



## Full wwPDB EM Validation Report ⓘ

Jul 21, 2025 – 10:32 am BST

PDB ID : 9G4Y / pdb\_00009g4y  
EMDB ID : EMD-51074  
Title : TRPC5 in complex with photoswitch E-AzHC  
Authors : Porav, S.A.; Bon, R.; Muench, S.  
Deposited on : 2024-07-16  
Resolution : 2.60 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.dev118  
Mogul : 1.8.4, CSD as541be (2020)  
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) : 2.44

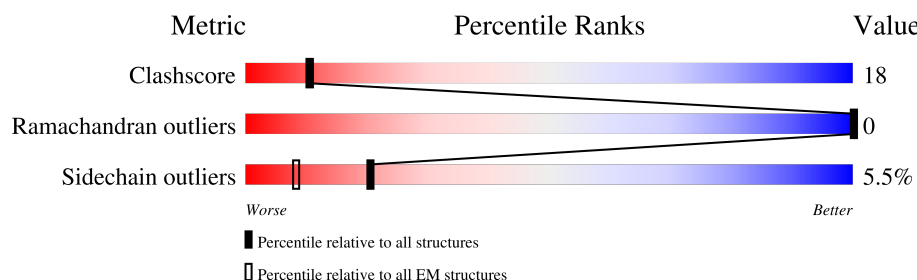
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.60 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	765	<div> <div>6%</div> <div>60%</div> <div>27%</div> <div>•</div> <div>12%</div> </div>
1	B	765	<div> <div>6%</div> <div>59%</div> <div>28%</div> <div>•</div> <div>12%</div> </div>
1	C	765	<div> <div>5%</div> <div>58%</div> <div>27%</div> <div>•</div> <div>12%</div> </div>
1	D	765	<div> <div>5%</div> <div>58%</div> <div>28%</div> <div>•</div> <div>12%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22291 atoms, of which 96 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 Short transient receptor potential channel 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	675	Total	C	N	O	S	0	0
			5503	3585	907	981	30		
1	B	676	Total	C	N	O	S	0	0
			5508	3587	908	983	30		
1	C	676	Total	C	N	O	S	0	0
			5508	3587	908	983	30		
1	D	677	Total	C	N	O	S	0	0
			5516	3593	909	984	30		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	MET	VAL	conflict	UNP Q9UL62
A	737	LEU	GLY	conflict	UNP Q9UL62
B	455	MET	VAL	conflict	UNP Q9UL62
B	737	LEU	GLY	conflict	UNP Q9UL62
C	455	MET	VAL	conflict	UNP Q9UL62
C	737	LEU	GLY	conflict	UNP Q9UL62
D	455	MET	VAL	conflict	UNP Q9UL62
D	737	LEU	GLY	conflict	UNP Q9UL62

- Molecule 2 is 8-[3-chloranyl-4-[( {E})-phenyldiazenyl]phenoxy]-7-[(4-chlorophenyl)methyl]-3-methyl-1-(3-oxidanylpropyl)purine-2,6-dione (CCD ID: A1IIE) (formula: C<sub>28</sub>H<sub>24</sub>Cl<sub>2</sub>N<sub>6</sub>O<sub>4</sub>).

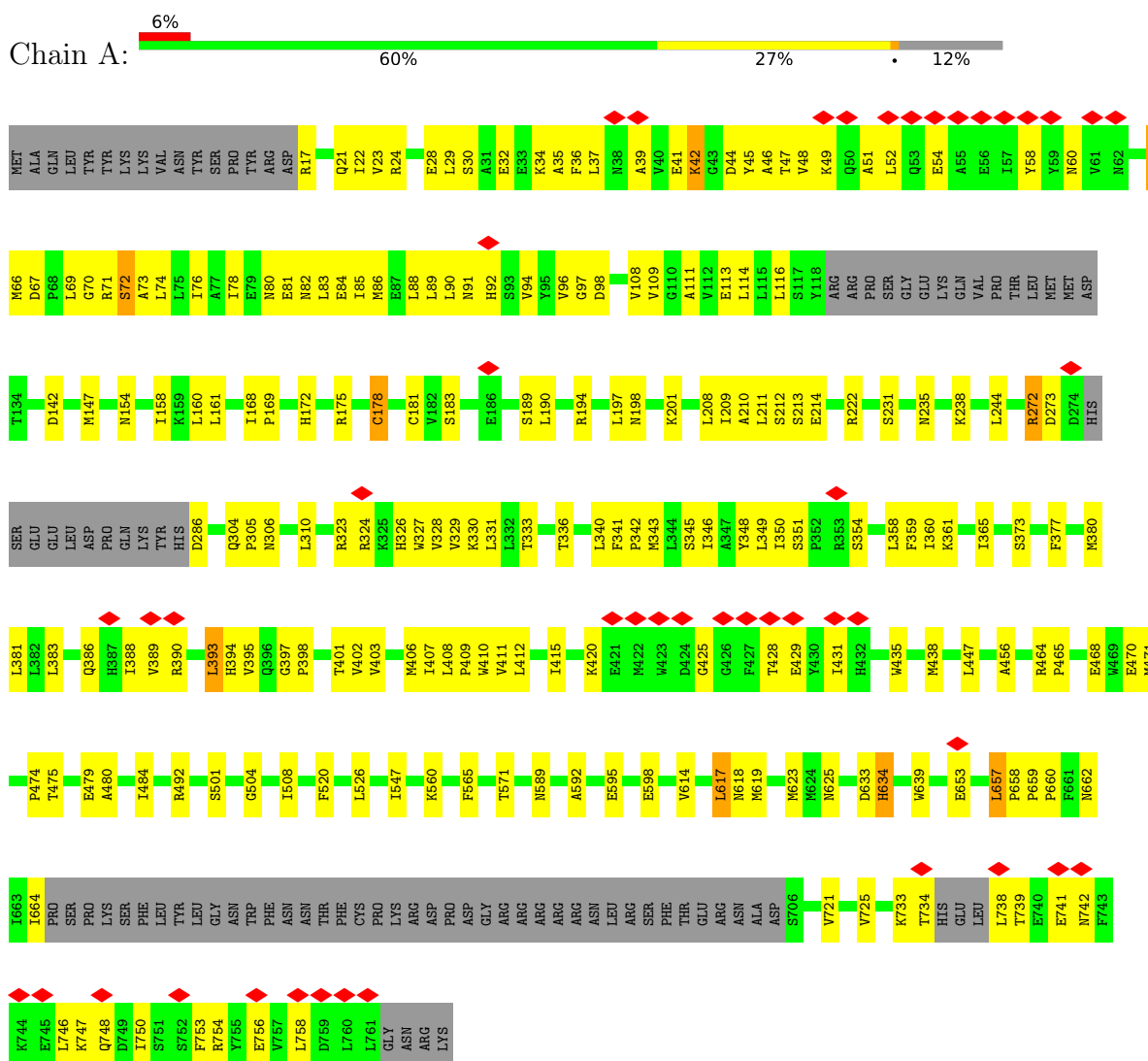


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 64	C 28	Cl 2	H 24	N 6	O 4	0
2	B	1	Total 64	C 28	Cl 2	H 24	N 6	O 4	0
2	C	1	Total 64	C 28	Cl 2	H 24	N 6	O 4	0
2	D	1	Total 64	C 28	Cl 2	H 24	N 6	O 4	0

### 3 Residue-property plots

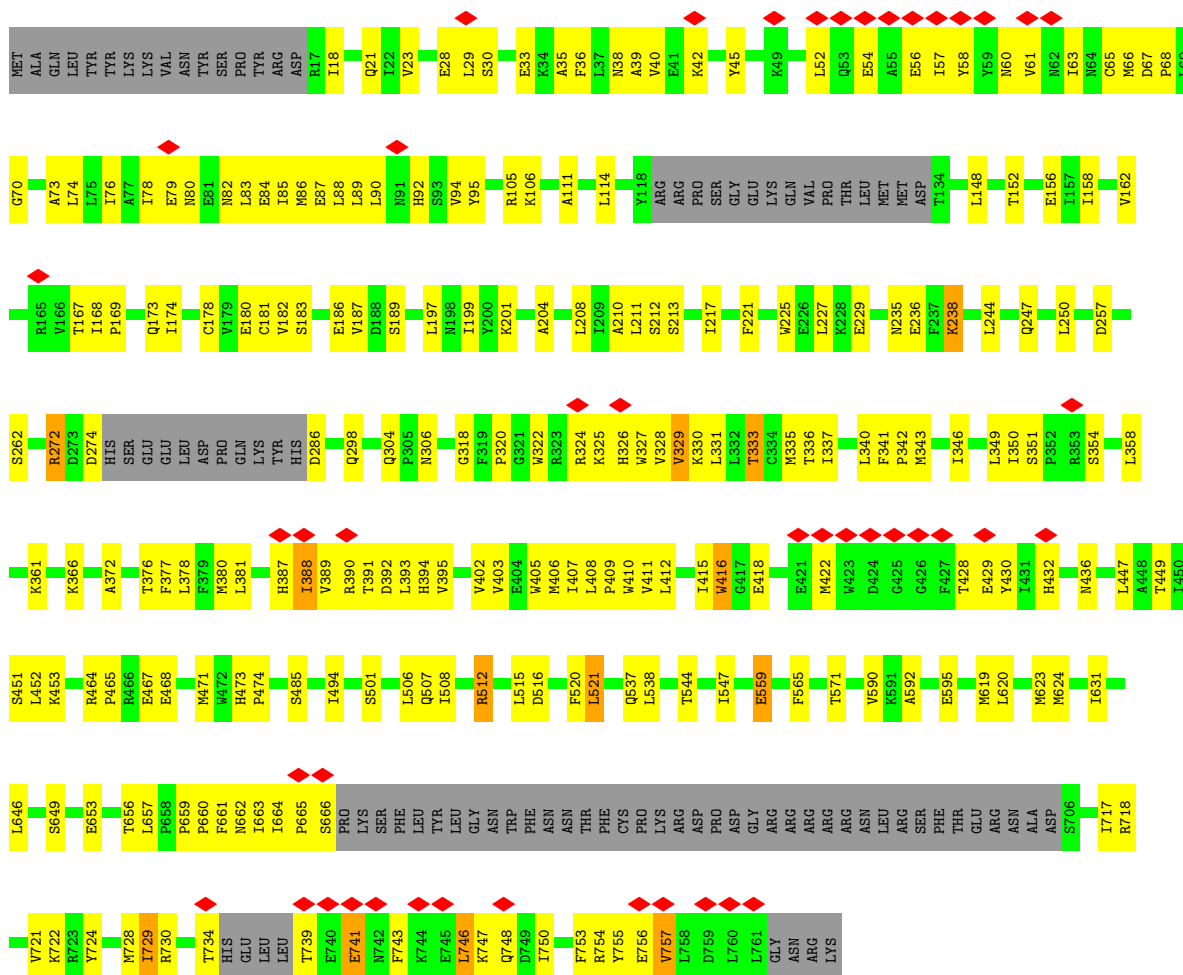
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Short transient receptor potential channel 5

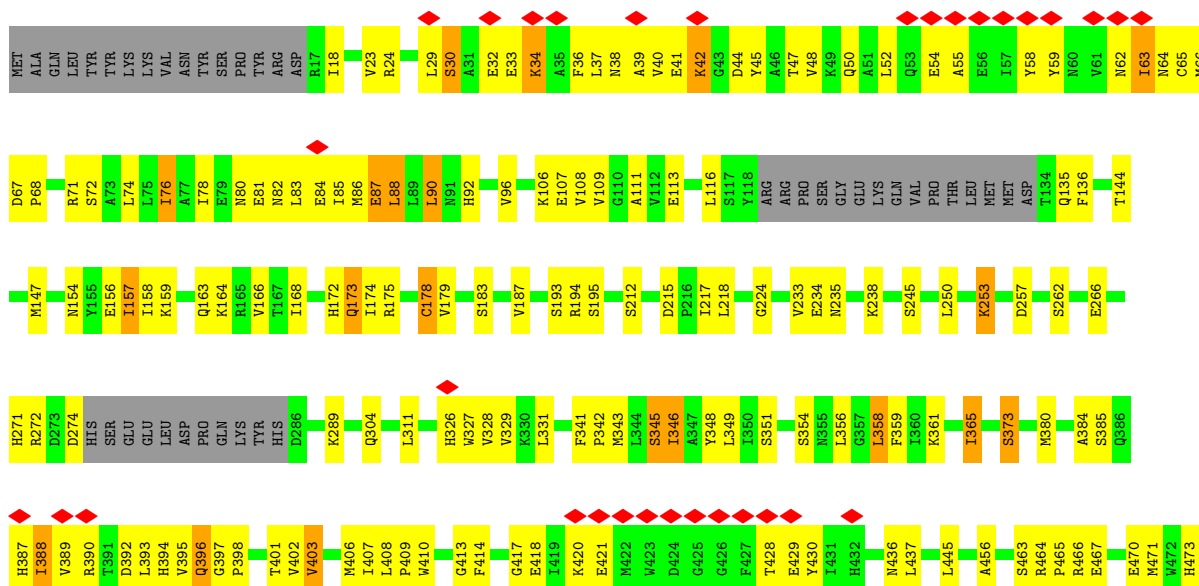


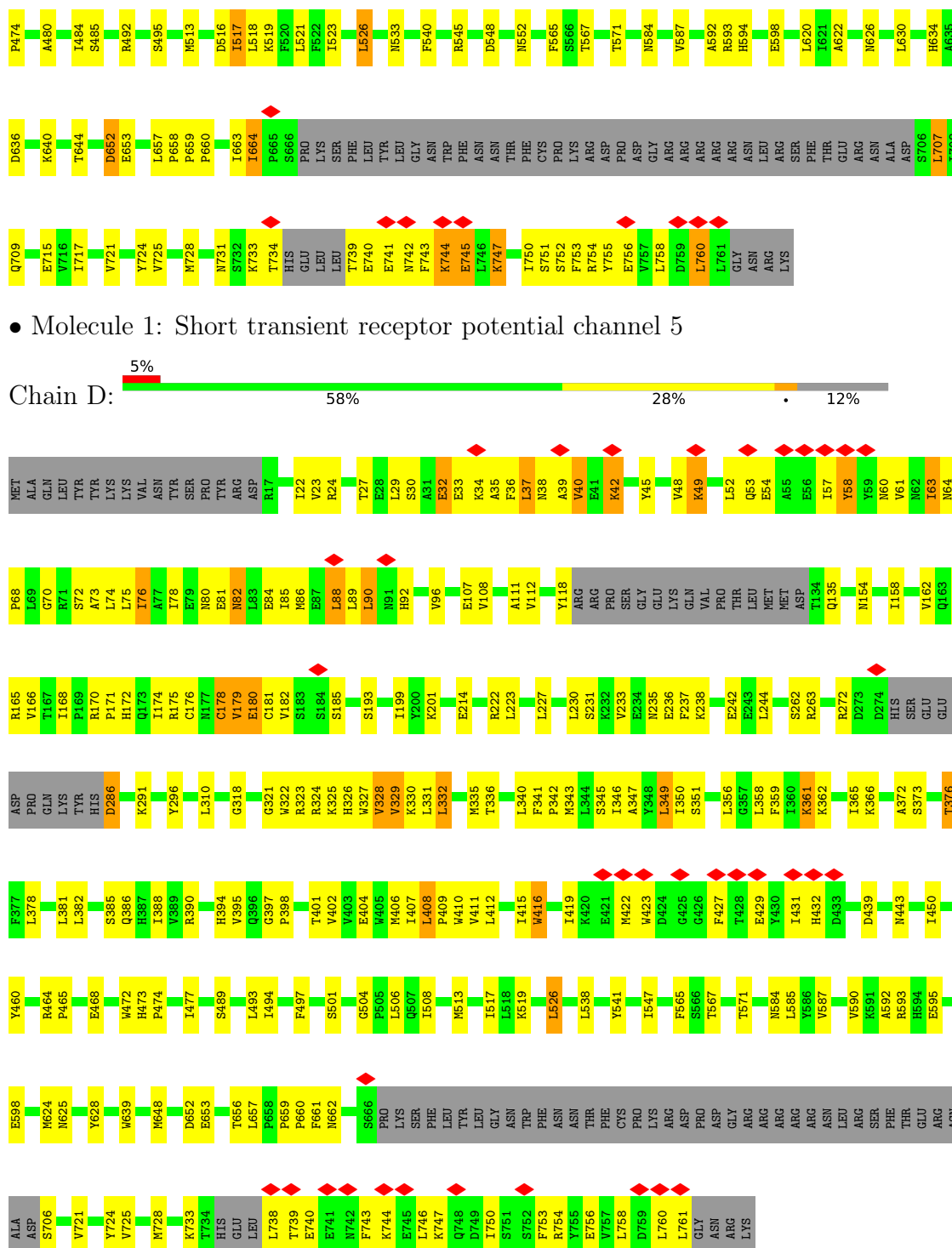
- Molecule 1: Short transient receptor potential channel 5





• Molecule 1: Short transient receptor potential channel 5





• Molecule 1: Short transient receptor potential channel 5

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	89351	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	12.248	Depositor
Minimum map value	-8.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.220	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	319.68, 319.68, 319.68	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1IIE

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	0.22	0/5632	0.31	0/7637
1	B	0.17	0/5638	0.24	0/7646
1	C	0.17	0/5638	0.23	0/7646
1	D	0.16	0/5646	0.23	0/7657
All	All	0.18	0/22554	0.25	0/30586

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	ARG	Sidechain
1	B	272	ARG	Sidechain
1	D	272	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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	5503	0	5547	219	0
1	B	5508	0	5549	228	0
1	C	5508	0	5548	215	0
1	D	5516	0	5560	238	0
2	A	40	24	0	0	0
2	B	40	24	0	1	0
2	C	40	24	0	0	0
2	D	40	24	0	0	0
All	All	22195	96	22204	820	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 (820) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:VAL:HA	1:C:406:MET:HE3	1.36	1.07
1:A:22:ILE:HD13	1:B:211:LEU:HD21	1.39	1.00
1:C:380:MET:HE3	1:C:407:ILE:HD12	1.42	0.99
1:D:66:MET:HE3	1:D:66:MET:HA	1.45	0.97
1:D:517:ILE:HD11	1:D:624:MET:HE3	1.45	0.97
1:C:39:ALA:HB1	1:C:44:ASP:HB2	1.46	0.94
1:B:52:LEU:HD22	1:B:92:HIS:HB3	1.49	0.94
1:B:74:LEU:HD21	1:B:90:LEU:HD11	1.50	0.93
1:D:82:ASN:HB2	1:D:85:ILE:HG12	1.50	0.92
1:A:324:ARG:HH21	1:D:175:ARG:HA	1.31	0.91
1:C:174:ILE:HD12	1:C:174:ILE:H	1.36	0.91
1:B:467:GLU:OE2	1:B:467:GLU:N	2.07	0.87
1:C:82:ASN:HB3	1:C:85:ILE:HB	1.57	0.87
1:D:547:ILE:H	1:D:547:ILE:HD12	1.40	0.84
1:D:81:GLU:HG2	1:D:108:VAL:HG21	1.60	0.84
1:A:738:LEU:HD21	1:D:740:GLU:HA	1.60	0.84
1:C:74:LEU:HD21	1:C:96:VAL:HG23	1.58	0.83
1:B:659:PRO:HA	1:B:662:ASN:HB2	1.59	0.83
1:D:439:ASP:O	1:D:443:ASN:ND2	2.11	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:ILE:HG22	1:C:390:ARG:HH22	1.45	0.81
1:D:517:ILE:HD11	1:D:624:MET:CE	2.10	0.80
1:B:380:MET:HE3	1:B:407:ILE:HG12	1.64	0.79
1:B:388:ILE:HG22	1:B:390:ARG:HH22	1.47	0.79
1:A:72:SER:O	1:A:76:ILE:HD12	1.82	0.79
1:B:35:ALA:O	1:B:39:ALA:N	2.17	0.78
1:B:464:ARG:HG3	1:B:465:PRO:HD2	1.66	0.78
1:D:394:HIS:ND1	1:D:465:PRO:HA	2.00	0.77
1:B:82:ASN:HB3	1:B:85:ILE:CD1	2.14	0.77
1:A:190:LEU:HD23	1:A:190:LEU:O	1.84	0.77
1:D:36:PHE:HA	1:D:39:ALA:HB3	1.66	0.77
1:B:90:LEU:HD22	1:B:114:LEU:HD22	1.65	0.77
1:D:39:ALA:HA	1:D:42:LYS:HB2	1.67	0.77
1:C:52:LEU:HD22	1:C:92:HIS:HB3	1.66	0.76
1:A:435:TRP:HB3	1:A:492:ARG:HH21	1.51	0.76
1:D:336:THR:O	1:D:340:LEU:HD12	1.86	0.76
1:A:406:MET:O	1:A:409:PRO:HD2	1.85	0.76
1:B:619:MET:HG2	1:C:513:MET:CE	2.15	0.76
1:D:386:GLN:OE1	1:D:386:GLN:N	2.18	0.76
1:B:89:LEU:HD23	1:B:94:VAL:HG21	1.67	0.76
1:C:346:ILE:HA	1:C:349:LEU:HD12	1.68	0.76
1:A:35:ALA:O	1:A:39:ALA:N	2.19	0.75
1:B:38:ASN:O	1:B:42:LYS:HG2	1.85	0.75
1:A:172:HIS:ND1	1:A:181:CYS:SG	2.59	0.75
1:D:653:GLU:O	1:D:656:THR:OG1	2.03	0.75
1:B:83:LEU:O	1:B:87:GLU:N	2.14	0.75
1:C:52:LEU:HD23	1:C:63:ILE:HD11	1.67	0.75
1:A:82:ASN:HB3	1:A:85:ILE:HD13	1.69	0.74
1:D:40:VAL:HG11	1:D:76:ILE:HB	1.68	0.74
1:A:526:LEU:CD2	1:B:494:ILE:HG13	2.17	0.74
1:A:324:ARG:NH2	1:D:174:ILE:O	2.21	0.73
1:A:82:ASN:OD1	1:A:748:GLN:NE2	2.22	0.73
1:A:212:SER:HA	1:D:23:VAL:HG23	1.70	0.73
1:B:73:ALA:HB1	1:B:89:LEU:HD11	1.70	0.73
1:A:560:LYS:NZ	1:B:559:GLU:HG3	2.03	0.73
1:C:380:MET:CE	1:C:407:ILE:HD12	2.18	0.73
1:B:663:ILE:HD12	1:B:663:ILE:O	1.88	0.72
1:A:738:LEU:HD22	1:A:742:ASN:HD22	1.54	0.72
1:D:48:VAL:HG22	1:D:52:LEU:HD11	1.71	0.72
1:D:411:VAL:O	1:D:415:ILE:HG13	1.90	0.72
1:B:52:LEU:CD2	1:B:92:HIS:HB3	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:O	1:B:201:LYS:HG3	1.90	0.71
1:D:36:PHE:O	1:D:40:VAL:N	2.23	0.71
1:D:135:GLN:OE1	1:D:135:GLN:N	2.23	0.71
1:A:109:VAL:O	1:A:113:GLU:HG3	1.90	0.71
1:A:89:LEU:H	1:A:89:LEU:HD12	1.54	0.71
1:D:227:LEU:HD13	1:D:244:LEU:HB3	1.72	0.71
1:D:81:GLU:HG2	1:D:108:VAL:CG2	2.20	0.70
1:B:89:LEU:CD2	1:B:94:VAL:HG21	2.21	0.70
1:D:659:PRO:HA	1:D:662:ASN:ND2	2.06	0.70
1:A:738:LEU:HD11	1:D:743:PHE:HB2	1.74	0.70
1:B:174:ILE:HD12	1:B:174:ILE:H	1.55	0.70
1:C:74:LEU:CD2	1:C:96:VAL:HG23	2.21	0.70
1:C:135:GLN:HG3	1:C:136:PHE:H	1.56	0.70
1:C:48:VAL:HG22	1:C:52:LEU:HD11	1.74	0.69
1:D:82:ASN:OD1	1:D:82:ASN:N	2.24	0.69
1:B:429:GLU:HA	1:B:432:HIS:CD2	2.28	0.69
1:C:144:THR:OG1	1:C:147:MET:HG3	1.92	0.69
1:D:29:LEU:HD23	1:D:34:LYS:HG2	1.74	0.69
1:B:178:CYS:HB2	1:B:180:GLU:OE1	1.92	0.69
1:C:721:VAL:O	1:C:725:VAL:HG23	1.93	0.69
1:B:23:VAL:HG23	1:C:212:SER:HA	1.75	0.68
1:A:327:TRP:HA	1:A:330:LYS:HE2	1.76	0.68
1:B:741:GLU:HG2	1:C:733:LYS:O	1.94	0.68
1:D:52:LEU:HD22	1:D:92:HIS:HB3	1.75	0.68
1:B:180:GLU:OE1	1:B:180:GLU:N	2.21	0.68
1:B:664:ILE:HG23	1:B:665:PRO:HD2	1.75	0.68
1:A:66:MET:CE	1:A:70:GLY:HA2	2.24	0.68
1:B:619:MET:HG2	1:C:513:MET:HE1	1.74	0.68
1:D:38:ASN:O	1:D:42:LYS:N	2.26	0.68
1:A:214:GLU:OE2	1:A:214:GLU:HA	1.94	0.67
1:B:236:GLU:N	1:B:236:GLU:OE1	2.27	0.67
1:A:464:ARG:HG3	1:A:465:PRO:HD2	1.74	0.67
1:C:754:ARG:NH2	1:D:756:GLU:OE2	2.21	0.67
1:D:63:ILE:HD13	1:D:63:ILE:H	1.59	0.67
1:D:286:ASP:O	1:D:291:LYS:NZ	2.27	0.67
1:C:565:PHE:HD1	1:C:571:THR:HG23	1.58	0.67
1:A:66:MET:HE1	1:A:70:GLY:HA2	1.75	0.67
1:B:82:ASN:HB3	1:B:85:ILE:HD13	1.77	0.67
1:B:377:PHE:HA	1:B:380:MET:HE2	1.77	0.67
1:C:234:GLU:HA	1:D:323:ARG:HH12	1.59	0.67
1:D:378:LEU:HD11	1:D:493:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ASN:HB3	1:B:85:ILE:HD12	1.77	0.67
1:B:333:THR:O	1:B:337:ILE:HD12	1.95	0.66
1:A:326:HIS:O	1:A:329:VAL:HG12	1.95	0.66
1:C:30:SER:OG	1:C:32:GLU:HG3	1.96	0.66
1:D:659:PRO:HA	1:D:662:ASN:HD21	1.58	0.66
1:D:231:SER:OG	1:D:242:GLU:HG3	1.95	0.66
1:A:341:PHE:CD1	1:A:342:PRO:HD3	2.30	0.66
1:A:754:ARG:O	1:A:758:LEU:HG	1.96	0.66
1:D:73:ALA:HA	1:D:76:ILE:HD12	1.77	0.66
1:D:385:SER:O	1:D:388:ILE:HG22	1.95	0.66
1:C:361:LYS:HE2	1:C:653:GLU:OE2	1.95	0.66
1:B:183:SER:O	1:B:187:VAL:HG23	1.96	0.66
1:C:41:GLU:OE1	1:C:42:LYS:NZ	2.20	0.65
1:C:394:HIS:ND1	1:C:465:PRO:HA	2.11	0.65
1:C:48:VAL:HG22	1:C:52:LEU:CD1	2.27	0.65
1:B:411:VAL:O	1:B:415:ILE:HG13	1.96	0.65
1:A:211:LEU:O	1:A:212:SER:OG	2.13	0.65
1:A:323:ARG:HD3	1:D:233:VAL:O	1.95	0.65
1:B:336:THR:O	1:B:340:LEU:HG	1.97	0.65
1:B:341:PHE:CD2	1:B:342:PRO:HD3	2.31	0.65
1:B:350:ILE:HG13	1:B:351:SER:N	2.10	0.65
1:D:82:ASN:HB2	1:D:85:ILE:CG1	2.25	0.65
1:C:37:LEU:HD11	1:C:65:CYS:SG	2.37	0.65
1:C:66:MET:SD	1:C:66:MET:N	2.70	0.65
1:B:86:MET:O	1:B:90:LEU:HD13	1.96	0.64
1:C:108:VAL:HG23	1:C:111:ALA:HB3	1.79	0.64
1:C:354:SER:O	1:C:358:LEU:HD22	1.96	0.64
1:B:718:ARG:O	1:B:722:LYS:HG3	1.98	0.64
1:A:48:VAL:HG12	1:A:52:LEU:CD1	2.26	0.64
1:C:403:VAL:HA	1:C:406:MET:CE	2.21	0.64
1:D:48:VAL:HG22	1:D:52:LEU:CD1	2.28	0.64
1:B:754:ARG:HD2	1:C:753:PHE:HB2	1.80	0.64
1:C:593:ARG:NH1	1:C:598:GLU:OE1	2.31	0.64
1:D:107:GLU:OE1	1:D:154:ASN:ND2	2.30	0.64
1:A:361:LYS:NZ	1:A:653:GLU:HG3	2.13	0.64
1:B:257:ASP:OD1	1:B:304:GLN:NE2	2.31	0.63
1:C:63:ILE:HG22	1:C:64:ASN:OD1	1.97	0.63
1:D:108:VAL:O	1:D:112:VAL:HG23	1.98	0.63
1:D:341:PHE:CD2	1:D:342:PRO:HD3	2.34	0.63
1:D:74:LEU:HD21	1:D:90:LEU:CD1	2.29	0.63
1:B:322:TRP:HA	1:B:325:LYS:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:MET:O	1:B:409:PRO:HD2	1.98	0.63
1:B:520:PHE:HB2	1:B:623:MET:HE1	1.81	0.63
1:B:66:MET:CA	1:B:66:MET:HE3	2.29	0.63
1:B:66:MET:HE3	1:B:66:MET:HA	1.81	0.62
1:D:567:THR:O	1:D:571:THR:OG1	2.17	0.62
1:B:327:TRP:NE1	1:B:328:VAL:HG23	2.13	0.62
1:B:422:MET:HB2	1:B:430:TYR:CE2	2.33	0.62
1:C:55:ALA:O	1:C:59:TYR:N	2.32	0.62
1:A:29:LEU:HD23	1:A:34:LYS:HG2	1.80	0.62
1:B:74:LEU:HD21	1:B:90:LEU:CD1	2.28	0.62
1:A:324:ARG:NH2	1:D:175:ARG:HA	2.10	0.62
1:B:66:MET:HE1	1:B:70:GLY:O	2.00	0.62
1:D:326:HIS:HB3	1:D:329:VAL:HG12	1.81	0.62
1:D:359:PHE:CE2	1:D:365:ILE:HD13	2.34	0.62
1:D:35:ALA:O	1:D:39:ALA:N	2.28	0.62
1:D:45:TYR:HD2	1:D:88:LEU:HG	1.63	0.62
1:D:72:SER:O	1:D:76:ILE:HG13	1.99	0.62
1:D:171:PRO:HG3	1:D:199:ILE:HG21	1.82	0.62
1:D:326:HIS:O	1:D:329:VAL:HG13	2.00	0.62
1:A:41:GLU:OE1	1:A:42:LYS:NZ	2.28	0.62
1:C:388:ILE:O	1:C:390:ARG:NH2	2.33	0.62
1:A:52:LEU:HD22	1:A:92:HIS:CG	2.35	0.62
1:A:74:LEU:CD2	1:A:96:VAL:HG12	2.29	0.62
1:A:74:LEU:HD22	1:A:96:VAL:HG12	1.79	0.61
1:D:347:ALA:CB	1:D:356:LEU:HD23	2.31	0.61
1:A:42:LYS:NZ	1:A:42:LYS:HA	2.14	0.61
1:A:42:LYS:HZ2	1:A:42:LYS:HA	1.63	0.61
1:B:329:VAL:O	1:B:333:THR:OG1	2.18	0.61
1:D:54:GLU:O	1:D:58:TYR:HB2	1.99	0.61
1:A:78:ILE:HG12	1:A:86:MET:SD	2.40	0.61
1:D:66:MET:HA	1:D:66:MET:CE	2.27	0.61
1:A:46:ALA:HA	1:A:49:LYS:HE2	1.82	0.61
1:A:48:VAL:HG12	1:A:52:LEU:HD12	1.81	0.61
1:B:342:PRO:O	1:B:346:ILE:HG12	2.01	0.61
1:B:407:ILE:O	1:B:411:VAL:HG23	2.01	0.61
1:A:231:SER:O	1:A:238:LYS:HG3	2.01	0.61
1:D:73:ALA:HA	1:D:76:ILE:CD1	2.31	0.61
1:B:619:MET:HG2	1:C:513:MET:HE3	1.83	0.61
1:C:154:ASN:OD1	1:C:157:ILE:HG13	2.01	0.61
1:A:738:LEU:CD1	1:D:743:PHE:HB2	2.31	0.60
1:D:343:MET:HA	1:D:346:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ALA:HB2	1:D:356:LEU:HD23	1.83	0.60
1:D:409:PRO:HG2	1:D:410:TRP:HD1	1.65	0.60
1:C:754:ARG:HG2	1:C:755:TYR:HD1	1.64	0.60
1:A:664:ILE:HD12	1:A:664:ILE:H	1.65	0.60
1:C:622:ALA:HA	1:D:625:ASN:OD1	2.01	0.60
1:D:415:ILE:HG22	1:D:419:ILE:HD11	1.84	0.60
1:B:30:SER:HB2	1:B:33:GLU:HG3	1.82	0.60
1:D:359:PHE:HE2	1:D:365:ILE:HD13	1.66	0.60
1:B:521:LEU:HD23	2:B:801:A1IE:N12	2.16	0.60
1:C:389:VAL:HG12	1:C:392:ASP:OD2	2.02	0.60
1:A:154:ASN:O	1:A:158:ILE:HG13	2.01	0.59
1:C:343:MET:HA	1:C:346:ILE:HD11	1.84	0.59
1:B:74:LEU:CD2	1:B:90:LEU:HD11	2.29	0.59
1:B:659:PRO:N	1:B:660:PRO:HD2	2.17	0.59
1:C:159:LYS:O	1:C:163:GLN:HG3	2.03	0.59
1:A:52:LEU:HD13	1:A:92:HIS:CE1	2.37	0.59
1:B:74:LEU:HD12	1:B:95:TYR:O	2.02	0.59
1:C:341:PHE:CZ	1:C:373:SER:HB2	2.38	0.59
1:B:743:PHE:HZ	1:C:745:GLU:HG2	1.67	0.59
1:C:52:LEU:HD13	1:C:92:HIS:CG	2.38	0.59
1:C:175:ARG:HA	1:D:324:ARG:HD3	1.85	0.59
1:A:22:ILE:CD1	1:B:211:LEU:HD21	2.25	0.59
1:A:342:PRO:O	1:A:346:ILE:HG12	2.03	0.59
1:B:449:THR:O	1:B:453:LYS:HG3	2.03	0.59
1:B:36:PHE:HA	1:B:39:ALA:HB3	1.85	0.59
1:A:324:ARG:HH21	1:D:175:ARG:CA	2.09	0.58
1:A:194:ARG:HH21	1:A:197:LEU:HD23	1.67	0.58
1:A:211:LEU:HD11	1:D:22:ILE:HD12	1.84	0.58
1:A:738:LEU:HD22	1:A:742:ASN:ND2	2.16	0.58
1:C:480:ALA:O	1:C:484:ILE:HG13	2.03	0.58
1:C:348:TYR:CD2	1:C:657:LEU:HD21	2.38	0.58
1:A:361:LYS:HZ3	1:A:653:GLU:HG3	1.67	0.58
1:B:56:GLU:N	1:B:56:GLU:OE1	2.37	0.58
1:B:60:ASN:HD22	1:B:61:VAL:HG23	1.69	0.58
1:B:318:GLY:O	1:B:320:PRO:HD3	2.03	0.58
1:A:397:GLY:N	1:A:398:PRO:HD3	2.18	0.58
1:D:48:VAL:O	1:D:52:LEU:HD12	2.04	0.58
1:D:52:LEU:HD13	1:D:92:HIS:CD2	2.38	0.58
1:B:516:ASP:OD1	1:B:623:MET:HE2	2.04	0.58
1:C:470:GLU:CD	1:C:470:GLU:H	2.11	0.58
1:A:395:VAL:O	1:A:398:PRO:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:GLY:N	1:C:398:PRO:HD3	2.19	0.58
1:D:30:SER:O	1:D:34:LYS:HG3	2.03	0.58
1:A:623:MET:HE2	1:B:506:LEU:HD11	1.86	0.58
1:C:154:ASN:O	1:C:158:ILE:HG13	2.04	0.58
1:D:52:LEU:HD22	1:D:92:HIS:CB	2.33	0.57
1:D:429:GLU:HA	1:D:432:HIS:CE1	2.39	0.57
1:A:28:GLU:OE1	1:A:29:LEU:N	2.30	0.57
1:D:373:SER:O	1:D:410:TRP:HZ3	1.88	0.57
1:B:331:LEU:O	1:B:335:MET:HG3	2.04	0.57
1:D:465:PRO:HD2	1:D:468:GLU:OE1	2.05	0.57
1:C:327:TRP:NE1	1:C:328:VAL:HG23	2.20	0.57
1:D:547:ILE:H	1:D:547:ILE:CD1	2.14	0.57
1:C:172:HIS:ND1	1:C:178:CYS:SG	2.77	0.57
1:D:472:TRP:HE3	1:D:477:ILE:HD11	1.68	0.57
1:D:36:PHE:CZ	1:D:48:VAL:HG23	2.39	0.57
1:D:593:ARG:NH1	1:D:598:GLU:OE1	2.38	0.57
1:B:595:GLU:HG3	1:C:471:MET:CE	2.34	0.57
1:A:209:ILE:O	1:A:213:SER:HB2	2.05	0.57
1:A:560:LYS:HZ1	1:B:559:GLU:HG3	1.68	0.56
1:B:754:ARG:HG2	1:C:753:PHE:CG	2.40	0.56
1:D:401:THR:HG22	1:D:404:GLU:HB2	1.87	0.56
1:D:409:PRO:HG2	1:D:410:TRP:CD1	2.40	0.56
1:D:74:LEU:HD21	1:D:90:LEU:HD13	1.87	0.56
1:D:464:ARG:HG2	1:D:465:PRO:HD2	1.87	0.56
1:A:17:ARG:HB3	1:B:167:THR:HG21	1.87	0.56
1:B:178:CYS:SG	1:B:181:CYS:HB2	2.45	0.56
1:C:48:VAL:O	1:C:52:LEU:HD12	2.05	0.56
1:C:71:ARG:HH21	1:C:76:ILE:HD11	1.70	0.56
1:D:172:HIS:ND1	1:D:181:CYS:SG	2.79	0.56
1:D:372:ALA:O	1:D:376:THR:HG23	2.05	0.56
1:D:416:TRP:HA	1:D:416:TRP:CE3	2.40	0.56
1:C:358:LEU:O	1:C:361:LYS:HB2	2.05	0.56
1:B:90:LEU:HD22	1:B:114:LEU:CD2	2.34	0.56
1:B:377:PHE:HB2	1:B:410:TRP:CD1	2.40	0.56
1:B:418:GLU:OE1	1:B:430:TYR:OH	2.12	0.56
1:C:346:ILE:HA	1:C:349:LEU:CD1	2.35	0.56
1:D:63:ILE:HG12	1:D:64:ASN:N	2.19	0.56
1:D:756:GLU:C	1:D:760:LEU:HD12	2.30	0.56
1:C:164:LYS:O	1:C:166:VAL:HG13	2.06	0.56
1:B:361:LYS:HE2	1:B:653:GLU:HG2	1.87	0.56
1:D:327:TRP:NE1	1:D:328:VAL:HG23	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:ILE:HD12	1:D:547:ILE:N	2.15	0.56
1:D:653:GLU:H	1:D:653:GLU:CD	2.14	0.56
1:C:664:ILE:HD13	1:C:664:ILE:H	1.71	0.55
1:B:351:SER:HB2	1:B:354:SER:HB3	1.88	0.55
1:C:106:LYS:HD2	1:C:106:LYS:O	2.06	0.55
1:B:422:MET:HB2	1:B:430:TYR:HE2	1.70	0.55
1:D:504:GLY:O	1:D:508:ILE:HG12	2.06	0.55
1:A:168:ILE:HG13	1:A:169:PRO:HD2	1.87	0.55
1:C:388:ILE:HG22	1:C:390:ARG:NH2	2.18	0.55
1:A:189:SER:O	1:B:262:SER:OG	2.14	0.55
1:C:66:MET:HE2	1:C:66:MET:H	1.72	0.55
1:A:30:SER:O	1:A:34:LYS:HG3	2.07	0.55
1:D:154:ASN:O	1:D:158:ILE:HG13	2.07	0.55
1:B:416:TRP:HA	1:B:416:TRP:CE3	2.42	0.55
1:C:395:VAL:O	1:C:398:PRO:HG3	2.06	0.55
1:A:30:SER:OG	1:A:32:GLU:HG3	2.07	0.54
1:C:740:GLU:OE1	1:D:733:LYS:HA	2.07	0.54
1:A:410:TRP:H	1:A:410:TRP:CD1	2.25	0.54
1:C:756:GLU:O	1:C:760:LEU:N	2.40	0.54
1:D:657:LEU:HD12	1:D:661:PHE:HB2	1.89	0.54
1:A:659:PRO:HA	1:A:662:ASN:HB2	1.89	0.54
1:B:74:LEU:O	1:B:78:ILE:HG13	2.08	0.54
1:D:342:PRO:O	1:D:346:ILE:HG12	2.07	0.54
1:A:71:ARG:O	1:A:76:ILE:HD11	2.07	0.54
1:D:164:LYS:O	1:D:166:VAL:HG13	2.08	0.54
1:A:345:SER:OG	1:A:657:LEU:HD22	2.08	0.54
1:B:45:TYR:CD2	1:B:88:LEU:HD22	2.42	0.54
1:B:169:PRO:HG2	1:B:199:ILE:CD1	2.38	0.54
1:C:326:HIS:HB3	1:C:329:VAL:HG23	1.88	0.54
1:C:743:PHE:CE1	1:C:747:LYS:HD3	2.43	0.54
1:D:416:TRP:HA	1:D:416:TRP:HE3	1.71	0.54
1:A:415:ILE:HD13	1:A:447:LEU:HD11	1.88	0.54
1:B:754:ARG:HG2	1:C:753:PHE:CD1	2.43	0.54
1:A:377:PHE:HB2	1:A:410:TRP:CE3	2.43	0.54
1:B:85:ILE:HD12	1:B:85:ILE:H	1.73	0.54
1:B:590:VAL:HG23	1:B:592:ALA:O	2.08	0.54
1:C:44:ASP:HB3	1:C:47:THR:OG1	2.07	0.54
1:C:183:SER:O	1:C:187:VAL:HG23	2.08	0.54
1:C:747:LYS:O	1:C:750:ILE:HG13	2.08	0.54
1:A:73:ALA:HB1	1:A:89:LEU:CD2	2.38	0.53
1:A:172:HIS:ND1	1:A:178:CYS:SG	2.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:TRP:HA	1:B:416:TRP:HE3	1.73	0.53
1:C:82:ASN:HB3	1:C:85:ILE:CB	2.35	0.53
1:D:30:SER:OG	1:D:32:GLU:OE2	2.24	0.53
1:D:84:GLU:HG2	1:D:85:ILE:H	1.72	0.53
1:D:350:ILE:HD12	1:D:351:SER:N	2.23	0.53
1:B:354:SER:O	1:B:358:LEU:HD22	2.07	0.53
1:C:52:LEU:HD22	1:C:92:HIS:CB	2.37	0.53
1:C:652:ASP:OD1	1:C:652:ASP:N	2.39	0.53
1:D:513:MET:HE2	1:D:628:TYR:HD1	1.72	0.53
1:B:36:PHE:O	1:B:40:VAL:N	2.31	0.53
1:B:57:ILE:HD12	1:B:58:TYR:N	2.23	0.53
1:B:322:TRP:CZ2	1:B:330:LYS:HG2	2.43	0.53
1:B:56:GLU:HG2	1:B:57:ILE:HG23	1.91	0.53
1:B:182:VAL:O	1:B:186:GLU:HG3	2.08	0.53
1:C:71:ARG:NH2	1:C:76:ILE:HD11	2.24	0.53
1:B:326:HIS:HB3	1:B:329:VAL:CG1	2.39	0.53
1:A:526:LEU:HD22	1:B:494:ILE:HG13	1.90	0.53
1:B:178:CYS:HB2	1:B:180:GLU:CD	2.34	0.53
1:B:739:THR:HG23	1:B:741:GLU:HG3	1.91	0.53
1:D:52:LEU:HD13	1:D:92:HIS:CE1	2.44	0.53
1:C:393:LEU:HD21	1:C:466:ARG:HD2	1.91	0.53
1:D:49:LYS:HD2	1:D:53:GLN:HG3	1.90	0.53
1:D:381:LEU:HD23	1:D:407:ILE:HD11	1.90	0.53
1:A:80:ASN:O	1:A:81:GLU:HB3	2.07	0.53
1:B:372:ALA:O	1:B:376:THR:HG23	2.08	0.53
1:A:393:LEU:HD12	1:D:541:TYR:HD1	1.74	0.53
1:A:734:THR:N	1:D:740:GLU:OE1	2.41	0.53
1:D:78:ILE:HG12	1:D:86:MET:SD	2.48	0.53
1:D:402:VAL:O	1:D:406:MET:HG2	2.09	0.53
1:A:82:ASN:CB	1:A:85:ILE:HD13	2.39	0.52
1:C:545:ARG:HB2	1:C:548:ASP:OD2	2.09	0.52
1:B:225:TRP:O	1:B:229:GLU:HG2	2.09	0.52
1:D:366:LYS:HE2	1:D:656:THR:HG23	1.90	0.52
1:D:408:LEU:CD1	1:D:412:LEU:HD11	2.40	0.52
1:D:747:LYS:HZ3	1:D:747:LYS:HB2	1.74	0.52
1:B:79:GLU:O	1:B:106:LYS:HE3	2.09	0.52
1:B:430:TYR:CD1	1:B:436:ASN:HB3	2.44	0.52
1:D:178:CYS:SG	1:D:181:CYS:HB2	2.49	0.52
1:D:359:PHE:HE2	1:D:365:ILE:CD1	2.22	0.52
1:B:343:MET:O	1:B:346:ILE:HG13	2.09	0.52
1:B:464:ARG:HG3	1:B:465:PRO:CD	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ILE:HG12	1:D:170:ARG:NH2	2.25	0.52
1:C:29:LEU:HD23	1:C:34:LYS:HG2	1.92	0.52
1:D:659:PRO:N	1:D:660:PRO:HD2	2.25	0.52
1:A:213:SER:O	1:D:24:ARG:NH2	2.37	0.52
1:A:560:LYS:HZ2	1:B:559:GLU:HG3	1.75	0.52
1:A:750:ILE:HG13	1:D:750:ILE:HD13	1.91	0.52
1:C:33:GLU:O	1:C:37:LEU:HD13	2.10	0.52
1:B:18:ILE:HB	1:C:168:ILE:HG22	1.91	0.52
1:D:60:ASN:OD1	1:D:60:ASN:N	2.41	0.52
1:A:37:LEU:HD11	1:A:65:CYS:SG	2.49	0.52
1:A:235:ASN:OD1	1:A:235:ASN:N	2.41	0.52
1:A:435:TRP:HB3	1:A:492:ARG:NH2	2.22	0.52
1:B:381:LEU:HD23	1:B:407:ILE:CD1	2.40	0.52
1:A:66:MET:HE1	1:A:70:GLY:CA	2.40	0.52
1:C:754:ARG:HA	1:D:753:PHE:CZ	2.45	0.52
1:B:54:GLU:O	1:B:58:TYR:HB2	2.10	0.52
1:D:37:LEU:HD11	1:D:65:CYS:SG	2.50	0.52
1:C:345:SER:O	1:C:349:LEU:HD12	2.10	0.51
1:C:406:MET:O	1:C:409:PRO:HD2	2.10	0.51
1:A:210:ALA:HB1	1:A:721:VAL:HG13	1.91	0.51
1:A:380:MET:HE3	1:A:407:ILE:HG13	1.91	0.51
1:A:739:THR:OG1	1:B:734:THR:HA	2.10	0.51
1:A:82:ASN:ND2	1:A:85:ILE:HD13	2.25	0.51
1:D:84:GLU:HG2	1:D:85:ILE:N	2.26	0.51
1:A:410:TRP:CD1	1:A:410:TRP:N	2.79	0.51
1:C:45:TYR:CD2	1:C:88:LEU:HG	2.45	0.51
1:D:291:LYS:HG2	1:D:648:MET:HE1	1.92	0.51
1:A:52:LEU:HD13	1:A:92:HIS:ND1	2.26	0.51
1:D:52:LEU:HD23	1:D:63:ILE:HG21	1.92	0.51
1:B:349:LEU:HG	1:B:657:LEU:HD11	1.92	0.51
1:D:39:ALA:CA	1:D:42:LYS:HB2	2.39	0.51
1:D:721:VAL:O	1:D:725:VAL:HG23	2.11	0.51
1:A:36:PHE:HA	1:A:39:ALA:HB3	1.93	0.51
1:A:595:GLU:HG3	1:B:471:MET:CE	2.41	0.51
1:C:262:SER:O	1:C:266:GLU:HG3	2.10	0.51
1:C:636:ASP:OD2	1:C:640:LYS:NZ	2.40	0.51
1:B:392:ASP:HA	1:B:395:VAL:HG23	1.92	0.51
1:A:44:ASP:C	1:A:44:ASP:OD1	2.55	0.51
1:C:144:THR:HG1	1:C:147:MET:HG3	1.75	0.51
1:A:408:LEU:HD13	1:A:412:LEU:HD23	1.93	0.50
1:C:311:LEU:HD13	1:C:644:THR:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:MET:HE1	1:D:427:PHE:HB2	1.92	0.50
1:C:533:ASN:OD1	1:D:382:LEU:HD23	2.12	0.50
1:A:756:GLU:OE1	1:D:754:ARG:NH1	2.45	0.50
1:B:665:PRO:O	1:B:666:SER:HB3	2.11	0.50
1:B:724:TYR:CE1	1:B:728:MET:HE3	2.47	0.50
1:D:590:VAL:HG23	1:D:592:ALA:O	2.11	0.50
1:A:595:GLU:HB2	1:B:471:MET:SD	2.51	0.50
1:C:410:TRP:CD1	1:C:410:TRP:H	2.27	0.50
1:A:480:ALA:O	1:A:484:ILE:HG13	2.12	0.50
1:A:520:PHE:HD1	1:A:623:MET:HE1	1.75	0.50
1:A:659:PRO:N	1:A:660:PRO:HD2	2.27	0.50
1:A:739:THR:CG2	1:A:741:GLU:HG2	2.42	0.50
1:C:72:SER:O	1:C:76:ILE:HB	2.11	0.50
1:D:171:PRO:HG3	1:D:199:ILE:CG2	2.42	0.50
1:A:373:SER:O	1:A:410:TRP:HZ3	1.94	0.50
1:A:754:ARG:HA	1:B:753:PHE:CZ	2.47	0.50
1:B:392:ASP:HA	1:B:395:VAL:CG2	2.41	0.50
1:A:336:THR:O	1:A:340:LEU:HG	2.12	0.50
1:B:595:GLU:HG3	1:C:471:MET:HE2	1.93	0.50
1:C:526:LEU:HD12	1:D:494:ILE:HG13	1.94	0.50
1:A:658:PRO:O	1:A:662:ASN:N	2.45	0.49
1:A:623:MET:HE2	1:B:506:LEU:CD1	2.42	0.49
1:D:410:TRP:CD1	1:D:410:TRP:N	2.79	0.49
1:C:37:LEU:O	1:C:40:VAL:HG22	2.11	0.49
1:A:464:ARG:HG3	1:A:465:PRO:CD	2.42	0.49
1:A:733:LYS:HE3	1:D:744:LYS:NZ	2.27	0.49
1:B:746:LEU:O	1:B:750:ILE:HD12	2.13	0.49
1:C:50:GLN:O	1:C:54:GLU:HB2	2.13	0.49
1:A:310:LEU:C	1:A:310:LEU:HD23	2.38	0.49
1:A:359:PHE:HD2	1:A:365:ILE:HD13	1.76	0.49
1:B:389:VAL:HB	1:B:392:ASP:OD2	2.11	0.49
1:C:754:ARG:HG2	1:C:755:TYR:N	2.26	0.49
1:D:513:MET:HE2	1:D:628:TYR:CD1	2.48	0.49
1:C:750:ILE:HD12	1:C:751:SER:N	2.27	0.49
1:C:373:SER:O	1:C:410:TRP:HZ3	1.95	0.49
1:C:445:LEU:HB2	1:C:485:SER:OG	2.13	0.49
1:D:408:LEU:O	1:D:412:LEU:HG	2.13	0.49
1:A:619:MET:HG3	1:B:624:MET:CE	2.43	0.49
1:C:109:VAL:O	1:C:113:GLU:HG3	2.12	0.49
1:C:272:ARG:H	1:C:709:GLN:HE22	1.60	0.49
1:D:86:MET:HE1	1:D:111:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:MET:HA	1:A:346:ILE:HD11	1.94	0.49
1:D:322:TRP:CZ2	1:D:330:LYS:HG2	2.47	0.49
1:A:526:LEU:HD23	1:B:494:ILE:HG13	1.95	0.49
1:C:403:VAL:O	1:C:407:ILE:HD13	2.13	0.49
1:C:752:SER:O	1:C:756:GLU:HG3	2.13	0.49
1:A:465:PRO:HD2	1:A:468:GLU:OE1	2.13	0.48
1:B:89:LEU:HD23	1:B:94:VAL:CG2	2.41	0.48
1:C:351:SER:O	1:C:354:SER:OG	2.24	0.48
1:D:174:ILE:HD12	1:D:175:ARG:N	2.28	0.48
1:A:23:VAL:HG12	1:A:24:ARG:HG3	1.94	0.48
1:B:36:PHE:CE1	1:B:40:VAL:HG23	2.47	0.48
1:C:253:LYS:HE3	1:C:257:ASP:OD1	2.12	0.48
1:C:430:TYR:CE1	1:C:436:ASN:HB3	2.48	0.48
1:A:42:LYS:HD2	1:A:42:LYS:N	2.27	0.48
1:A:201:LYS:HG2	1:A:244:LEU:HD11	1.95	0.48
1:D:565:PHE:HD1	1:D:571:THR:HG23	1.78	0.48
1:A:304:GLN:OE1	1:A:306:ASN:HB2	2.12	0.48
1:A:403:VAL:HG12	1:A:407:ILE:HD12	1.95	0.48
1:A:470:GLU:HG2	1:A:471:MET:H	1.79	0.48
1:A:592:ALA:HB2	1:B:467:GLU:HG3	1.94	0.48
1:A:617:LEU:HD13	1:A:617:LEU:O	2.13	0.48
1:A:754:ARG:HG2	1:B:753:PHE:CG	2.48	0.48
1:C:71:ARG:HE	1:C:76:ILE:HG12	1.78	0.48
1:C:217:ILE:HD12	1:C:717:ILE:HD11	1.95	0.48
1:C:523:ILE:HD13	1:D:497:PHE:HE2	1.79	0.48
1:C:584:ASN:O	1:C:587:VAL:HG22	2.13	0.48
1:A:222:ARG:NH1	1:A:222:ARG:HB2	2.28	0.48
1:D:263:ARG:HH11	1:D:263:ARG:HB3	1.77	0.48
1:D:395:VAL:HG12	1:D:398:PRO:HG3	1.96	0.48
1:B:52:LEU:HD11	1:B:63:ILE:HG12	1.94	0.48
1:B:67:ASP:OD1	1:B:68:PRO:HD2	2.14	0.48
1:C:395:VAL:HG22	1:C:463:SER:OG	2.14	0.48
1:A:45:TYR:CE2	1:A:88:LEU:HG	2.49	0.48
1:B:66:MET:HE3	1:B:67:ASP:N	2.28	0.48
1:C:731:ASN:O	1:C:734:THR:HG22	2.13	0.48
1:A:208:LEU:O	1:A:208:LEU:HG	2.13	0.48
1:B:512:ARG:HB2	1:B:631:ILE:HD13	1.96	0.48
1:C:78:ILE:HG13	1:C:86:MET:SD	2.54	0.47
1:C:81:GLU:HG2	1:C:108:VAL:HG11	1.96	0.47
1:D:45:TYR:CD2	1:D:88:LEU:HG	2.47	0.47
1:A:402:VAL:O	1:A:406:MET:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:SER:HA	1:A:639:TRP:CZ2	2.49	0.47
1:A:565:PHE:HD1	1:A:571:THR:HG23	1.79	0.47
1:B:547:ILE:HG13	1:B:547:ILE:O	2.13	0.47
1:D:341:PHE:CG	1:D:342:PRO:HD3	2.50	0.47
1:C:62:ASN:OD1	1:C:63:ILE:N	2.48	0.47
1:C:88:LEU:HD13	1:C:92:HIS:HE1	1.78	0.47
1:C:456:ALA:HB2	1:C:474:PRO:HB2	1.96	0.47
1:D:756:GLU:O	1:D:760:LEU:HD12	2.13	0.47
1:A:754:ARG:HG2	1:B:753:PHE:CD2	2.48	0.47
1:B:238:LYS:HE3	1:B:238:LYS:HB2	1.43	0.47
1:B:39:ALA:HA	1:B:42:LYS:CG	2.44	0.47
1:B:565:PHE:HD1	1:B:571:THR:HG23	1.80	0.47
1:C:215:ASP:OD2	1:C:218:LEU:HB2	2.15	0.47
1:D:74:LEU:HD21	1:D:90:LEU:HD11	1.97	0.47
1:A:211:LEU:HD11	1:D:22:ILE:CD1	2.44	0.47
1:C:341:PHE:HB3	1:C:342:PRO:HD3	1.97	0.47
1:C:410:TRP:CD1	1:C:410:TRP:N	2.83	0.47
1:D:38:ASN:HB3	1:D:42:LYS:HE2	1.96	0.47
1:D:52:LEU:HD13	1:D:92:HIS:CG	2.50	0.47
1:D:67:ASP:CG	1:D:68:PRO:HD2	2.40	0.47
1:D:158:ILE:O	1:D:162:VAL:HG23	2.15	0.47
1:D:165:ARG:HG2	1:D:165:ARG:HH11	1.80	0.47
1:D:473:HIS:ND1	1:D:474:PRO:HD2	2.29	0.47
1:A:51:ALA:O	1:A:54:GLU:HG3	2.15	0.47
1:B:148:LEU:O	1:B:152:THR:HG23	2.14	0.47
1:B:390:ARG:HA	1:B:390:ARG:HD3	1.62	0.47
1:C:38:ASN:O	1:C:42:LYS:N	2.44	0.47
1:C:135:GLN:HG3	1:C:136:PHE:N	2.26	0.47
1:C:224:GLY:O	1:C:245:SER:OG	2.33	0.47
1:C:567:THR:O	1:C:571:THR:OG1	2.24	0.47
1:A:388:ILE:HD13	1:A:401:THR:HG21	1.97	0.47
1:C:420:LYS:HB2	1:C:420:LYS:NZ	2.30	0.47
1:D:227:LEU:HD13	1:D:244:LEU:CB	2.41	0.47
1:C:83:LEU:O	1:C:87:GLU:N	2.32	0.47
1:C:359:PHE:O	1:C:365:ILE:HG21	2.15	0.47
1:A:350:ILE:HG13	1:A:351:SER:N	2.30	0.46
1:A:471:MET:CE	1:D:595:GLU:HB2	2.46	0.46
1:B:29:LEU:HD11	1:B:65:CYS:SG	2.55	0.46
1:B:663:ILE:O	1:B:663:ILE:CD1	2.59	0.46
1:C:401:THR:HG22	1:C:402:VAL:H	1.79	0.46
1:D:32:GLU:OE2	1:D:33:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:GLU:OE2	1:D:61:VAL:HG13	2.15	0.46
1:D:40:VAL:HG22	1:D:89:LEU:HD21	1.97	0.46
1:D:96:VAL:O	1:D:96:VAL:HG12	2.15	0.46
1:D:263:ARG:HB3	1:D:263:ARG:NH1	2.30	0.46
1:D:397:GLY:N	1:D:398:PRO:HD3	2.30	0.46
1:A:746:LEU:HD23	1:D:743:PHE:CE1	2.50	0.46
1:B:28:GLU:HG3	1:B:29:LEU:N	2.29	0.46
1:B:473:HIS:ND1	1:B:474:PRO:HD2	2.31	0.46
1:D:39:ALA:O	1:D:42:LYS:HB2	2.15	0.46
1:D:406:MET:O	1:D:409:PRO:HD2	2.14	0.46
1:A:108:VAL:HG23	1:A:108:VAL:O	2.14	0.46
1:B:78:ILE:HG12	1:B:86:MET:SD	2.55	0.46
1:B:408:LEU:HD23	1:B:412:LEU:HG	1.98	0.46
1:C:82:ASN:CB	1:C:85:ILE:HB	2.37	0.46
1:C:724:TYR:CE1	1:C:728:MET:HE3	2.49	0.46
1:A:48:VAL:HG12	1:A:52:LEU:HD11	1.96	0.46
1:A:733:LYS:O	1:A:734:THR:OG1	2.26	0.46
1:B:366:LYS:NZ	1:B:656:THR:HG22	2.30	0.46
1:D:42:LYS:HD3	1:D:42:LYS:HA	1.40	0.46
1:D:54:GLU:HG3	1:D:58:TYR:HB2	1.98	0.46
1:D:236:GLU:HB2	1:D:237:PHE:CD1	2.51	0.46
1:D:331:LEU:O	1:D:335:MET:HG3	2.15	0.46
1:C:526:LEU:HD22	1:C:526:LEU:HA	1.74	0.46
1:A:66:MET:SD	1:A:70:GLY:HA2	2.56	0.46
1:B:66:MET:HE1	1:B:70:GLY:C	2.39	0.46
1:C:257:ASP:OD2	1:C:304:GLN:NE2	2.47	0.46
1:C:418:GLU:OE2	1:C:430:TYR:OH	2.19	0.46
1:C:467:GLU:CD	1:C:467:GLU:H	2.24	0.46
1:D:85:ILE:O	1:D:89:LEU:HD12	2.15	0.46
1:A:377:PHE:HE1	1:A:407:ILE:HG23	1.81	0.46
1:A:475:THR:O	1:A:479:GLU:HG3	2.16	0.46
1:B:66:MET:HE3	1:B:66:MET:C	2.41	0.46
1:C:34:LYS:HB3	1:C:34:LYS:HE3	1.51	0.46
1:C:109:VAL:HG11	1:C:156:GLU:OE2	2.15	0.46
1:C:754:ARG:O	1:C:758:LEU:HG	2.15	0.46
1:D:222:ARG:NH1	1:D:296:TYR:OH	2.49	0.46
1:A:45:TYR:O	1:A:49:LYS:HD3	2.16	0.46
1:B:169:PRO:HG2	1:B:199:ILE:HD11	1.98	0.46
1:D:401:THR:CG2	1:D:404:GLU:H	2.29	0.46
1:A:52:LEU:HD22	1:A:92:HIS:CB	2.46	0.46
1:A:83:LEU:HA	1:A:86:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD11	1:A:161:LEU:HD23	1.98	0.46
1:A:326:HIS:ND1	1:A:328:VAL:HB	2.31	0.46
1:B:158:ILE:O	1:B:162:VAL:HG23	2.16	0.46
1:C:414:PHE:CE1	1:C:659:PRO:HG2	2.50	0.46
1:C:234:GLU:CA	1:D:323:ARG:HH12	2.29	0.45
1:A:97:GLY:O	1:A:98:ASP:HB2	2.16	0.45
1:A:756:GLU:OE2	1:D:758:LEU:HD21	2.16	0.45
1:B:57:ILE:CD1	1:B:58:TYR:HD1	2.30	0.45
1:D:343:MET:HA	1:D:346:ILE:CD1	2.46	0.45
1:A:69:LEU:N	1:A:69:LEU:HD23	2.31	0.45
1:B:54:GLU:O	1:B:54:GLU:HG3	2.15	0.45
1:B:82:ASN:O	1:B:86:MET:HB2	2.16	0.45
1:B:756:GLU:HG3	1:B:757:VAL:N	2.31	0.45
1:C:380:MET:HE3	1:C:407:ILE:CD1	2.31	0.45
1:D:350:ILE:HD12	1:D:351:SER:CB	2.47	0.45
1:A:116:LEU:HD11	1:A:161:LEU:CD2	2.47	0.45
1:A:348:TYR:HB2	1:A:360:ILE:HG21	1.97	0.45
1:B:754:ARG:CZ	1:B:754:ARG:HB3	2.47	0.45
1:A:45:TYR:OH	1:A:84:GLU:HB3	2.17	0.45
1:A:58:TYR:HB3	1:A:60:ASN:OD1	2.16	0.45
1:A:211:LEU:HD21	1:D:22:ILE:CD1	2.47	0.45
1:A:214:GLU:OE2	1:A:214:GLU:CA	2.64	0.45
1:A:331:LEU:HD23	1:A:331:LEU:O	2.17	0.45
1:C:517:ILE:HG12	1:C:620:LEU:HD11	1.98	0.45
1:D:332:LEU:H	1:D:332:LEU:HG	1.53	0.45
1:D:526:LEU:HD22	1:D:526:LEU:HA	1.74	0.45
1:A:108:VAL:CG2	1:A:111:ALA:HB3	2.46	0.45
1:A:114:LEU:HD23	1:A:114:LEU:O	2.16	0.45
1:C:271:HIS:HA	1:C:709:GLN:NE2	2.31	0.45
1:C:348:TYR:HD2	1:C:657:LEU:HD21	1.79	0.45
1:C:744:LYS:HE3	1:C:744:LYS:HB3	1.33	0.45
1:A:614:VAL:O	1:A:618:ASN:ND2	2.40	0.45
1:A:721:VAL:O	1:A:725:VAL:HG23	2.16	0.45
1:C:116:LEU:HD23	1:C:116:LEU:HA	1.83	0.45
1:C:396:GLN:NE2	1:C:464:ARG:HG2	2.31	0.45
1:D:358:LEU:O	1:D:361:LYS:HB2	2.17	0.45
1:D:652:ASP:OD1	1:D:652:ASP:N	2.39	0.45
1:A:44:ASP:OD1	1:A:47:THR:HB	2.16	0.45
1:A:425:GLY:O	1:A:429:GLU:HB3	2.16	0.45
1:B:537:GLN:O	1:B:537:GLN:HG3	2.17	0.45
1:B:659:PRO:CD	1:B:660:PRO:HD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:PHE:CD1	1:B:661:PHE:N	2.85	0.45
1:C:401:THR:HG22	1:C:402:VAL:N	2.32	0.45
1:A:44:ASP:OD1	1:A:44:ASP:O	2.35	0.45
1:B:520:PHE:CD2	1:B:620:LEU:HD13	2.51	0.45
1:D:381:LEU:HD23	1:D:407:ILE:CD1	2.46	0.45
1:D:422:MET:HE1	1:D:427:PHE:CB	2.47	0.45
1:A:190:LEU:HG	1:B:306:ASN:OD1	2.17	0.45
1:B:178:CYS:O	1:B:182:VAL:HG23	2.17	0.45
1:C:341:PHE:HE1	1:C:658:PRO:HG2	1.81	0.45
1:C:384:ALA:HA	1:C:403:VAL:HG11	1.99	0.45
1:A:407:ILE:O	1:A:411:VAL:HG23	2.17	0.44
1:B:227:LEU:HD13	1:B:244:LEU:HB3	1.98	0.44
1:B:408:LEU:CD2	1:B:412:LEU:HD11	2.48	0.44
1:C:173:GLN:OE1	1:C:173:GLN:HA	2.18	0.44
1:C:348:TYR:HE1	1:C:361:LYS:HE3	1.82	0.44
1:D:349:LEU:HD23	1:D:349:LEU:HA	1.79	0.44
1:D:423:TRP:CE3	1:D:423:TRP:HA	2.52	0.44
1:B:210:ALA:HB1	1:B:721:VAL:HG13	1.99	0.44
1:C:659:PRO:N	1:C:660:PRO:HD2	2.32	0.44
1:A:351:SER:O	1:A:354:SER:HB3	2.16	0.44
1:B:156:GLU:OE1	1:B:156:GLU:O	2.35	0.44
1:D:36:PHE:HA	1:D:39:ALA:CB	2.40	0.44
1:D:326:HIS:HB3	1:D:329:VAL:CG1	2.47	0.44
1:D:429:GLU:HA	1:D:432:HIS:ND1	2.32	0.44
1:D:464:ARG:HG2	1:D:465:PRO:CD	2.47	0.44
1:A:381:LEU:HD23	1:A:407:ILE:CD1	2.48	0.44
1:B:45:TYR:CD2	1:B:88:LEU:HD13	2.53	0.44
1:B:465:PRO:HG2	1:B:468:GLU:OE2	2.18	0.44
1:C:41:GLU:CD	1:C:42:LYS:HD3	2.42	0.44
1:C:346:ILE:H	1:C:346:ILE:HG12	1.56	0.44
1:D:318:GLY:CA	1:D:362:LYS:HD3	2.47	0.44
1:D:459:LYS:HD2	1:D:460:TYR:CZ	2.52	0.44
1:A:410:TRP:H	1:A:410:TRP:HD1	1.64	0.44
1:A:415:ILE:HD13	1:A:447:LEU:CD1	2.47	0.44
1:B:180:GLU:HG2	1:B:181:CYS:N	2.32	0.44
1:C:715:GLU:OE1	1:C:715:GLU:HA	2.17	0.44
1:C:733:LYS:O	1:C:733:LYS:HG3	2.18	0.44
1:A:471:MET:HE2	1:D:595:GLU:HB2	2.00	0.44
1:A:753:PHE:CD1	1:D:754:ARG:HG2	2.52	0.44
1:A:753:PHE:CE1	1:D:754:ARG:HG2	2.52	0.44
1:B:39:ALA:HA	1:B:42:LYS:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLU:H	1:B:84:GLU:HG2	1.64	0.44
1:B:515:LEU:HD13	1:B:515:LEU:HA	1.81	0.44
1:B:82:ASN:CB	1:B:85:ILE:HD13	2.46	0.44
1:B:447:LEU:HD23	1:B:447:LEU:HA	1.80	0.44
1:C:82:ASN:O	1:C:86:MET:HB2	2.17	0.44
1:D:52:LEU:HD23	1:D:63:ILE:CG2	2.48	0.44
1:C:90:LEU:HD13	1:C:90:LEU:HA	1.83	0.44
1:C:707:LEU:HD22	1:C:707:LEU:HA	1.76	0.44
1:C:739:THR:CG2	1:C:742:ASN:H	2.31	0.44
1:D:32:GLU:OE1	1:D:61:VAL:HG21	2.18	0.44
1:D:75:LEU:N	1:D:75:LEU:HD12	2.33	0.44
1:D:408:LEU:N	1:D:409:PRO:HD2	2.32	0.44
1:C:540:PHE:CE2	1:D:388:ILE:HG21	2.53	0.44
1:D:80:ASN:HB2	1:D:82:ASN:OD1	2.17	0.44
1:A:465:PRO:HG2	1:A:468:GLU:OE2	2.17	0.43
1:A:589:ASN:HA	1:A:598:GLU:HG2	2.00	0.43
1:B:21:GLN:O	1:C:212:SER:HA	2.18	0.43
1:B:173:GLN:HG2	1:B:174:ILE:H	1.83	0.43
1:B:405:TRP:HA	1:B:405:TRP:CE3	2.52	0.43
1:C:63:ILE:HD13	1:C:63:ILE:HA	1.62	0.43
1:D:584:ASN:O	1:D:587:VAL:HG22	2.18	0.43
1:A:42:LYS:HA	1:A:42:LYS:CE	2.46	0.43
1:A:750:ILE:HD13	1:B:750:ILE:HG13	1.99	0.43
1:C:74:LEU:O	1:C:78:ILE:HD12	2.18	0.43
1:A:333:THR:O	1:A:336:THR:HG22	2.18	0.43
1:A:659:PRO:HA	1:A:662:ASN:CB	2.48	0.43
1:B:663:ILE:O	1:B:664:ILE:HG12	2.19	0.43
1:D:180:GLU:OE1	1:D:180:GLU:HA	2.18	0.43
1:A:383:LEU:HA	1:A:386:GLN:OE1	2.18	0.43
1:B:80:ASN:HB2	1:B:82:ASN:OD1	2.18	0.43
1:D:29:LEU:HD11	1:D:33:GLU:HB3	2.00	0.43
1:D:724:TYR:CE1	1:D:728:MET:HE3	2.53	0.43
1:D:740:GLU:CD	1:D:740:GLU:H	2.27	0.43
1:A:142:ASP:OD2	1:A:198:ASN:ND2	2.45	0.43
1:B:208:LEU:O	1:B:211:LEU:O	2.36	0.43
1:C:387:HIS:O	1:C:387:HIS:ND1	2.51	0.43
1:C:410:TRP:H	1:C:410:TRP:HD1	1.66	0.43
1:C:428:THR:HG23	1:C:429:GLU:N	2.33	0.43
1:D:86:MET:HG3	1:D:90:LEU:HD22	2.00	0.43
1:D:450:ILE:HD13	1:D:450:ILE:HA	1.87	0.43
1:C:657:LEU:N	1:C:657:LEU:HD22	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:TYR:O	1:D:49:LYS:HB3	2.18	0.43
1:A:381:LEU:HD23	1:A:407:ILE:HD13	2.01	0.43
1:B:52:LEU:O	1:B:56:GLU:N	2.41	0.43
1:B:167:THR:HG22	1:B:168:ILE:N	2.32	0.43
1:C:194:ARG:HE	1:C:194:ARG:HB2	1.67	0.43
1:C:289:LYS:HE2	1:C:289:LYS:HB2	1.90	0.43
1:D:179:VAL:HA	1:D:182:VAL:HG22	1.99	0.43
1:D:52:LEU:HD13	1:D:92:HIS:NE2	2.34	0.43
1:A:408:LEU:HB3	1:A:409:PRO:HD3	1.99	0.43
1:B:57:ILE:HD12	1:B:57:ILE:C	2.44	0.43
1:C:67:ASP:CG	1:C:68:PRO:HD2	2.44	0.43
1:C:233:VAL:HG12	1:D:323:ARG:HH11	1.84	0.43
1:C:516:ASP:OD1	1:C:519:LYS:HE2	2.19	0.43
1:A:81:GLU:CG	1:A:81:GLU:O	2.66	0.43
1:A:389:VAL:HG12	1:A:390:ARG:N	2.34	0.43
1:B:538:LEU:O	1:B:538:LEU:HG	2.17	0.43
1:C:739:THR:HG23	1:C:741:GLU:N	2.33	0.43
1:D:66:MET:HE3	1:D:66:MET:CA	2.32	0.43
1:D:238:LYS:HE2	1:D:242:GLU:OE2	2.19	0.43
1:A:21:GLN:O	1:B:212:SER:HA	2.19	0.42
1:A:94:VAL:O	1:A:96:VAL:HG13	2.19	0.42
1:A:354:SER:O	1:A:358:LEU:HD23	2.19	0.42
1:A:438:MET:HE3	1:A:438:MET:HB2	1.81	0.42
1:C:331:LEU:HD12	1:C:331:LEU:HA	1.86	0.42
1:C:380:MET:HB3	1:C:407:ILE:HD11	2.00	0.42
1:D:585:LEU:HG	1:D:585:LEU:O	2.19	0.42
1:A:739:THR:HG21	1:A:741:GLU:HG2	2.00	0.42
1:B:56:GLU:CD	1:B:57:ILE:HG13	2.44	0.42
1:B:221:PHE:CD1	1:B:298:GLN:HG3	2.54	0.42
1:B:741:GLU:HG3	1:B:741:GLU:H	1.48	0.42
1:C:80:ASN:O	1:C:81:GLU:HB2	2.20	0.42
1:B:729:ILE:HD12	1:B:729:ILE:HA	1.67	0.42
1:C:66:MET:H	1:C:66:MET:CE	2.32	0.42
1:C:437:LEU:HD23	1:C:437:LEU:HA	1.79	0.42
1:C:108:VAL:CG2	1:C:111:ALA:HB3	2.48	0.42
1:C:147:MET:HB3	1:C:147:MET:HE3	1.70	0.42
1:A:456:ALA:HB2	1:A:474:PRO:HB2	2.02	0.42
1:A:756:GLU:OE2	1:D:754:ARG:HD3	2.19	0.42
1:B:82:ASN:OD1	1:B:748:GLN:NE2	2.52	0.42
1:D:431:ILE:O	1:D:431:ILE:HG22	2.19	0.42
1:A:175:ARG:HA	1:B:324:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:VAL:HG12	1:B:76:ILE:CG2	2.50	0.42
1:B:45:TYR:HA	1:B:88:LEU:HD21	2.01	0.42
1:B:335:MET:HE2	1:B:335:MET:HB3	1.87	0.42
1:B:393:LEU:HB3	1:B:394:HIS:HD2	1.84	0.42
1:C:164:LYS:H	1:C:164:LYS:HG2	1.60	0.42
1:C:403:VAL:CA	1:C:406:MET:HE3	2.26	0.42
1:B:86:MET:HE1	1:B:111:ALA:HB1	2.00	0.42
1:C:342:PRO:O	1:C:346:ILE:HG12	2.19	0.42
1:C:365:ILE:HD12	1:C:365:ILE:HA	1.85	0.42
1:C:626:ASN:O	1:C:630:LEU:HG	2.20	0.42
1:C:733:LYS:O	1:C:734:THR:HB	2.20	0.42
1:D:422:MET:HE1	1:D:427:PHE:CA	2.49	0.42
1:C:341:PHE:CB	1:C:342:PRO:HD3	2.50	0.42
1:A:108:VAL:O	1:A:108:VAL:CG2	2.67	0.42
1:B:52:LEU:HD22	1:B:92:HIS:CB	2.36	0.42
1:B:430:TYR:CE1	1:B:436:ASN:HB3	2.55	0.42
1:B:739:THR:CG2	1:B:741:GLU:HG3	2.50	0.42
1:C:64:ASN:ND2	1:C:66:MET:SD	2.77	0.42
1:C:739:THR:HG22	1:C:742:ASN:HB2	2.02	0.42
1:D:318:GLY:HA2	1:D:362:LYS:HE3	2.01	0.42
1:A:49:LYS:HE2	1:A:49:LYS:HB2	1.75	0.41
1:A:304:GLN:HG2	1:A:305:PRO:HD2	2.01	0.41
1:A:428:THR:O	1:A:431:ILE:HG12	2.20	0.41
1:C:408:LEU:N	1:C:409:PRO:HD2	2.35	0.41
1:C:492:ARG:NH1	1:C:495:SER:OG	2.52	0.41
1:A:634:HIS:ND1	1:A:634:HIS:N	2.67	0.41
1:B:90:LEU:CD2	1:B:114:LEU:HD22	2.44	0.41
1:B:337:ILE:HD12	1:B:337:ILE:H	1.85	0.41
1:B:366:LYS:HD3	1:B:656:THR:HA	2.02	0.41
1:B:389:VAL:HG12	1:B:391:THR:H	1.85	0.41
1:B:422:MET:HE2	1:B:430:TYR:CE2	2.54	0.41
1:B:201:LYS:HE3	1:B:201:LYS:HB3	1.68	0.41
1:B:402:VAL:HG23	1:B:403:VAL:N	2.36	0.41
1:D:201:LYS:HE2	1:D:201:LYS:HB3	1.69	0.41
1:D:341:PHE:O	1:D:345:SER:OG	2.26	0.41
1:A:147:MET:HE3	1:A:198:ASN:HB3	2.01	0.41
1:A:504:GLY:O	1:A:508:ILE:HG12	2.21	0.41
1:B:42:LYS:NZ	1:B:755:TYR:OH	2.30	0.41
1:B:340:LEU:HD13	1:B:343:MET:CE	2.50	0.41
1:C:23:VAL:HG12	1:C:24:ARG:HG3	2.02	0.41
1:D:321:GLY:O	1:D:325:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:LEU:O	1:D:408:LEU:HD13	2.21	0.41
1:B:57:ILE:CD1	1:B:58:TYR:CD1	3.03	0.41
1:B:595:GLU:HB2	1:C:471:MET:SD	2.61	0.41
1:D:73:ALA:HB1	1:D:89:LEU:HD23	2.03	0.41
1:A:420:LYS:HB3	1:A:420:LYS:HE3	1.65	0.41
1:B:452:LEU:HD23	1:B:452:LEU:HA	1.82	0.41
1:C:663:ILE:HG13	1:C:664:ILE:N	2.36	0.41
1:A:36:PHE:O	1:A:39:ALA:HB3	2.21	0.41
1:A:324:ARG:NH2	1:D:176:CYS:H	2.19	0.41
1:A:747:LYS:HB3	1:A:747:LYS:HE3	1.61	0.41
1:C:36:PHE:O	1:C:39:ALA:N	2.54	0.41
1:C:233:VAL:HG12	1:D:323:ARG:NH1	2.36	0.41
1:C:473:HIS:ND1	1:C:474:PRO:HD2	2.36	0.41
1:C:760:LEU:HD22	1:C:760:LEU:HA	1.78	0.41
1:A:88:LEU:HA	1:A:88:LEU:HD23	1.81	0.41
1:A:428:THR:HG23	1:A:429:GLU:N	2.36	0.41
1:B:94:VAL:HG12	1:B:95:TYR:N	2.36	0.41
1:D:66:MET:HE2	1:D:70:GLY:HA2	2.02	0.41
1:A:74:LEU:HD11	1:A:90:LEU:CD2	2.51	0.41
1:A:82:ASN:HD22	1:A:85:ILE:HD13	1.86	0.41
1:A:113:GLU:HG2	1:A:160:LEU:HD21	2.02	0.41
1:A:349:LEU:HD21	1:A:657:LEU:HD11	2.01	0.41
1:A:520:PHE:HD1	1:A:623:MET:CE	2.34	0.41
1:B:73:ALA:HB1	1:B:89:LEU:CD1	2.46	0.41
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.87	0.41
1:B:659:PRO:HD2	1:B:660:PRO:HD2	2.02	0.41
1:C:106:LYS:HG3	1:C:108:VAL:HG13	2.01	0.41
1:C:341:PHE:CD1	1:C:341:PHE:C	2.97	0.41
1:D:501:SER:HA	1:D:639:TRP:CZ2	2.55	0.41
1:C:413:GLY:O	1:C:417:GLY:N	2.40	0.41
1:D:223:LEU:HD12	1:D:223:LEU:HA	1.87	0.41
1:D:341:PHE:CD1	1:D:341:PHE:C	2.99	0.41
1:D:406:MET:HE3	1:D:406:MET:HB3	1.82	0.41
1:D:657:LEU:HD12	1:D:661:PHE:CB	2.50	0.41
1:A:403:VAL:HG12	1:A:407:ILE:CD1	2.52	0.40
1:B:217:ILE:HD12	1:B:717:ILE:HD11	2.03	0.40
1:B:394:HIS:N	1:B:394:HIS:CD2	2.89	0.40
1:B:646:LEU:O	1:B:649:SER:HB2	2.22	0.40
1:C:393:LEU:CD2	1:C:466:ARG:HB2	2.50	0.40
1:A:45:TYR:CD2	1:A:88:LEU:HD11	2.56	0.40
1:A:750:ILE:CD1	1:B:750:ILE:HG13	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:ILE:O	1:B:512:ARG:HG2	2.20	0.40
1:C:39:ALA:HA	1:C:42:LYS:HB2	2.03	0.40
1:C:40:VAL:O	1:C:85:ILE:HG21	2.21	0.40
1:C:106:LYS:O	1:C:107:GLU:HB2	2.20	0.40
1:C:592:ALA:O	1:C:594:HIS:N	2.53	0.40
1:A:36:PHE:HE1	1:A:48:VAL:HG22	1.87	0.40
1:A:739:THR:HG23	1:A:741:GLU:HG2	2.03	0.40
1:D:310:LEU:C	1:D:310:LEU:HD23	2.46	0.40
1:A:74:LEU:HD12	1:A:74:LEU:HA	1.84	0.40
1:A:394:HIS:ND1	1:A:465:PRO:HA	2.36	0.40
1:B:57:ILE:HD12	1:B:58:TYR:HD1	1.87	0.40
1:B:204:ALA:O	1:B:247:GLN:NE2	2.54	0.40
1:B:388:ILE:CG2	1:B:390:ARG:HH12	2.34	0.40
1:C:523:ILE:HD13	1:D:497:PHE:CE2	2.56	0.40
1:D:57:ILE:HD13	1:D:57:ILE:HA	1.86	0.40
1:A:738:LEU:HD23	1:A:738:LEU:HA	1.91	0.40
1:B:94:VAL:HG12	1:B:95:TYR:H	1.86	0.40
1:B:340:LEU:HB3	1:B:343:MET:HE2	2.03	0.40
1:C:634:HIS:ND1	1:C:634:HIS:N	2.69	0.40
1:D:82:ASN:HB2	1:D:85:ILE:CD1	2.52	0.40
1:D:326:HIS:CE1	1:D:327:TRP:HD1	2.39	0.40
1:D:538:LEU:O	1:D:538:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	665/765 (87%)	652 (98%)	13 (2%)	0	100	100
1	B	666/765 (87%)	650 (98%)	16 (2%)	0	100	100
1	C	666/765 (87%)	649 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	667/765 (87%)	655 (98%)	12 (2%)	0	100	100
All	All	2664/3060 (87%)	2606 (98%)	58 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	604/688 (88%)	587 (97%)	17 (3%)	38	65
1	B	605/688 (88%)	576 (95%)	29 (5%)	21	44
1	C	605/688 (88%)	561 (93%)	44 (7%)	11	25
1	D	606/688 (88%)	563 (93%)	43 (7%)	12	26
All	All	2420/2752 (88%)	2287 (94%)	133 (6%)	20	38

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	65	CYS
1	A	67	ASP
1	A	72	SER
1	A	91	ASN
1	A	178	CYS
1	A	183	SER
1	A	272	ARG
1	A	273	ASP
1	A	286	ASP
1	A	393	LEU
1	A	547	ILE
1	A	617	LEU
1	A	625	ASN
1	A	633	ASP
1	A	634	HIS

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Mol	Chain	Res	Type
1	A	657	LEU
1	B	105	ARG
1	B	189	SER
1	B	213	SER
1	B	235	ASN
1	B	238	LYS
1	B	250	LEU
1	B	272	ARG
1	B	274	ASP
1	B	286	ASP
1	B	329	VAL
1	B	333	THR
1	B	387	HIS
1	B	388	ILE
1	B	416	TRP
1	B	428	THR
1	B	451	SER
1	B	485	SER
1	B	501	SER
1	B	507	GLN
1	B	512	ARG
1	B	521	LEU
1	B	544	THR
1	B	559	GLU
1	B	729	ILE
1	B	730	ARG
1	B	741	GLU
1	B	746	LEU
1	B	747	LYS
1	B	757	VAL
1	C	30	SER
1	C	34	LYS
1	C	42	LYS
1	C	58	TYR
1	C	63	ILE
1	C	76	ILE
1	C	84	GLU
1	C	87	GLU
1	C	88	LEU
1	C	90	LEU
1	C	157	ILE
1	C	173	GLN

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Mol	Chain	Res	Type
1	C	178	CYS
1	C	179	VAL
1	C	193	SER
1	C	195	SER
1	C	235	ASN
1	C	238	LYS
1	C	250	LEU
1	C	253	LYS
1	C	274	ASP
1	C	345	SER
1	C	346	ILE
1	C	356	LEU
1	C	358	LEU
1	C	365	ILE
1	C	373	SER
1	C	385	SER
1	C	388	ILE
1	C	396	GLN
1	C	403	VAL
1	C	421	GLU
1	C	517	ILE
1	C	518	LEU
1	C	521	LEU
1	C	526	LEU
1	C	552	ASN
1	C	652	ASP
1	C	664	ILE
1	C	707	LEU
1	C	744	LYS
1	C	745	GLU
1	C	747	LYS
1	C	760	LEU
1	D	27	THR
1	D	32	GLU
1	D	37	LEU
1	D	40	VAL
1	D	42	LYS
1	D	49	LYS
1	D	58	TYR
1	D	63	ILE
1	D	76	ILE
1	D	82	ASN

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Mol	Chain	Res	Type
1	D	88	LEU
1	D	90	LEU
1	D	118	TYR
1	D	168	ILE
1	D	178	CYS
1	D	179	VAL
1	D	180	GLU
1	D	185	SER
1	D	193	SER
1	D	214	GLU
1	D	230	LEU
1	D	235	ASN
1	D	262	SER
1	D	286	ASP
1	D	328	VAL
1	D	329	VAL
1	D	332	LEU
1	D	349	LEU
1	D	361	LYS
1	D	376	THR
1	D	390	ARG
1	D	408	LEU
1	D	416	TRP
1	D	453	LYS
1	D	489	SER
1	D	506	LEU
1	D	519	LYS
1	D	526	LEU
1	D	706	SER
1	D	738	LEU
1	D	739	THR
1	D	746	LEU
1	D	761	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	297	HIS
1	A	742	ASN
1	B	80	ASN
1	B	297	HIS

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Mol	Chain	Res	Type
1	B	394	HIS
1	B	432	HIS
1	B	436	ASN
1	B	573	GLN
1	B	748	GLN
1	C	50	GLN
1	C	92	HIS
1	C	235	ASN
1	C	297	HIS
1	C	551	ASN
1	C	573	GLN
1	C	709	GLN
1	D	50	GLN
1	D	258	GLN
1	D	533	ASN
1	D	710	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are 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
2	A1IIE	C	801	-	40,44,44	5.25	17 (42%)	46,62,62	4.04	19 (41%)
2	A1IIE	A	801	-	40,44,44	5.24	16 (40%)	46,62,62	4.01	19 (41%)
2	A1IIE	B	801	-	40,44,44	5.29	17 (42%)	46,62,62	4.00	19 (41%)
2	A1IIE	D	801	-	40,44,44	5.24	18 (45%)	46,62,62	4.00	20 (43%)

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
2	A1IIE	C	801	-	-	2/15/17/17	0/5/5/5
2	A1IIE	A	801	-	-	2/15/17/17	0/5/5/5
2	A1IIE	B	801	-	-	2/15/17/17	0/5/5/5
2	A1IIE	D	801	-	-	2/15/17/17	0/5/5/5

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	A1IIE	C1E-CL	-18.84	1.29	1.73
2	D	801	A1IIE	C1E-CL	-18.84	1.29	1.73
2	C	801	A1IIE	C1E-CL	-18.84	1.29	1.73
2	A	801	A1IIE	C1E-CL	-18.82	1.29	1.73
2	A	801	A1IIE	C1K-CL1	-18.07	1.35	1.74
2	C	801	A1IIE	C1K-CL1	-18.01	1.35	1.74
2	B	801	A1IIE	C1K-CL1	-17.98	1.35	1.74
2	D	801	A1IIE	C1K-CL1	-17.97	1.35	1.74
2	C	801	A1IIE	C17-C1E	12.22	1.53	1.40
2	B	801	A1IIE	C17-C1E	12.12	1.53	1.40
2	A	801	A1IIE	C17-C1E	12.00	1.53	1.40
2	D	801	A1IIE	C17-C1E	11.90	1.53	1.40
2	A	801	A1IIE	C1F-C1E	9.77	1.54	1.38
2	C	801	A1IIE	C1F-C1E	9.74	1.54	1.38
2	B	801	A1IIE	C1F-C1E	9.64	1.54	1.38
2	D	801	A1IIE	C1F-C1E	9.63	1.54	1.38
2	B	801	A1IIE	C1P-N14	7.28	1.46	1.38
2	D	801	A1IIE	C1P-N14	6.56	1.46	1.38
2	C	801	A1IIE	C1P-N14	6.45	1.45	1.38
2	A	801	A1IIE	C1P-N14	6.37	1.45	1.38
2	B	801	A1IIE	C12-N14	4.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	A1IIE	C1M-C1K	4.24	1.46	1.38
2	A	801	A1IIE	C1M-C1K	4.23	1.46	1.38
2	D	801	A1IIE	C1M-C1K	4.22	1.46	1.38
2	C	801	A1IIE	C1M-C1K	4.20	1.46	1.38
2	C	801	A1IIE	C1L-C1K	4.18	1.45	1.38
2	A	801	A1IIE	C1L-C1K	4.17	1.45	1.38
2	D	801	A1IIE	C1L-C1K	4.01	1.45	1.38
2	B	801	A1IIE	C1L-C1K	3.98	1.45	1.38
2	D	801	A1IIE	C12-N14	3.86	1.43	1.38
2	B	801	A1IIE	C1O-N14	3.78	1.53	1.46
2	A	801	A1IIE	C1O-N14	3.70	1.52	1.46
2	D	801	A1IIE	C1Q-N15	3.64	1.55	1.47
2	C	801	A1IIE	C12-N14	3.61	1.42	1.38
2	B	801	A1IIE	C1Q-N15	3.58	1.55	1.47
2	C	801	A1IIE	C1Q-N15	3.43	1.54	1.47
2	D	801	A1IIE	C1O-N14	3.42	1.52	1.46
2	A	801	A1IIE	C1Q-N15	3.42	1.54	1.47
2	A	801	A1IIE	C12-N14	3.42	1.42	1.38
2	C	801	A1IIE	C1O-N14	3.22	1.52	1.46
2	B	801	A1IIE	C1P-N15	2.98	1.44	1.38
2	D	801	A1IIE	C1P-N15	2.94	1.44	1.38
2	C	801	A1IIE	C1P-N15	2.90	1.43	1.38
2	A	801	A1IIE	C1P-N15	2.84	1.43	1.38
2	A	801	A1IIE	C15-C14	2.57	1.43	1.38
2	B	801	A1IIE	C15-C14	2.57	1.43	1.38
2	D	801	A1IIE	C15-C14	2.51	1.43	1.38
2	C	801	A1IIE	C15-C14	2.50	1.43	1.38
2	B	801	A1IIE	C17-N1	2.29	1.47	1.42
2	B	801	A1IIE	O1-C14	2.28	1.44	1.39
2	C	801	A1IIE	C1G-C1H	2.26	1.56	1.51
2	D	801	A1IIE	C17-N1	2.23	1.47	1.42
2	B	801	A1IIE	C19-C18	2.18	1.43	1.39
2	D	801	A1IIE	C19-C18	2.17	1.43	1.39
2	D	801	A1IIE	O1-C14	2.17	1.44	1.39
2	B	801	A1IIE	C13-N13	2.15	1.42	1.36
2	C	801	A1IIE	O1-C14	2.15	1.44	1.39
2	A	801	A1IIE	O1-C14	2.15	1.44	1.39
2	C	801	A1IIE	C19-C18	2.14	1.43	1.39
2	A	801	A1IIE	C19-C18	2.14	1.43	1.39
2	D	801	A1IIE	C1G-C1H	2.13	1.56	1.51
2	C	801	A1IIE	C13-N13	2.10	1.41	1.36
2	A	801	A1IIE	C13-N13	2.10	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	A1IIE	C13-N13	2.09	1.41	1.36
2	D	801	A1IIE	C-N15	2.06	1.44	1.40
2	C	801	A1IIE	C17-N1	2.04	1.46	1.42
2	A	801	A1IIE	C1G-C1H	2.04	1.56	1.51
2	B	801	A1IIE	C1G-C1H	2.01	1.56	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	A1IIE	C1F-C1E-C17	-19.86	109.38	121.75
2	A	801	A1IIE	C1F-C1E-C17	-19.57	109.56	121.75
2	B	801	A1IIE	C1F-C1E-C17	-19.38	109.67	121.75
2	D	801	A1IIE	C1F-C1E-C17	-19.32	109.71	121.75
2	A	801	A1IIE	C1M-C1K-C1L	-7.76	111.18	121.24
2	D	801	A1IIE	C1M-C1K-C1L	-7.74	111.21	121.24
2	C	801	A1IIE	C1M-C1K-C1L	-7.74	111.21	121.24
2	B	801	A1IIE	C1M-C1K-C1L	-7.72	111.24	121.24
2	B	801	A1IIE	C1-C-N15	7.49	119.72	113.58
2	D	801	A1IIE	C1-C-N15	7.34	119.60	113.58
2	A	801	A1IIE	C1-C-N15	7.31	119.57	113.58
2	C	801	A1IIE	C1-C-N15	7.20	119.48	113.58
2	C	801	A1IIE	C17-C1E-CL	5.93	125.79	119.62
2	A	801	A1IIE	C17-C1E-CL	5.87	125.73	119.62
2	B	801	A1IIE	C17-C1E-CL	5.80	125.66	119.62
2	D	801	A1IIE	C17-C1E-CL	5.79	125.65	119.62
2	A	801	A1IIE	C1N-C1M-C1K	5.26	124.79	119.24
2	D	801	A1IIE	C1N-C1M-C1K	5.18	124.71	119.24
2	B	801	A1IIE	C1N-C1M-C1K	5.14	124.66	119.24
2	C	801	A1IIE	C1N-C1M-C1K	5.14	124.66	119.24
2	B	801	A1IIE	C1I-C1L-C1K	4.64	124.14	119.24
2	C	801	A1IIE	C1I-C1L-C1K	4.63	124.12	119.24
2	D	801	A1IIE	C1I-C1L-C1K	4.59	124.08	119.24
2	A	801	A1IIE	C1I-C1L-C1K	4.56	124.06	119.24
2	D	801	A1IIE	C14-C1F-C1E	4.51	125.75	118.51
2	B	801	A1IIE	C14-C1F-C1E	4.50	125.73	118.51
2	A	801	A1IIE	C14-C1F-C1E	4.48	125.70	118.51
2	C	801	A1IIE	C14-C1F-C1E	4.47	125.68	118.51
2	D	801	A1IIE	C1O-N14-C12	4.11	123.98	120.13
2	B	801	A1IIE	C1O-N14-C12	4.10	123.97	120.13
2	C	801	A1IIE	C1O-N14-C12	3.97	123.84	120.13
2	C	801	A1IIE	C1F-C1E-CL	3.93	124.83	118.49
2	A	801	A1IIE	C1F-C1E-CL	3.85	124.71	118.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	A1IIE	C1F-C1E-CL	3.83	124.67	118.49
2	A	801	A1IIE	C1O-N14-C12	3.82	123.71	120.13
2	D	801	A1IIE	C1F-C1E-CL	3.81	124.64	118.49
2	C	801	A1IIE	C16-C17-C1E	3.74	121.48	117.67
2	A	801	A1IIE	C16-C17-C1E	3.65	121.39	117.67
2	D	801	A1IIE	C1E-C17-N1	-3.65	113.83	117.70
2	D	801	A1IIE	C16-C17-C1E	3.55	121.29	117.67
2	B	801	A1IIE	C16-C17-C1E	3.53	121.27	117.67
2	B	801	A1IIE	C1E-C17-N1	-3.51	113.99	117.70
2	B	801	A1IIE	C1M-C1K-CL1	3.44	124.73	119.35
2	D	801	A1IIE	C1M-C1K-CL1	3.44	124.73	119.35
2	C	801	A1IIE	C1M-C1K-CL1	3.43	124.72	119.35
2	A	801	A1IIE	C1M-C1K-CL1	3.33	124.55	119.35
2	A	801	A1IIE	C1E-C17-N1	-3.32	114.19	117.70
2	A	801	A1IIE	C15-C16-C17	3.16	125.35	120.02
2	A	801	A1IIE	C1L-C1K-CL1	3.14	124.27	119.35
2	C	801	A1IIE	C15-C16-C17	3.11	125.27	120.02
2	D	801	A1IIE	C15-C16-C17	3.04	125.16	120.02
2	B	801	A1IIE	C15-C16-C17	3.04	125.15	120.02
2	C	801	A1IIE	C1L-C1K-CL1	3.02	124.07	119.35
2	D	801	A1IIE	C1L-C1K-CL1	3.01	124.06	119.35
2	B	801	A1IIE	C1L-C1K-CL1	2.99	124.03	119.35
2	C	801	A1IIE	C1E-C17-N1	-2.92	114.60	117.70
2	D	801	A1IIE	C17-N1-N12	2.88	121.20	114.56
2	D	801	A1IIE	C1Q-N15-C	2.84	121.61	117.58
2	C	801	A1IIE	C1Q-N15-C	2.80	121.56	117.58
2	B	801	A1IIE	C17-N1-N12	2.74	120.89	114.56
2	A	801	A1IIE	C1Q-N15-C	2.70	121.41	117.58
2	B	801	A1IIE	C12-N14-C1P	-2.67	119.65	122.20
2	B	801	A1IIE	C1Q-N15-C	2.66	121.36	117.58
2	A	801	A1IIE	C12-N14-C1P	-2.59	119.72	122.20
2	C	801	A1IIE	C12-N14-C1P	-2.56	119.75	122.20
2	A	801	A1IIE	C17-N1-N12	2.53	120.41	114.56
2	D	801	A1IIE	C12-N14-C1P	-2.52	119.79	122.20
2	C	801	A1IIE	C18-N12-N1	2.38	124.81	112.99
2	A	801	A1IIE	C16-C15-C14	-2.37	116.84	119.73
2	A	801	A1IIE	C18-N12-N1	2.28	124.33	112.99
2	D	801	A1IIE	C16-C15-C14	-2.28	116.95	119.73
2	C	801	A1IIE	C16-C15-C14	-2.24	117.00	119.73
2	C	801	A1IIE	C17-N1-N12	2.21	119.66	114.56
2	B	801	A1IIE	C18-N12-N1	2.20	123.92	112.99
2	B	801	A1IIE	C16-C15-C14	-2.19	117.05	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	A1HIE	C18-N12-N1	2.15	123.69	112.99
2	D	801	A1HIE	O-C-C1	-2.01	122.03	125.33

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	801	A1HIE	C1F-C14-O1-C13
2	A	801	A1HIE	C1F-C14-O1-C13
2	C	801	A1HIE	C15-C14-O1-C13
2	D	801	A1HIE	C1F-C14-O1-C13
2	A	801	A1HIE	C15-C14-O1-C13
2	B	801	A1HIE	C1F-C14-O1-C13
2	D	801	A1HIE	C15-C14-O1-C13
2	B	801	A1HIE	C15-C14-O1-C13

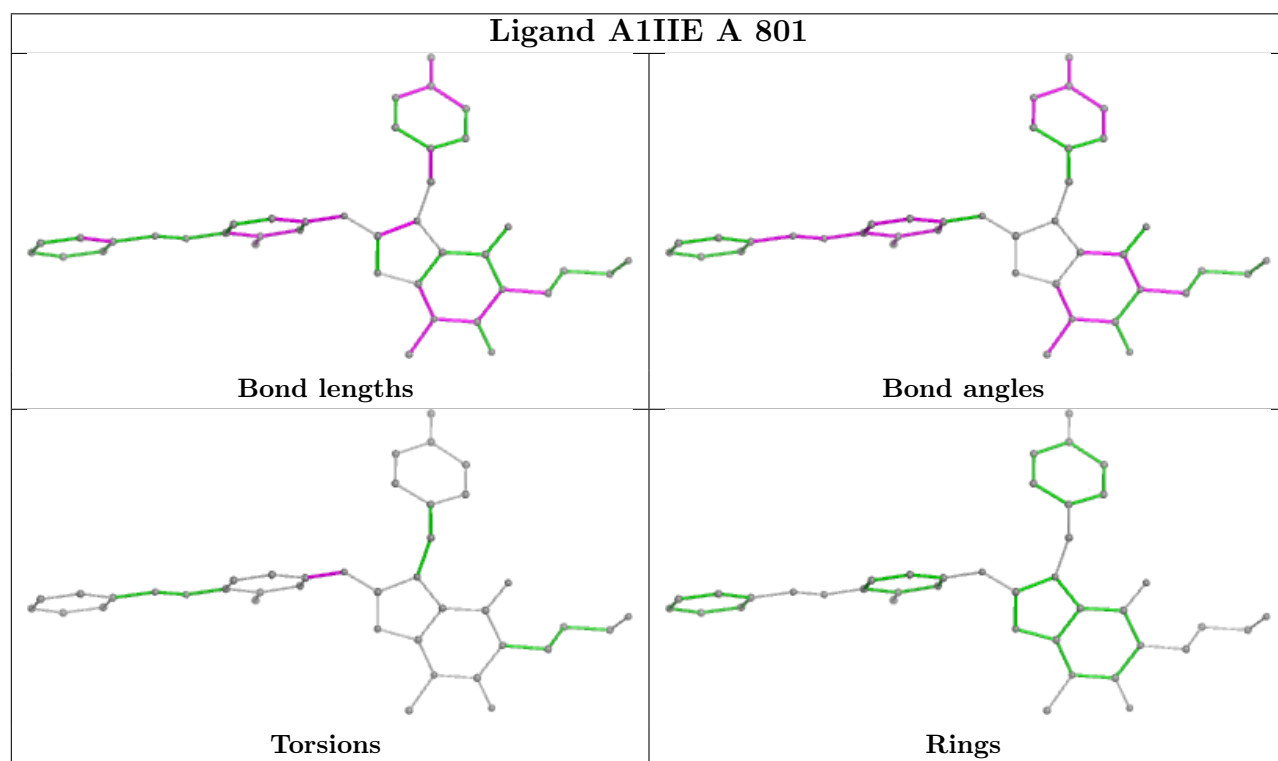
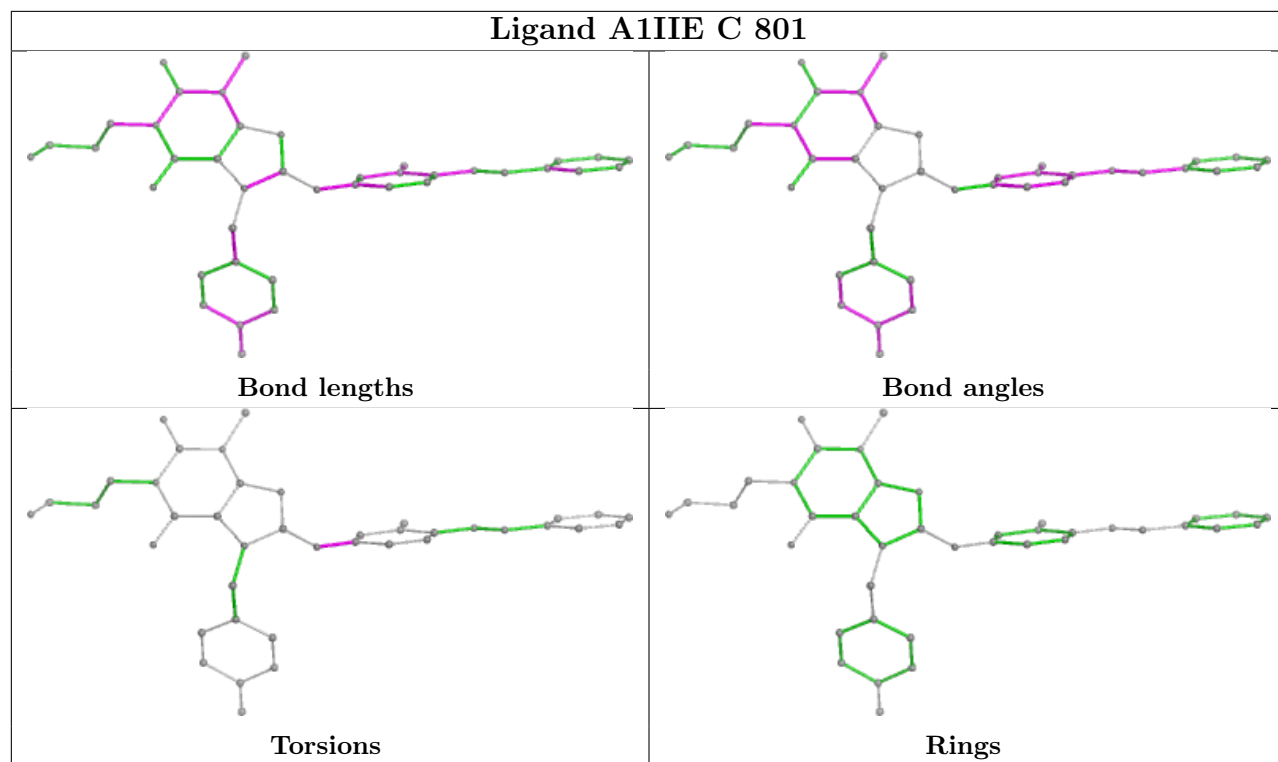
There are no ring outliers.

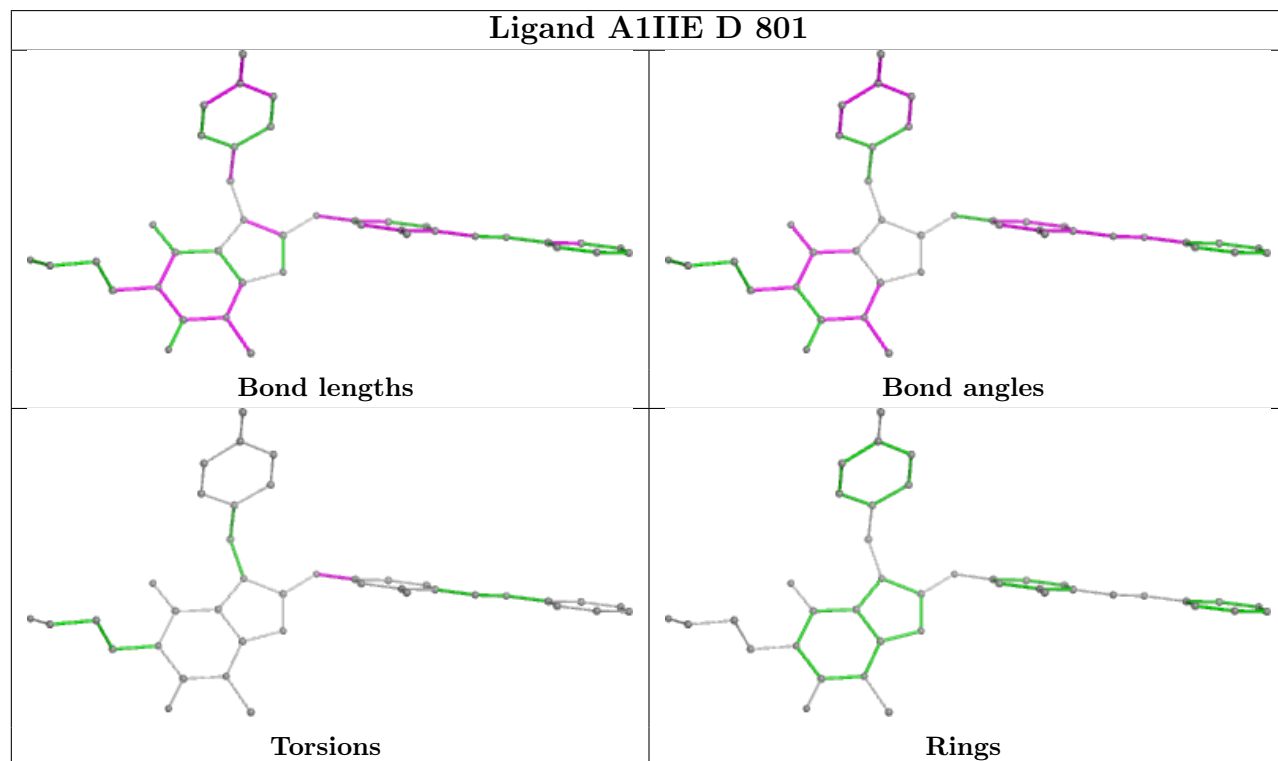
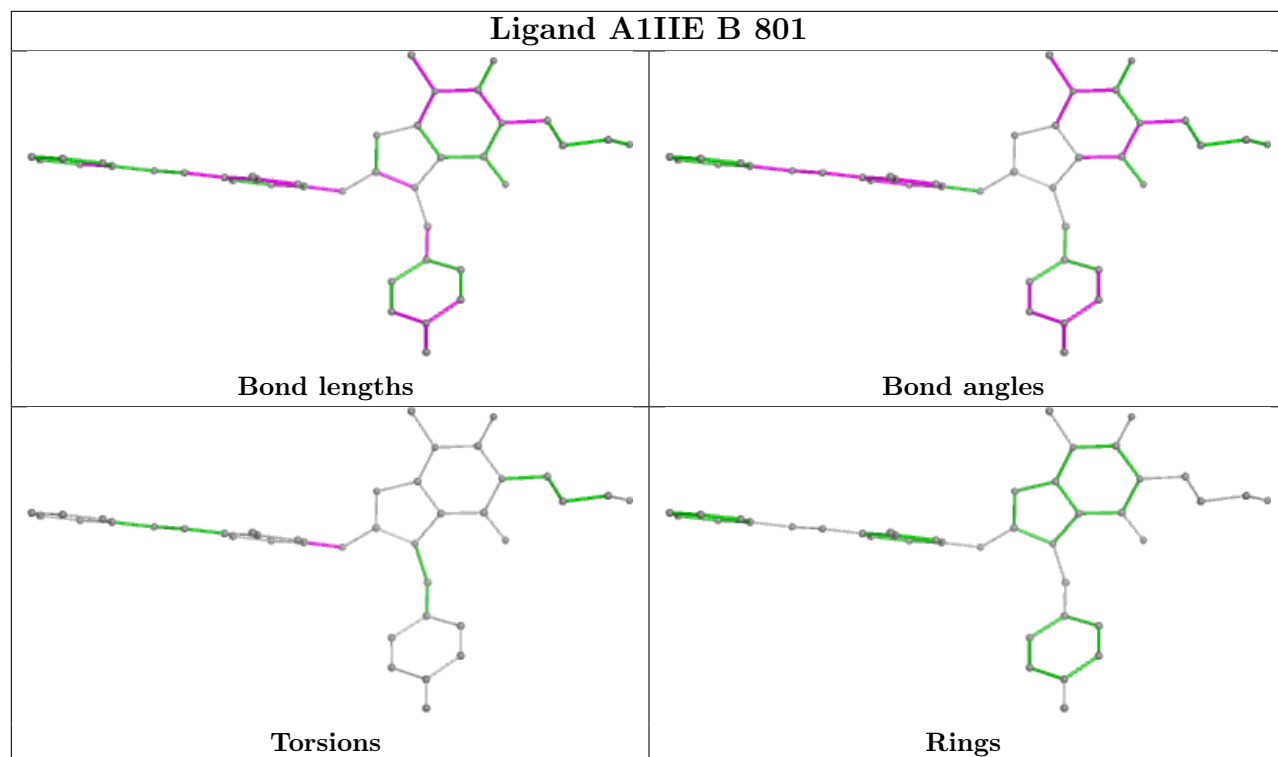
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	A1HIE	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.

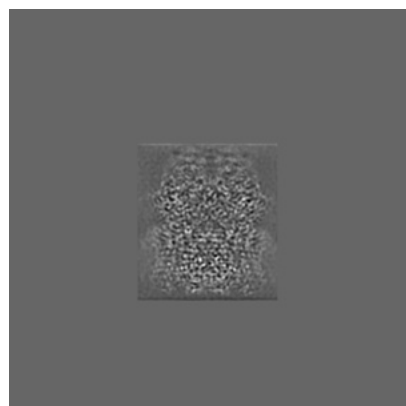
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51074. These allow visual inspection of the internal detail of the map and identification of artifacts.

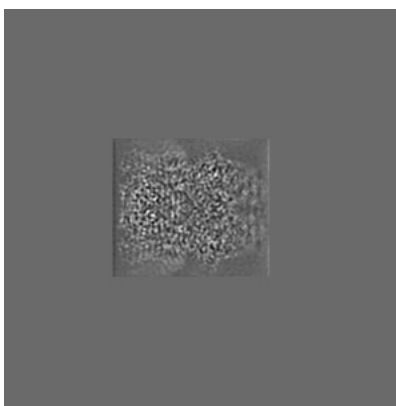
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

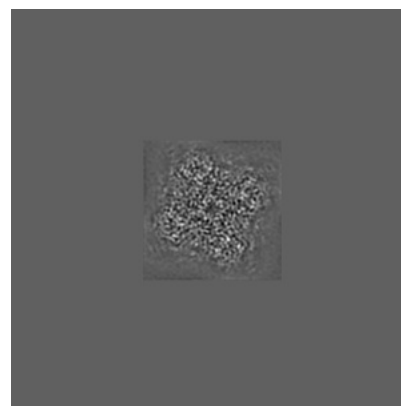
#### 6.1.1 Primary map



X

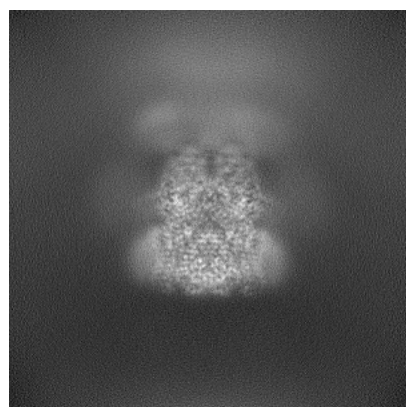


Y

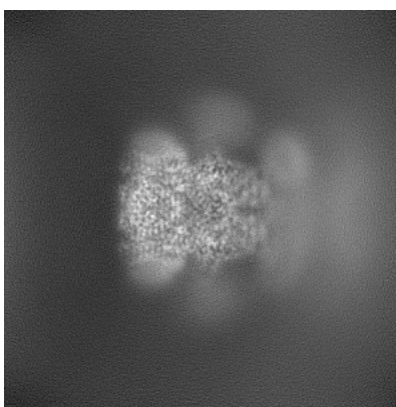


Z

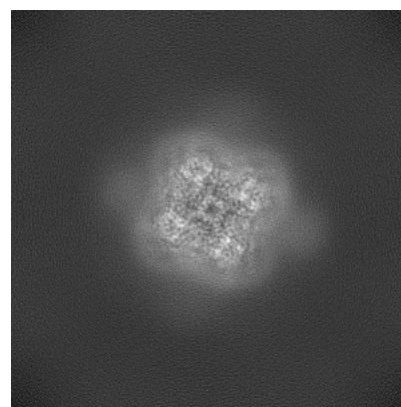
#### 6.1.2 Raw map



X



Y

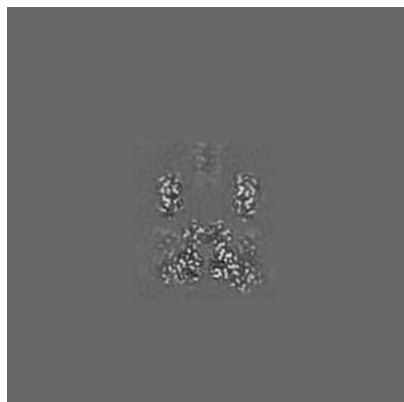


Z

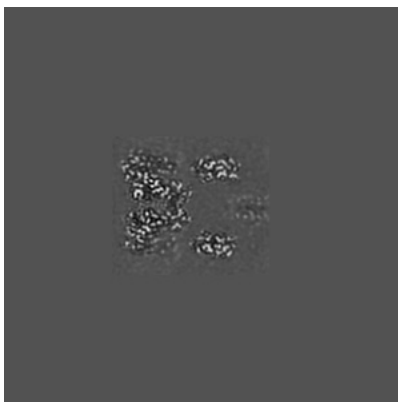
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

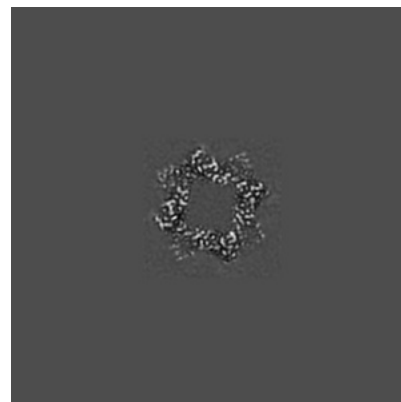
### 6.2.1 Primary map



X Index: 216

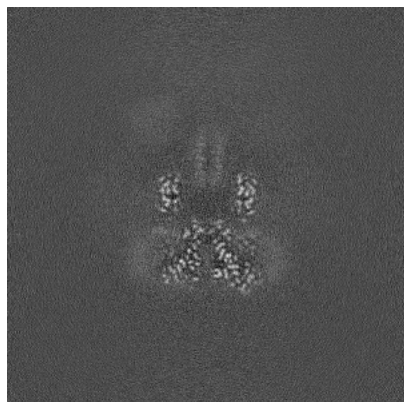


Y Index: 216

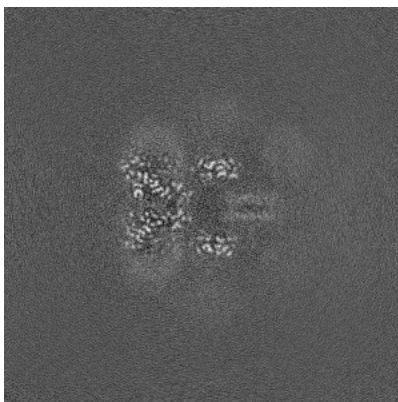


Z Index: 216

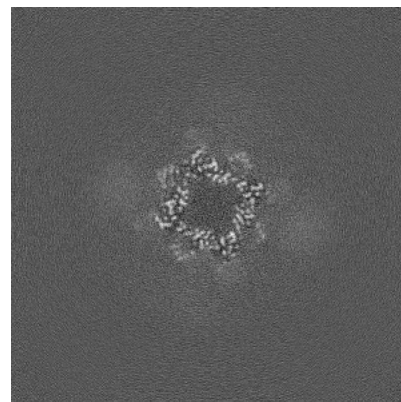
### 6.2.2 Raw map



X Index: 216



Y Index: 216

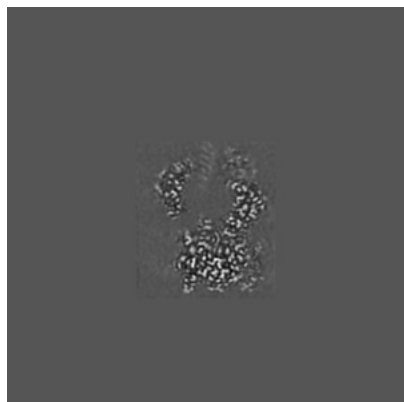


Z Index: 216

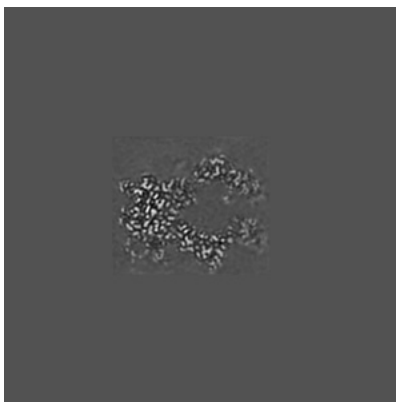
The images above show central slices of the map in three orthogonal directions.

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

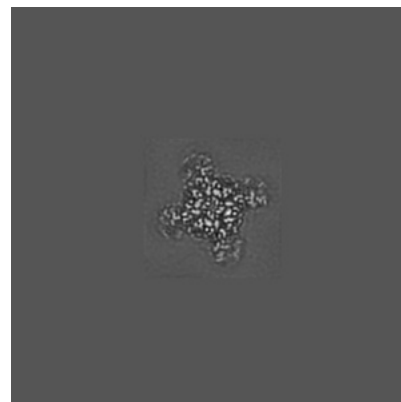
### 6.3.1 Primary map



X Index: 203

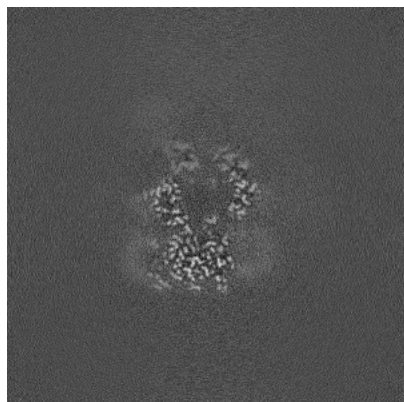


Y Index: 197

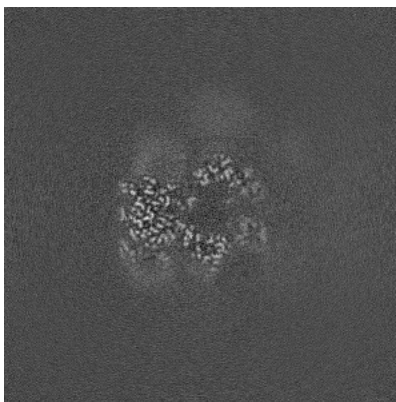


Z Index: 155

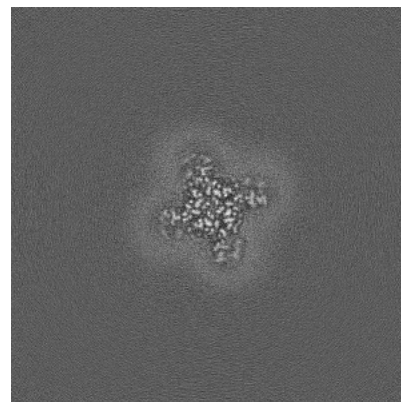
### 6.3.2 Raw map



X Index: 232



Y Index: 200

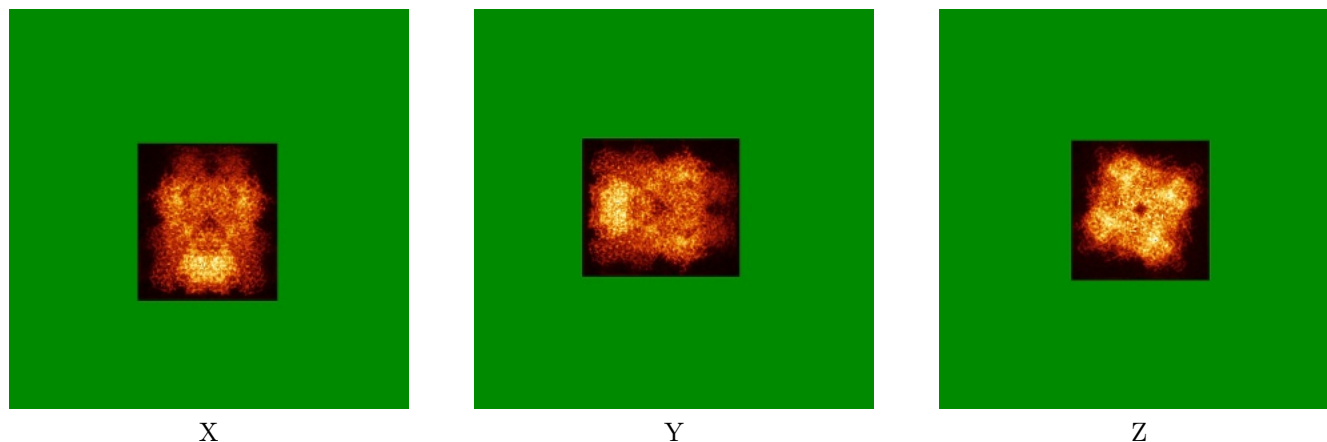


Z Index: 155

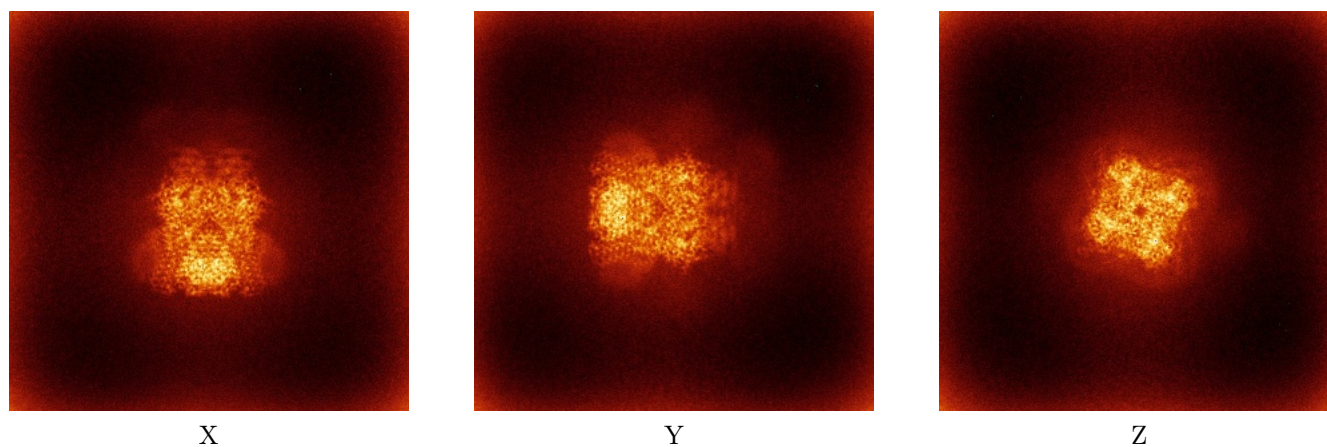
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map

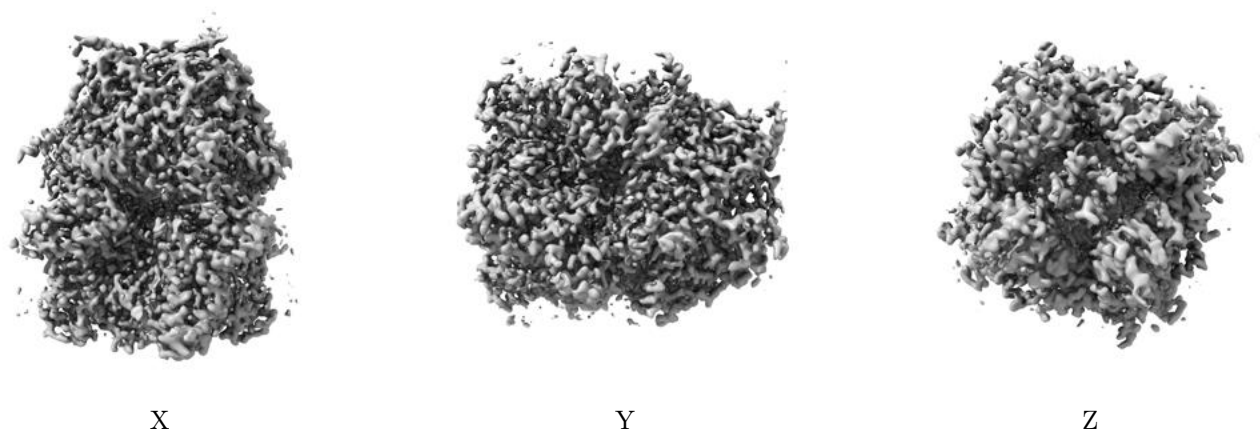


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



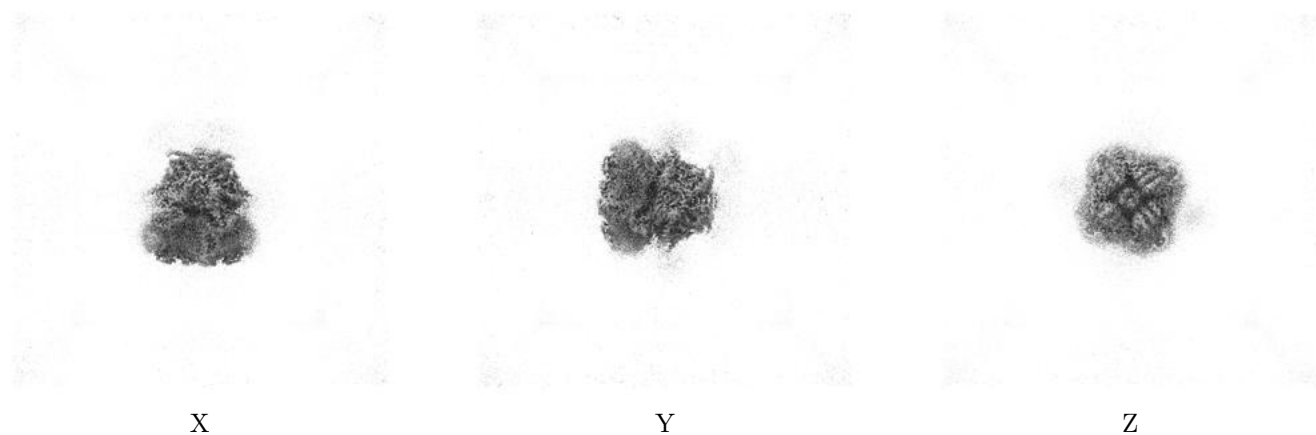
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. 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](#)

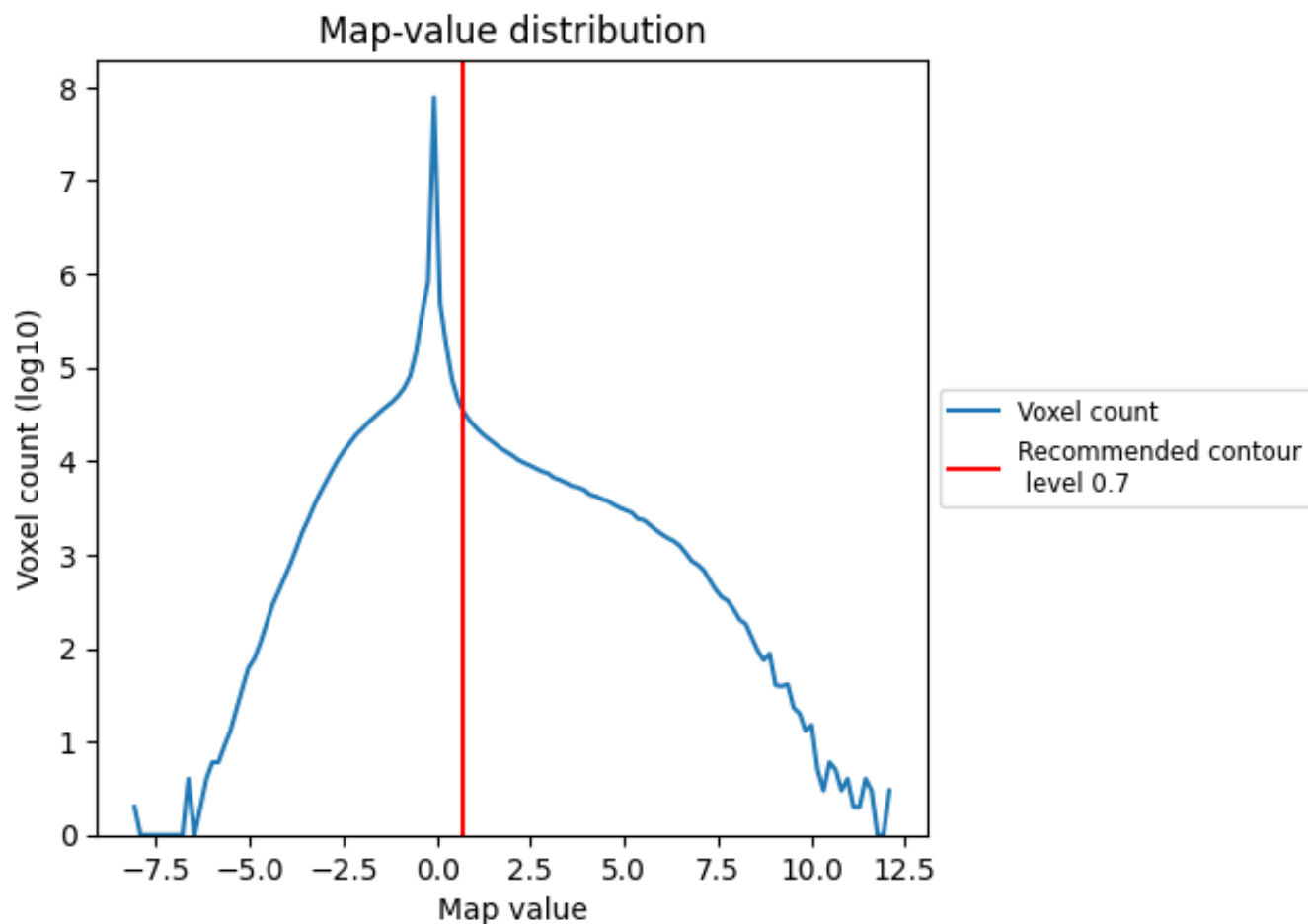
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

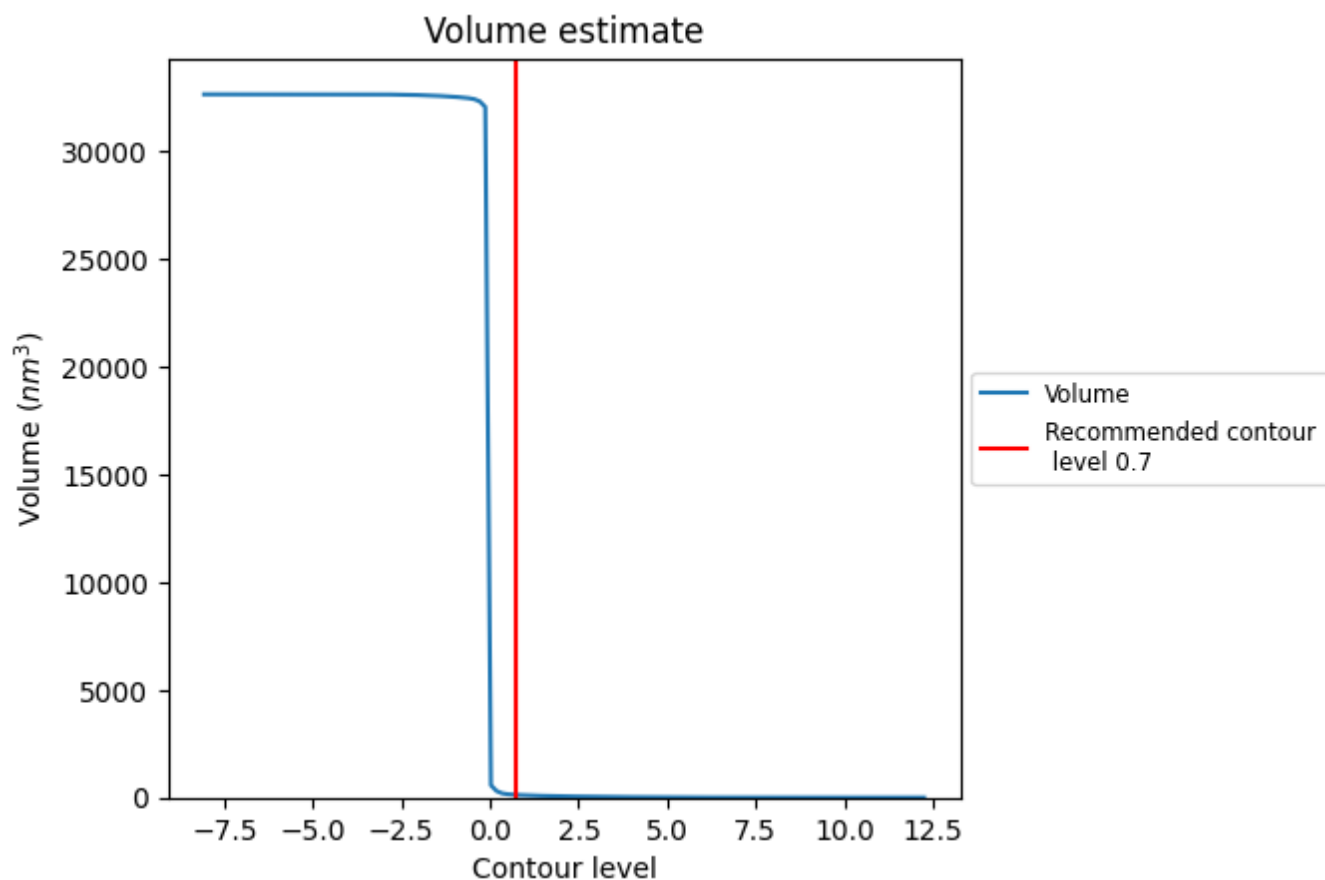
This section contains the results of statistical analysis of the map.

### 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.

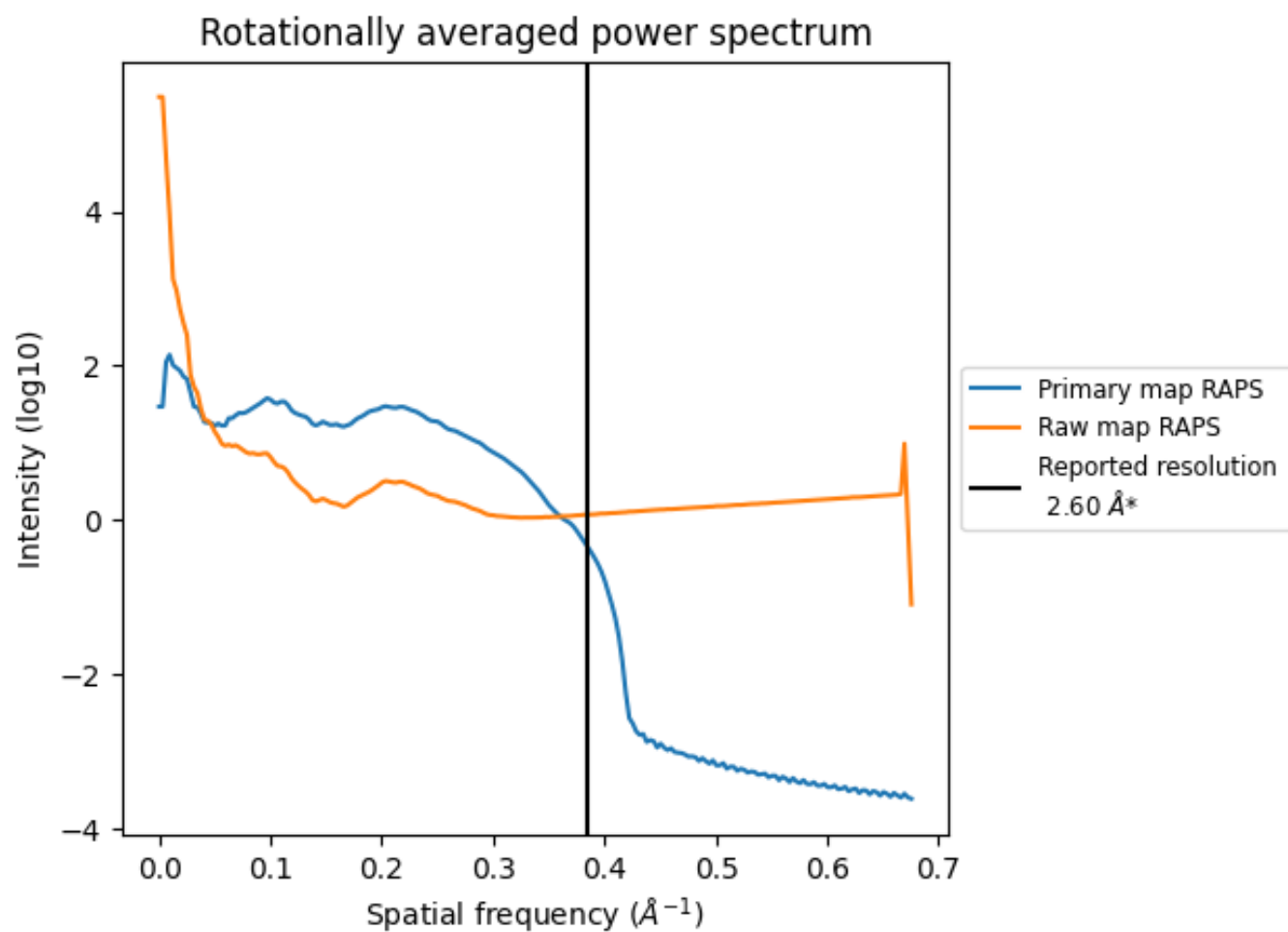
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm<sup>3</sup>; this corresponds to an approximate mass of 116 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 ⓘ

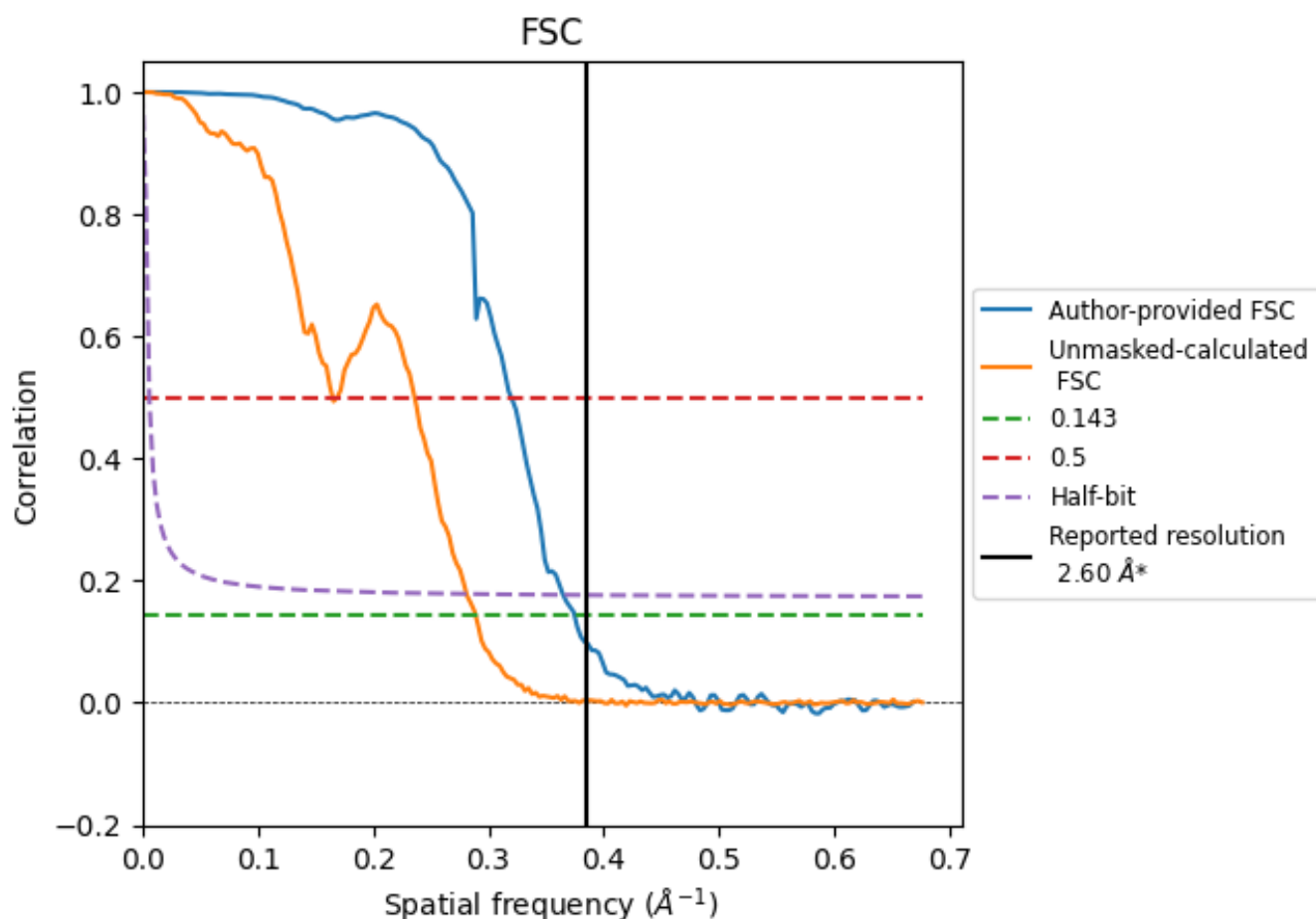


\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

## 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 0.385  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

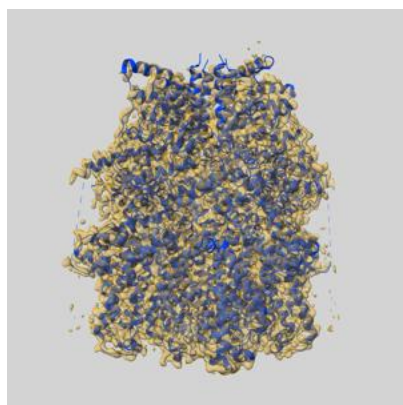
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.67	3.13	2.74
Unmasked-calculated*	3.46	6.06	3.56

\*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 3.46 differs from the reported value 2.6 by more than 10 %

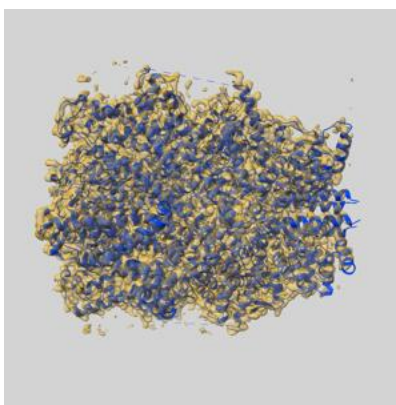
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51074 and PDB model 9G4Y. Per-residue inclusion information can be found in section 3 on page 5.

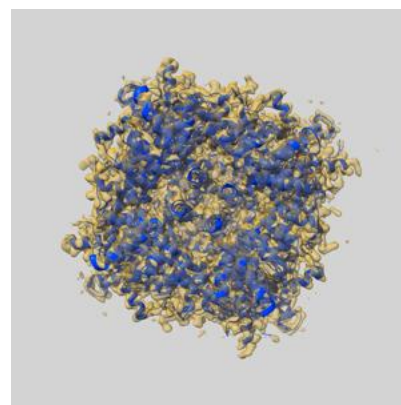
### 9.1 Map-model overlay [i](#)



X



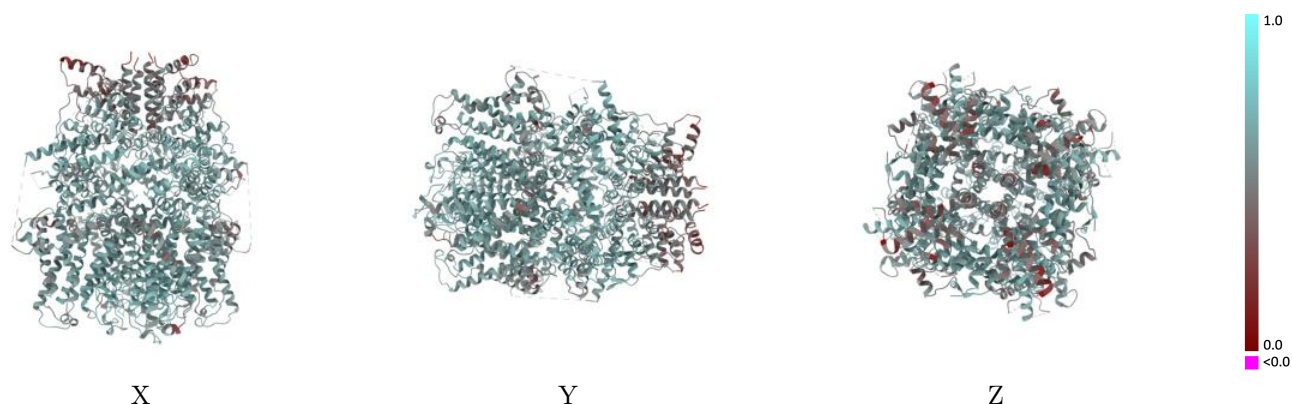
Y



Z

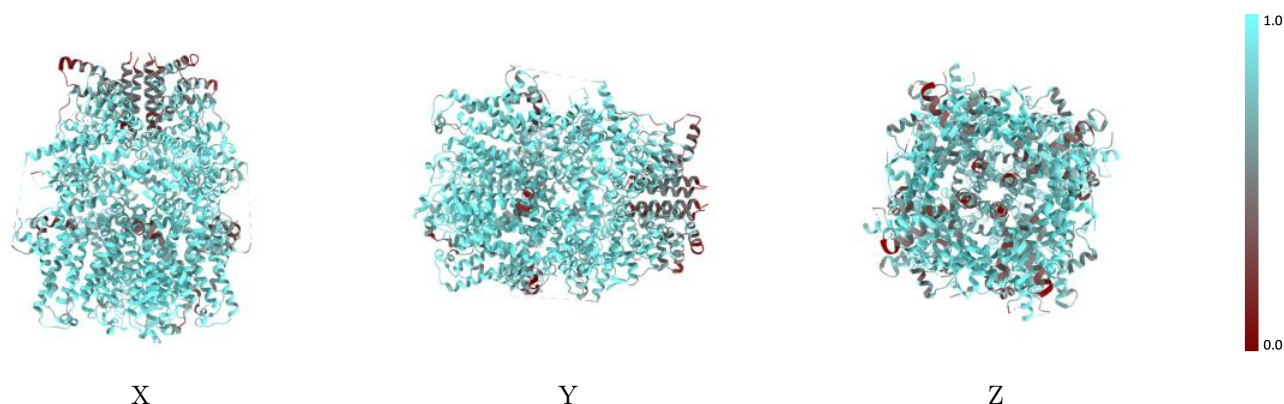
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



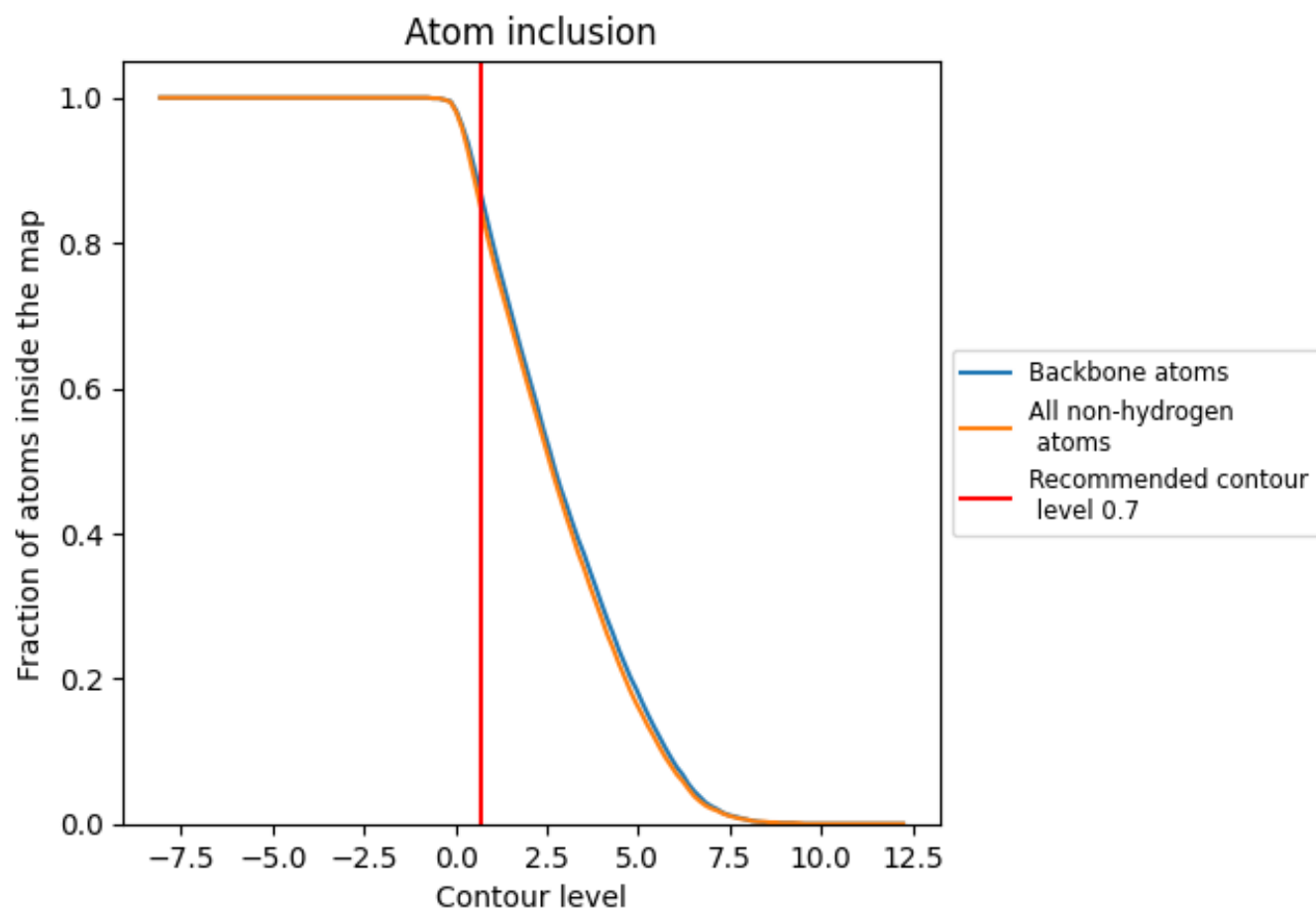
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 85% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8470	<div></div> 0.5910
A	<div></div> 0.8460	<div></div> 0.5910
B	<div></div> 0.8470	<div></div> 0.5900
C	<div></div> 0.8470	<div></div> 0.5920
D	<div></div> 0.8550	<div></div> 0.5930

