



## Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 02:41 AM UTC

PDB ID : 9DCA / pdb\_00009dca  
EMDB ID : EMD-46747  
Title : S. thermophilus class III ribonucleotide reductase with ATP and TTP  
Authors : Andree, G.A.; Drennan, C.L.  
Deposited on : 2024-08-25  
Resolution : 3.60 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>.

---

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

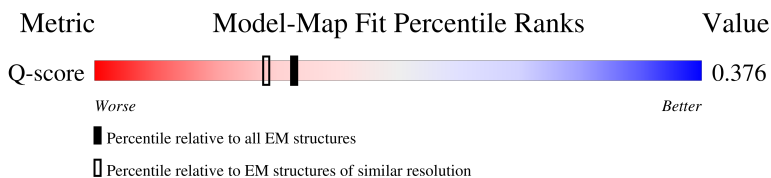
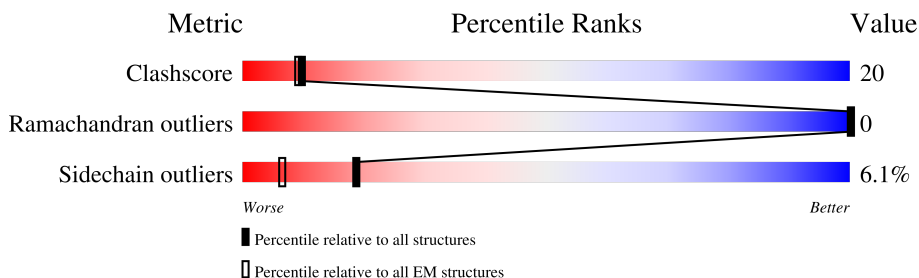
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 ( 3.10 - 4.10 )

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	734	
1	B	734	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11376 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 Anaerobic ribonucleoside-triphosphate reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	699	Total	C	N	O	S	0	0
			5588	3545	945	1071	27		
1	B	699	Total	C	N	O	S	0	0
			5597	3552	947	1071	27		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ILE	THR	conflict	UNP A0A3G6JS83
A	8	ARG	LYS	conflict	UNP A0A3G6JS83
A	56	GLY	GLU	conflict	UNP A0A3G6JS83
A	493	ASP	ASN	conflict	UNP A0A3G6JS83
B	3	ILE	THR	conflict	UNP A0A3G6JS83
B	8	ARG	LYS	conflict	UNP A0A3G6JS83
B	56	GLY	GLU	conflict	UNP A0A3G6JS83
B	493	ASP	ASN	conflict	UNP A0A3G6JS83

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
3	A	2	Total Mg 2 2	0
3	B	2	Total Mg 2 2	0

- Molecule 4 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula:  $\text{C}_{10}\text{H}_{17}\text{N}_2\text{O}_{14}\text{P}_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 29	C 10	N 2	O 14	P 3	0
4	B	1	Total 29	C 10	N 2	O 14	P 3	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

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

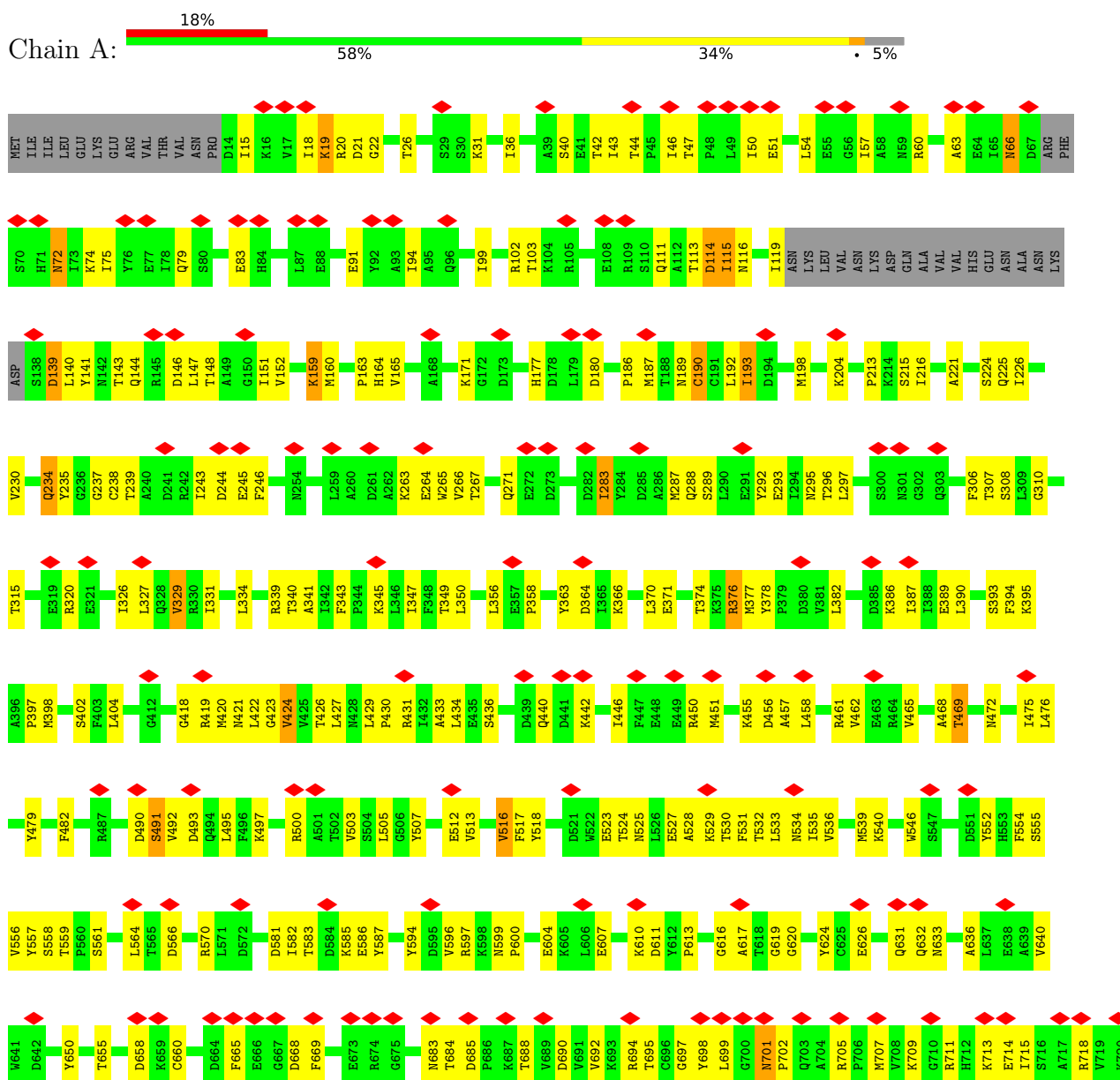
- Molecule 6 is water.

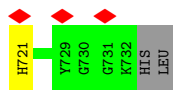
Mol	Chain	Residues	Atoms	AltConf
6	A	3	Total O 3 3	0
6	B	1	Total O 1 1	0

### 3 Residue-property plots [i](#)

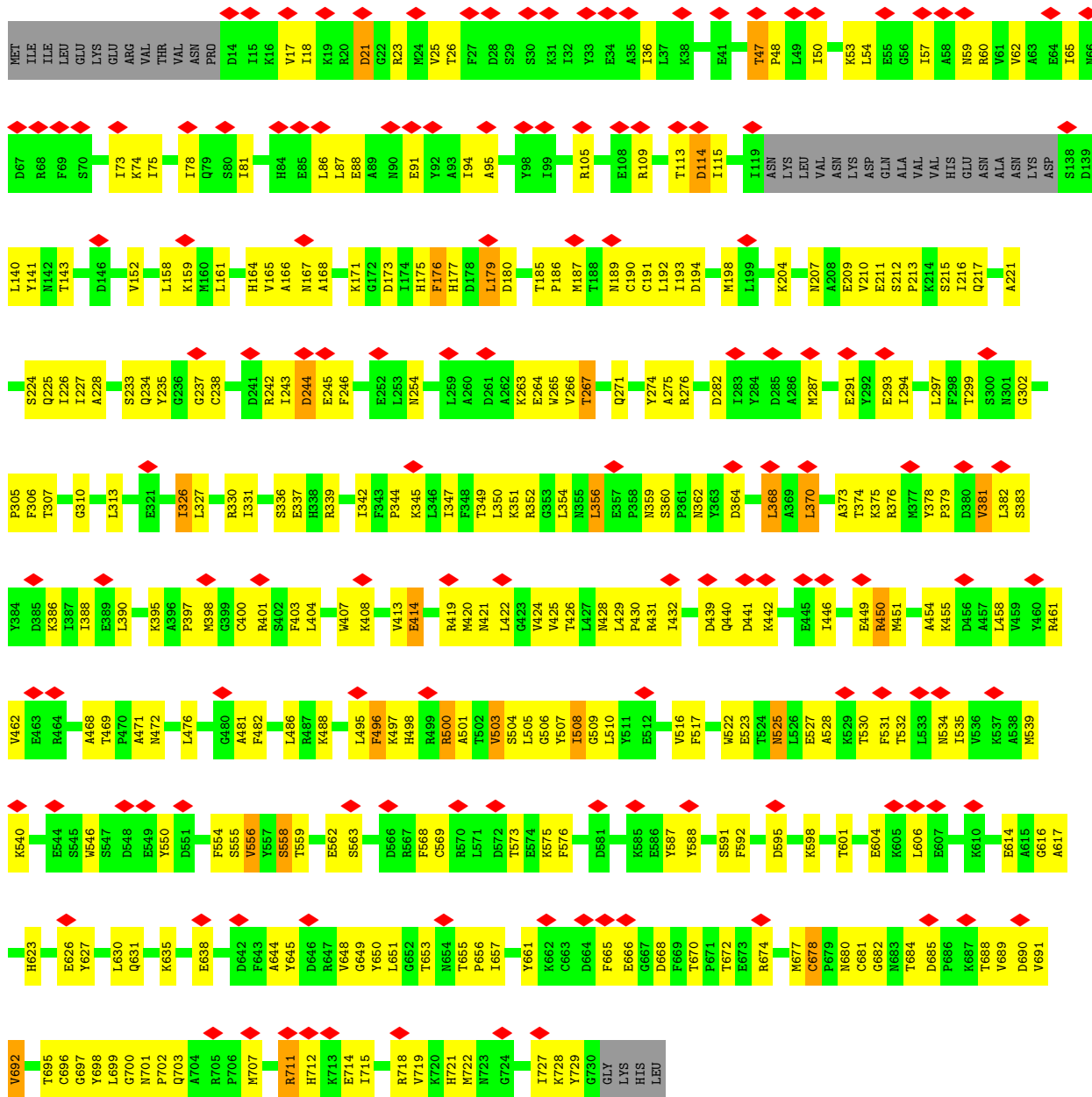
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Anaerobic ribonucleoside-triphosphate reductase





• Molecule 1: Anaerobic ribonucleoside-triphosphate reductase



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	290300	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 ( $e^-/\text{\AA}^2$ )	51.35	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	16.443	Depositor
Minimum map value	0.000	Depositor
Average map value	0.150	Depositor
Map value standard deviation	0.666	Depositor
Recommended contour level	5.33	Depositor
Map size ( $\text{\AA}$ )	212.992, 212.992, 212.992	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.832, 0.832, 0.832	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, ATP, TTP

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	0.28	0/5711	0.44	0/7723
1	B	0.42	0/5722	0.63	5/7740 (0.1%)
All	All	0.36	0/11433	0.54	5/15463 (0.0%)

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	7
All	All	0	8

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	503	VAL	CA-C-N	-9.29	107.92	122.87
1	B	503	VAL	C-N-CA	-9.29	107.92	122.87
1	B	503	VAL	CB-CA-C	-6.49	100.96	110.62
1	B	496	PHE	CA-CB-CG	5.32	119.12	113.80
1	B	176	PHE	N-CA-C	-5.24	103.97	110.41

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	ARG	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	105	ARG	Sidechain
1	B	109	ARG	Sidechain
1	B	376	ARG	Sidechain
1	B	450	ARG	Sidechain
1	B	500	ARG	Sidechain
1	B	711	ARG	Sidechain
1	B	718	ARG	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5588	0	5469	203	0
1	B	5597	0	5472	245	0
2	A	62	0	24	5	0
2	B	62	0	24	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	29	0	13	2	0
4	B	29	0	12	4	0
5	B	1	0	0	0	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0
All	All	11376	0	11014	441	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 20.

All (441) 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:B:339:ARG:HG3	1:B:690:ASP:OD2	1.55	1.06
1:B:595:ASP:HB3	1:B:598:LYS:HE2	1.43	1.01
1:B:17:VAL:HG22	1:B:73:ILE:CG2	1.97	0.94
1:B:432:ILE:HD11	1:B:450:ARG:HG3	1.58	0.85
1:A:306:PHE:HA	1:A:343:PHE:HE2	1.43	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ILE:HG13	1:B:699:LEU:HD12	1.63	0.81
1:B:337:GLU:HB3	1:B:661:TYR:HE2	1.47	0.80
1:A:221:ALA:O	1:A:225:GLN:HG3	1.81	0.80
1:B:36:ILE:CG2	1:B:54:LEU:HD22	2.13	0.78
1:B:36:ILE:HG21	1:B:54:LEU:HD22	1.66	0.76
1:B:595:ASP:HB3	1:B:598:LYS:CE	2.15	0.76
1:B:17:VAL:HG22	1:B:73:ILE:HG22	1.68	0.76
1:A:165:VAL:HG21	1:A:457:ALA:HB2	1.68	0.75
1:A:404:LEU:HB3	1:A:419:ARG:HH22	1.52	0.75
1:B:73:ILE:HG12	1:B:78:ILE:HD11	1.68	0.74
1:B:176:PHE:HA	1:B:425:VAL:HG23	1.67	0.74
1:B:562:GLU:HG2	1:B:563:SER:H	1.54	0.73
1:B:370:LEU:HD11	1:B:638:GLU:HB2	1.70	0.72
1:B:696:CYS:SG	1:B:697:GLY:N	2.64	0.71
1:B:400:CYS:SG	1:B:697:GLY:HA3	2.31	0.70
1:B:627:TYR:CD2	1:B:653:THR:HG23	2.27	0.70
1:B:627:TYR:CE2	1:B:653:THR:HG23	2.27	0.69
1:B:672:THR:HG21	1:B:677:MET:SD	2.32	0.69
1:B:540:LYS:HD2	1:B:616:GLY:HA3	1.74	0.69
1:A:512:GLU:OE2	1:A:585:LYS:NZ	2.25	0.69
1:B:420:MET:HE1	1:B:500:ARG:HH21	1.59	0.68
1:A:238:CYS:O	1:A:307:THR:HA	1.94	0.68
1:B:342:ILE:HD11	1:B:700:GLY:HA2	1.75	0.68
1:A:581:ASP:OD1	1:A:597:ARG:NH2	2.26	0.68
1:B:430:PRO:CG	1:B:588:TYR:HE2	2.07	0.68
1:B:442:LYS:O	1:B:446:ILE:HG13	1.94	0.68
1:A:581:ASP:CG	1:A:597:ARG:HH22	2.01	0.67
1:A:234:GLN:NE2	1:A:237:GLY:O	2.28	0.67
1:B:665:PHE:HE1	1:B:727:ILE:HG23	1.60	0.67
1:A:159:LYS:HB2	1:A:159:LYS:NZ	2.10	0.67
1:A:79:GLN:NE2	1:A:102:ARG:HD2	2.10	0.67
1:B:422:LEU:CD1	1:B:501:ALA:HB1	2.24	0.67
1:B:681:CYS:SG	1:B:682:GLY:N	2.62	0.67
1:A:692:VAL:HG11	1:A:699:LEU:HD23	1.76	0.67
1:B:263:LYS:HA	1:B:271:GLN:NE2	2.10	0.67
1:B:352:ARG:HB2	1:B:645:TYR:HE2	1.60	0.67
1:B:65:ILE:HD13	1:B:78:ILE:HD12	1.77	0.66
1:A:51:GLU:HA	1:A:54:LEU:HD12	1.77	0.66
1:A:582:ILE:HG22	1:A:583:THR:HG23	1.77	0.66
1:A:455:LYS:HB2	1:A:546:TRP:CZ2	2.30	0.66
1:B:508:ILE:HG22	1:B:591:SER:H	1.60	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:GLU:OE1	1:A:713:LYS:HE2	1.94	0.65
1:B:242:ARG:NH1	1:B:245:GLU:OE1	2.30	0.65
1:B:711:ARG:O	1:B:715:ILE:HG12	1.97	0.65
1:A:393:SER:O	1:A:395:LYS:NZ	2.27	0.65
1:A:193:ILE:HD11	1:A:238:CYS:SG	2.37	0.65
1:A:75:ILE:HD11	2:A:802:ATP:H5'1	1.78	0.65
1:A:339:ARG:NE	1:A:690:ASP:OD2	2.30	0.65
1:B:342:ILE:HG13	1:B:699:LEU:CD1	2.29	0.63
1:A:42:THR:OG1	2:A:801:ATP:N6	2.32	0.63
1:B:430:PRO:HG3	1:B:588:TYR:CE2	2.34	0.63
1:A:42:THR:HG22	1:A:43:ILE:HD12	1.80	0.63
1:B:244:ASP:OD1	1:B:244:ASP:N	2.29	0.62
1:B:91:GLU:HG3	1:B:94:ILE:HG12	1.81	0.62
1:A:386:LYS:NZ	1:A:389:GLU:OE2	2.32	0.62
1:B:672:THR:CG2	1:B:677:MET:SD	2.88	0.62
1:A:79:GLN:O	1:A:83:GLU:HG3	2.00	0.62
1:A:701:ASN:N	1:A:701:ASN:OD1	2.32	0.62
1:A:91:GLU:HG3	1:A:94:ILE:HG12	1.82	0.61
1:A:40:SER:O	1:A:44:THR:OG1	2.17	0.61
1:A:530:THR:O	1:A:534:ASN:ND2	2.33	0.61
1:A:458:LEU:HD11	1:A:505:LEU:HB2	1.81	0.61
1:A:177:HIS:HE1	1:A:564:LEU:HD11	1.66	0.61
1:A:119:ILE:O	1:A:119:ILE:HG22	2.01	0.60
1:B:719:VAL:O	1:B:721:HIS:CD2	2.54	0.60
1:B:215:SER:OG	1:B:216:ILE:N	2.34	0.60
1:B:623:HIS:NE2	1:B:648:VAL:HG21	2.15	0.60
1:B:114:ASP:N	1:B:114:ASP:OD1	2.28	0.60
1:A:57:ILE:HD13	1:A:60:ARG:HH21	1.64	0.60
1:B:440:GLN:HG2	1:B:517:PHE:CE2	2.36	0.60
1:A:422:LEU:HD22	1:A:465:VAL:HG11	1.83	0.60
1:B:306:PHE:HB3	1:B:698:TYR:HE2	1.66	0.60
1:B:306:PHE:HB3	1:B:698:TYR:CE2	2.37	0.60
1:B:310:GLY:HA2	1:B:347:ILE:HG12	1.84	0.60
1:B:243:ILE:HA	1:B:246:PHE:CE2	2.37	0.60
1:B:143:THR:HG22	1:B:302:GLY:HA3	1.84	0.60
1:B:684:THR:O	1:B:703:GLN:NE2	2.35	0.59
1:B:424:VAL:O	1:B:461:ARG:NH1	2.35	0.59
1:A:244:ASP:OD1	1:A:245:GLU:N	2.35	0.59
1:B:233:SER:O	1:B:233:SER:OG	2.18	0.59
1:B:587:TYR:CD2	1:B:714:GLU:CD	2.81	0.59
1:A:397:PRO:HG3	1:A:650:TYR:HE2	1.65	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LEU:HD13	1:A:503:VAL:HG12	1.85	0.59
1:B:21:ASP:OD2	1:B:167:ASN:ND2	2.35	0.59
1:B:65:ILE:HD13	1:B:78:ILE:CD1	2.33	0.58
1:B:204:LYS:HA	1:B:209:GLU:HA	1.84	0.58
1:A:288:GLN:HA	1:A:329:VAL:HG21	1.85	0.58
1:A:306:PHE:HB3	1:A:698:TYR:CZ	2.38	0.58
1:B:65:ILE:CD1	1:B:78:ILE:HD12	2.33	0.58
1:B:495:LEU:O	1:B:500:ARG:HG2	2.04	0.58
1:A:99:ILE:O	1:A:103:THR:HG23	2.03	0.58
1:B:401:ARG:HD2	1:B:558:SER:O	2.04	0.58
1:B:630:LEU:HD11	1:B:722:MET:HE1	1.86	0.58
1:A:20:ARG:HA	1:A:75:ILE:HG21	1.84	0.57
1:A:180:ASP:OD1	1:A:180:ASP:N	2.35	0.57
1:A:243:ILE:HA	1:A:246:PHE:CE2	2.40	0.57
1:B:451:MET:HE1	1:B:539:MET:HG3	1.85	0.57
1:B:440:GLN:CG	1:B:517:PHE:CE2	2.88	0.57
1:A:72:ASN:OD1	1:A:72:ASN:N	2.37	0.57
1:A:225:GLN:NE2	4:A:805:TTP:O4	2.37	0.57
1:A:287:MET:HG3	1:A:326:ILE:HG13	1.86	0.57
1:A:306:PHE:HA	1:A:343:PHE:CE2	2.32	0.57
1:B:177:HIS:O	1:B:461:ARG:NH2	2.36	0.57
1:B:497:LYS:HG2	1:B:498:HIS:CD2	2.39	0.57
1:A:345:LYS:HA	1:A:378:TYR:CE2	2.40	0.57
1:A:714:GLU:OE2	1:A:718:ARG:NH2	2.38	0.57
1:B:458:LEU:HD13	1:B:554:PHE:CE2	2.39	0.56
1:A:442:LYS:O	1:A:446:ILE:HG12	2.05	0.56
1:B:692:VAL:HG21	1:B:699:LEU:HD13	1.85	0.56
1:B:287:MET:HG3	1:B:326:ILE:HG12	1.88	0.56
1:A:529:LYS:NZ	1:A:611:ASP:OD2	2.37	0.56
1:B:176:PHE:HB3	1:B:179:LEU:HD21	1.88	0.56
1:B:225:GLN:HE22	4:B:801:TTP:HN3	1.53	0.56
1:B:227:ILE:HG12	1:B:238:CYS:SG	2.46	0.56
1:B:234:GLN:NE2	1:B:237:GLY:O	2.38	0.56
1:B:439:ASP:OD1	1:B:441:ASP:N	2.38	0.56
1:B:601:THR:N	1:B:604:GLU:OE2	2.37	0.56
1:A:213:PRO:HA	4:A:805:TTP:H5'1	1.88	0.56
1:A:350:LEU:HB3	1:A:356:LEU:HD21	1.88	0.56
1:A:398:MET:HE3	1:A:404:LEU:HD11	1.88	0.56
1:A:561:SER:O	1:A:561:SER:OG	2.22	0.56
1:B:422:LEU:HD13	1:B:501:ALA:HB1	1.87	0.56
1:B:349:THR:HG22	1:B:382:LEU:HB2	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:THR:HG23	1:A:50:ILE:H	1.70	0.55
1:B:458:LEU:O	1:B:462:VAL:HG12	2.06	0.55
1:B:228:ALA:HB2	1:B:297:LEU:HD11	1.88	0.55
1:B:381:VAL:HG22	1:B:651:LEU:HB3	1.88	0.55
1:B:692:VAL:CG2	1:B:699:LEU:HD13	2.35	0.55
1:A:289:SER:HA	4:B:801:TTP:HM52	1.88	0.55
1:A:558:SER:OG	1:A:620:GLY:O	2.24	0.55
1:A:685:ASP:OD1	1:A:688:THR:OG1	2.24	0.55
1:B:213:PRO:HA	4:B:801:TTP:H5'1	1.88	0.55
1:B:569:CYS:O	1:B:573:THR:HG22	2.07	0.55
1:B:383:SER:OG	1:B:649:GLY:HA2	2.06	0.55
1:B:398:MET:HE1	1:B:421:ASN:HB2	1.88	0.55
1:B:386:LYS:NZ	1:B:614:GLU:OE2	2.30	0.55
1:B:674:ARG:HA	1:B:712:HIS:CD2	2.42	0.55
1:B:345:LYS:HD2	1:B:378:TYR:CE1	2.41	0.55
1:B:670:THR:HG23	1:B:670:THR:O	2.06	0.55
1:A:141:TYR:HB3	1:B:187:MET:HE1	1.88	0.55
1:A:694:ARG:NH1	1:A:697:GLY:O	2.40	0.55
1:B:497:LYS:HE3	1:B:498:HIS:CE1	2.42	0.54
1:A:683:ASN:OD1	1:A:684:THR:N	2.40	0.54
1:B:471:ALA:HB2	1:B:488:LYS:HG2	1.89	0.54
1:B:711:ARG:NH2	1:B:714:GLU:OE1	2.40	0.54
1:A:607:GLU:HA	1:A:610:LYS:HD3	1.88	0.54
1:B:364:ASP:OD1	1:B:364:ASP:N	2.40	0.54
1:B:161:LEU:HB3	1:B:166:ALA:HB2	1.90	0.54
1:A:47:THR:HG22	1:A:50:ILE:HB	1.90	0.54
1:A:446:ILE:O	1:A:450:ARG:HG2	2.07	0.54
1:A:709:LYS:CE	1:A:713:LYS:HZ3	2.21	0.54
1:B:345:LYS:HD2	1:B:378:TYR:HE1	1.72	0.54
1:B:430:PRO:CG	1:B:588:TYR:CE2	2.87	0.54
1:A:19:LYS:HZ3	2:A:802:ATP:PB	2.30	0.54
1:B:352:ARG:HA	1:B:356:LEU:HB2	1.89	0.54
1:B:510:LEU:HD12	1:B:592:PHE:HB3	1.90	0.54
1:A:187:MET:HE2	1:A:187:MET:HA	1.89	0.53
1:B:187:MET:HB3	1:B:235:TYR:CE1	2.43	0.53
1:B:370:LEU:CD1	1:B:638:GLU:HB2	2.38	0.53
1:B:291:GLU:OE2	1:B:330:ARG:NH2	2.41	0.53
1:A:63:ALA:O	1:A:66:ASN:ND2	2.42	0.53
1:B:345:LYS:NZ	1:B:650:TYR:OH	2.41	0.53
1:B:217:GLN:NE2	1:B:282:ASP:OD1	2.42	0.53
1:A:171:LYS:O	1:A:431:ARG:NH2	2.41	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:VAL:HG11	1:A:617:ALA:HA	1.91	0.53
1:B:327:LEU:HB3	1:B:368:LEU:HD22	1.91	0.53
1:A:404:LEU:HB3	1:A:419:ARG:NH2	2.22	0.53
1:B:186:PRO:HB2	1:B:468:ALA:HB2	1.90	0.52
1:A:143:THR:O	1:A:146:ASP:N	2.41	0.52
1:A:433:ALA:O	1:A:436:SER:OG	2.28	0.52
1:A:586:GLU:OE1	1:A:713:LYS:CE	2.57	0.52
1:B:458:LEU:HD13	1:B:554:PHE:CD2	2.44	0.52
1:A:709:LYS:NZ	1:A:713:LYS:NZ	2.58	0.52
1:B:523:GLU:OE1	1:B:523:GLU:N	2.29	0.52
1:B:672:THR:HG21	1:B:677:MET:CE	2.39	0.52
1:B:496:PHE:HB3	1:B:501:ALA:HB2	1.90	0.52
1:A:420:MET:SD	1:A:420:MET:N	2.83	0.52
1:A:517:PHE:HB3	1:A:518:TYR:HD1	1.74	0.52
1:B:509:GLY:O	1:B:510:LEU:C	2.53	0.52
1:B:175:HIS:HB3	1:B:426:THR:HB	1.92	0.52
1:B:266:VAL:HG12	1:B:267:THR:N	2.24	0.52
1:B:354:LEU:O	1:B:362:ASN:HB2	2.10	0.52
1:A:264:GLU:HG2	1:A:265:TRP:CD1	2.45	0.51
1:A:398:MET:HG3	1:A:402:SER:OG	2.09	0.51
1:B:528:ALA:O	1:B:532:THR:HG23	2.09	0.51
1:A:532:THR:O	1:A:536:VAL:HG23	2.10	0.51
1:A:345:LYS:HG3	1:A:378:TYR:CZ	2.45	0.51
1:A:421:ASN:OD1	1:A:422:LEU:N	2.42	0.51
1:A:523:GLU:HG2	1:A:524:THR:N	2.23	0.51
1:B:440:GLN:CG	1:B:517:PHE:HE2	2.22	0.51
1:B:672:THR:HG21	1:B:677:MET:HE3	1.92	0.51
1:B:691:VAL:HG23	1:B:702:PRO:HD2	1.91	0.51
1:A:594:TYR:CE2	1:A:600:PRO:HG3	2.45	0.51
1:A:177:HIS:O	1:A:461:ARG:NH2	2.43	0.51
1:A:516:VAL:HG23	1:A:582:ILE:HG13	1.91	0.51
1:B:238:CYS:HB3	1:B:307:THR:HG22	1.91	0.51
1:B:419:ARG:NH2	1:B:500:ARG:O	2.43	0.51
1:B:695:THR:HG23	1:B:696:CYS:H	1.75	0.51
1:B:455:LYS:HB2	1:B:546:TRP:CZ2	2.46	0.51
1:A:540:LYS:HD3	1:A:616:GLY:HA3	1.92	0.51
1:B:294:ILE:HD11	1:B:344:PRO:HD3	1.92	0.51
1:B:271:GLN:O	1:B:274:TYR:HB3	2.11	0.51
1:B:562:GLU:HG2	1:B:563:SER:N	2.22	0.51
1:B:198:MET:HE2	1:B:481:ALA:HA	1.94	0.50
1:B:342:ILE:CD1	1:B:700:GLY:HA2	2.41	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:THR:O	1:B:534:ASN:ND2	2.44	0.50
1:A:495:LEU:O	1:A:495:LEU:HD12	2.11	0.50
1:A:462:VAL:HG21	1:A:552:TYR:HD2	1.76	0.50
1:B:496:PHE:HB3	1:B:501:ALA:CB	2.41	0.50
1:B:630:LEU:HD11	1:B:722:MET:CE	2.41	0.50
1:A:469:THR:H	1:A:472:ASN:HD22	1.59	0.50
1:B:656:PRO:HB3	1:B:668:ASP:HB2	1.93	0.50
1:B:428:ASN:O	1:B:432:ILE:HD13	2.12	0.50
1:B:345:LYS:HD3	1:B:698:TYR:CD1	2.47	0.49
1:B:626:GLU:HB2	1:B:721:HIS:CG	2.47	0.49
1:A:20:ARG:HB2	2:A:802:ATP:O1B	2.12	0.49
1:A:364:ASP:N	1:A:364:ASP:OD1	2.44	0.49
1:A:531:PHE:CE1	1:A:535:ILE:HD11	2.47	0.49
1:A:177:HIS:CD2	1:A:424:VAL:HB	2.46	0.49
1:B:458:LEU:HD11	1:B:505:LEU:HD12	1.93	0.49
1:A:147:LEU:O	1:A:151:ILE:HG23	2.13	0.49
1:A:370:LEU:O	1:A:374:THR:HG22	2.12	0.49
1:B:198:MET:HG3	1:B:226:ILE:CD1	2.43	0.49
1:A:308:SER:HA	1:A:345:LYS:HB3	1.95	0.49
1:B:359:ASN:OD1	1:B:360:SER:N	2.45	0.49
1:A:148:THR:O	1:A:151:ILE:HG12	2.13	0.48
1:B:375:LYS:HE2	1:B:631:GLN:NE2	2.27	0.48
1:B:167:ASN:O	1:B:171:LYS:HG2	2.12	0.48
1:B:482:PHE:HB2	1:B:495:LEU:HD21	1.95	0.48
1:A:451:MET:HE3	1:A:546:TRP:CH2	2.48	0.48
1:A:490:ASP:OD1	1:A:491:SER:N	2.46	0.48
1:B:424:VAL:HG12	1:B:504:SER:HB2	1.95	0.48
1:B:506:GLY:HA3	1:B:559:THR:HG23	1.96	0.48
1:A:143:THR:O	1:A:144:GLN:C	2.56	0.48
1:A:517:PHE:HB3	1:A:518:TYR:CD1	2.49	0.48
1:B:221:ALA:O	1:B:225:GLN:HG3	2.14	0.47
1:A:422:LEU:HB2	1:A:503:VAL:HG22	1.96	0.47
1:A:497:LYS:HA	1:A:552:TYR:CE1	2.49	0.47
1:A:566:ASP:OD1	1:A:570:ARG:NH2	2.46	0.47
1:B:349:THR:HG22	1:B:382:LEU:CB	2.44	0.47
1:B:420:MET:SD	1:B:420:MET:N	2.87	0.47
1:A:531:PHE:O	1:A:535:ILE:HG12	2.14	0.47
1:B:36:ILE:HG22	1:B:54:LEU:HD13	1.96	0.47
1:B:330:ARG:NH2	1:B:344:PRO:HD2	2.30	0.47
1:A:297:LEU:HD12	1:A:297:LEU:HA	1.72	0.47
1:A:525:ASN:OD1	1:A:527:GLU:N	2.48	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASN:HA	1:B:62:VAL:HG12	1.96	0.47
1:B:65:ILE:CD1	1:B:78:ILE:CD1	2.93	0.47
1:B:403:PHE:HZ	1:B:650:TYR:CD1	2.32	0.47
1:A:114:ASP:OD1	1:A:114:ASP:N	2.45	0.47
1:A:636:ALA:O	1:A:640:VAL:HG12	2.14	0.47
1:B:224:SER:OG	1:B:293:GLU:HG2	2.15	0.47
1:B:685:ASP:O	1:B:689:VAL:HG12	2.15	0.47
1:A:356:LEU:HA	1:A:366:LYS:NZ	2.30	0.46
1:A:382:LEU:HD11	1:A:397:PRO:HD3	1.96	0.46
1:A:596:VAL:HG12	1:A:718:ARG:HA	1.96	0.46
1:B:21:ASP:OD1	1:B:21:ASP:N	2.46	0.46
1:A:430:PRO:HB3	1:A:512:GLU:HB3	1.96	0.46
1:B:666:GLU:O	1:B:728:LYS:HB2	2.15	0.46
1:A:177:HIS:HD2	1:A:424:VAL:HB	1.79	0.46
1:B:36:ILE:HD13	1:B:57:ILE:HD11	1.97	0.46
1:B:47:THR:O	1:B:48:PRO:C	2.58	0.46
1:B:47:THR:O	1:B:50:ILE:N	2.49	0.46
1:A:702:PRO:HG3	1:A:707:MET:HE1	1.95	0.46
1:B:408:LYS:HA	1:B:414:GLU:HA	1.97	0.46
1:B:522:TRP:N	1:B:523:GLU:OE1	2.48	0.46
1:B:522:TRP:O	1:B:525:ASN:ND2	2.49	0.46
1:A:377:MET:HB2	1:A:699:LEU:HD21	1.98	0.46
1:B:25:VAL:HG12	1:B:26:THR:N	2.31	0.46
1:B:497:LYS:HG2	1:B:498:HIS:N	2.31	0.46
1:B:531:PHE:O	1:B:535:ILE:HG22	2.15	0.46
1:A:709:LYS:NZ	1:A:713:LYS:HZ3	2.12	0.46
1:B:190:CYS:HB3	1:B:237:GLY:H	1.79	0.46
1:A:21:ASP:HB2	1:A:163:PRO:HB2	1.98	0.46
1:A:566:ASP:OD1	1:A:566:ASP:C	2.59	0.46
1:B:21:ASP:HB3	1:B:164:HIS:HB3	1.97	0.46
1:A:462:VAL:HG21	1:A:552:TYR:CD2	2.51	0.46
1:B:707:MET:SD	1:B:711:ARG:HB3	2.56	0.46
1:A:164:HIS:NE2	1:A:456:ASP:OD2	2.46	0.45
1:A:320:ARG:NH2	1:A:364:ASP:OD2	2.50	0.45
1:B:711:ARG:HD3	1:B:711:ARG:HA	1.78	0.45
1:A:265:TRP:CZ3	1:B:274:TYR:HA	2.50	0.45
1:A:267:THR:O	1:A:271:GLN:HG3	2.17	0.45
1:B:198:MET:HG3	1:B:226:ILE:HD13	1.98	0.45
1:A:238:CYS:N	1:A:306:PHE:O	2.46	0.45
1:A:482:PHE:HB3	1:A:495:LEU:HD11	1.98	0.45
1:B:88:GLU:O	1:B:88:GLU:HG2	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:VAL:CG1	1:B:267:THR:N	2.79	0.45
1:B:211:GLU:O	1:B:212:SER:C	2.60	0.45
1:A:709:LYS:HE3	1:A:713:LYS:HZ3	1.81	0.45
1:B:419:ARG:HD2	1:B:500:ARG:HE	1.81	0.45
1:A:189:ASN:ND2	1:A:190:CYS:SG	2.90	0.45
1:A:497:LYS:HA	1:A:552:TYR:HE1	1.81	0.45
1:B:428:ASN:CG	1:B:431:ARG:HB3	2.42	0.45
1:A:334:LEU:HD11	1:A:341:ALA:HB2	1.98	0.45
1:B:264:GLU:HB3	1:B:265:TRP:CD1	2.52	0.45
1:B:378:TYR:HD1	1:B:379:PRO:HA	1.82	0.45
1:A:421:ASN:OD1	1:A:423:GLY:N	2.48	0.45
1:A:434:LEU:HD12	1:A:516:VAL:HG21	1.99	0.45
1:B:36:ILE:HG22	1:B:54:LEU:HD22	1.97	0.45
1:A:334:LEU:CD1	1:A:341:ALA:HB2	2.47	0.44
1:B:430:PRO:HG3	1:B:588:TYR:CD2	2.51	0.44
1:A:115:ILE:O	1:A:116:ASN:C	2.60	0.44
1:B:678:CYS:O	1:B:678:CYS:SG	2.74	0.44
1:A:239:THR:HG21	1:A:398:MET:HA	1.99	0.44
1:A:186:PRO:HB2	1:A:468:ALA:HB2	1.99	0.44
1:A:266:VAL:HG23	1:A:271:GLN:HG2	2.00	0.44
1:B:458:LEU:HD22	1:B:503:VAL:HG11	2.00	0.44
1:B:728:LYS:HB3	1:B:728:LYS:HE2	1.70	0.44
1:A:192:LEU:O	1:A:418:GLY:N	2.49	0.44
1:B:665:PHE:HA	1:B:729:TYR:O	2.18	0.44
1:A:295:ASN:HD21	1:B:207:ASN:H	1.66	0.44
1:A:152:VAL:HG21	1:B:152:VAL:HG21	1.99	0.44
1:B:606:LEU:HD22	1:B:648:VAL:CG1	2.47	0.44
1:A:347:ILE:HD13	1:A:397:PRO:HD2	2.00	0.44
1:A:585:LYS:HB2	1:A:587:TYR:CD2	2.52	0.44
1:B:575:LYS:HG3	1:B:576:PHE:CD1	2.53	0.44
1:A:159:LYS:HB2	1:A:159:LYS:HZ2	1.81	0.43
1:A:599:ASN:HA	1:A:721:HIS:CD2	2.53	0.43
1:B:50:ILE:O	1:B:53:LYS:HG2	2.18	0.43
1:B:440:GLN:HG3	1:B:517:PHE:CE2	2.53	0.43
1:A:40:SER:HA	1:A:94:ILE:HG22	2.00	0.43
1:A:292:TYR:O	1:A:296:THR:HG22	2.18	0.43
1:B:175:HIS:O	1:B:425:VAL:HG23	2.17	0.43
1:B:189:ASN:HA	1:B:235:TYR:CZ	2.53	0.43
1:B:429:LEU:HD11	1:B:507:TYR:HB2	2.01	0.43
1:A:198:MET:SD	1:A:226:ILE:HD13	2.58	0.43
1:A:528:ALA:O	1:A:532:THR:HG22	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:HD11	1:B:95:ALA:HB2	2.00	0.43
1:B:173:ASP:OD1	1:B:450:ARG:NH1	2.50	0.43
1:A:529:LYS:O	1:A:533:LEU:HD23	2.18	0.43
1:B:187:MET:HB3	1:B:235:TYR:CD1	2.53	0.43
1:B:350:LEU:HB3	1:B:356:LEU:HD21	2.01	0.43
1:A:187:MET:HB3	1:A:235:TYR:HD1	1.84	0.43
1:A:469:THR:H	1:A:472:ASN:ND2	2.16	0.43
1:B:47:THR:HB	1:B:50:ILE:HG12	2.01	0.43
1:B:525:ASN:OD1	1:B:527:GLU:N	2.51	0.43
1:A:358:PRO:HA	1:A:363:TYR:CD1	2.53	0.43
1:A:557:TYR:CE2	1:A:559:THR:HA	2.53	0.43
1:B:454:ALA:HB1	1:B:505:LEU:HD11	2.00	0.43
1:B:510:LEU:HD23	1:B:510:LEU:HA	1.88	0.43
1:A:331:ILE:HD12	1:A:371:GLU:HG2	2.00	0.43
1:A:472:ASN:HB3	1:B:141:TYR:CZ	2.54	0.43
1:B:192:LEU:HB2	1:B:398:MET:HG3	2.01	0.43
1:A:243:ILE:HG22	1:A:310:GLY:O	2.19	0.43
1:A:327:LEU:O	1:A:331:ILE:HG22	2.19	0.43
1:A:554:PHE:N	1:A:554:PHE:CD1	2.86	0.43
1:A:604:GLU:O	1:A:607:GLU:HG2	2.19	0.43
1:A:382:LEU:HD22	1:A:387:ILE:HG13	2.00	0.43
1:A:613:PRO:HA	1:A:617:ALA:HB3	2.01	0.43
1:B:193:ILE:HG22	1:B:194:ASP:N	2.34	0.43
1:B:210:VAL:HG13	4:B:801:TTP:H1'	2.01	0.43
1:B:193:ILE:CD1	1:B:238:CYS:SG	3.07	0.43
1:A:705:ARG:HD2	1:A:705:ARG:C	2.44	0.42
1:B:168:ALA:HB1	1:B:173:ASP:HB3	2.01	0.42
1:A:74:LYS:HE2	1:A:74:LYS:HB2	1.75	0.42
1:A:139:ASP:OD1	1:A:139:ASP:N	2.49	0.42
1:B:398:MET:HE2	1:B:398:MET:HB3	1.81	0.42
1:B:373:ALA:HA	1:B:378:TYR:O	2.19	0.42
1:A:20:ARG:NH2	2:A:802:ATP:O3G	2.49	0.42
1:A:115:ILE:HD12	1:A:115:ILE:HA	1.69	0.42
1:B:627:TYR:HD1	1:B:722:MET:CE	2.32	0.42
1:B:18:ILE:HG22	1:B:74:LYS:HA	2.01	0.42
1:B:175:HIS:HB2	1:B:568:PHE:CE2	2.53	0.42
1:B:351:LYS:C	1:B:356:LEU:HD23	2.44	0.42
1:B:441:ASP:N	1:B:441:ASP:OD1	2.52	0.42
1:B:627:TYR:HD1	1:B:722:MET:HE2	1.84	0.42
1:A:216:ILE:HD12	1:A:283:ILE:HD13	2.01	0.42
1:A:263:LYS:HB2	1:A:263:LYS:HE2	1.78	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ILE:HD12	1:B:18:ILE:HA	1.82	0.42
1:B:429:LEU:N	1:B:430:PRO:HD2	2.35	0.42
1:A:187:MET:HB3	1:A:235:TYR:CD1	2.55	0.42
1:A:665:PHE:CD1	1:A:665:PHE:C	2.96	0.42
1:A:555:SER:OG	1:A:556:VAL:O	2.35	0.42
1:B:497:LYS:CG	1:B:498:HIS:N	2.83	0.42
1:A:224:SER:OG	1:A:293:GLU:HG2	2.19	0.42
1:A:429:LEU:N	1:A:430:PRO:HD2	2.34	0.42
1:A:556:VAL:O	1:A:619:GLY:HA3	2.19	0.42
1:B:173:ASP:OD2	1:B:450:ARG:HD2	2.20	0.42
1:B:476:LEU:HA	1:B:481:ALA:HB3	2.01	0.42
1:B:505:LEU:HD23	1:B:506:GLY:N	2.35	0.42
1:B:556:VAL:HG13	1:B:617:ALA:HA	2.01	0.42
1:B:575:LYS:HG3	1:B:576:PHE:CE1	2.55	0.42
1:B:670:THR:O	1:B:670:THR:CG2	2.68	0.42
1:A:419:ARG:HG2	1:A:500:ARG:HG2	2.02	0.42
1:B:407:TRP:O	1:B:408:LYS:C	2.61	0.41
1:A:239:THR:OG1	1:A:308:SER:HB2	2.19	0.41
1:B:354:LEU:O	1:B:360:SER:OG	2.38	0.41
1:B:397:PRO:HG3	1:B:650:TYR:HE1	1.85	0.41
1:B:113:THR:OG1	1:B:114:ASP:OD1	2.38	0.41
1:A:18:ILE:HG23	1:A:74:LYS:HA	2.01	0.41
1:A:186:PRO:HG2	1:B:141:TYR:OH	2.21	0.41
1:A:539:MET:HE3	1:A:539:MET:HB3	1.71	0.41
1:B:655:THR:O	1:B:657:ILE:HG23	2.21	0.41
1:B:661:TYR:HB2	1:B:688:THR:O	2.19	0.41
1:A:340:THR:HB	1:A:376:ARG:HH11	1.85	0.41
1:A:440:GLN:HG2	1:A:517:PHE:HE2	1.84	0.41
1:A:535:ILE:HG12	1:A:535:ILE:H	1.71	0.41
1:B:75:ILE:HD11	2:B:803:ATP:H5'1	2.02	0.41
1:B:606:LEU:CD1	1:B:644:ALA:HB2	2.51	0.41
1:A:140:LEU:HA	1:B:472:ASN:O	2.21	0.41
1:A:530:THR:HG22	1:A:534:ASN:HD21	1.86	0.41
1:A:624:TYR:CE1	1:A:694:ARG:HD3	2.56	0.41
1:B:275:ALA:O	1:B:276:ARG:C	2.64	0.41
1:B:657:ILE:HD12	1:B:657:ILE:O	2.20	0.41
1:A:426:THR:HG21	1:A:559:THR:HG21	2.02	0.41
1:A:631:GLN:O	1:A:633:ASN:ND2	2.53	0.41
1:B:57:ILE:HA	1:B:60:ARG:HB2	2.03	0.41
1:B:115:ILE:HD12	1:B:115:ILE:HA	1.89	0.41
1:B:327:LEU:O	1:B:331:ILE:HG22	2.19	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:LYS:HE3	1:B:550:TYR:HE2	1.84	0.41
1:A:21:ASP:OD1	1:A:22:GLY:N	2.45	0.41
1:A:192:LEU:HD23	1:A:398:MET:HB3	2.03	0.41
1:A:429:LEU:HD21	1:A:507:TYR:HB2	2.03	0.41
1:A:475:ILE:HG23	1:A:476:LEU:N	2.36	0.41
1:A:660:CYS:HB2	1:A:669:PHE:HZ	1.85	0.41
1:A:668:ASP:OD1	1:A:669:PHE:N	2.52	0.41
1:B:87:LEU:HD12	1:B:87:LEU:HA	1.91	0.41
1:B:623:HIS:CE1	1:B:648:VAL:HG21	2.55	0.41
1:A:493:ASP:OD1	1:A:552:TYR:OH	2.39	0.41
1:A:711:ARG:O	1:A:715:ILE:HD12	2.21	0.41
1:B:50:ILE:HA	1:B:53:LYS:HG2	2.03	0.41
1:A:356:LEU:HD13	1:A:366:LYS:NZ	2.35	0.40
1:A:434:LEU:HD11	1:A:582:ILE:HG21	2.03	0.40
1:B:159:LYS:HE2	1:B:159:LYS:HB2	1.70	0.40
1:B:185:THR:O	1:B:187:MET:N	2.52	0.40
1:B:299:THR:HG23	1:B:305:PRO:HD3	2.03	0.40
1:A:349:THR:HG21	1:A:394:PHE:HZ	1.87	0.40
1:A:631:GLN:HB3	1:A:632:GLN:NE2	2.36	0.40
1:B:73:ILE:HG12	1:B:78:ILE:CD1	2.44	0.40
1:A:531:PHE:CZ	1:A:535:ILE:HD11	2.57	0.40
1:A:692:VAL:HG13	1:A:699:LEU:HB3	2.02	0.40
1:B:23:ARG:NH2	1:B:449:GLU:OE2	2.54	0.40
1:A:204:LYS:HB3	1:A:479:TYR:CZ	2.57	0.40
1:B:274:TYR:O	1:B:275:ALA:C	2.64	0.40
1:B:395:LYS:HE3	1:B:404:LEU:HB2	2.02	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	693/734 (94%)	640 (92%)	53 (8%)	0	100	100
1	B	695/734 (95%)	629 (90%)	66 (10%)	0	100	100
All	All	1388/1468 (95%)	1269 (91%)	119 (9%)	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	604/637 (95%)	568 (94%)	36 (6%)	17	45
1	B	605/637 (95%)	567 (94%)	38 (6%)	16	44
All	All	1209/1274 (95%)	1135 (94%)	74 (6%)	19	45

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	19	LYS
1	A	26	THR
1	A	31	LYS
1	A	36	ILE
1	A	46	ILE
1	A	66	ASN
1	A	72	ASN
1	A	111	GLN
1	A	113	THR
1	A	114	ASP
1	A	115	ILE
1	A	139	ASP
1	A	159	LYS
1	A	160	MET
1	A	190	CYS
1	A	193	ILE
1	A	215	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	230	VAL
1	A	234	GLN
1	A	283	ILE
1	A	315	THR
1	A	329	VAL
1	A	390	LEU
1	A	424	VAL
1	A	427	LEU
1	A	469	THR
1	A	491	SER
1	A	492	VAL
1	A	513	VAL
1	A	516	VAL
1	A	626	GLU
1	A	655	THR
1	A	658	ASP
1	A	695	THR
1	A	701	ASN
1	B	21	ASP
1	B	47	THR
1	B	81	ILE
1	B	114	ASP
1	B	140	LEU
1	B	158	LEU
1	B	165	VAL
1	B	179	LEU
1	B	180	ASP
1	B	191	CYS
1	B	244	ASP
1	B	254	ASN
1	B	267	THR
1	B	313	LEU
1	B	326	ILE
1	B	336	SER
1	B	356	LEU
1	B	368	LEU
1	B	370	LEU
1	B	374	THR
1	B	381	VAL
1	B	388	ILE
1	B	390	LEU
1	B	413	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	414	GLU
1	B	469	THR
1	B	486	LEU
1	B	508	ILE
1	B	516	VAL
1	B	525	ASN
1	B	555	SER
1	B	556	VAL
1	B	558	SER
1	B	635	LYS
1	B	678	CYS
1	B	680	ASN
1	B	692	VAL
1	B	701	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	116	ASN
1	A	175	HIS
1	A	177	HIS
1	A	189	ASN
1	A	295	ASN
1	A	328	GLN
1	A	472	ASN
1	A	478	GLN
1	A	534	ASN
1	A	632	GLN
1	A	633	ASN
1	B	71	HIS
1	B	72	ASN
1	B	169	HIS
1	B	177	HIS
1	B	225	GLN
1	B	367	GLN
1	B	421	ASN
1	B	472	ASN
1	B	498	HIS
1	B	534	ASN
1	B	680	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\# Z  > 2$
2	ATP	B	803	3	32,33,33	0.75	0	48,52,52	1.02	2 (4%)
4	TTP	A	805	3	29,30,30	0.57	0	43,47,47	0.81	2 (4%)
2	ATP	A	801	3	32,33,33	0.52	0	48,52,52	0.59	0
2	ATP	B	802	3	32,33,33	0.97	2 (6%)	48,52,52	1.49	5 (10%)
4	TTP	B	801	3	29,30,30	1.30	4 (13%)	43,47,47	1.52	9 (20%)
2	ATP	A	802	3	32,33,33	0.51	0	48,52,52	0.66	0

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	ATP	B	803	3	-	7/22/38/38	0/3/3/3
4	TTP	A	805	3	-	2/22/34/34	0/2/2/2
2	ATP	A	801	3	-	6/22/38/38	0/3/3/3

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	802	3	-	7/22/38/38	0/3/3/3
4	TTP	B	801	3	-	4/22/34/34	0/2/2/2
2	ATP	A	802	3	-	5/22/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	TTP	C5'-C4'	-4.16	1.39	1.51
2	B	802	ATP	PA-O3A	3.55	1.63	1.59
2	B	802	ATP	PB-O3A	2.72	1.62	1.59
4	B	801	TTP	PB-O3A	-2.53	1.56	1.59
4	B	801	TTP	C4-C5	2.51	1.48	1.44
4	B	801	TTP	O5'-C5'	-2.13	1.36	1.44

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	ATP	O2B-PB-O3B	5.92	123.28	107.27
4	B	801	TTP	O5'-C5'-C4'	-4.33	94.26	108.99
2	B	802	ATP	O3A-PA-O1A	4.07	122.94	110.70
4	B	801	TTP	O4'-C4'-C3'	3.25	113.06	105.65
4	B	801	TTP	C1'-N1-C6	3.15	126.02	120.74
2	B	802	ATP	O2B-PB-O3A	2.97	115.30	107.27
4	B	801	TTP	C5-C4-N3	2.94	117.88	115.32
2	B	802	ATP	O3A-PB-O1B	-2.93	101.90	110.70
4	B	801	TTP	C4-N3-C2	-2.89	123.55	127.34
4	B	801	TTP	O4'-C4'-C5'	2.76	118.17	109.33
2	B	803	ATP	PA-O5'-C5'	-2.64	106.25	121.35
2	B	802	ATP	O3B-PB-O1B	-2.57	102.96	110.70
4	B	801	TTP	C1'-N1-C2	-2.40	112.97	117.66
2	B	803	ATP	C4-C5-N7	-2.30	107.96	110.58
4	A	805	TTP	O2-C2-N1	-2.18	119.96	122.80
4	A	805	TTP	O2-C2-N3	2.17	125.48	121.49
4	B	801	TTP	C4'-O4'-C1'	-2.14	104.42	109.51
4	B	801	TTP	N3-C2-N1	2.08	117.60	114.89

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801	TTP	PB-O3B-PG-O3G

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	801	ATP	C4'-C5'-O5'-PA
2	A	801	ATP	O4'-C1'-N9-C4
2	B	802	ATP	O4'-C1'-N9-C4
2	B	802	ATP	O4'-C4'-C5'-O5'
2	B	802	ATP	O4'-C1'-N9-C8
2	B	803	ATP	C3'-C4'-C5'-O5'
4	B	801	TTP	C3'-C4'-C5'-O5'
2	A	801	ATP	O4'-C1'-N9-C8
2	B	803	ATP	O4'-C4'-C5'-O5'
2	A	802	ATP	C2'-C1'-N9-C8
2	B	803	ATP	C2'-C1'-N9-C8
2	A	801	ATP	C5'-O5'-PA-O1A
2	B	802	ATP	C5'-O5'-PA-O1A
2	B	802	ATP	C5'-O5'-PA-O2A
2	B	802	ATP	C5'-O5'-PA-O3A
2	B	802	ATP	C4'-C5'-O5'-PA
2	A	801	ATP	O4'-C4'-C5'-O5'
4	A	805	TTP	PG-O3B-PB-O1B
2	A	802	ATP	C2'-C1'-N9-C4
2	A	802	ATP	C3'-C4'-C5'-O5'
2	A	802	ATP	PG-O3B-PB-O2B
2	B	803	ATP	PG-O3B-PB-O2B
4	A	805	TTP	PG-O3B-PB-O2B
4	B	801	TTP	PB-O3B-PG-O2G
2	A	802	ATP	O4'-C1'-N9-C8
2	B	803	ATP	O4'-C1'-N9-C8
2	A	801	ATP	PG-O3B-PB-O2B
2	B	803	ATP	C2'-C1'-N9-C4
2	B	803	ATP	PG-O3B-PB-O1B
4	B	801	TTP	PA-O3A-PB-O2B

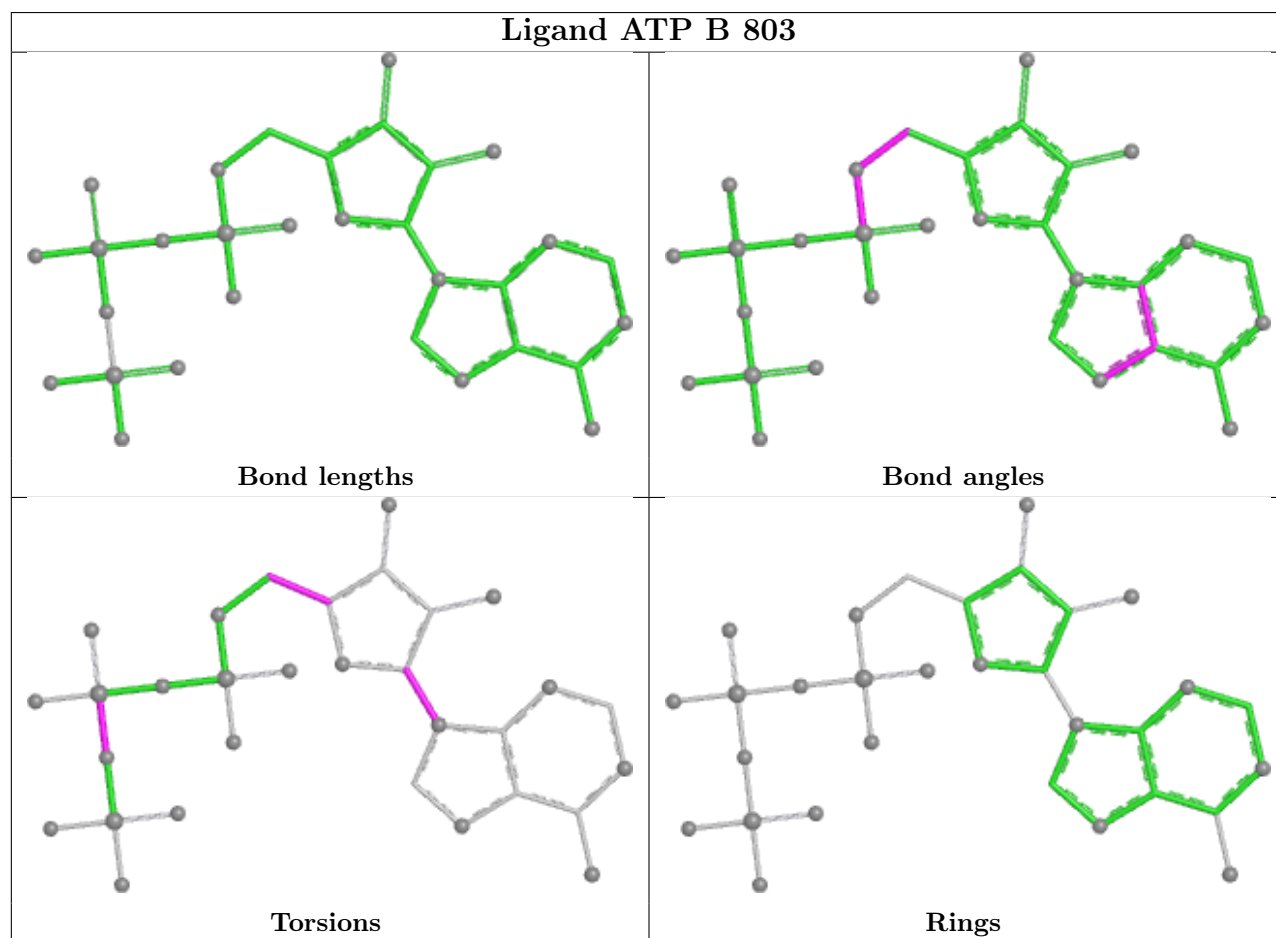
There are no ring outliers.

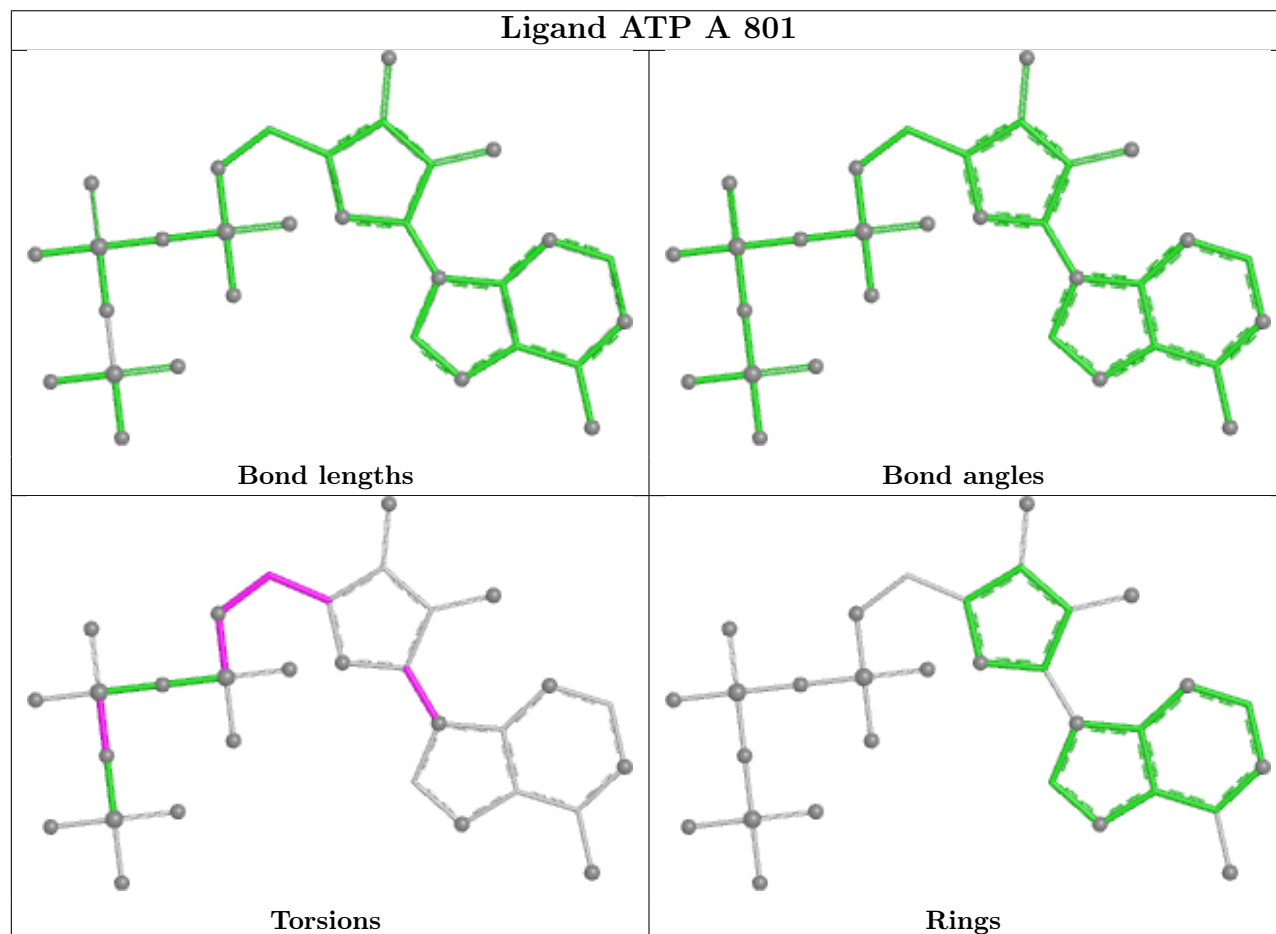
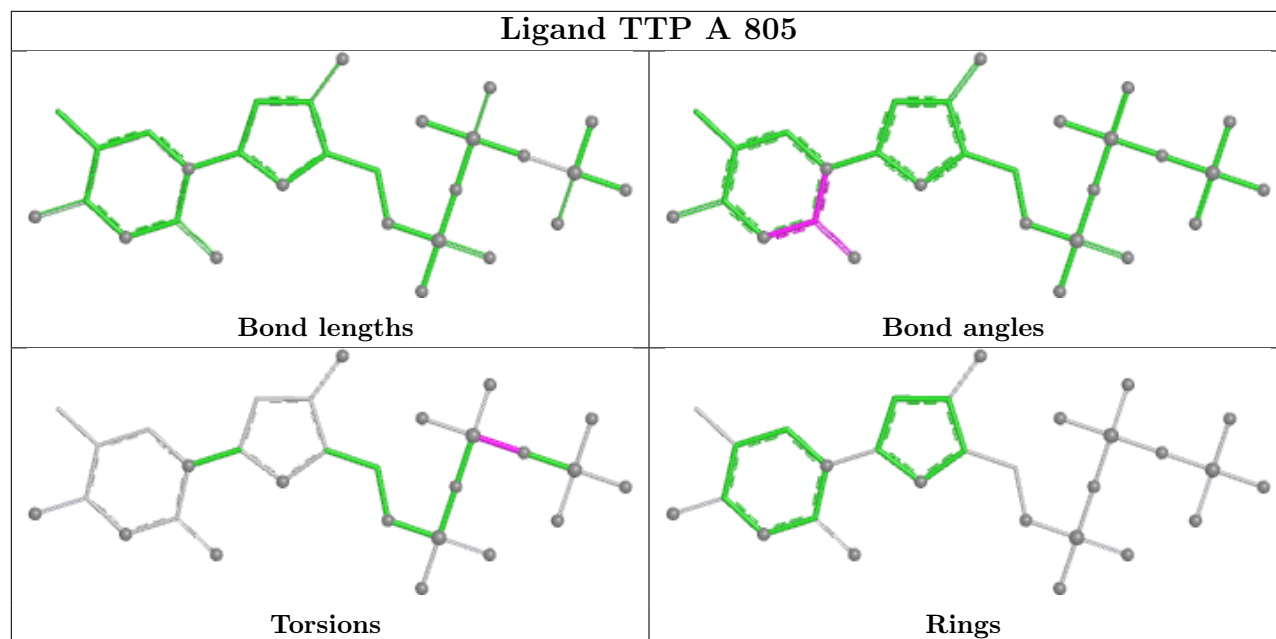
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	803	ATP	1	0
4	A	805	TTP	2	0
2	A	801	ATP	1	0
4	B	801	TTP	4	0
2	A	802	ATP	4	0

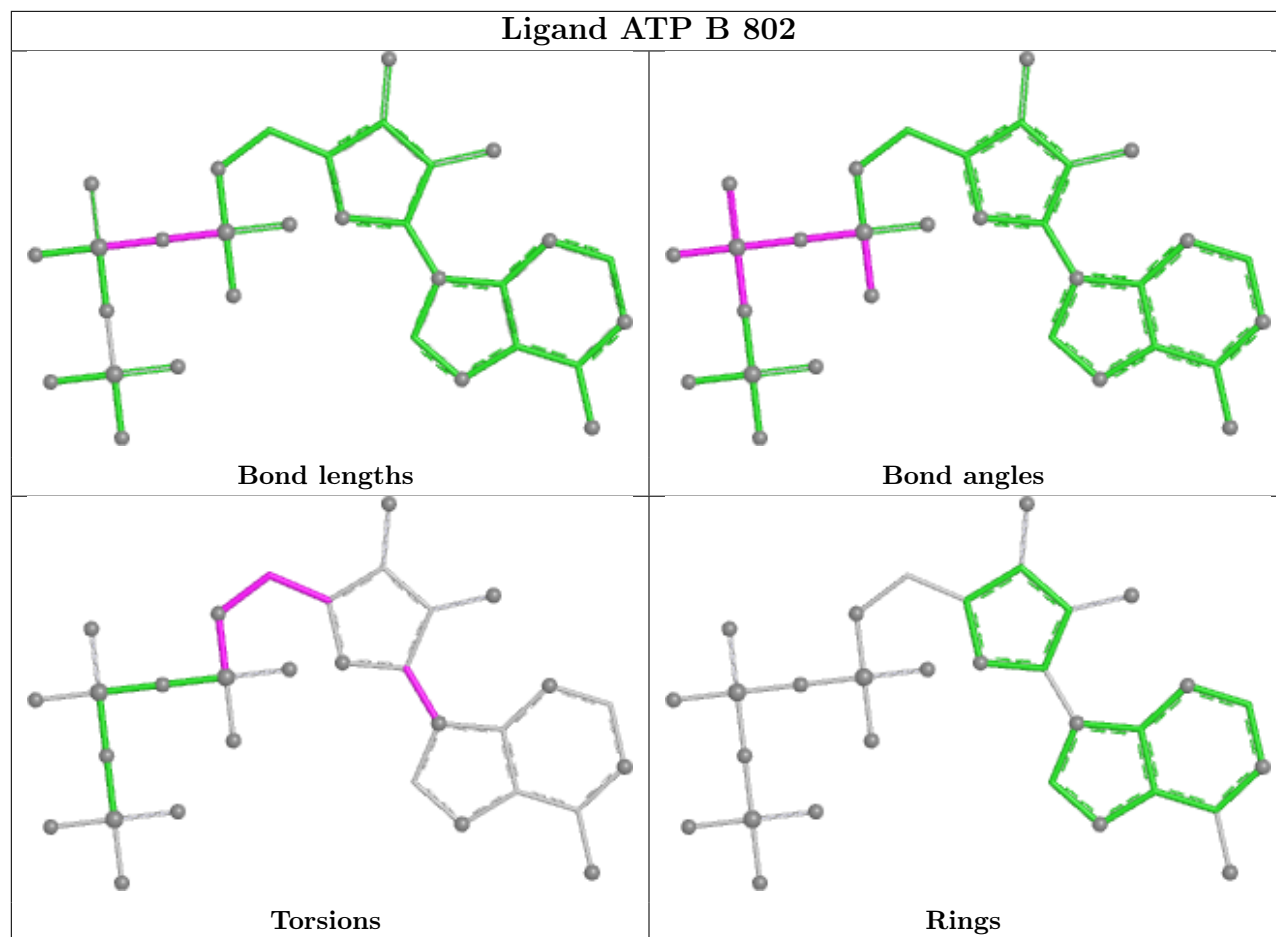
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

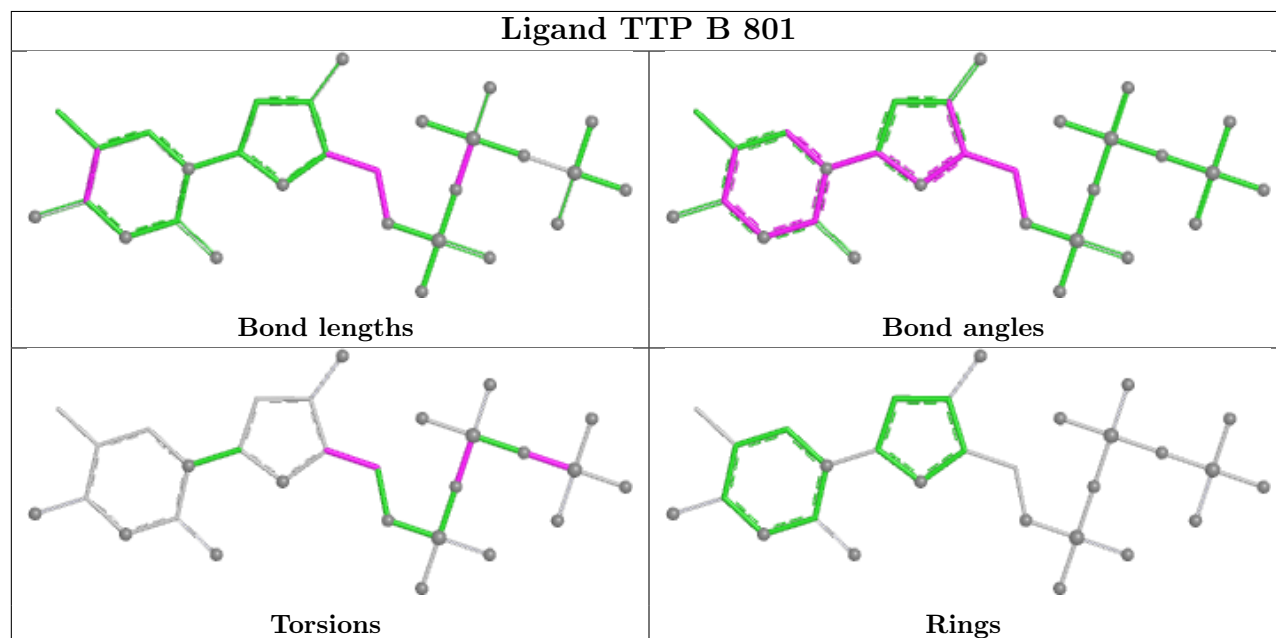


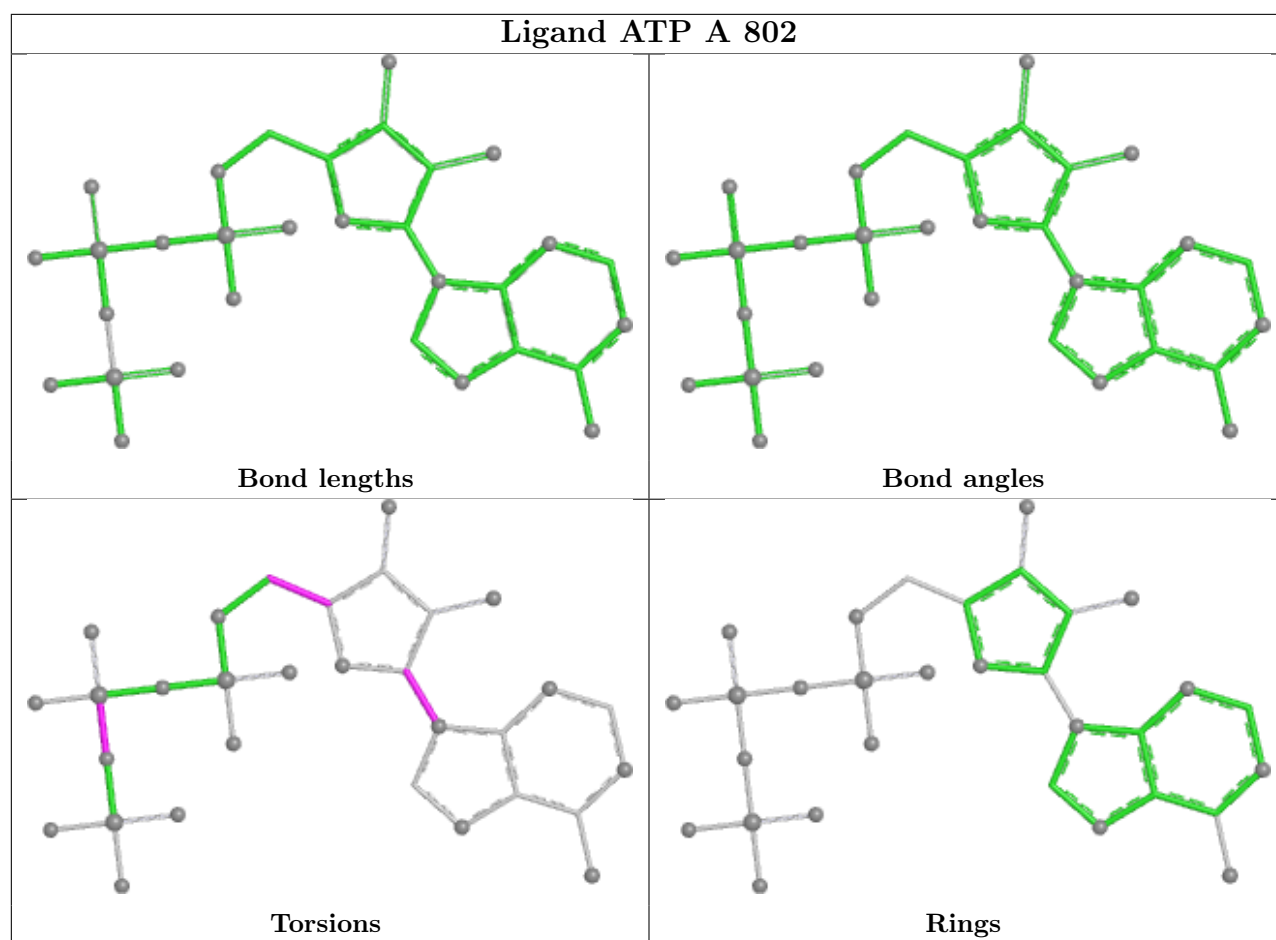


## Ligand ATP B 802



## Ligand TTP B 801





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

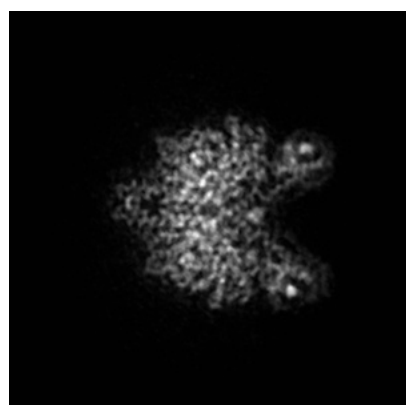
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46747. These allow visual inspection of the internal detail of the map and identification of artifacts.

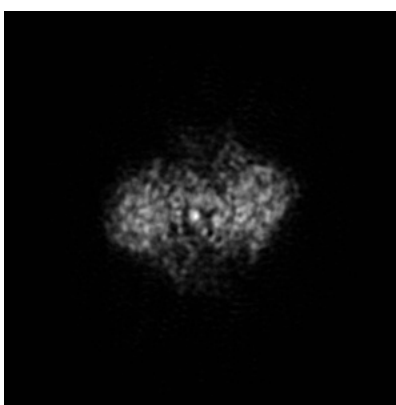
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

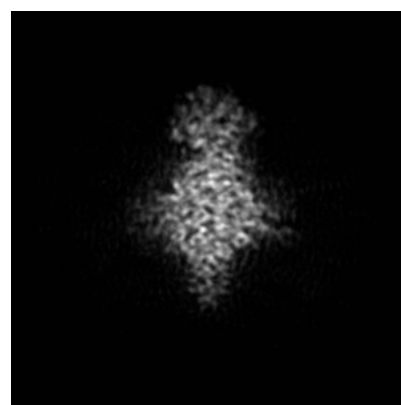
#### 6.1.1 Primary map



X



Y

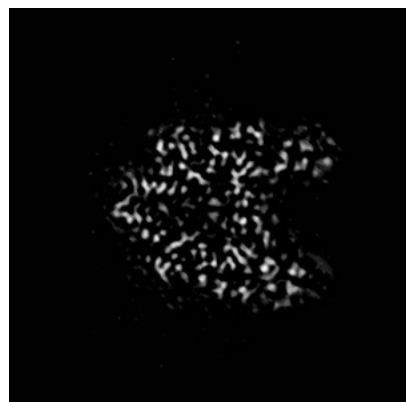


Z

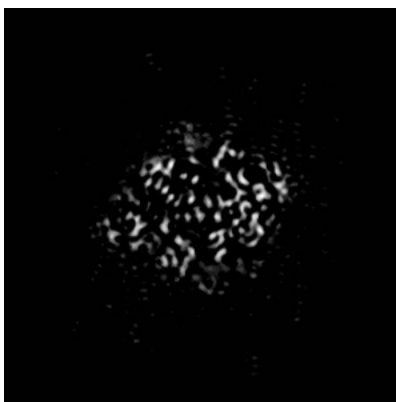
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 128



Y Index: 128



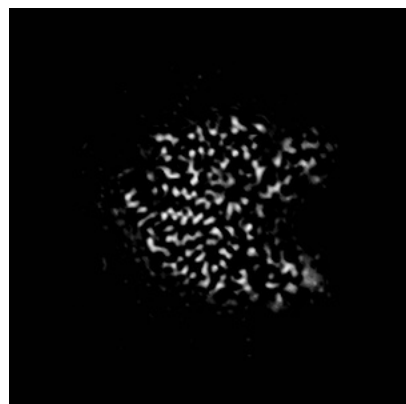
Z Index: 128



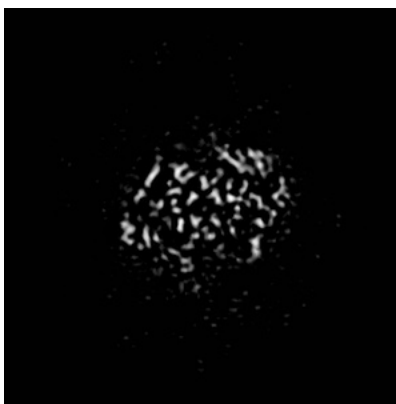
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 133



Y Index: 118

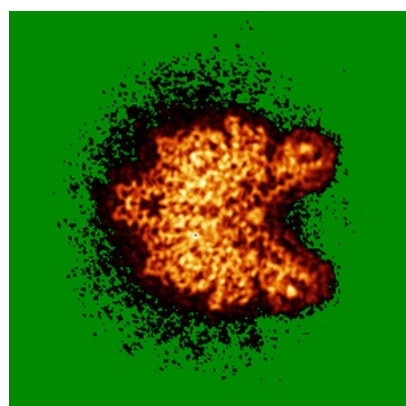


Z Index: 91

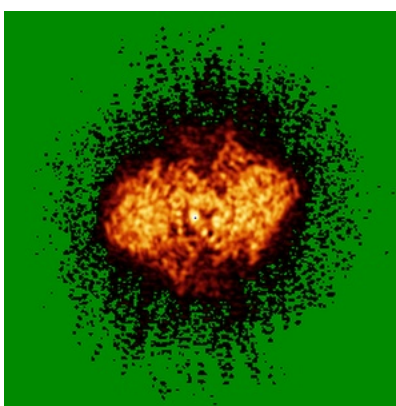
The images above show the largest variance slices of the map in three orthogonal directions.

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

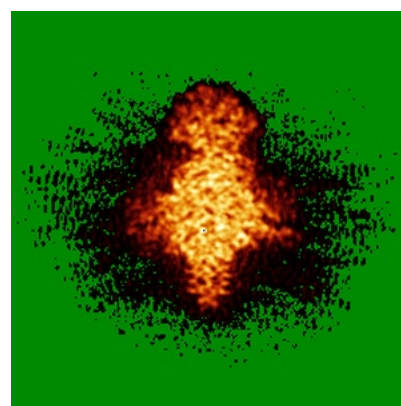
### 6.4.1 Primary map



X



Y



Z

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 5.33. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

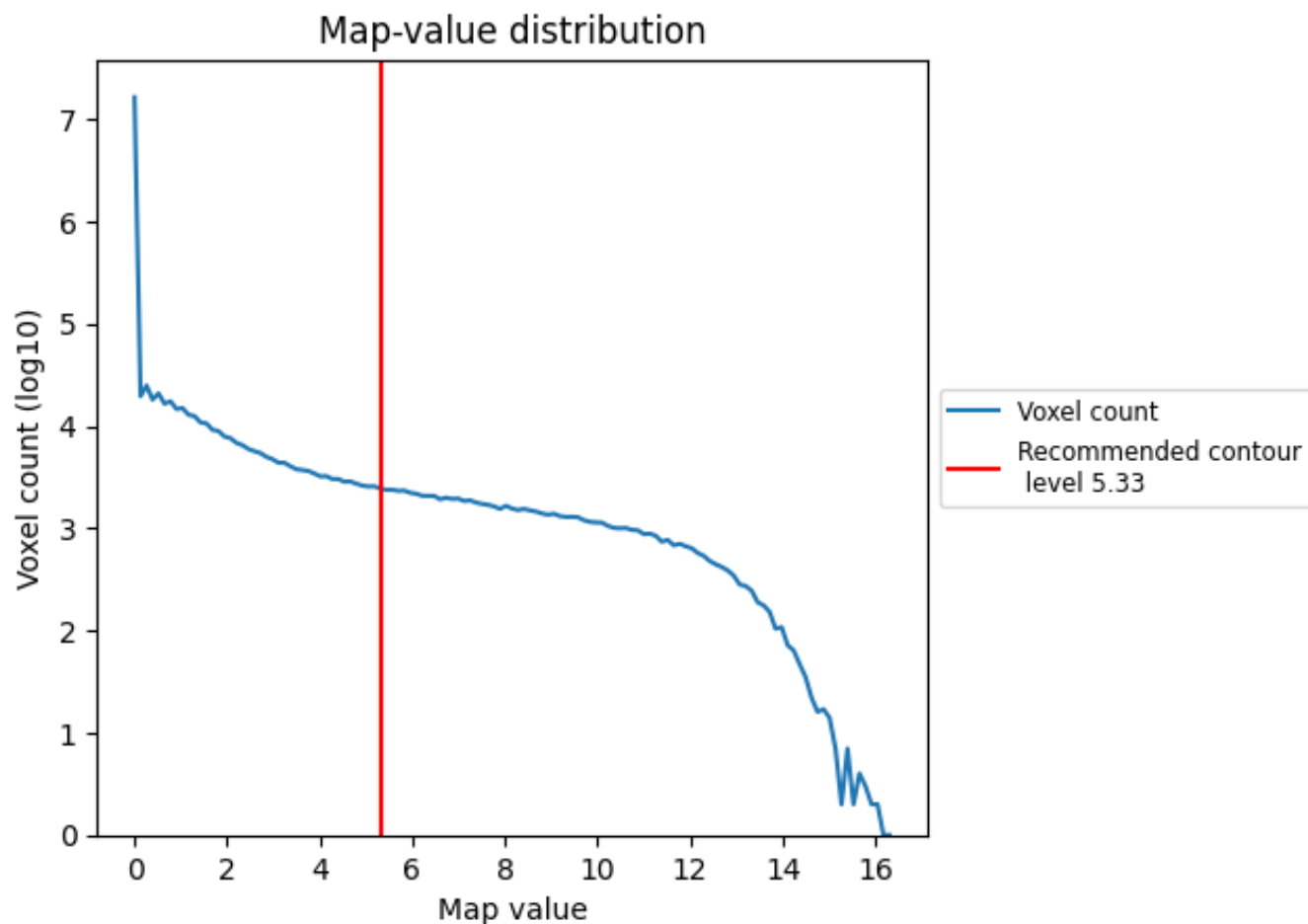
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

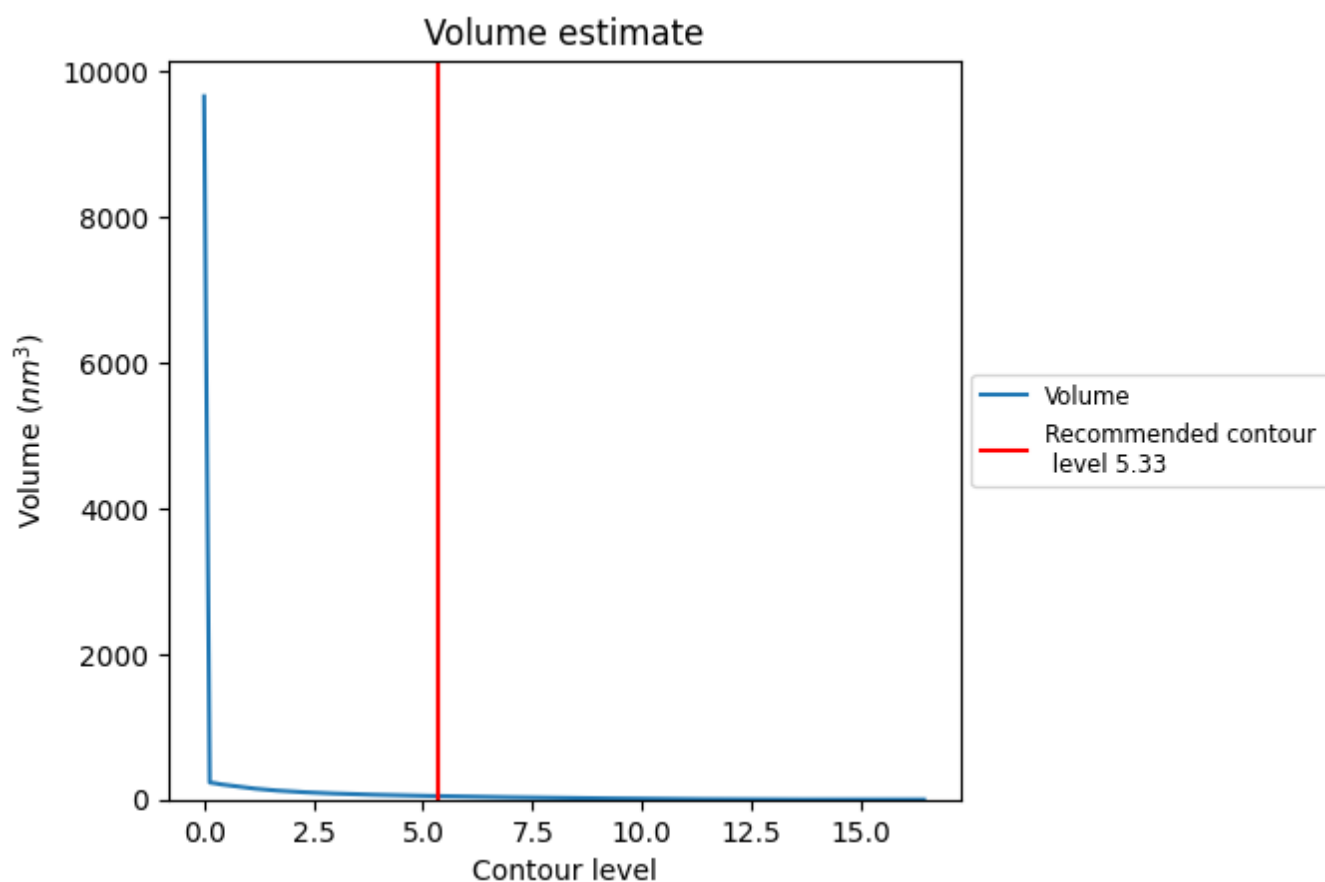
This section contains the results of statistical analysis of the map.

### 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.

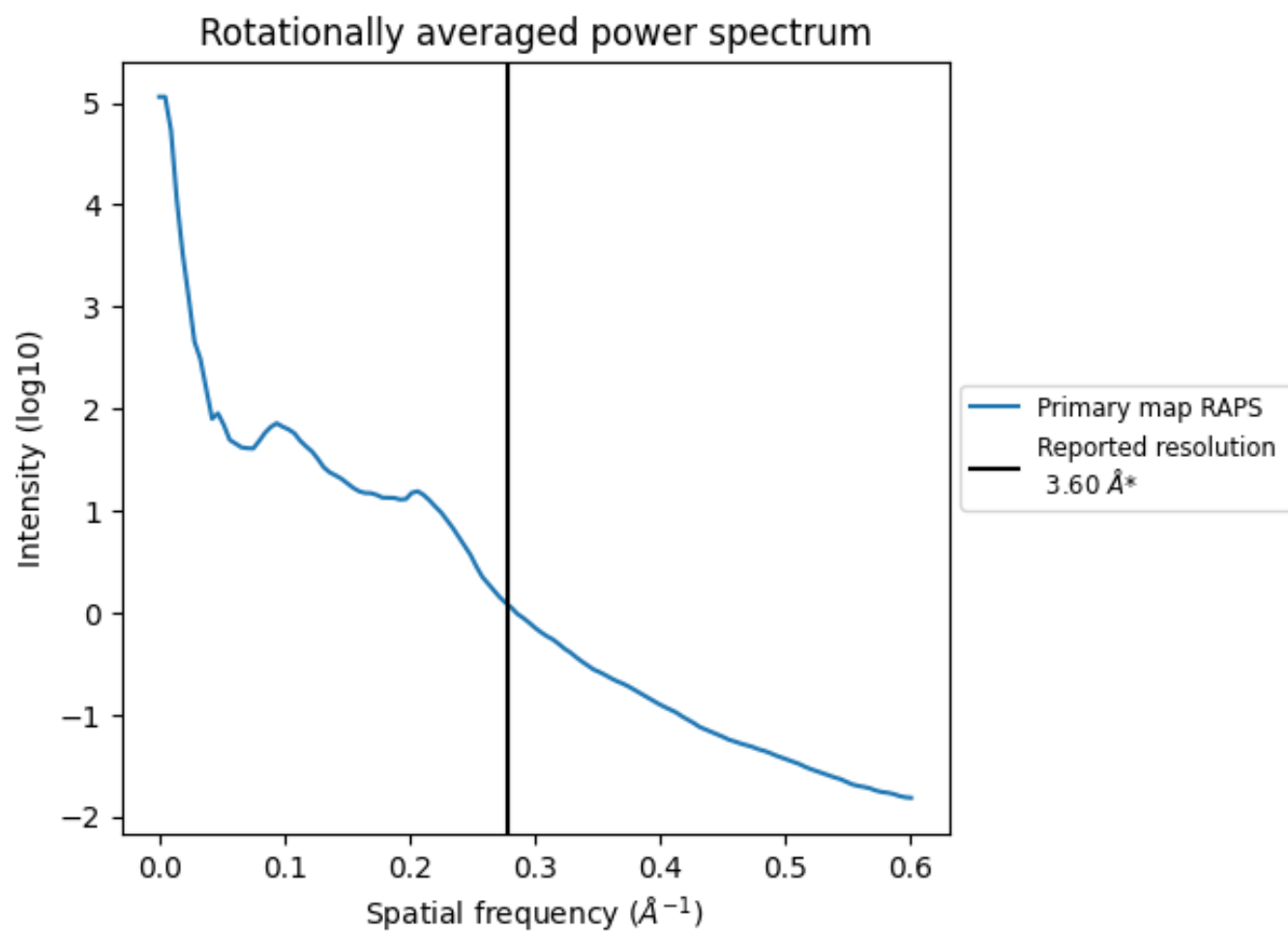
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $48 \text{ nm}^3$ ; this corresponds to an approximate mass of 43 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 0.278 Å<sup>-1</sup>

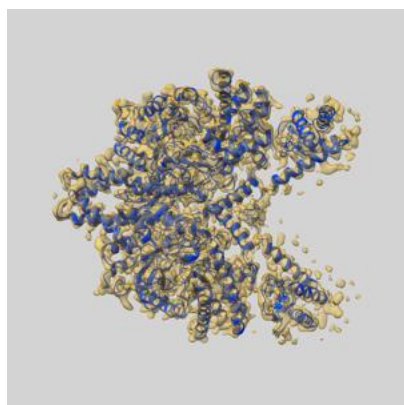
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

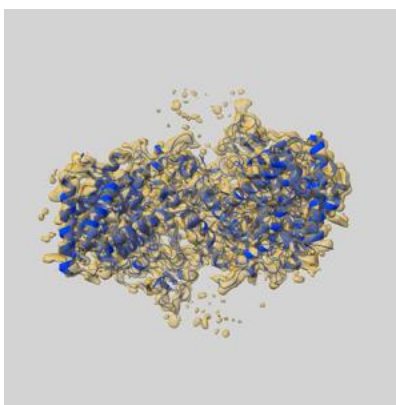
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46747 and PDB model 9DCA. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

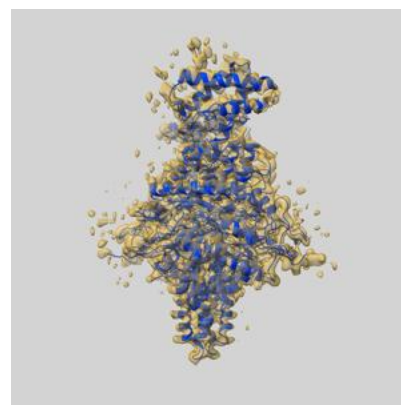
### 9.1 Map-model overlay [i](#)



X



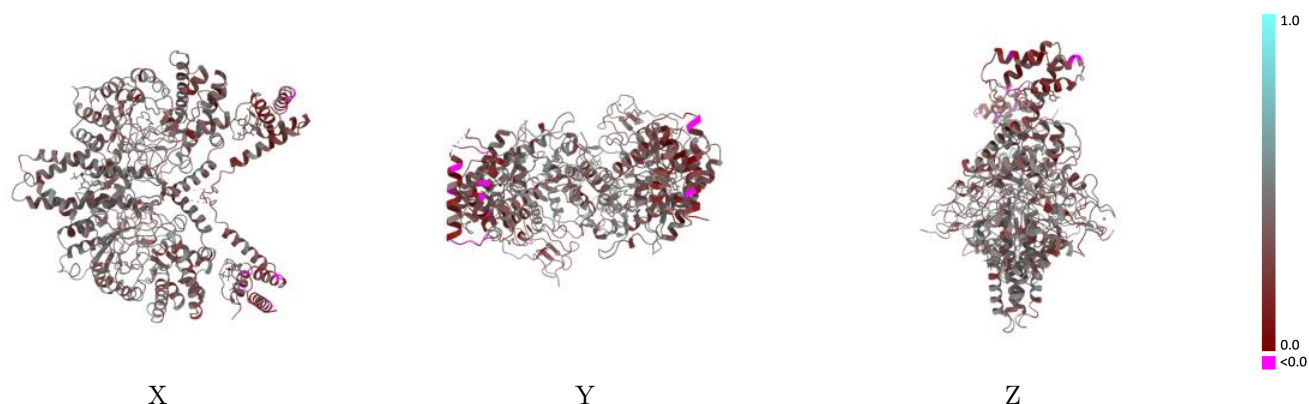
Y



Z

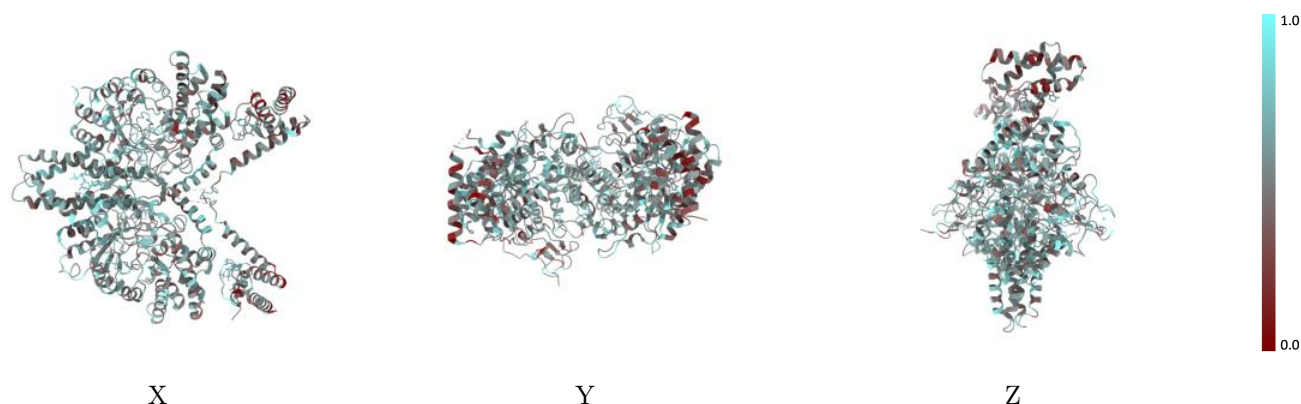
The images above show the 3D surface view of the map at the recommended contour level 5.33 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

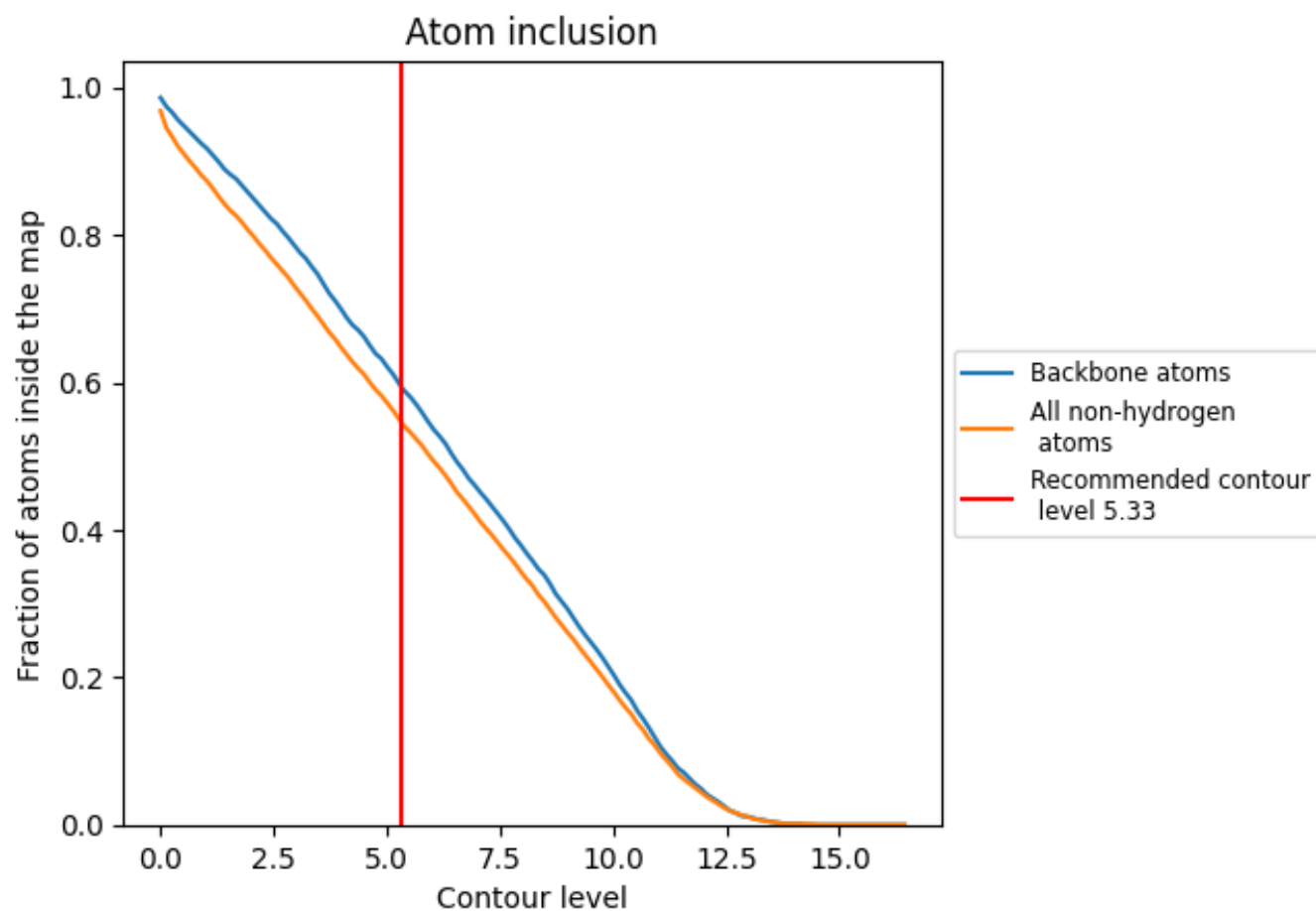
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (5.33).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 55% 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 (5.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5450	<div></div> 0.3760
A	<div></div> 0.5520	<div></div> 0.3740
B	<div></div> 0.5550	<div></div> 0.3780

