0.40
3:C:230:VAL:HA	3:C:233:MET:HG3	2.03	0.40
4:D:114:GLU:O	4:D:118:LYS:HE2	2.21	0.40
4:D:133:PHE:CD2	4:D:177:MET:HB2	2.56	0.40
1:A:3:TYR:N	1:A:3:TYR:CD1	2.89	0.40
1:A:258:ILE:HD13	1:A:275:ASP:HB3	2.03	0.40
1:A:315:THR:CG2	1:A:323:PHE:HB3	2.51	0.40
1:A:951:PRO:HG2	2:B:188:CYS:SG	2.61	0.40
1:A:1080:ARG:NH2	2:B:190:LEU:HD12	2.36	0.40
2:B:291:ASP:OD1	2:B:291:ASP:C	2.60	0.40
3:C:270:ASP:OD1	3:C:273:LYS:HB2	2.21	0.40
1:A:1112:LEU:HG	1:A:1113:GLN:H	1.87	0.40
2:B:89:MET:SD	2:B:97:LEU:HD13	2.61	0.40
2:B:404:ALA:HB1	2:B:409:MET:HE3	2.03	0.40
4:D:113:ARG:NH1	4:D:113:ARG:HG3	2.36	0.40
4:D:282:LEU:HD23	4:D:282:LEU:HA	1.91	0.40
1:A:330:ASP:HA	1:A:355:ASN:HB3	2.03	0.40
1:A:334:VAL:HG12	1:A:349:ALA:HA	2.03	0.40
1:A:718:TYR:HB2	1:A:755:SER:HA	2.03	0.40
1:A:756:ALA:HB1	1:A:801:VAL:HG21	2.04	0.40
2:B:269:LYS:HD2	2:B:270:ASP:H	1.85	0.40
3:C:86:ASP:HA	3:C:134:LEU:HA	2.02	0.40
4:D:103:SER:HB3	4:D:113:ARG:NH1	2.35	0.40
4:D:113:ARG:HG3	4:D:113:ARG:HH11	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	816/1148 (71%)	746 (91%)	64 (8%)	6 (1%)	19	41
2	B	380/405 (94%)	346 (91%)	31 (8%)	3 (1%)	16	39
3	C	295/298 (99%)	277 (94%)	16 (5%)	2 (1%)	19	41
4	D	274/286 (96%)	258 (94%)	15 (6%)	1 (0%)	30	54
All	All	1765/2137 (83%)	1627 (92%)	126 (7%)	12 (1%)	21	41

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1122	ARG
2	B	154	ILE
3	C	164	VAL
4	D	263	HIS
1	A	773	SER
1	A	1118	SER
3	C	161	HIS
2	B	213	VAL
1	A	1115	ASP
1	A	982	ALA
1	A	126	PRO
2	B	208	PHE

### 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	717/1007 (71%)	655 (91%)	62 (9%)	8	23
2	B	346/367 (94%)	306 (88%)	40 (12%)	4	13
3	C	262/262 (100%)	243 (93%)	19 (7%)	11	29
4	D	249/256 (97%)	227 (91%)	22 (9%)	8	22
All	All	1574/1892 (83%)	1431 (91%)	143 (9%)	10	20

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	57	MET
1	A	63	VAL
1	A	72	GLU
1	A	80	LEU
1	A	81	THR
1	A	134	ARG
1	A	139	LEU
1	A	148	ASP
1	A	163	HIS
1	A	181	VAL
1	A	198	ARG
1	A	199	GLU
1	A	210	GLU
1	A	234	GLN
1	A	255	GLN
1	A	279	ARG
1	A	286	GLU
1	A	288	GLU
1	A	290	GLN
1	A	313	CYS
1	A	335	LYS
1	A	350	MET
1	A	367	LEU
1	A	369	ARG
1	A	370	GLN
1	A	372	GLN
1	A	391	ARG
1	A	713	ARG
1	A	753	ARG
1	A	758	THR

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Mol	Chain	Res	Type
1	A	766	SER
1	A	771	PHE
1	A	775	THR
1	A	784	GLU
1	A	796	GLN
1	A	812	TYR
1	A	831	VAL
1	A	854	SER
1	A	857	LYS
1	A	860	THR
1	A	864	LYS
1	A	865	GLU
1	A	895	THR
1	A	936	LYS
1	A	947	ARG
1	A	957	VAL
1	A	962	ASP
1	A	966	LEU
1	A	1004	VAL
1	A	1005	ASN
1	A	1007	PHE
1	A	1012	LEU
1	A	1014	MET
1	A	1025	GLN
1	A	1046	SER
1	A	1061	VAL
1	A	1104	LYS
1	A	1115	ASP
1	A	1116	ASP
1	A	1121	LYS
1	A	1122	ARG
2	B	46	ILE
2	B	48	ASN
2	B	52	SER
2	B	56	SER
2	B	64	MET
2	B	68	HIS
2	B	74	ASP
2	B	86	GLN
2	B	88	MET
2	B	116	LYS
2	B	131	ARG

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Mol	Chain	Res	Type
2	B	138	THR
2	B	142	TYR
2	B	144	TYR
2	B	162	ARG
2	B	210	SER
2	B	222	LYS
2	B	229	LYS
2	B	230	ARG
2	B	259	LYS
2	B	260	GLN
2	B	269	LYS
2	B	279	ASP
2	B	291	ASP
2	B	292	ASP
2	B	303	SER
2	B	316	ASN
2	B	318	CYS
2	B	321	LEU
2	B	325	GLN
2	B	366	CYS
2	B	367	ASN
2	B	373	ARG
2	B	377	GLU
2	B	391	CYS
2	B	396	SER
2	B	406	LYS
2	B	410	SER
2	B	413	LYS
2	B	426	ILE
3	C	1	MET
3	C	22	ARG
3	C	41	THR
3	C	46	SER
3	C	86	ASP
3	C	92	ASP
3	C	157	ARG
3	C	162	GLU
3	C	177	CYS
3	C	180	TYR
3	C	195	GLU
3	C	200	ARG
3	C	209	ILE

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Mol	Chain	Res	Type
3	C	235	ASP
3	C	255	LEU
3	C	295	HIS
3	C	296	LEU
3	C	297	ARG
3	C	298	LEU
4	D	118	LYS
4	D	125	LYS
4	D	129	ARG
4	D	141	GLN
4	D	144	MET
4	D	170	GLN
4	D	242	SER
4	D	248	SER
4	D	262	LEU
4	D	265	VAL
4	D	273	GLN
4	D	280	GLU
4	D	283	ASP
4	D	286	VAL
4	D	291	CYS
4	D	310	SER
4	D	321	TRP
4	D	322	CYS
4	D	323	ASP
4	D	344	SER
4	D	367	LEU
4	D	371	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	A	1034	ASN
2	B	100	GLN
2	B	178	GLN
2	B	260	GLN
4	D	306	HIS



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	TPO	C	160	3	8,10,11	1.08	0	10,14,16	2.04	1 (10%)

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	TPO	C	160	3	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	160	TPO	P-OG1-CB	-5.85	107.43	123.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	A1A1I	B	502	-	70,72,72	0.52	0	89,110,110	1.07	6 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A1A1I	B	502	-	-	10/32/84/84	1/10/10/10

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	502	A1A1I	C17-N2-C19	4.34	126.49	116.19
6	B	502	A1A1I	C36-N9-C41	-3.35	120.25	121.90
6	B	502	A1A1I	C19-C31-C23	-2.68	119.47	123.61
6	B	502	A1A1I	C31-C19-N2	-2.46	117.54	120.41
6	B	502	A1A1I	C42-N9-C41	2.12	120.68	117.73
6	B	502	A1A1I	C17-N2-C16	2.11	116.32	111.57

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	502	A1A1I	C26-C25-N4-C22
6	B	502	A1A1I	C20-C19-N2-C16
6	B	502	A1A1I	C31-C19-N2-C16
6	B	502	A1A1I	N1-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
6	B	502	A1A1I	N1-C13-C14-C18
6	B	502	A1A1I	C6-C5-S1-O1
6	B	502	A1A1I	C14-C13-N1-C10
6	B	502	A1A1I	C14-C13-N1-C11
6	B	502	A1A1I	C26-C25-N4-C24
6	B	502	A1A1I	C6-C5-S1-O5

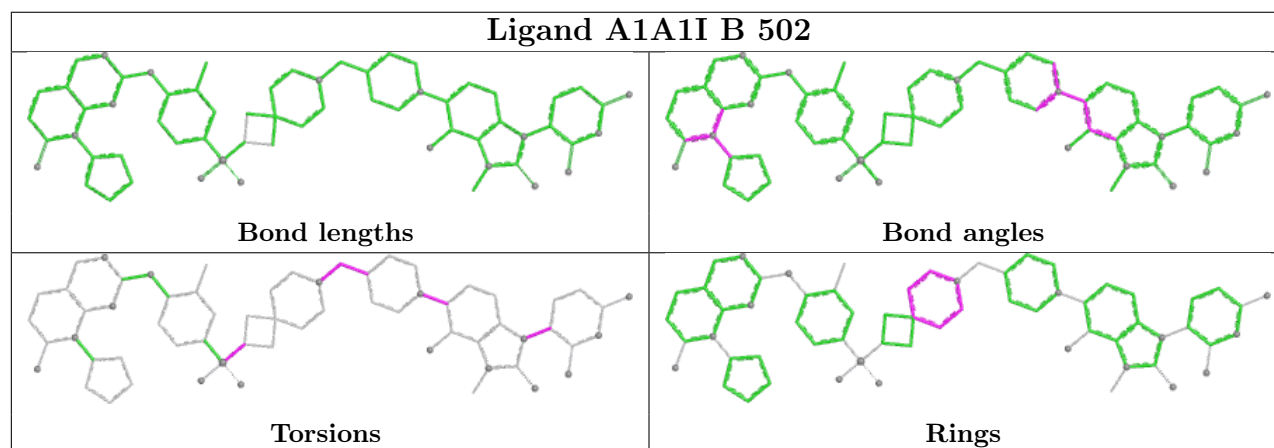
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	502	A1A1I	C10-C11-C12-C7-C9-N1

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	502	A1A1I	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

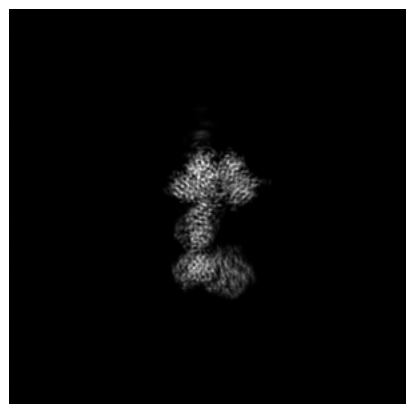
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46464. These allow visual inspection of the internal detail of the map and identification of artifacts.

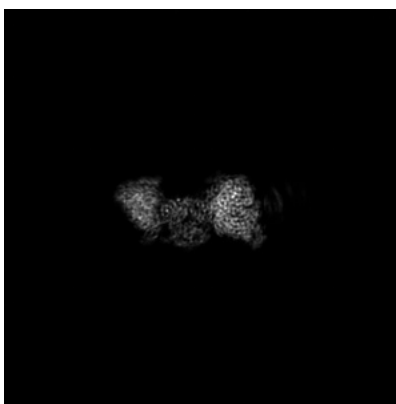
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

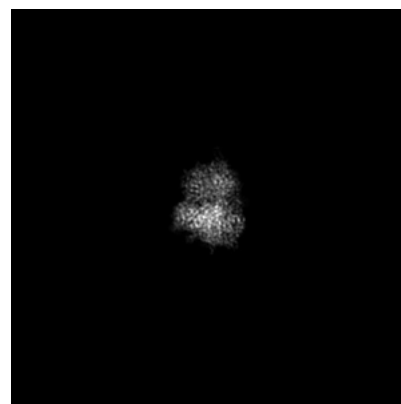
#### 6.1.1 Primary map



X

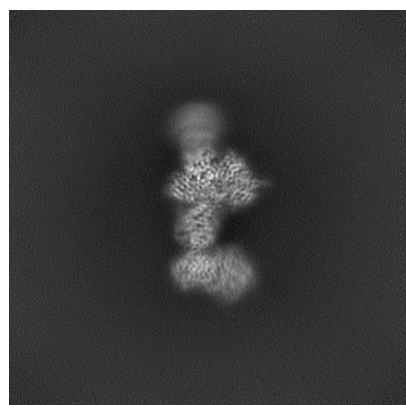


Y

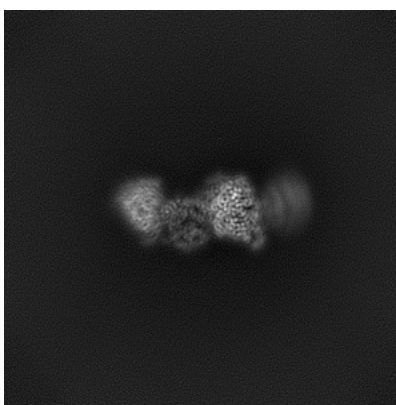


Z

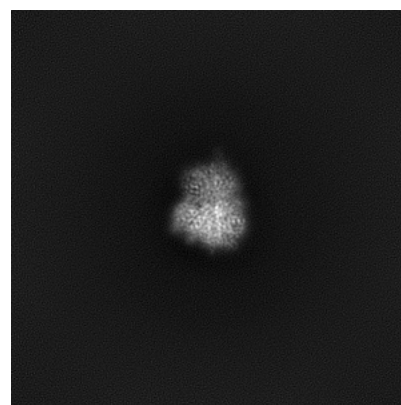
#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

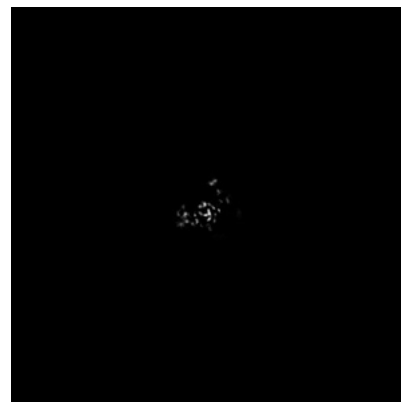
### 6.2.1 Primary map



X Index: 176

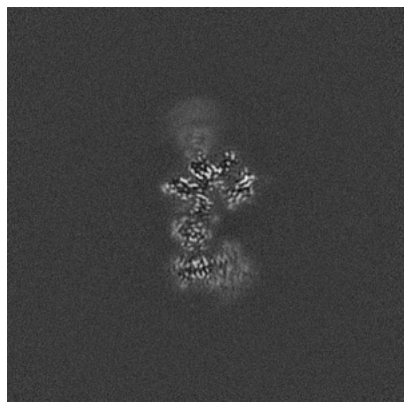


Y Index: 176

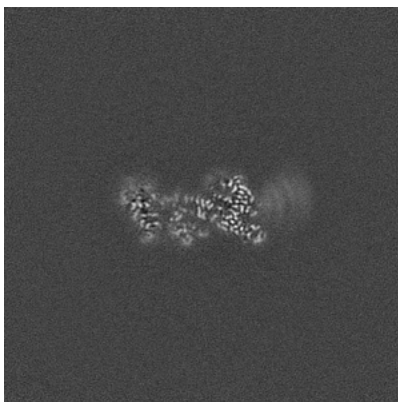


Z Index: 176

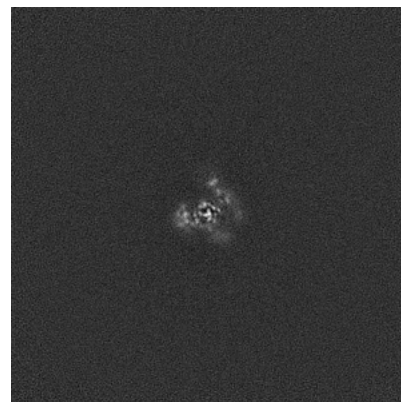
### 6.2.2 Raw map



X Index: 176



Y Index: 176

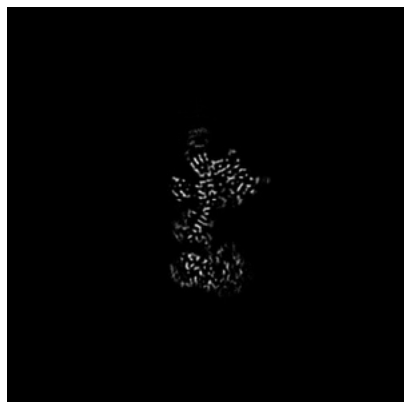


Z Index: 176

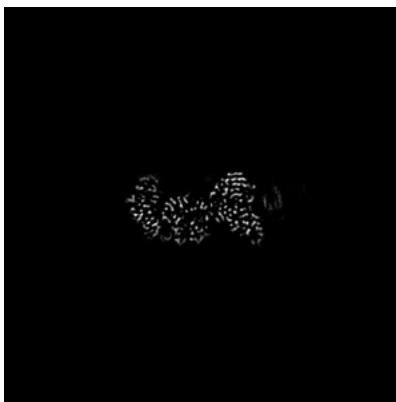
The images above show central slices of the map in three orthogonal directions.

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

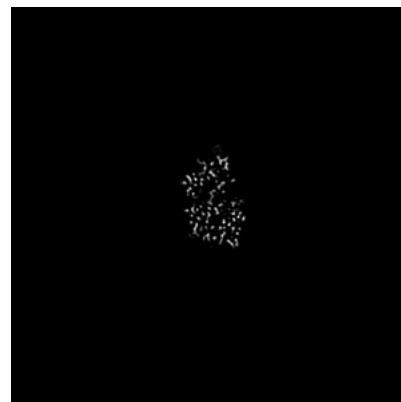
### 6.3.1 Primary map



X Index: 181

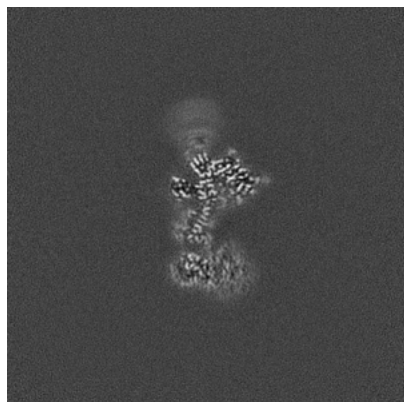


Y Index: 166

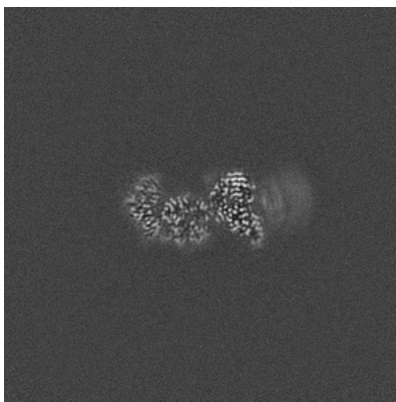


Z Index: 197

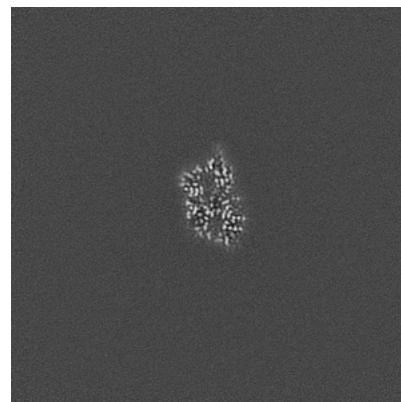
### 6.3.2 Raw map



X Index: 181



Y Index: 166



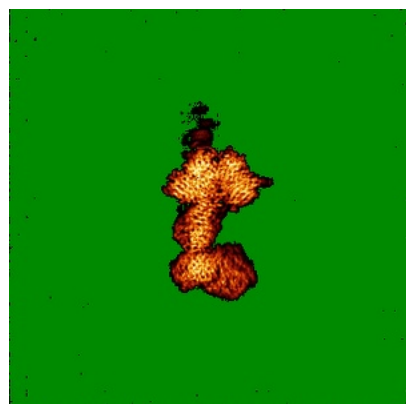
Z Index: 202

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

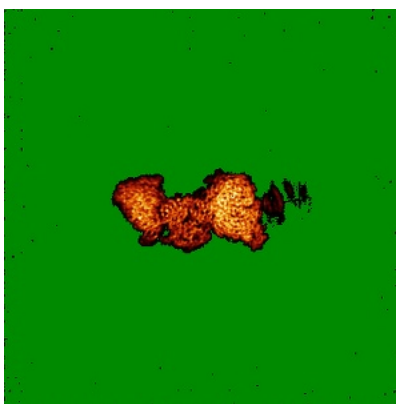


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

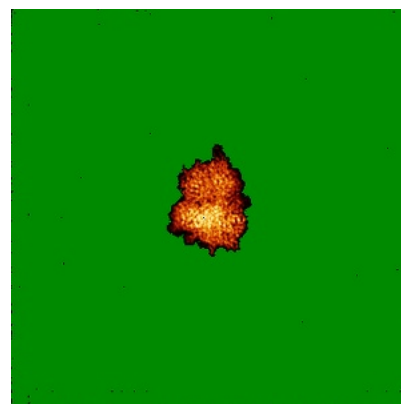
### 6.4.1 Primary map



X

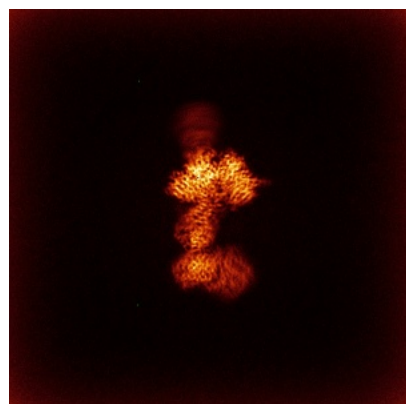


Y

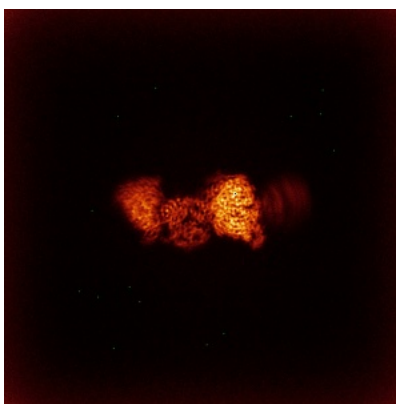


Z

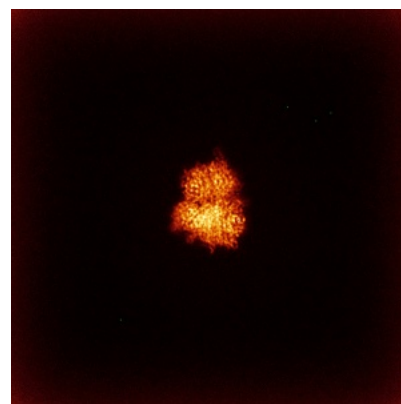
### 6.4.2 Raw map



X



Y



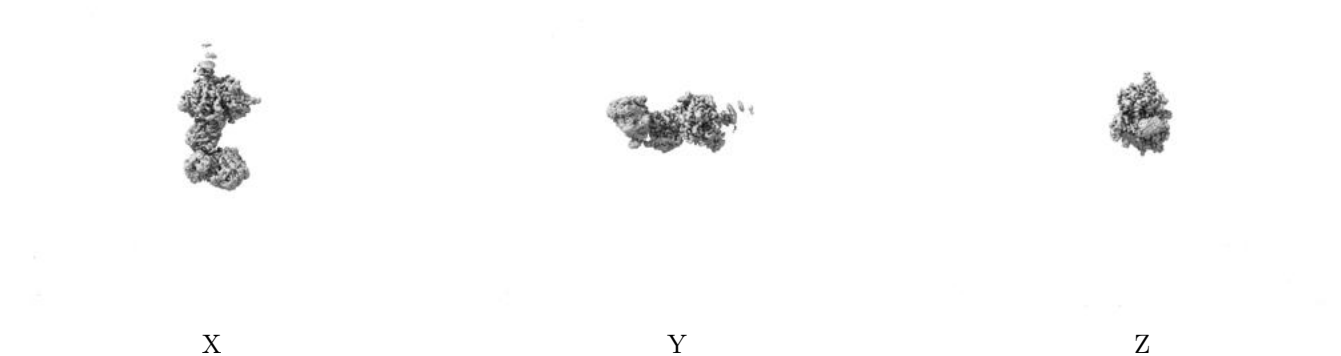
Z

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.



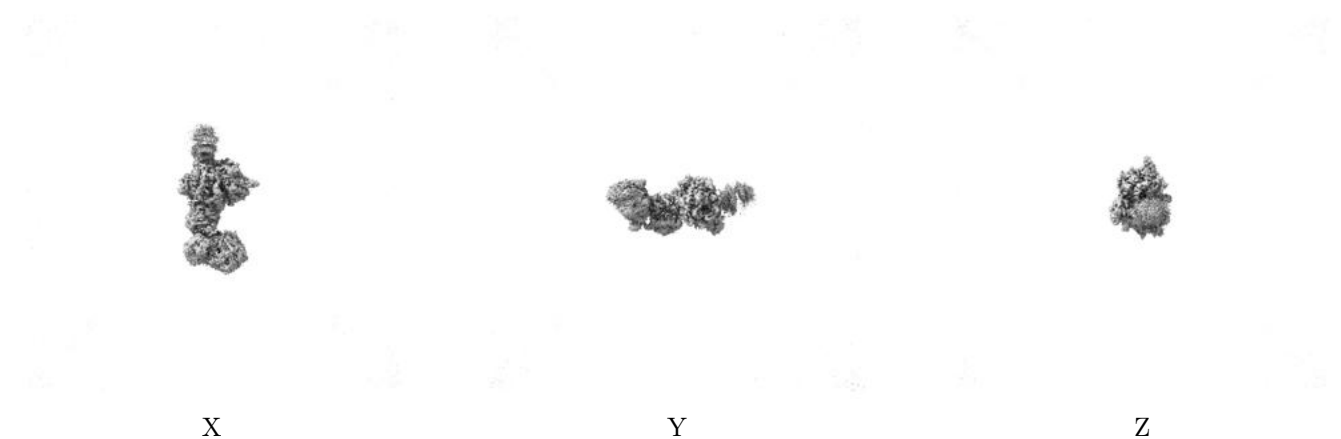
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

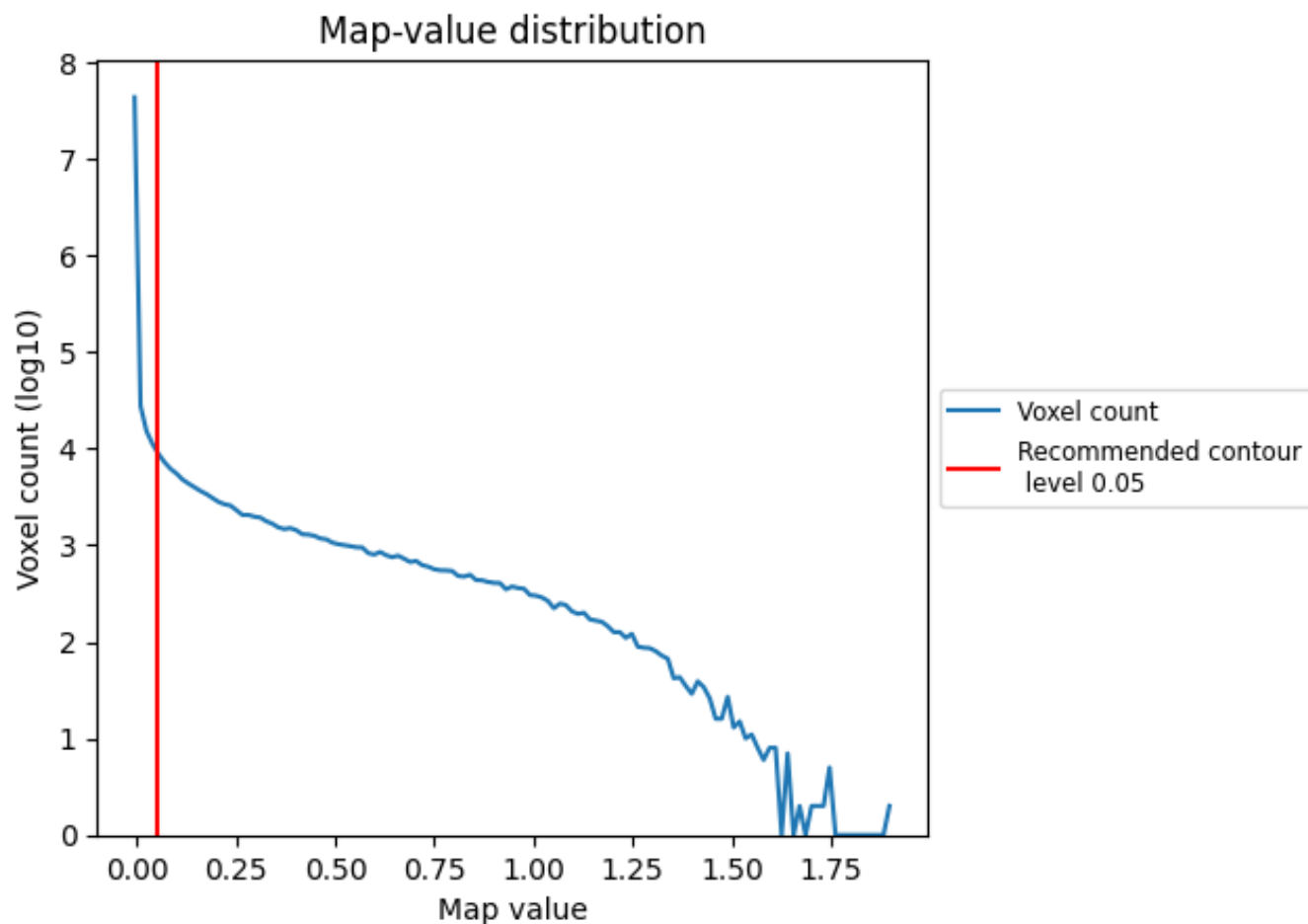
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

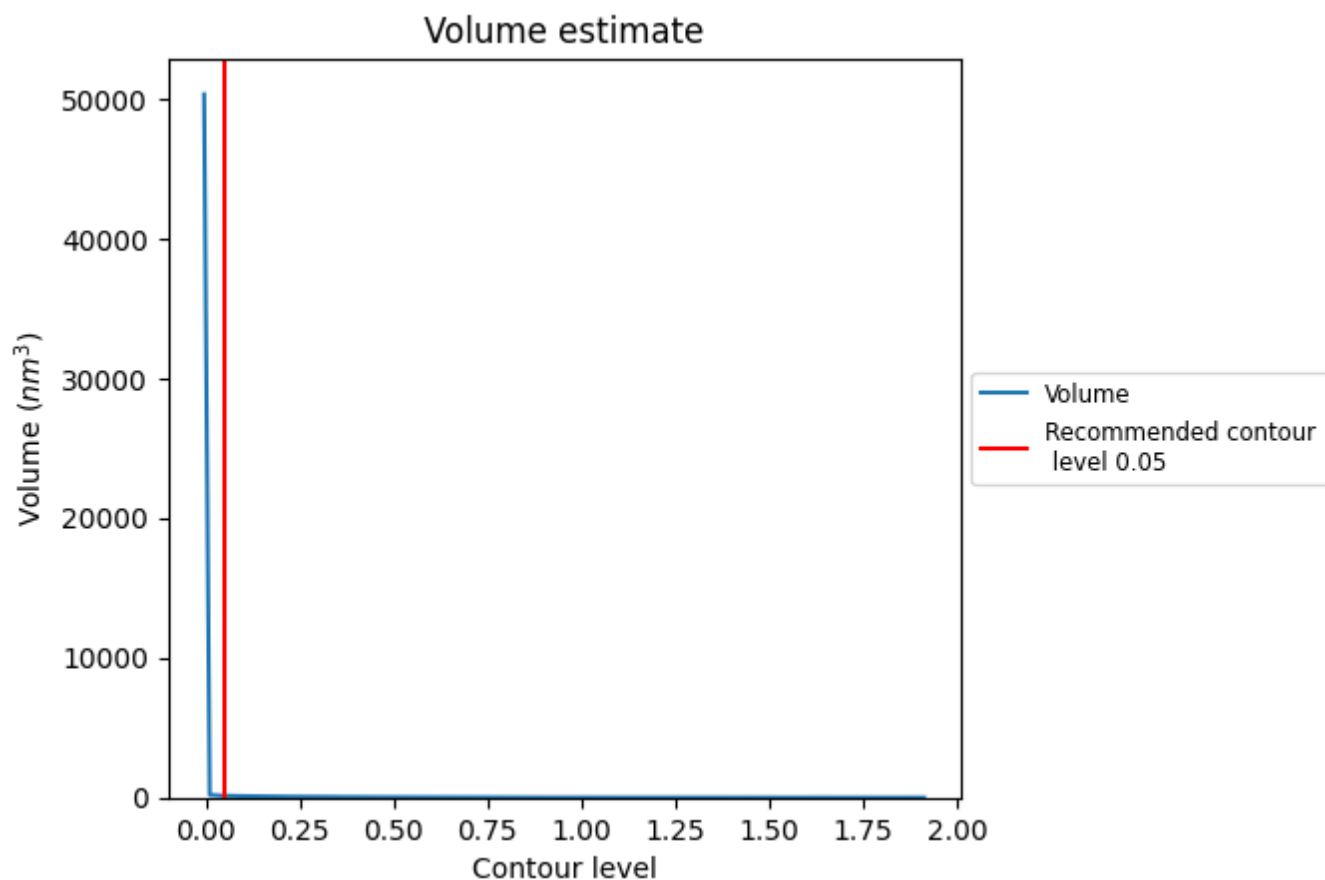
This section contains the results of statistical analysis of the map.

### 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.

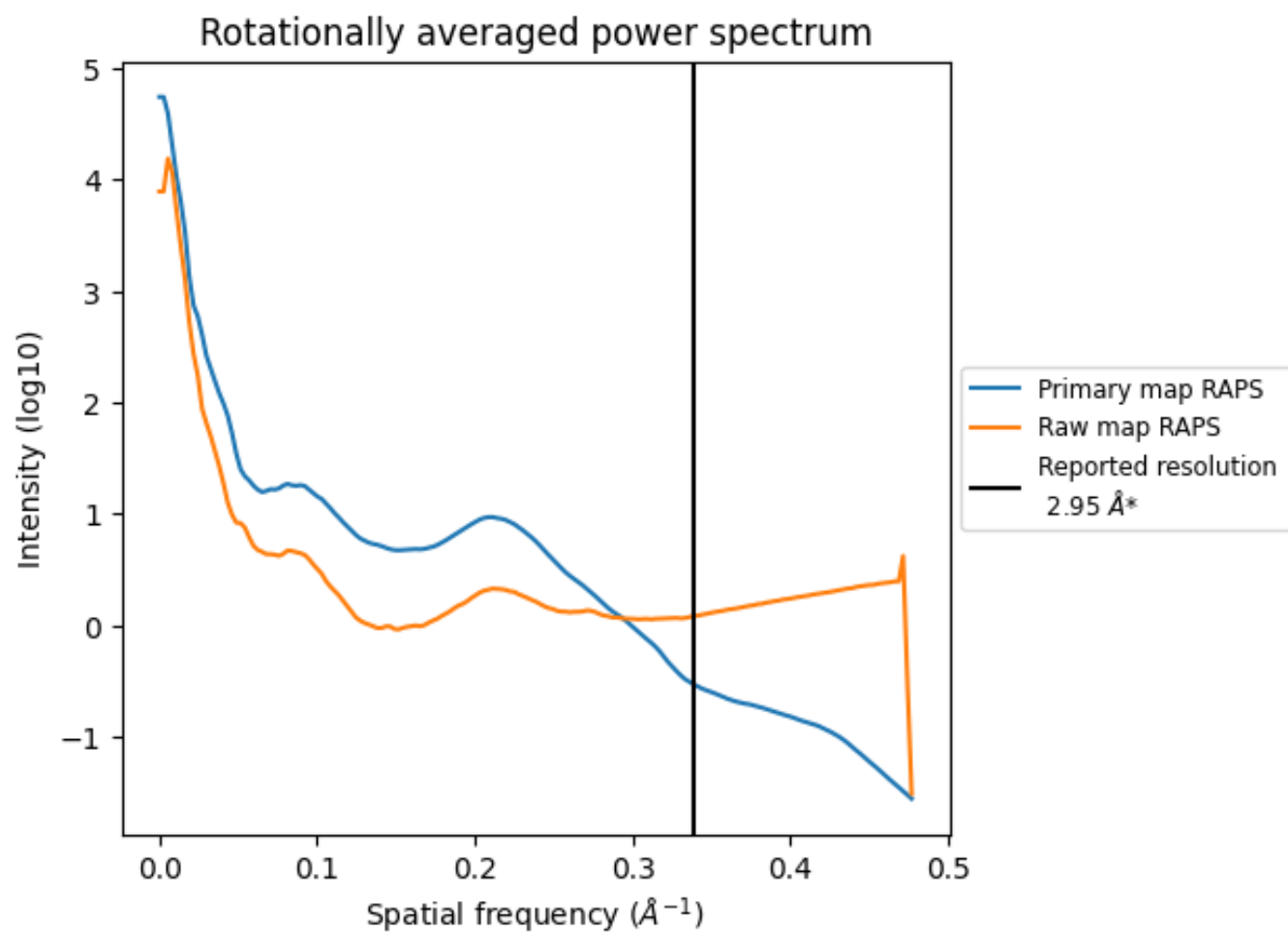
## 7.2 Volume estimate [i](#)



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 ⓘ

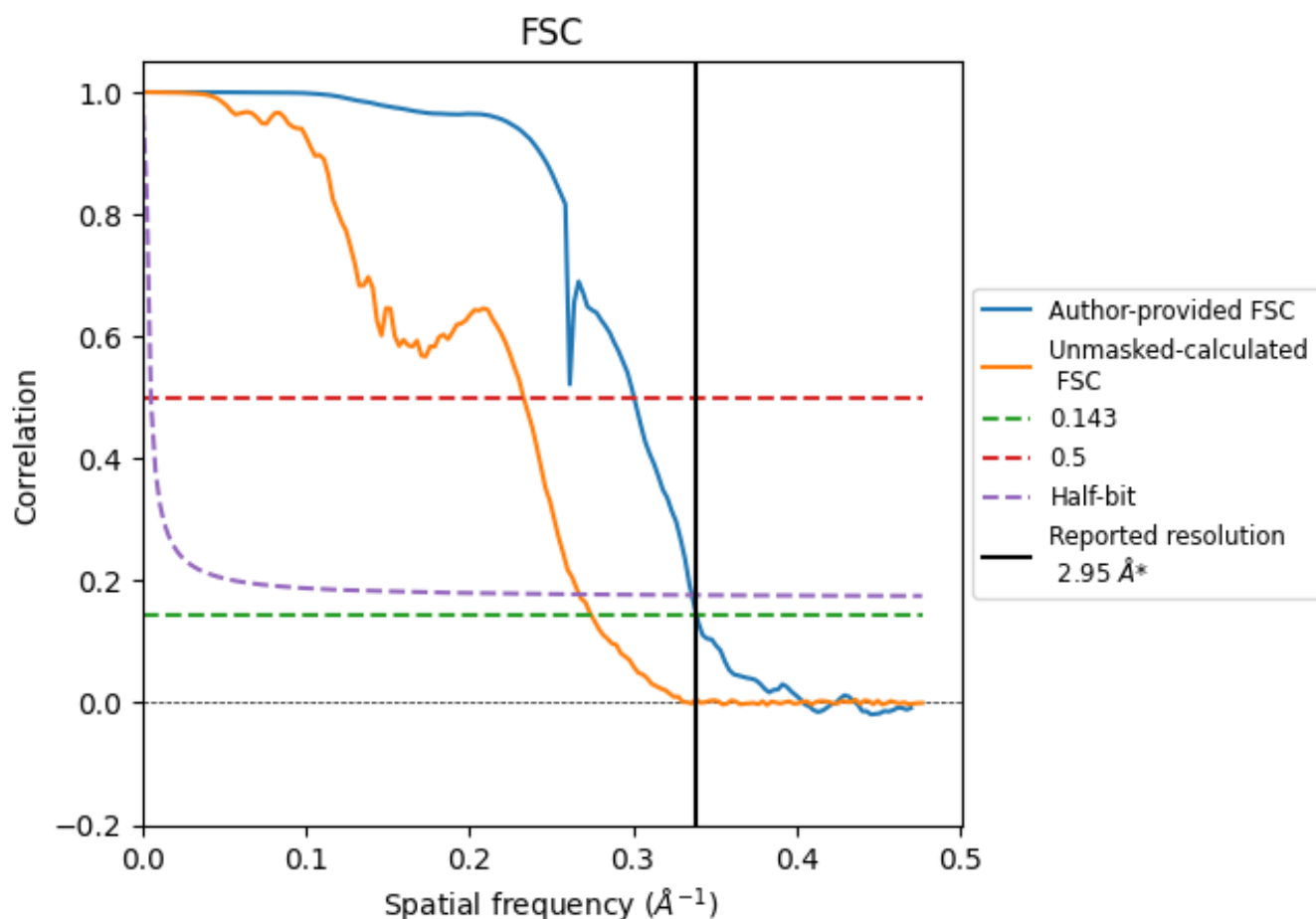


\*Reported resolution corresponds to spatial frequency of 0.339 Å<sup>-1</sup>

## 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 0.339 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

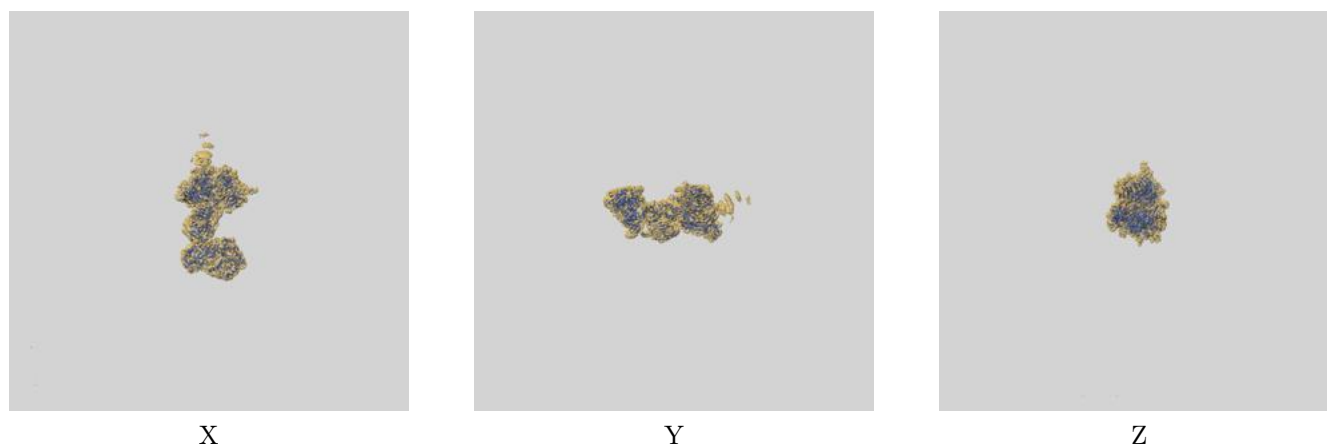
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.33	2.98
Unmasked-calculated*	3.64	4.29	3.74

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.64 differs from the reported value 2.95 by more than 10 %

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

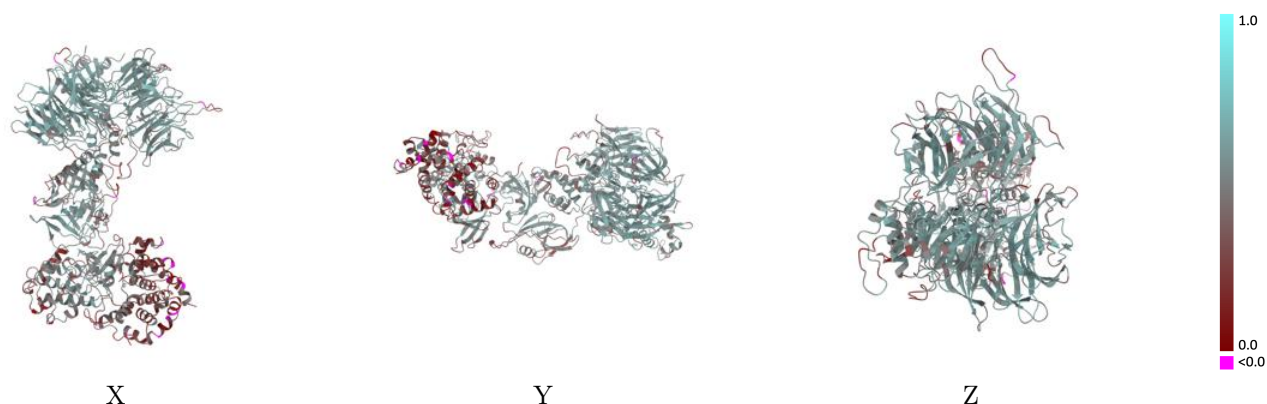
This section contains information regarding the fit between EMDB map EMD-46464 and PDB model 9D0W. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

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



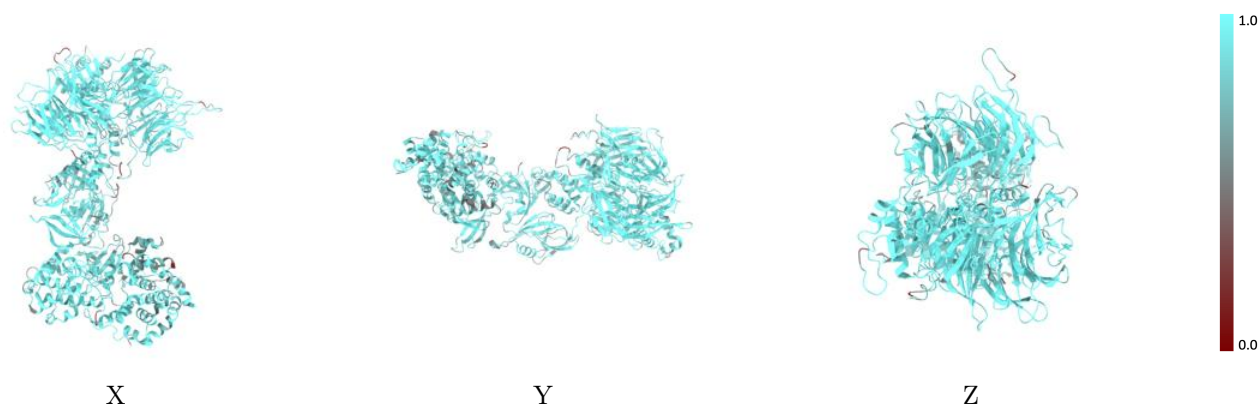
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

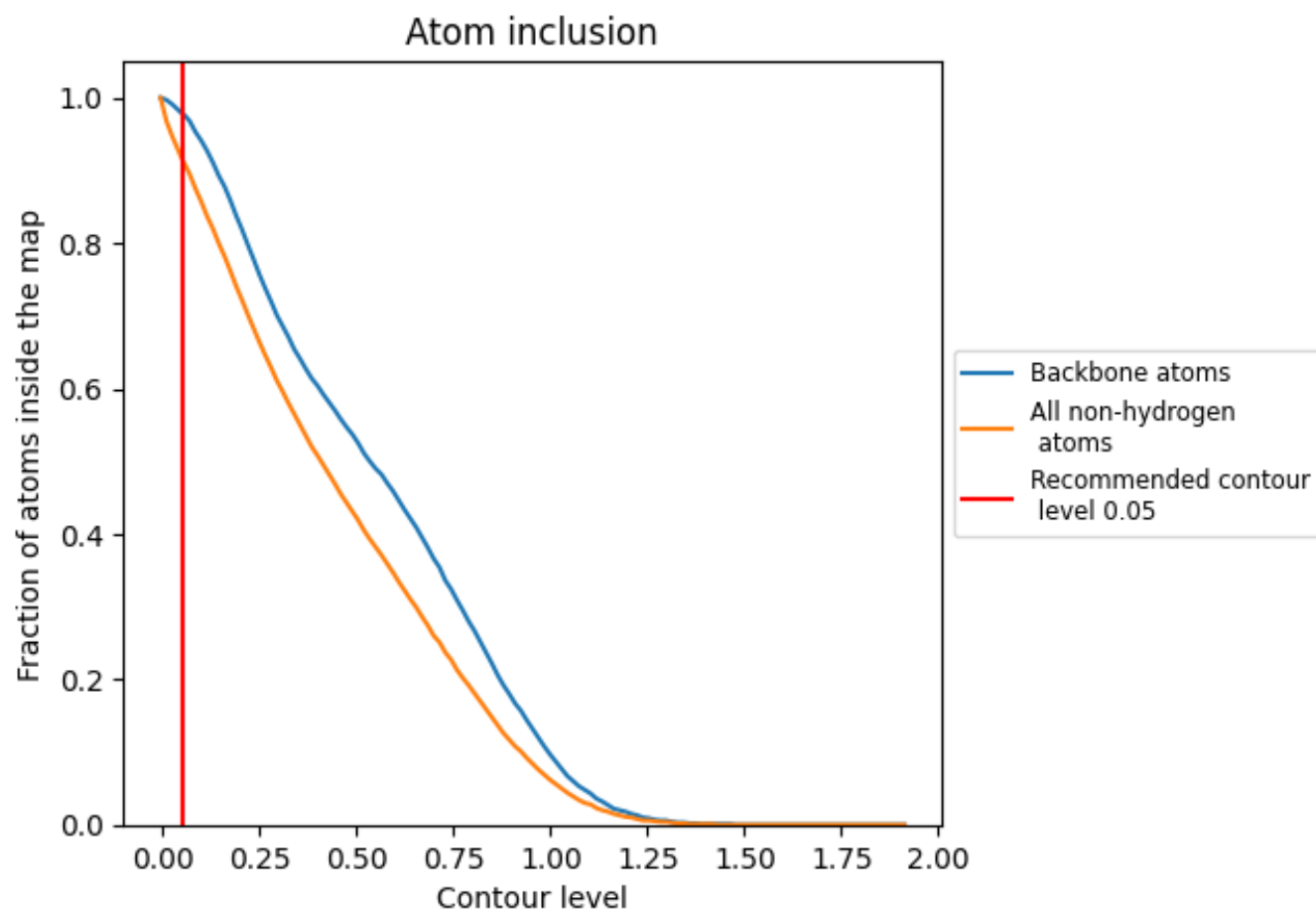
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.05).



## 9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 92% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9150	<div></div> 0.4750
A	<div></div> 0.9430	<div></div> 0.5450
B	<div></div> 0.9080	<div></div> 0.4780
C	<div></div> 0.9260	<div></div> 0.4590
D	<div></div> 0.8320	<div></div> 0.2860

