



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 12:24 PM EST

PDB ID : 2P8Y
EMDB ID : EMD-1344
Title : Fitted structure of ADPR-eEF2 in the 80S:ADPR-eEF2:GDP:sordarin cryo-EM reconstruction
Authors : Taylor, D.J.; Nilsson, J.; Merrill, A.R.; Andersen, G.R.; Nissen, P.; Frank, J.
Deposited on : 2007-03-23
Resolution : 11.70 Å(reported)
Based on initial model : 1U2R

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

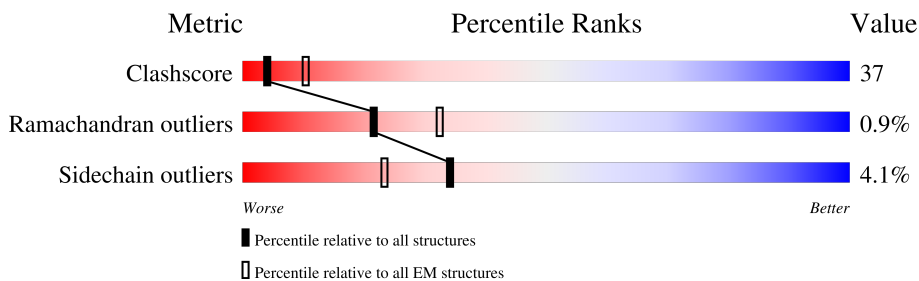
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.70 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	842	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	DDE	T	699	-	-	X	-
2	APR	T	1699	X	-	-	-
3	SO1	T	1700	X	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6440 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.

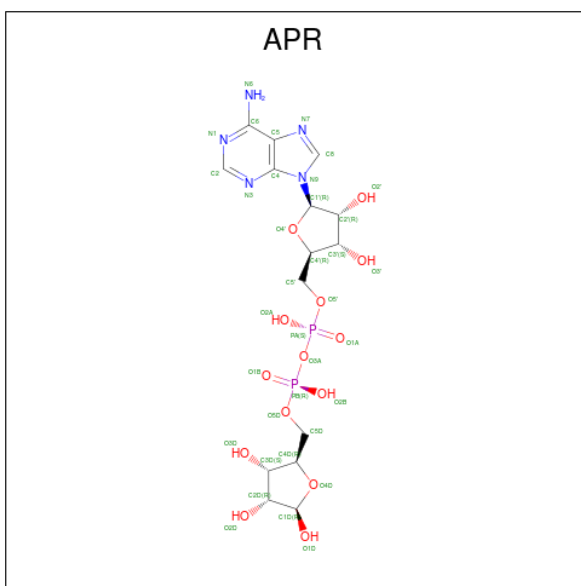
- Molecule 1 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	T	814	6342	4035	1082	1195	30	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	699	DDE	HIS	modified residue	UNP P32324

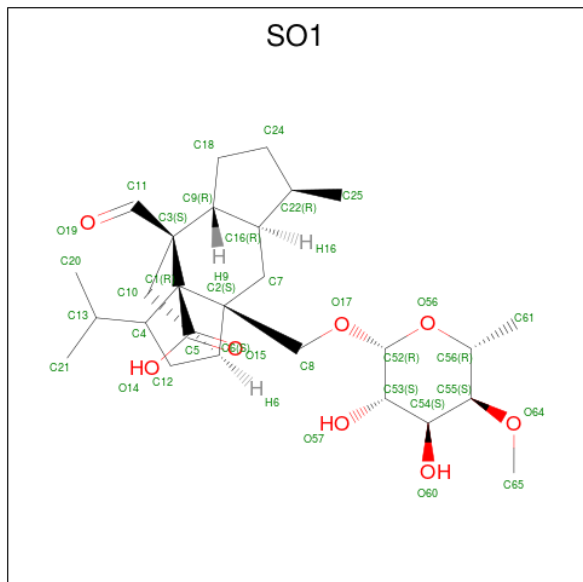
- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	T	1	35	15	5	13	2	0

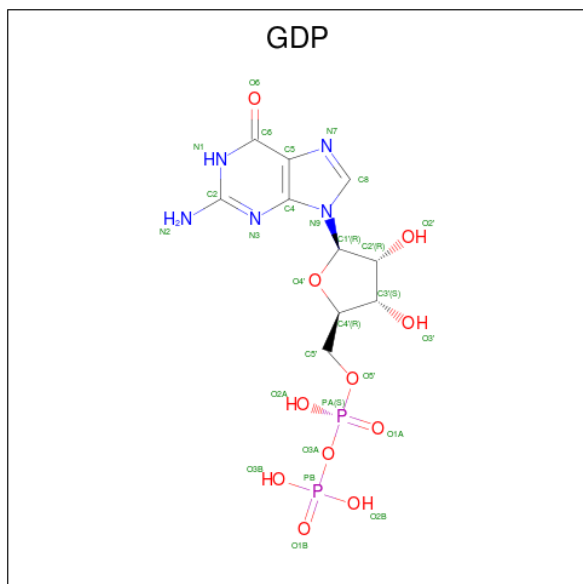
- Molecule 3 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.B.ETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-M

ETHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (three-letter code: SO1) (formula: $C_{27}H_{42}O_8$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	T	1	35	27	8	0

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

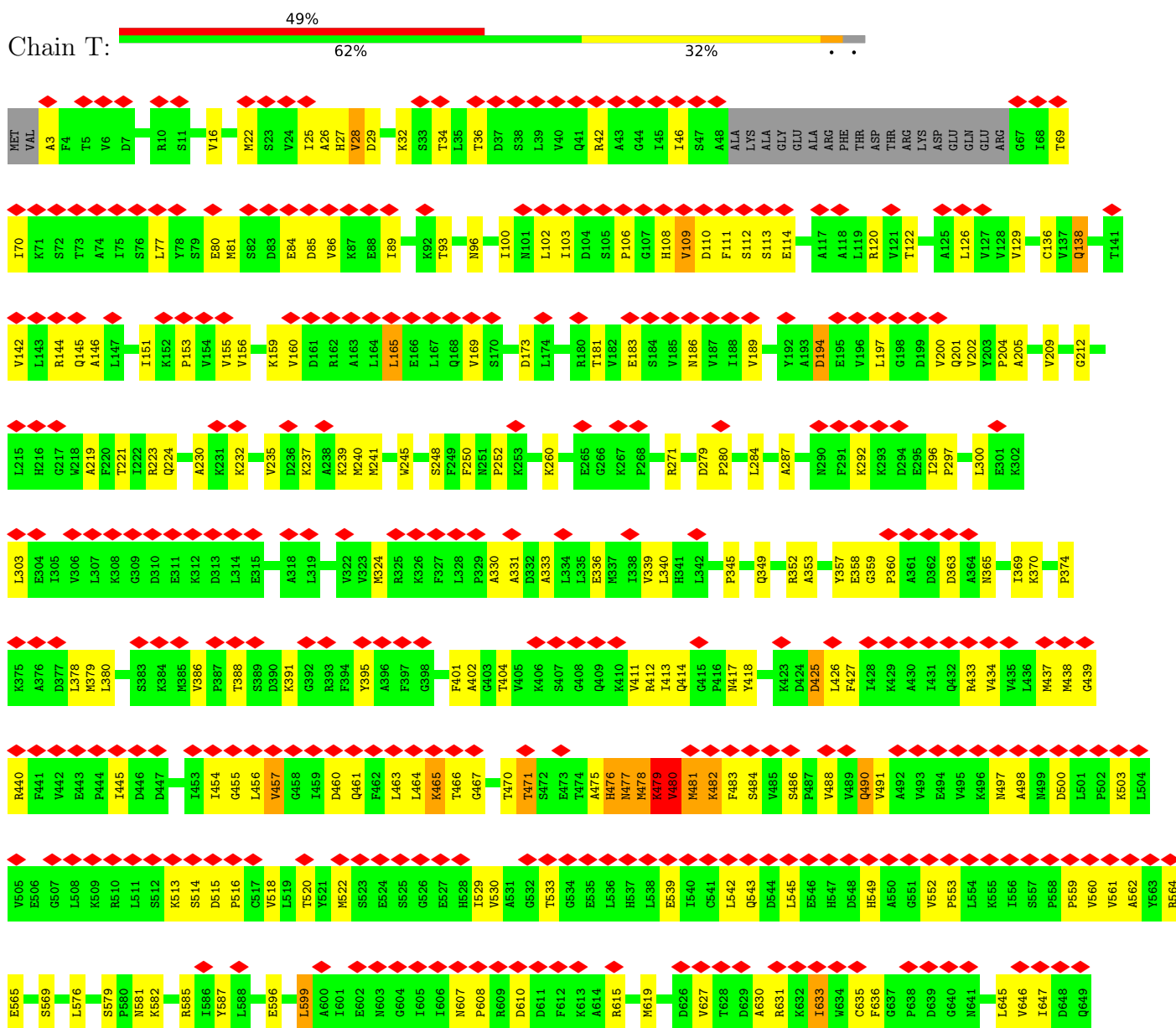


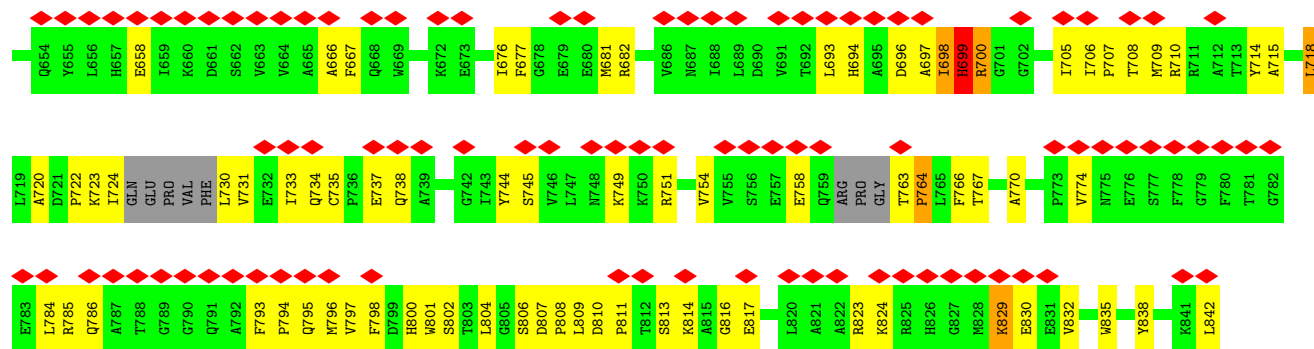
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	T	1	28	10	5	11	2	0

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: Elongation factor 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70510	Depositor
Resolution determination method	Not provided	
CTF correction method	CTF correction of 3D-maps by Wiener filtration	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	37642	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	240.079	Depositor
Minimum map value	-83.236	Depositor
Average map value	7.515	Depositor
Map value standard deviation	24.161	Depositor
Recommended contour level	66.6	Depositor
Map size (\AA)	381.3, 381.3, 381.3	wwPDB
Map dimensions	205, 205, 205	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	1.86, 1.86, 1.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: APR, SO1, DDE, GDP

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	T	1.03	11/6431 (0.2%)	0.80	17/8688 (0.2%)

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	T	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	481	MET	N-CA	35.95	2.18	1.46
1	T	480	VAL	N-CA	32.97	2.12	1.46
1	T	480	VAL	CA-C	30.56	2.32	1.52
1	T	479	LYS	C-N	28.36	1.99	1.34
1	T	479	LYS	N-CA	22.20	1.90	1.46
1	T	479	LYS	CA-C	21.18	2.08	1.52
1	T	481	MET	CA-C	14.97	1.91	1.52
1	T	478	MET	C-N	14.95	1.68	1.34
1	T	482	LYS	N-CA	14.21	1.74	1.46
1	T	478	MET	CA-C	9.71	1.78	1.52
1	T	478	MET	N-CA	6.00	1.58	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	480	VAL	N-CA-C	19.14	162.66	111.00
1	T	481	MET	CB-CA-C	-14.71	80.97	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	479	LYS	CA-C-N	13.31	146.49	117.20
1	T	479	LYS	N-CA-C	12.82	145.61	111.00
1	T	481	MET	N-CA-C	11.71	142.62	111.00
1	T	480	VAL	N-CA-CB	-11.47	86.27	111.50
1	T	479	LYS	C-N-CA	10.03	146.76	121.70
1	T	479	LYS	O-C-N	-9.17	108.02	122.70
1	T	481	MET	N-CA-CB	9.10	126.98	110.60
1	T	480	VAL	CA-C-O	-8.95	101.31	120.10
1	T	478	MET	C-N-CA	8.68	143.40	121.70
1	T	482	LYS	N-CA-CB	7.96	124.93	110.60
1	T	479	LYS	N-CA-CB	-7.66	96.80	110.60
1	T	478	MET	CA-C-N	7.17	132.97	117.20
1	T	482	LYS	CB-CA-C	-7.04	96.32	110.40
1	T	479	LYS	CA-C-O	-6.96	105.48	120.10
1	T	478	MET	O-C-N	-5.75	113.50	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	T	698	ILE	Mainchain
1	T	699	DDE	Peptide,Mainchain

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	T	6342	0	6400	471	0
2	T	35	0	19	7	0
3	T	35	0	40	67	0
4	T	28	0	12	3	0
All	All	6440	0	6471	471	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 37.

All (471) 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:T:798:PHE:CB	3:T:1700:SO1:H6	1.24	1.61
1:T:145:GLN:HA	1:T:481:MET:CB	1.12	1.60
1:T:798:PHE:CD1	3:T:1700:SO1:H102	1.06	1.57
1:T:144:ARG:CD	1:T:482:LYS:N	1.69	1.53
1:T:798:PHE:CG	3:T:1700:SO1:H102	1.44	1.53
1:T:798:PHE:HB2	3:T:1700:SO1:C6	1.35	1.53
1:T:800:HIS:HB2	1:T:801:TRP:CA	1.35	1.52
1:T:111:PHE:CD1	1:T:483:PHE:HZ	1.24	1.51
1:T:798:PHE:CZ	3:T:1700:SO1:H182	1.47	1.50
1:T:111:PHE:CD1	1:T:483:PHE:CZ	2.00	1.49
1:T:481:MET:C	1:T:481:MET:HG3	1.24	1.48
1:T:145:GLN:CG	1:T:481:MET:HB3	1.39	1.47
1:T:478:MET:C	1:T:478:MET:CA	1.78	1.47
1:T:145:GLN:CA	1:T:481:MET:HB2	0.99	1.47
1:T:482:LYS:N	1:T:482:LYS:CA	1.74	1.47
1:T:478:MET:C	1:T:479:LYS:N	1.68	1.44
1:T:800:HIS:CB	1:T:801:TRP:N	1.80	1.44
1:T:111:PHE:CE1	1:T:483:PHE:HZ	1.38	1.42
1:T:800:HIS:HB2	1:T:801:TRP:N	1.11	1.42
1:T:798:PHE:CD2	3:T:1700:SO1:H16	0.87	1.40
1:T:221:THR:HG21	1:T:336:GLU:CD	1.40	1.40
1:T:481:MET:C	1:T:481:MET:CA	1.91	1.37
1:T:144:ARG:HD3	1:T:482:LYS:N	1.13	1.36
1:T:113:SER:OG	1:T:516:PRO:CG	1.74	1.35
1:T:798:PHE:CE2	3:T:1700:SO1:H182	1.61	1.35
1:T:479:LYS:N	1:T:479:LYS:CA	1.90	1.32
1:T:561:VAL:CG2	1:T:774:VAL:CG1	2.07	1.32
1:T:111:PHE:HD1	1:T:483:PHE:CZ	1.40	1.29
1:T:481:MET:C	1:T:481:MET:CG	2.01	1.29
1:T:561:VAL:HG21	1:T:774:VAL:CB	1.62	1.29
1:T:465:LYS:HE3	1:T:513:LYS:O	1.30	1.27
1:T:221:THR:HG21	1:T:336:GLU:OE1	1.35	1.26
1:T:70:ILE:HD11	1:T:439:GLY:O	1.08	1.24
1:T:120:ARG:HH22	1:T:480:VAL:CA	1.48	1.24
1:T:561:VAL:CG2	1:T:774:VAL:HG11	1.68	1.22
1:T:70:ILE:CD1	1:T:439:GLY:O	1.88	1.22
1:T:479:LYS:CA	1:T:479:LYS:C	2.08	1.22
1:T:798:PHE:CE2	3:T:1700:SO1:H16	1.74	1.21
1:T:114:GLU:OE1	1:T:516:PRO:HD3	1.06	1.21
1:T:798:PHE:CE2	3:T:1700:SO1:C18	2.23	1.20
1:T:145:GLN:CG	1:T:481:MET:CB	2.19	1.20
1:T:798:PHE:CE1	3:T:1700:SO1:H102	1.76	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:144:ARG:NH1	1:T:482:LYS:N	1.88	1.18
1:T:113:SER:OG	1:T:516:PRO:HG3	1.30	1.17
1:T:561:VAL:CG2	1:T:774:VAL:CB	2.22	1.17
1:T:797:VAL:HG23	3:T:1700:SO1:O57	1.41	1.16
1:T:561:VAL:CG2	1:T:774:VAL:HB	1.75	1.16
1:T:114:GLU:OE1	1:T:516:PRO:CD	1.93	1.16
1:T:221:THR:HG21	1:T:336:GLU:OE2	1.42	1.15
1:T:479:LYS:C	1:T:480:VAL:N	1.99	1.15
1:T:800:HIS:HB2	1:T:801:TRP:HA	1.27	1.14
1:T:70:ILE:H	1:T:440:ARG:HB3	1.10	1.13
1:T:480:VAL:CA	1:T:480:VAL:N	2.12	1.13
1:T:120:ARG:NH2	1:T:480:VAL:HA	1.65	1.12
1:T:221:THR:CG2	1:T:336:GLU:OE1	1.96	1.12
1:T:480:VAL:N	1:T:480:VAL:CG2	2.12	1.12
1:T:798:PHE:CG	3:T:1700:SO1:C10	2.13	1.12
1:T:798:PHE:CG	3:T:1700:SO1:H16	1.84	1.11
1:T:797:VAL:HG22	3:T:1700:SO1:O57	1.43	1.10
1:T:111:PHE:CE1	1:T:483:PHE:CZ	2.25	1.10
1:T:120:ARG:NH2	1:T:480:VAL:CA	2.13	1.10
1:T:798:PHE:CE2	3:T:1700:SO1:C16	2.32	1.10
1:T:480:VAL:C	1:T:481:MET:N	2.05	1.10
1:T:464:LEU:HD13	1:T:513:LYS:NZ	1.66	1.09
1:T:561:VAL:HG22	1:T:774:VAL:HG11	1.12	1.09
1:T:481:MET:HE3	1:T:482:LYS:N	1.65	1.07
1:T:69:THR:HB	1:T:440:ARG:NH1	1.70	1.07
1:T:481:MET:CA	1:T:481:MET:N	2.18	1.07
1:T:561:VAL:HG22	1:T:774:VAL:CG1	1.78	1.05
1:T:798:PHE:CB	3:T:1700:SO1:C6	2.08	1.04
1:T:798:PHE:CG	3:T:1700:SO1:C6	2.38	1.04
1:T:560:VAL:O	3:T:1700:SO1:C20	2.06	1.04
1:T:113:SER:H	1:T:516:PRO:HG2	1.23	1.03
1:T:109:VAL:HG21	1:T:138:GLN:HG2	1.37	1.02
1:T:219:ALA:HB1	1:T:333:ALA:HB2	1.42	1.02
1:T:145:GLN:CB	1:T:481:MET:CB	2.39	1.01
1:T:481:MET:CB	1:T:481:MET:C	2.29	1.01
1:T:111:PHE:CZ	1:T:482:LYS:N	2.30	1.00
1:T:111:PHE:HZ	1:T:482:LYS:N	1.59	1.00
1:T:126:LEU:HD11	1:T:156:VAL:HG23	1.43	0.99
1:T:800:HIS:CB	1:T:801:TRP:CA	2.27	0.99
1:T:480:VAL:N	1:T:480:VAL:HG22	1.75	0.99
1:T:480:VAL:CA	1:T:480:VAL:C	2.32	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:145:GLN:CB	1:T:481:MET:HB2	1.93	0.98
1:T:145:GLN:HG2	1:T:481:MET:HB3	0.97	0.97
1:T:798:PHE:CZ	3:T:1700:SO1:C18	2.43	0.97
1:T:465:LYS:CE	1:T:513:LYS:O	2.12	0.97
1:T:481:MET:CE	1:T:482:LYS:N	2.28	0.96
1:T:464:LEU:HD13	1:T:513:LYS:HZ3	1.22	0.96
1:T:800:HIS:CB	1:T:801:TRP:HA	1.94	0.96
1:T:113:SER:HG	1:T:516:PRO:HG3	1.31	0.96
1:T:797:VAL:HG23	3:T:1700:SO1:C53	1.96	0.96
1:T:221:THR:CG2	1:T:336:GLU:CD	2.32	0.95
1:T:724:ILE:HD11	1:T:804:LEU:HD12	1.50	0.94
1:T:145:GLN:CA	1:T:481:MET:CB	1.89	0.94
1:T:561:VAL:HG21	1:T:774:VAL:HB	0.94	0.93
1:T:144:ARG:CZ	1:T:482:LYS:N	2.32	0.93
1:T:481:MET:N	1:T:481:MET:HA	1.84	0.93
1:T:145:GLN:HG3	1:T:481:MET:HB3	1.49	0.92
1:T:70:ILE:HD11	1:T:439:GLY:C	1.81	0.92
1:T:144:ARG:HD2	1:T:482:LYS:N	1.84	0.92
1:T:798:PHE:CE2	3:T:1700:SO1:C24	2.53	0.91
1:T:113:SER:OG	1:T:516:PRO:HG2	1.71	0.91
1:T:798:PHE:CG	3:T:1700:SO1:H6	2.02	0.90
1:T:145:GLN:HG2	1:T:481:MET:CB	1.93	0.90
1:T:70:ILE:O	1:T:440:ARG:CG	2.19	0.89
1:T:27:HIS:CD2	1:T:138:GLN:HB2	2.07	0.89
1:T:800:HIS:HB3	1:T:801:TRP:N	1.87	0.89
1:T:70:ILE:O	1:T:440:ARG:HD2	1.73	0.88
1:T:463:LEU:HD21	1:T:467:GLY:HA3	1.55	0.88
1:T:126:LEU:HD11	1:T:156:VAL:CG2	2.03	0.88
1:T:70:ILE:HG23	1:T:440:ARG:O	1.73	0.87
1:T:144:ARG:NE	1:T:482:LYS:N	2.21	0.87
1:T:798:PHE:CD1	3:T:1700:SO1:H101	2.07	0.87
1:T:797:VAL:HG23	3:T:1700:SO1:C54	2.06	0.86
1:T:797:VAL:HA	3:T:1700:SO1:H53	1.58	0.84
1:T:111:PHE:HE1	1:T:483:PHE:CZ	1.94	0.84
1:T:221:THR:CG2	1:T:336:GLU:OE2	2.24	0.84
1:T:70:ILE:N	1:T:440:ARG:HB3	1.93	0.83
1:T:145:GLN:HG3	1:T:481:MET:CB	2.05	0.83
1:T:562:ALA:CB	3:T:1700:SO1:C11	2.56	0.83
1:T:113:SER:N	1:T:516:PRO:HG2	1.93	0.82
1:T:560:VAL:O	3:T:1700:SO1:H203	1.79	0.82
1:T:145:GLN:CB	1:T:481:MET:HB3	2.08	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:145:GLN:HG3	1:T:481:MET:HG2	1.59	0.82
1:T:70:ILE:O	1:T:440:ARG:CD	2.28	0.82
1:T:798:PHE:CE2	3:T:1700:SO1:C22	2.63	0.81
1:T:562:ALA:CB	3:T:1700:SO1:H11	2.10	0.81
1:T:109:VAL:CG2	1:T:138:GLN:HG2	2.11	0.81
1:T:111:PHE:CE2	1:T:481:MET:HG2	2.16	0.81
1:T:111:PHE:HE2	1:T:481:MET:HG2	1.45	0.81
1:T:488:VAL:CG1	1:T:796:MET:HE2	2.11	0.80
1:T:798:PHE:HD2	3:T:1700:SO1:H16	0.97	0.80
1:T:70:ILE:O	1:T:440:ARG:HG2	1.79	0.80
1:T:486:SER:OG	1:T:795:GLN:HG3	1.82	0.79
1:T:120:ARG:HH21	1:T:480:VAL:HA	1.45	0.79
1:T:145:GLN:HA	1:T:481:MET:CA	2.13	0.79
1:T:562:ALA:HB3	3:T:1700:SO1:C11	2.13	0.78
1:T:562:ALA:HB2	3:T:1700:SO1:H11	1.64	0.78
1:T:488:VAL:HG12	1:T:796:MET:HE2	1.65	0.78
1:T:798:PHE:CD2	3:T:1700:SO1:C7	2.67	0.78
1:T:120:ARG:NH2	1:T:480:VAL:N	2.33	0.77
1:T:698:ILE:HG23	1:T:699:DDE:CG	2.13	0.77
1:T:751:ARG:HD2	1:T:814:LYS:HZ2	1.50	0.77
1:T:813:SER:O	1:T:817:GLU:HG3	1.84	0.76
1:T:69:THR:CB	1:T:440:ARG:NH1	2.47	0.76
1:T:114:GLU:CD	1:T:516:PRO:HD3	2.04	0.76
1:T:560:VAL:O	3:T:1700:SO1:H201	1.86	0.76
1:T:145:GLN:HG3	1:T:481:MET:CG	2.16	0.76
1:T:561:VAL:HG21	1:T:774:VAL:CG1	1.97	0.76
1:T:798:PHE:CD2	3:T:1700:SO1:C22	2.69	0.76
1:T:22:MET:SD	1:T:102:LEU:HD12	2.26	0.75
1:T:120:ARG:HH22	1:T:480:VAL:N	1.85	0.75
1:T:576:LEU:HD21	1:T:842:LEU:HG	1.69	0.74
1:T:34:THR:HG23	4:T:843:GDP:O2A	1.86	0.74
1:T:205:ALA:HB2	1:T:245:TRP:CD1	2.22	0.74
1:T:698:ILE:HG23	1:T:699:DDE:CD2	2.18	0.74
1:T:751:ARG:CD	1:T:814:LYS:NZ	2.50	0.73
1:T:219:ALA:HB1	1:T:333:ALA:CB	2.16	0.73
1:T:698:ILE:HG23	1:T:699:DDE:CE1	2.19	0.73
1:T:378:LEU:H	1:T:471:THR:HG22	1.54	0.73
1:T:219:ALA:HB2	1:T:330:ALA:HA	1.70	0.72
1:T:111:PHE:HE2	1:T:481:MET:CG	2.01	0.72
1:T:221:THR:HG22	1:T:336:GLU:OE1	1.89	0.72
1:T:797:VAL:HG23	3:T:1700:SO1:H54	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:464:LEU:O	1:T:465:LYS:HB2	1.90	0.72
1:T:145:GLN:CA	1:T:481:MET:CG	2.67	0.72
1:T:480:VAL:N	1:T:480:VAL:HG23	2.02	0.72
1:T:219:ALA:CB	1:T:333:ALA:HB2	2.19	0.71
1:T:353:ALA:CB	1:T:370:LYS:HG2	2.19	0.71
1:T:561:VAL:HG22	1:T:774:VAL:CB	2.07	0.71
1:T:694:HIS:O	1:T:700:ARG:HD3	1.89	0.71
1:T:70:ILE:CG2	1:T:440:ARG:O	2.39	0.71
1:T:798:PHE:HE2	3:T:1700:SO1:C24	2.01	0.70
1:T:698:ILE:CG2	1:T:699:DDE:CD2	2.70	0.70
1:T:699:DDE:HAA1	2:T:1699:APR:H5'2	1.74	0.70
1:T:488:VAL:HB	1:T:796:MET:HE1	1.73	0.70
1:T:798:PHE:CD2	3:T:1700:SO1:H102	2.22	0.70
1:T:223:ARG:HH11	1:T:223:ARG:HG2	1.57	0.70
1:T:32:LYS:O	1:T:36:THR:HG23	1.92	0.69
1:T:479:LYS:N	1:T:479:LYS:CB	2.56	0.69
1:T:374:PRO:O	1:T:404:THR:HG23	1.92	0.69
1:T:111:PHE:HD1	1:T:483:PHE:CE1	2.07	0.69
1:T:488:VAL:HB	1:T:796:MET:CE	2.23	0.68
1:T:189:VAL:CG1	1:T:200:VAL:HG13	2.22	0.68
1:T:480:VAL:N	1:T:480:VAL:CB	2.56	0.67
1:T:561:VAL:HG23	1:T:774:VAL:CG1	2.19	0.67
1:T:798:PHE:CE1	3:T:1700:SO1:C10	2.57	0.67
1:T:630:ALA:O	1:T:633:ILE:HG23	1.94	0.67
1:T:103:ILE:HD12	1:T:122:THR:HG22	1.77	0.67
1:T:559:PRO:HB2	3:T:1700:SO1:C20	2.24	0.67
1:T:478:MET:C	1:T:478:MET:HA	2.08	0.67
1:T:699:DDE:HAA1	2:T:1699:APR:C5'	2.26	0.66
1:T:751:ARG:HD2	1:T:814:LYS:NZ	2.10	0.66
1:T:731:VAL:HG12	1:T:770:ALA:O	1.95	0.66
1:T:737:GLU:HB2	1:T:766:PHE:CE2	2.30	0.66
1:T:490:GLN:H	1:T:559:PRO:HD3	1.62	0.65
1:T:763:THR:N	1:T:764:PRO:HD3	2.12	0.65
1:T:798:PHE:CB	3:T:1700:SO1:C2	2.75	0.65
1:T:798:PHE:HZ	1:T:801:TRP:CH2	2.14	0.64
1:T:829:LYS:CE	1:T:830:GLU:H	2.11	0.64
1:T:800:HIS:CG	1:T:801:TRP:N	2.62	0.64
1:T:829:LYS:HE3	1:T:829:LYS:HA	1.78	0.64
1:T:284:LEU:HD13	1:T:324:MET:HE1	1.80	0.63
1:T:800:HIS:HD2	1:T:802:SER:N	1.95	0.63
1:T:237:LYS:O	1:T:241:MET:HG2	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:113:SER:OG	1:T:516:PRO:CB	2.45	0.63
1:T:627:VAL:O	1:T:631:ARG:HG3	1.98	0.63
1:T:798:PHE:CE2	3:T:1700:SO1:C9	2.81	0.63
1:T:633:ILE:HD12	1:T:635:CYS:N	2.14	0.63
1:T:734:GLN:HG3	1:T:767:THR:HG22	1.80	0.63
1:T:86:VAL:HG13	1:T:93:THR:HG21	1.81	0.63
1:T:698:ILE:HG23	1:T:699:DDE:ND1	2.14	0.62
1:T:433:ARG:HB3	1:T:457:VAL:CG1	2.30	0.62
1:T:718:LEU:HB3	1:T:835:TRP:HB3	1.82	0.62
1:T:204:PRO:HB2	1:T:245:TRP:CZ2	2.35	0.61
1:T:797:VAL:HA	3:T:1700:SO1:C53	2.30	0.61
1:T:520:THR:HG22	1:T:530:VAL:HG22	1.81	0.61
1:T:559:PRO:HB2	3:T:1700:SO1:H201	1.82	0.61
1:T:284:LEU:CD1	1:T:324:MET:HE1	2.31	0.61
1:T:576:LEU:HD11	1:T:585:ARG:HD3	1.82	0.61
1:T:561:VAL:HG23	1:T:774:VAL:HG11	1.77	0.61
1:T:694:HIS:CD2	1:T:696:ASP:H	2.19	0.61
1:T:698:ILE:CG2	1:T:699:DDE:NE2	2.64	0.61
1:T:798:PHE:HB3	3:T:1700:SO1:H72	1.83	0.61
1:T:324:MET:HE2	1:T:324:MET:HA	1.82	0.60
1:T:800:HIS:CD2	1:T:802:SER:N	2.69	0.60
1:T:800:HIS:CG	1:T:801:TRP:CA	2.84	0.60
1:T:284:LEU:HD13	1:T:324:MET:CE	2.32	0.60
1:T:564:ARG:HG3	1:T:682:ARG:HB2	1.83	0.60
1:T:126:LEU:CD1	1:T:156:VAL:HG23	2.25	0.59
1:T:379:MET:HB2	1:T:402:ALA:HB3	1.83	0.59
1:T:202:VAL:HG12	1:T:209:VAL:CG2	2.33	0.59
1:T:111:PHE:CD1	1:T:483:PHE:CE1	2.82	0.59
1:T:561:VAL:CG2	1:T:774:VAL:HG12	2.23	0.59
1:T:365:ASN:O	1:T:369:ILE:HG12	2.03	0.58
1:T:479:LYS:C	1:T:480:VAL:HG22	2.24	0.58
1:T:497:ASN:HB3	1:T:500:ASP:OD2	2.04	0.58
1:T:751:ARG:HD3	1:T:814:LYS:NZ	2.20	0.57
1:T:464:LEU:HD13	1:T:513:LYS:CE	2.33	0.57
1:T:464:LEU:CD1	1:T:513:LYS:HZ3	2.08	0.57
1:T:545:LEU:HA	1:T:549:HIS:HB2	1.85	0.57
1:T:797:VAL:CG2	3:T:1700:SO1:C53	2.65	0.57
1:T:386:VAL:HG11	1:T:437:MET:CE	2.34	0.57
1:T:581:ASN:O	1:T:582:LYS:HB2	2.05	0.57
1:T:296:ILE:O	1:T:300:LEU:HD13	2.05	0.57
1:T:3:ALA:HA	1:T:46:ILE:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:797:VAL:HG22	3:T:1700:SO1:H57	1.66	0.56
1:T:500:ASP:HB3	1:T:552:VAL:HG11	1.87	0.56
1:T:500:ASP:CB	1:T:552:VAL:HG11	2.35	0.56
1:T:106:PRO:HB3	1:T:108:HIS:NE2	2.21	0.56
1:T:751:ARG:CD	1:T:814:LYS:HZ3	2.17	0.56
1:T:798:PHE:HE2	3:T:1700:SO1:H242	1.71	0.56
1:T:89:ILE:HG12	1:T:340:LEU:HD23	1.88	0.56
1:T:615:ARG:HG2	1:T:619:MET:HE3	1.87	0.55
1:T:108:HIS:CE1	1:T:114:GLU:HB2	2.41	0.55
1:T:490:GLN:HG3	1:T:559:PRO:HG3	1.88	0.55
1:T:26:ALA:HB3	1:T:32:LYS:HB2	1.88	0.55
1:T:129:VAL:HG11	1:T:181:THR:CG2	2.36	0.55
1:T:829:LYS:HE3	1:T:830:GLU:H	1.71	0.55
1:T:698:ILE:HG23	1:T:699:DDE:NE2	2.21	0.55
1:T:800:HIS:C	1:T:801:TRP:HA	2.27	0.55
1:T:223:ARG:HA	1:T:241:MET:HE2	1.88	0.55
1:T:615:ARG:HG2	1:T:619:MET:CE	2.36	0.55
1:T:194:ASP:HB2	1:T:197:LEU:HD13	1.89	0.55
1:T:413:ILE:HB	1:T:427:PHE:HB2	1.88	0.54
1:T:490:GLN:HB2	1:T:559:PRO:HB3	1.89	0.54
1:T:700:ARG:O	1:T:705:ILE:HD12	2.08	0.54
1:T:296:ILE:HB	1:T:297:PRO:HD3	1.89	0.54
1:T:369:ILE:HD12	1:T:401:PHE:HB3	1.90	0.54
1:T:279:ASP:HB3	1:T:280:PRO:HD3	1.89	0.54
1:T:108:HIS:HE1	1:T:114:GLU:HB2	1.72	0.54
1:T:378:LEU:H	1:T:471:THR:CG2	2.21	0.54
1:T:520:THR:HA	1:T:529:ILE:O	2.08	0.53
1:T:560:VAL:O	3:T:1700:SO1:C13	2.55	0.53
1:T:798:PHE:CD2	3:T:1700:SO1:C9	2.85	0.53
1:T:360:PRO:O	1:T:363:ASP:HB3	2.08	0.53
1:T:798:PHE:CG	3:T:1700:SO1:C16	2.66	0.53
1:T:829:LYS:HE2	1:T:830:GLU:H	1.74	0.53
1:T:111:PHE:CE1	1:T:483:PHE:CE2	2.95	0.53
1:T:500:ASP:CG	1:T:552:VAL:HG11	2.29	0.53
1:T:806:SER:HB2	1:T:813:SER:HB2	1.90	0.53
1:T:109:VAL:HG11	1:T:142:VAL:CG2	2.38	0.52
1:T:515:ASP:HB3	1:T:518:VAL:CG1	2.39	0.52
1:T:798:PHE:H	3:T:1700:SO1:H53	1.74	0.52
1:T:28:VAL:HG22	1:T:138:GLN:OE1	2.08	0.52
1:T:646:VAL:C	1:T:647:ILE:HD12	2.29	0.52
1:T:129:VAL:HG11	1:T:181:THR:HG23	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:464:LEU:CD1	1:T:513:LYS:NZ	2.57	0.52
1:T:561:VAL:HA	3:T:1700:SO1:H203	1.91	0.52
1:T:693:LEU:HB3	1:T:700:ARG:HD2	1.92	0.52
1:T:745:SER:O	1:T:749:LYS:HG3	2.10	0.52
1:T:471:THR:HG23	1:T:471:THR:O	2.09	0.51
1:T:250:PHE:O	1:T:252:PRO:HD3	2.10	0.51
1:T:113:SER:CB	1:T:516:PRO:HG2	2.39	0.51
1:T:426:LEU:HD12	1:T:427:PHE:H	1.76	0.51
1:T:785:ARG:HG3	1:T:785:ARG:HH11	1.75	0.51
1:T:694:HIS:CD2	1:T:699:DDE:HD2	2.46	0.51
1:T:569:SER:O	1:T:720:ALA:HB1	2.10	0.51
1:T:559:PRO:C	3:T:1700:SO1:H201	2.31	0.51
1:T:479:LYS:N	1:T:479:LYS:HB2	2.26	0.51
1:T:751:ARG:HD3	1:T:814:LYS:HZ3	1.76	0.51
1:T:800:HIS:CG	1:T:801:TRP:HA	2.46	0.51
1:T:189:VAL:HG13	1:T:200:VAL:HG13	1.92	0.51
1:T:223:ARG:HG2	1:T:223:ARG:NH1	2.21	0.51
1:T:470:THR:HG21	1:T:475:ALA:HB1	1.93	0.51
1:T:718:LEU:HD12	1:T:722:PRO:HG2	1.92	0.51
1:T:576:LEU:HD21	1:T:585:ARG:HH11	1.76	0.50
1:T:360:PRO:HB2	1:T:363:ASP:HB2	1.94	0.50
1:T:414:GLN:HB2	1:T:477:ASN:HD21	1.77	0.50
1:T:562:ALA:HB3	3:T:1700:SO1:H181	1.93	0.50
1:T:706:ILE:HB	1:T:707:PRO:HD3	1.94	0.50
1:T:386:VAL:HG11	1:T:437:MET:HE1	1.94	0.50
1:T:576:LEU:HD21	1:T:585:ARG:NH1	2.27	0.50
1:T:798:PHE:H	3:T:1700:SO1:C53	2.25	0.50
1:T:576:LEU:HD13	1:T:587:TYR:CE1	2.46	0.50
1:T:607:ASN:HB2	1:T:610:ASP:OD2	2.11	0.50
1:T:539:GLU:O	1:T:543:GLN:HG3	2.12	0.49
1:T:345:PRO:O	1:T:349:GLN:HG3	2.11	0.49
1:T:411:VAL:HG12	1:T:412:ARG:N	2.27	0.49
1:T:488:VAL:CB	1:T:796:MET:HE2	2.43	0.49
1:T:699:DDE:HAA3	1:T:699:DDE:HAD2	1.77	0.49
1:T:552:VAL:HG13	1:T:553:PRO:HD2	1.95	0.49
1:T:111:PHE:CE2	1:T:481:MET:CG	2.86	0.49
1:T:202:VAL:CG1	1:T:209:VAL:CG2	2.91	0.49
1:T:464:LEU:HD13	1:T:513:LYS:HZ1	1.67	0.48
1:T:503:LYS:HD2	1:T:552:VAL:HG21	1.94	0.48
1:T:153:PRO:HD2	1:T:200:VAL:HG22	1.95	0.48
1:T:109:VAL:CG1	1:T:142:VAL:CG2	2.92	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:200:VAL:HG22	1:T:200:VAL:O	2.13	0.48
1:T:433:ARG:HB3	1:T:457:VAL:HG11	1.95	0.48
1:T:798:PHE:HB3	3:T:1700:SO1:C7	2.43	0.48
1:T:69:THR:CB	1:T:440:ARG:HH12	2.25	0.48
1:T:271:ARG:HG3	1:T:271:ARG:HH11	1.79	0.48
1:T:646:VAL:HG23	1:T:667:PHE:CD2	2.49	0.48
1:T:797:VAL:CA	3:T:1700:SO1:H53	2.39	0.48
1:T:186:ASN:HB3	1:T:201:GLN:OE1	2.14	0.48
1:T:360:PRO:HD2	1:T:363:ASP:HB2	1.96	0.48
1:T:699:DDE:HAC1	2:T:1699:APR:H5'1	1.96	0.48
1:T:699:DDE:HAB1	2:T:1699:APR:O3A	2.14	0.47
1:T:110:ASP:OD2	1:T:112:SER:HB3	2.14	0.47
1:T:461:GLN:CD	1:T:461:GLN:H	2.16	0.47
1:T:823:ARG:HE	1:T:832:VAL:HG22	1.79	0.47
1:T:237:LYS:HA	1:T:240:MET:HB2	1.95	0.47
1:T:114:GLU:CD	1:T:514:SER:O	2.53	0.47
1:T:807:ASP:OD1	1:T:809:LEU:N	2.44	0.47
1:T:784:LEU:HD23	1:T:794:PRO:HD3	1.97	0.47
1:T:80:GLU:HA	1:T:96:ASN:O	2.15	0.47
1:T:698:ILE:CG2	1:T:699:DDE:CE1	2.92	0.47
1:T:70:ILE:O	1:T:440:ARG:CB	2.64	0.46
1:T:106:PRO:HB3	1:T:108:HIS:CD2	2.50	0.46
1:T:823:ARG:NH1	1:T:829:LYS:O	2.47	0.46
1:T:84:GLU:HG3	1:T:85:ASP:N	2.30	0.46
1:T:515:ASP:O	1:T:518:VAL:HG12	2.15	0.46
1:T:565:GLU:O	1:T:681:MET:HA	2.14	0.46
1:T:454:ILE:HG13	1:T:455:GLY:N	2.30	0.46
1:T:480:VAL:HA	1:T:480:VAL:C	2.33	0.46
1:T:559:PRO:HB2	3:T:1700:SO1:C21	2.45	0.46
1:T:809:LEU:O	1:T:811:PRO:HD3	2.16	0.46
1:T:411:VAL:HG12	1:T:412:ARG:H	1.80	0.46
1:T:800:HIS:CD2	1:T:801:TRP:C	2.89	0.46
1:T:111:PHE:CE1	1:T:482:LYS:C	2.89	0.46
1:T:114:GLU:OE1	1:T:516:PRO:CG	2.62	0.46
1:T:126:LEU:HD11	1:T:156:VAL:HG21	1.93	0.46
1:T:113:SER:CB	1:T:516:PRO:CG	2.87	0.46
1:T:785:ARG:HG3	1:T:786:GLN:N	2.30	0.46
1:T:113:SER:CA	1:T:516:PRO:HG2	2.46	0.45
1:T:798:PHE:CG	3:T:1700:SO1:C7	2.99	0.45
1:T:42:ARG:HG2	1:T:331:ALA:CB	2.47	0.45
1:T:378:LEU:N	1:T:471:THR:HG22	2.28	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:434:VAL:HG12	1:T:445:ILE:HG22	1.98	0.45
1:T:483:PHE:N	1:T:793:PHE:HE1	2.15	0.45
1:T:202:VAL:CG1	1:T:209:VAL:HG22	2.47	0.45
1:T:221:THR:OG1	1:T:224:GLN:HG3	2.15	0.45
1:T:733:ILE:O	1:T:767:THR:HA	2.17	0.45
1:T:202:VAL:HG12	1:T:209:VAL:HG23	1.98	0.45
1:T:800:HIS:C	1:T:801:TRP:CE3	2.90	0.45
1:T:81:MET:HG3	1:T:339:VAL:HG11	1.99	0.45
1:T:699:DDE:HAB2	1:T:699:DDE:HAU3	1.71	0.45
1:T:109:VAL:HG12	1:T:142:VAL:HG22	1.99	0.45
1:T:699:DDE:CAB	2:T:1699:APR:H5R1	2.47	0.45
1:T:479:LYS:C	1:T:479:LYS:HA	2.25	0.44
1:T:560:VAL:O	3:T:1700:SO1:H13	2.16	0.44
1:T:25:ILE:HG23	1:T:142:VAL:HB	2.00	0.44
1:T:515:ASP:HB3	1:T:518:VAL:HG12	2.00	0.44
1:T:29:ASP:HA	4:T:843:GDP:H5'	2.00	0.44
1:T:561:VAL:HG22	1:T:774:VAL:CG2	2.47	0.44
1:T:718:LEU:HA	1:T:722:PRO:HG3	2.00	0.44
1:T:159:LYS:HG3	4:T:843:GDP:C2	2.53	0.44
1:T:479:LYS:C	1:T:479:LYS:CB	2.81	0.44
1:T:607:ASN:HA	1:T:608:PRO:HD3	1.83	0.44
1:T:715:ALA:HB2	1:T:838:TYR:HB2	2.00	0.44
1:T:763:THR:N	1:T:764:PRO:CD	2.79	0.44
1:T:490:GLN:OE1	3:T:1700:SO1:H213	2.18	0.44
1:T:564:ARG:HG3	1:T:682:ARG:CB	2.47	0.44
1:T:16:VAL:HB	1:T:345:PRO:HD2	2.00	0.44
1:T:560:VAL:C	3:T:1700:SO1:C20	2.82	0.44
1:T:633:ILE:O	1:T:633:ILE:HG13	2.18	0.44
1:T:28:VAL:O	1:T:29:ASP:HB2	2.17	0.43
1:T:737:GLU:HB2	1:T:766:PHE:HE2	1.79	0.43
1:T:699:DDE:HAB1	2:T:1699:APR:H5'2	1.99	0.43
1:T:69:THR:CG2	1:T:440:ARG:NH1	2.81	0.43
1:T:380:LEU:HD13	1:T:456:LEU:HD11	2.00	0.43
1:T:77:LEU:HB2	1:T:100:ILE:HB	2.00	0.43
1:T:235:VAL:HG12	1:T:239:LYS:HB3	2.01	0.43
1:T:414:GLN:CB	1:T:477:ASN:HD21	2.31	0.43
1:T:491:VAL:HG21	1:T:542:LEU:HD11	2.01	0.43
1:T:108:HIS:CE1	1:T:112:SER:HG	2.36	0.43
1:T:114:GLU:OE1	1:T:515:ASP:HA	2.19	0.43
1:T:153:PRO:HD2	1:T:200:VAL:CG2	2.49	0.43
1:T:798:PHE:CB	3:T:1700:SO1:C7	2.97	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:800:HIS:CD2	1:T:801:TRP:CA	3.02	0.43
1:T:357:TYR:OH	1:T:476:HIS:HB2	2.19	0.43
1:T:798:PHE:CD1	3:T:1700:SO1:C6	2.78	0.43
1:T:465:LYS:HB3	1:T:466:THR:H	1.67	0.42
1:T:478:MET:CA	1:T:478:MET:O	2.54	0.42
1:T:697:ALA:C	1:T:699:DDE:N	2.63	0.42
1:T:763:THR:HG22	1:T:763:THR:O	2.19	0.42
1:T:69:THR:CG2	1:T:440:ARG:NH2	2.82	0.42
1:T:114:GLU:OE1	1:T:514:SER:O	2.37	0.42
1:T:197:LEU:HD12	1:T:197:LEU:N	2.34	0.42
1:T:386:VAL:HG11	1:T:437:MET:HE3	2.00	0.42
1:T:810:ASP:O	1:T:816:GLY:HA3	2.19	0.42
1:T:426:LEU:HD12	1:T:427:PHE:N	2.34	0.42
1:T:378:LEU:HD11	1:T:380:LEU:HB2	2.02	0.42
1:T:798:PHE:HD2	3:T:1700:SO1:C16	1.73	0.42
1:T:69:THR:HG21	1:T:440:ARG:HH22	1.84	0.42
1:T:205:ALA:HB2	1:T:245:TRP:NE1	2.35	0.42
1:T:560:VAL:C	3:T:1700:SO1:H203	2.37	0.42
1:T:552:VAL:CG1	1:T:553:PRO:HD2	2.50	0.42
1:T:388:THR:HG21	1:T:395:TYR:CD1	2.55	0.42
1:T:230:ALA:C	1:T:232:LYS:H	2.23	0.41
1:T:284:LEU:HD11	1:T:303:LEU:CD1	2.50	0.41
1:T:353:ALA:HB3	1:T:370:LYS:HG2	1.99	0.41
1:T:417:ASN:HB2	1:T:425:ASP:OD2	2.20	0.41
1:T:763:THR:O	1:T:764:PRO:O	2.38	0.41
1:T:744:TYR:CE1	1:T:754:VAL:HG21	2.55	0.41
1:T:710:ARG:NH1	1:T:714:TYR:OH	2.54	0.41
1:T:369:ILE:HD13	1:T:402:ALA:HB2	2.01	0.41
1:T:454:ILE:HG13	1:T:455:GLY:H	1.84	0.41
1:T:636:PHE:CE1	1:T:645:LEU:HD21	2.55	0.41
1:T:658:GLU:OE1	1:T:700:ARG:NH2	2.54	0.41
1:T:666:ALA:CB	1:T:709:MET:HB3	2.51	0.41
1:T:698:ILE:HG21	2:T:1699:APR:O4D	2.21	0.41
1:T:731:VAL:O	1:T:731:VAL:HG13	2.21	0.41
1:T:106:PRO:CB	1:T:108:HIS:NE2	2.84	0.41
1:T:287:ALA:HA	1:T:292:LYS:HD2	2.02	0.41
1:T:490:GLN:N	1:T:559:PRO:HD3	2.32	0.41
1:T:576:LEU:CD2	1:T:842:LEU:HG	2.45	0.41
1:T:110:ASP:O	1:T:111:PHE:HB2	2.21	0.41
1:T:169:VAL:HG12	1:T:173:ASP:HB2	2.03	0.41
1:T:418:TYR:CD1	1:T:418:TYR:C	2.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:599:LEU:HD12	1:T:599:LEU:HA	1.88	0.41
1:T:800:HIS:CA	1:T:801:TRP:HA	2.49	0.41
1:T:69:THR:HB	1:T:440:ARG:CZ	2.45	0.40
1:T:824:LYS:HD3	1:T:830:GLU:OE1	2.22	0.40
1:T:260:LYS:HE2	1:T:260:LYS:HB3	1.80	0.40
1:T:358:GLU:OE2	1:T:479:LYS:HG3	2.21	0.40
1:T:484:SER:HB3	1:T:533:THR:HG23	2.03	0.40
1:T:579:SER:HB3	1:T:708:THR:OG1	2.20	0.40
1:T:565:GLU:CD	1:T:676:ILE:HB	2.41	0.40
1:T:751:ARG:HD3	1:T:814:LYS:CE	2.50	0.40
1:T:27:HIS:CD2	1:T:136:CYS:HB2	2.57	0.40
1:T:155:VAL:CG1	1:T:156:VAL:N	2.84	0.40
1:T:722:PRO:O	1:T:723:LYS:HD2	2.20	0.40
1:T:807:ASP:HA	1:T:808:PRO:HD3	1.96	0.40
1:T:146:ALA:HA	1:T:151:ILE:HD12	2.04	0.40
1:T:160:VAL:HG23	1:T:212:GLY:O	2.22	0.40
1:T:165:LEU:HD12	1:T:165:LEU:HA	1.90	0.40
1:T:633:ILE:HD12	1:T:633:ILE:C	2.42	0.40
1:T:718:LEU:HA	1:T:722:PRO:CG	2.51	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	T	791/842 (94%)	746 (94%)	38 (5%)	7 (1%)	17 57

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	700	ARG
1	T	764	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	391	LYS
1	T	465	LYS
1	T	425	ASP
1	T	498	ALA
1	T	359	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	T	691/714 (97%)	663 (96%)	28 (4%)	30 55

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	28	VAL
1	T	109	VAL
1	T	138	GLN
1	T	165	LEU
1	T	183	GLU
1	T	194	ASP
1	T	248	SER
1	T	352	ARG
1	T	438	MET
1	T	457	VAL
1	T	460	ASP
1	T	471	THR
1	T	476	HIS
1	T	477	ASN
1	T	479	LYS
1	T	480	VAL
1	T	490	GLN
1	T	522	MET
1	T	596	GLU
1	T	599	LEU
1	T	633	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	677	PHE
1	T	718	LEU
1	T	730	LEU
1	T	735	CYS
1	T	738	GLN
1	T	758	GLU
1	T	829	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	21	ASN
1	T	27	HIS
1	T	101	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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	DDE	T	699	2,1	14,20,21	2.05	4 (28%)	14,28,30	2.39	4 (28%)

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
1	DDE	T	699	2,1	-	2/20/21/23	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	699	DDE	OAG-CBI	4.99	1.33	1.23
1	T	699	DDE	CAT-CE1	3.62	1.55	1.50
1	T	699	DDE	CAC-NCB	2.92	1.60	1.50
1	T	699	DDE	CBW-CBI	2.01	1.56	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	699	DDE	OAG-CBI-CBW	-6.19	112.65	120.49
1	T	699	DDE	OAG-CBI-NAD	4.73	131.22	123.00
1	T	699	DDE	CG-ND1-CE1	2.18	109.50	103.05
1	T	699	DDE	CAT-CE1-ND1	2.17	128.62	122.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	T	699	DDE	CAU-CAT-CE1-ND1
1	T	699	DDE	CE1-CAT-CAU-CBW

There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	T	699	DDE	18	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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
4	GDP	T	843	-	24,30,30	1.08	3 (12%)	30,47,47	0.82	1 (3%)
3	SO1	T	1700	1	35,39,39	2.02	9 (25%)	39,64,64	2.17	7 (17%)
2	APR	T	1699	1	33,38,39	1.47	6 (18%)	37,58,60	1.76	7 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDP	T	843	-	-	0/12/32/32	0/3/3/3
3	SO1	T	1700	1	1/1/15/16	7/21/104/104	0/7/5/5
2	APR	T	1699	1	1/1/9/10	3/18/51/54	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	1700	SO1	C7-C2	6.30	1.64	1.54
3	T	1700	SO1	C12-C4	-5.00	1.42	1.54
2	T	1699	APR	C2-N1	4.16	1.41	1.33
3	T	1700	SO1	C1-C5	3.90	1.59	1.50
3	T	1700	SO1	C55-C56	3.29	1.58	1.52
2	T	1699	APR	C3'-C4'	2.89	1.60	1.53
4	T	843	GDP	C6-N1	2.80	1.42	1.37
2	T	1699	APR	O2'-C2'	2.74	1.49	1.43
3	T	1700	SO1	O56-C52	2.64	1.48	1.41
3	T	1700	SO1	C10-C3	2.60	1.59	1.55
3	T	1700	SO1	C52-C53	2.35	1.59	1.52
3	T	1700	SO1	C8-C2	2.33	1.57	1.53
3	T	1700	SO1	C10-C6	2.32	1.58	1.53
2	T	1699	APR	C4-N3	2.29	1.38	1.35
2	T	1699	APR	O4D-C4D	2.24	1.48	1.44
4	T	843	GDP	O3'-C3'	2.16	1.48	1.43
4	T	843	GDP	C5-C4	-2.13	1.37	1.43
2	T	1699	APR	O4D-C1D	2.08	1.48	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	1700	SO1	C1-C4-C13	9.04	128.15	118.44
3	T	1700	SO1	C10-C6-C2	6.52	112.00	104.16
2	T	1699	APR	O2D-C2D-C3D	-4.93	101.92	111.27
3	T	1700	SO1	C7-C2-C6	4.26	120.25	112.17
2	T	1699	APR	PB-O3A-PA	-4.10	118.76	132.83
2	T	1699	APR	C1D-C2D-C3D	3.74	107.33	101.63
3	T	1700	SO1	C18-C9-C16	-3.65	98.41	103.64
2	T	1699	APR	C1D-O4D-C4D	3.25	115.75	108.16
2	T	1699	APR	O4D-C1D-C2D	-2.75	100.67	105.99
2	T	1699	APR	C5-C6-N6	2.67	124.40	120.35
2	T	1699	APR	C3'-C2'-C1'	2.40	104.59	100.98
3	T	1700	SO1	C12-C6-C10	-2.24	106.13	107.91
4	T	843	GDP	O3'-C3'-C4'	-2.23	104.61	111.05
3	T	1700	SO1	O17-C52-C53	2.15	111.67	108.30
3	T	1700	SO1	C24-C18-C9	-2.08	101.02	105.13

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	1699	APR	C1D
3	T	1700	SO1	C4

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	1700	SO1	C2-C1-C5-O14
3	T	1700	SO1	C2-C1-C5-O15
2	T	1699	APR	C3'-C4'-C5'-O5'
2	T	1699	APR	O4'-C4'-C5'-O5'
3	T	1700	SO1	C21-C13-C4-C12
3	T	1700	SO1	C20-C13-C4-C1
3	T	1700	SO1	C21-C13-C4-C1
3	T	1700	SO1	C20-C13-C4-C12
2	T	1699	APR	C5D-O5D-PB-O1B
3	T	1700	SO1	C1-C2-C8-O17

There are no ring outliers.

3 monomers are involved in 77 short contacts:

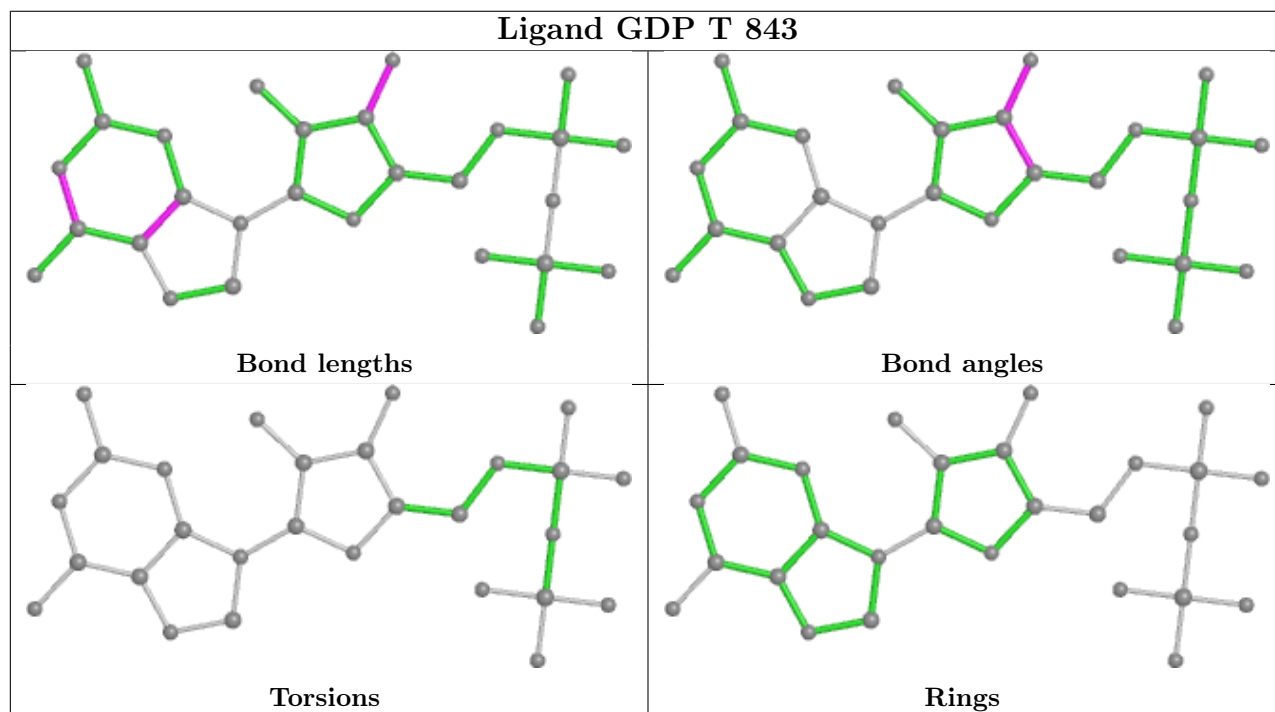
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	T	843	GDP	3	0

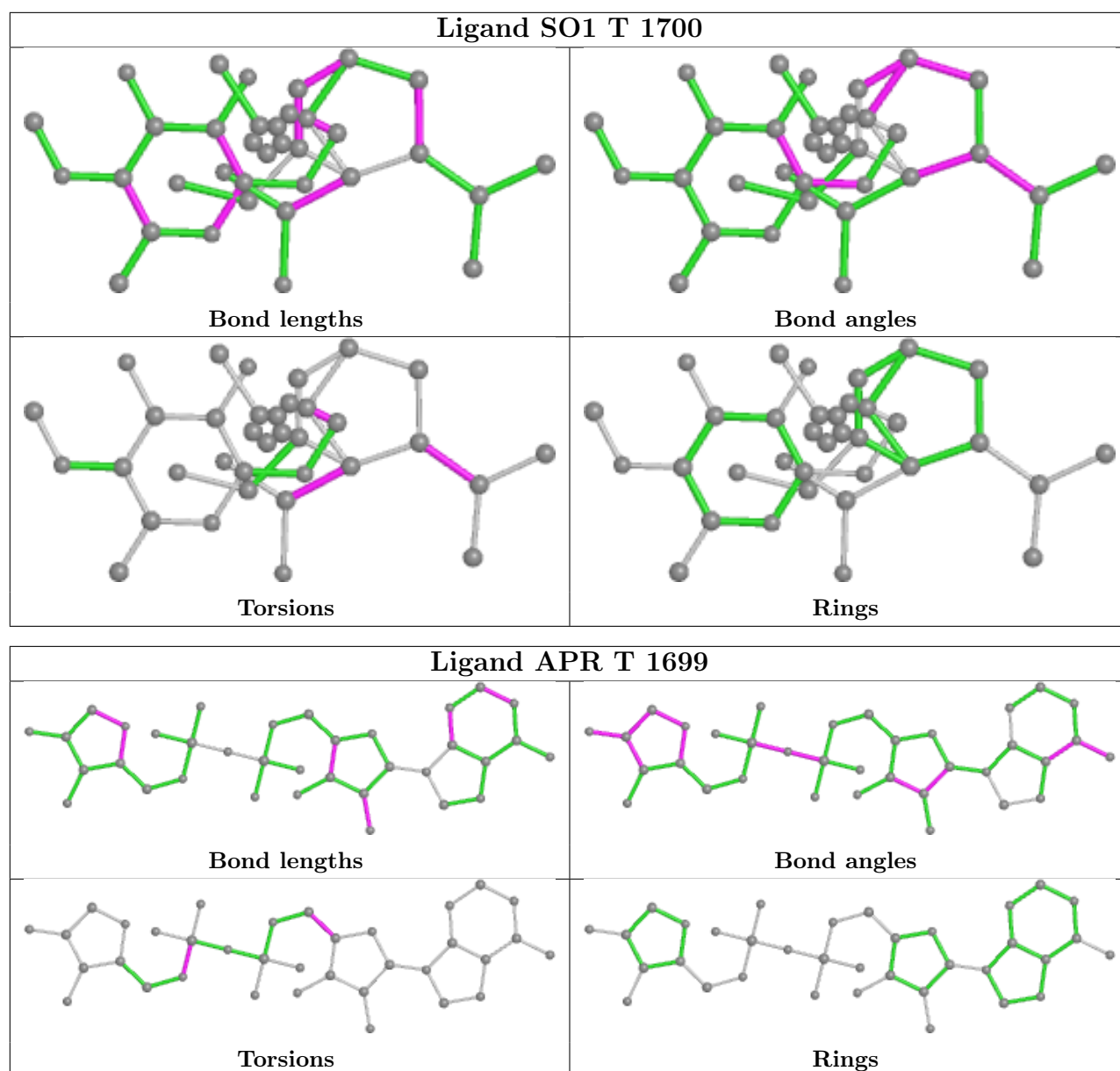
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	1700	SO1	67	0
2	T	1699	APR	7	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	T	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	482:LYS	C	483:PHE	N	6.62
1	T	558:PRO	C	559:PRO	N	5.80
1	T	481:MET	C	482:LYS	N	4.59
1	T	329:PRO	C	330:ALA	N	4.46
1	T	800:HIS	C	801:TRP	N	3.75
1	T	344:SER	C	345:PRO	N	3.47
1	T	216:HIS	C	217:GLY	N	3.23
1	T	480:VAL	C	481:MET	N	2.05
1	T	479:LYS	C	480:VAL	N	1.99
1	T	478:MET	C	479:LYS	N	1.68
1	T	698:ILE	C	699:DDE	N	0.89
1	T	699:DDE	C	700:ARG	N	0.85

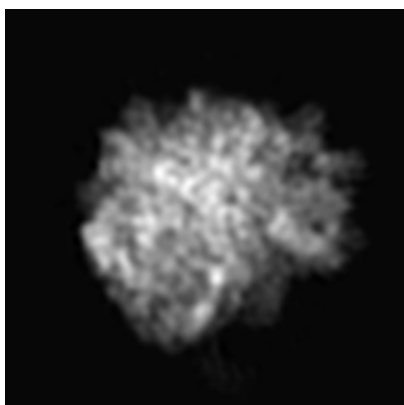
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1344. These allow visual inspection of the internal detail of the map and identification of artifacts.

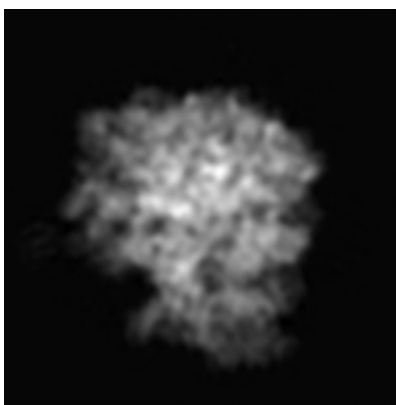
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

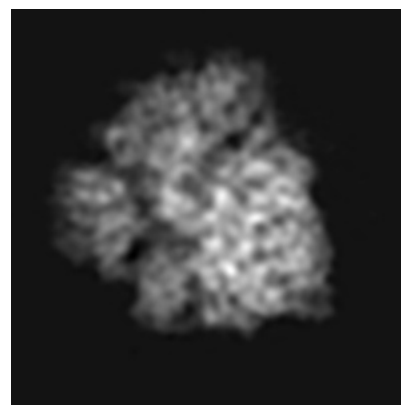
6.1.1 Primary map



X



Y

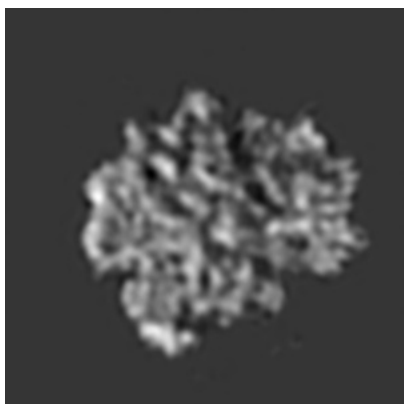


Z

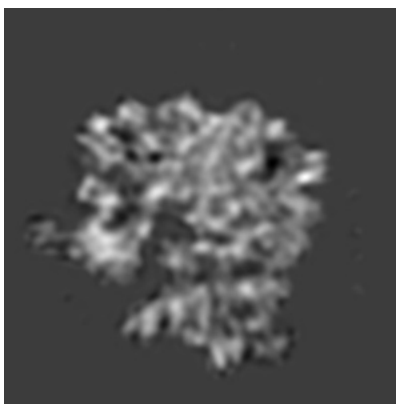
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

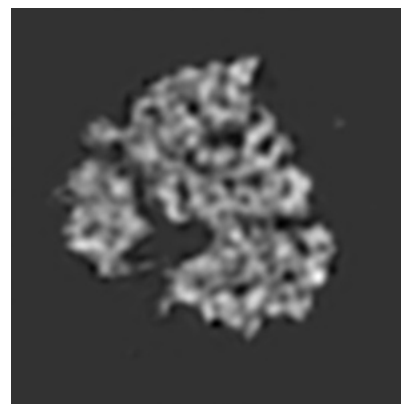
6.2.1 Primary map



X Index: 102



Y Index: 102

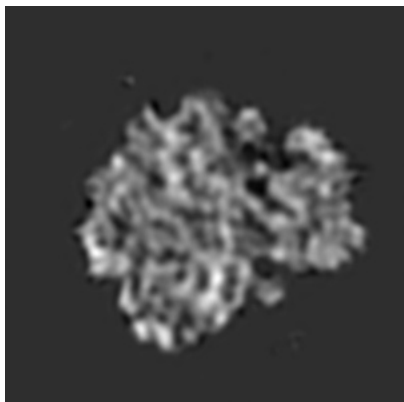


Z Index: 102

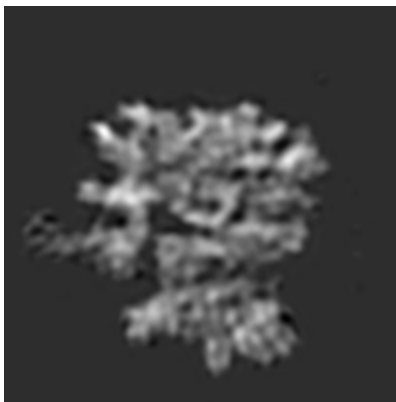
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

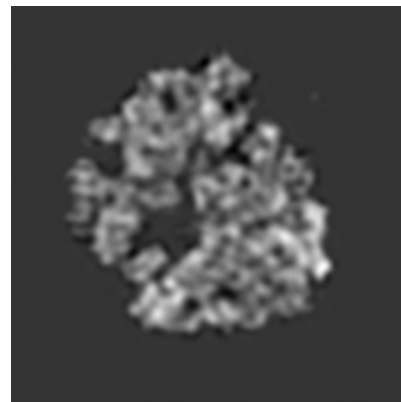
6.3.1 Primary map



X Index: 106



Y Index: 107

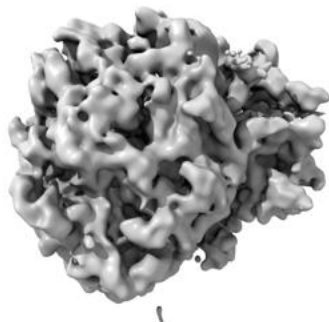


Z Index: 94

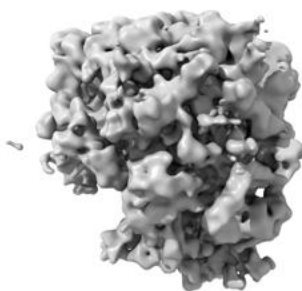
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

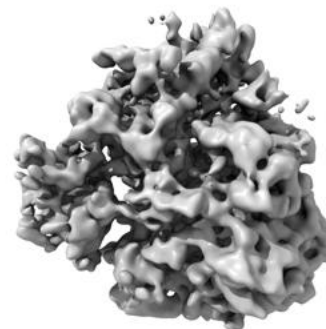
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 66.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

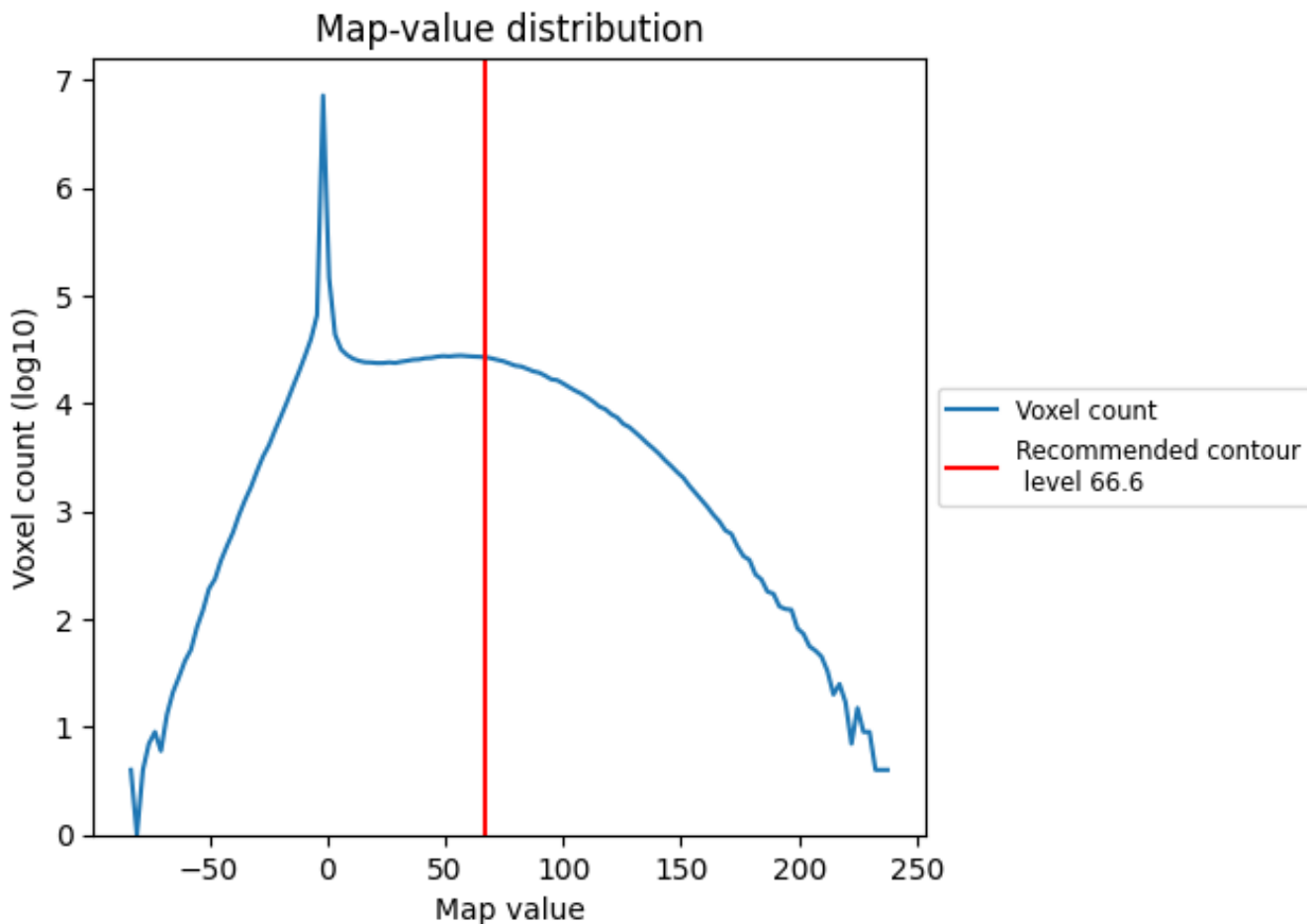
6.5 Mask visualisation

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

7 Map analysis [i](#)

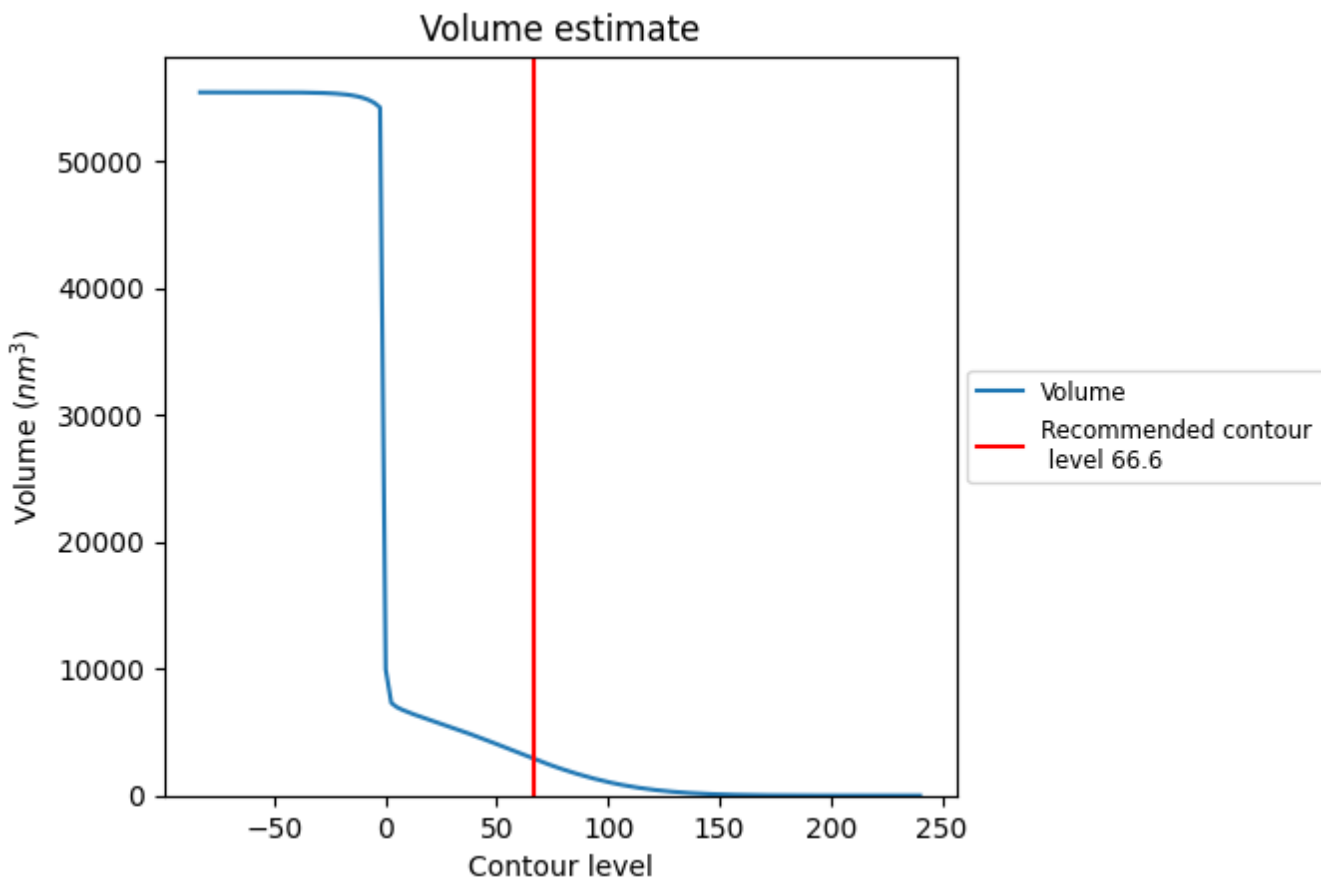
This section contains the results of statistical analysis of the map.

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.

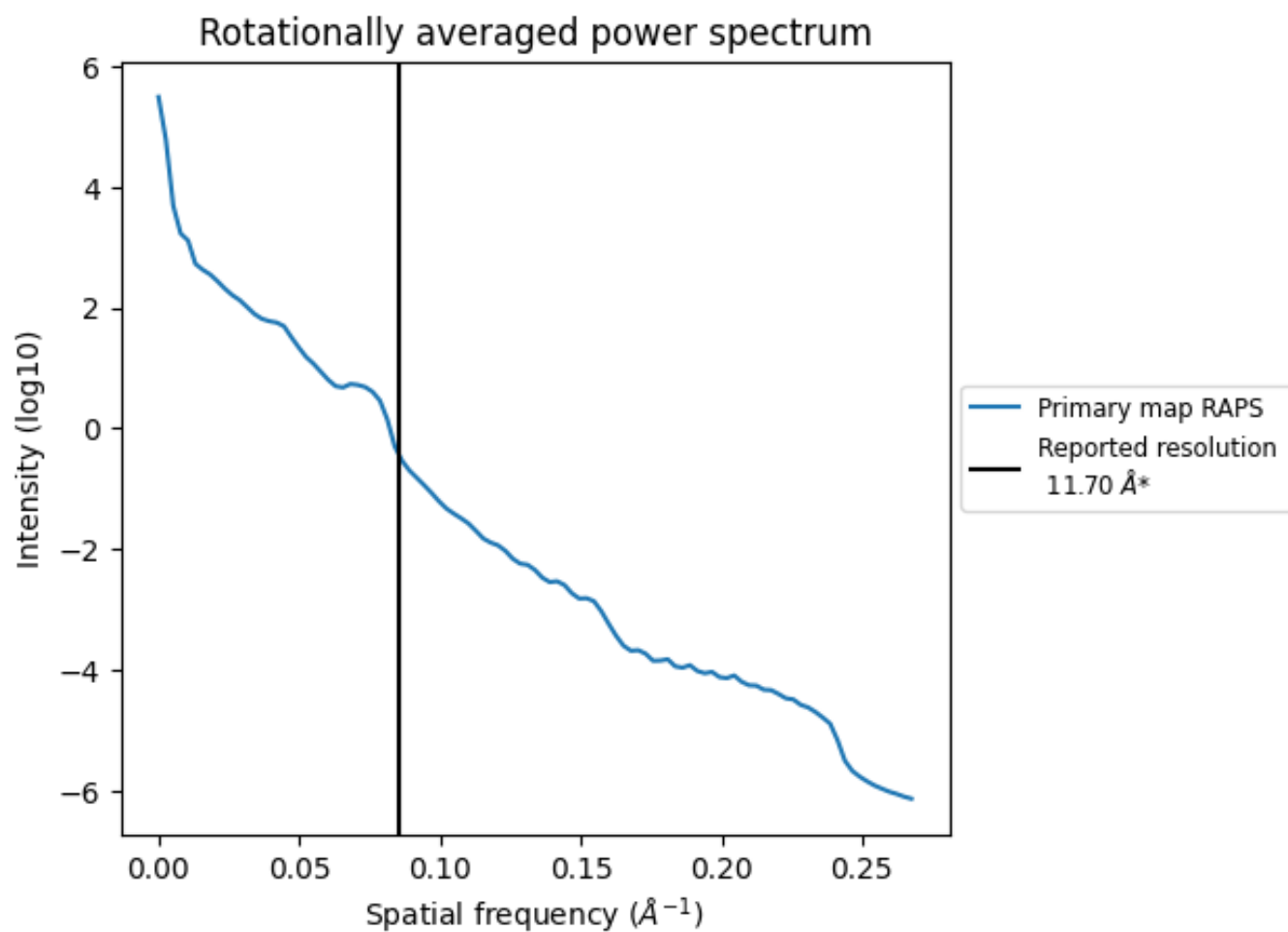
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2905 nm³; this corresponds to an approximate mass of 2624 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.085\AA^{-1}

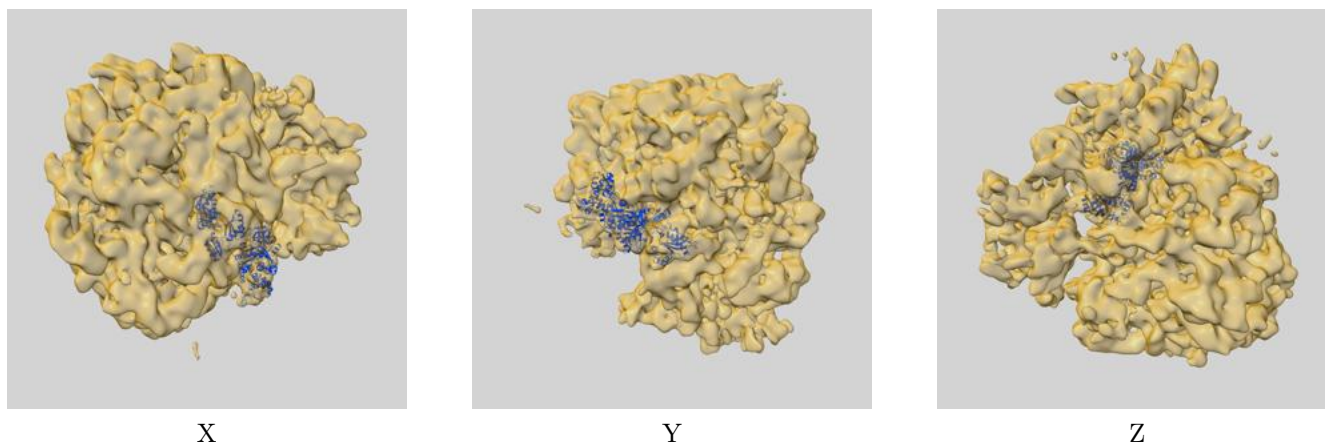
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

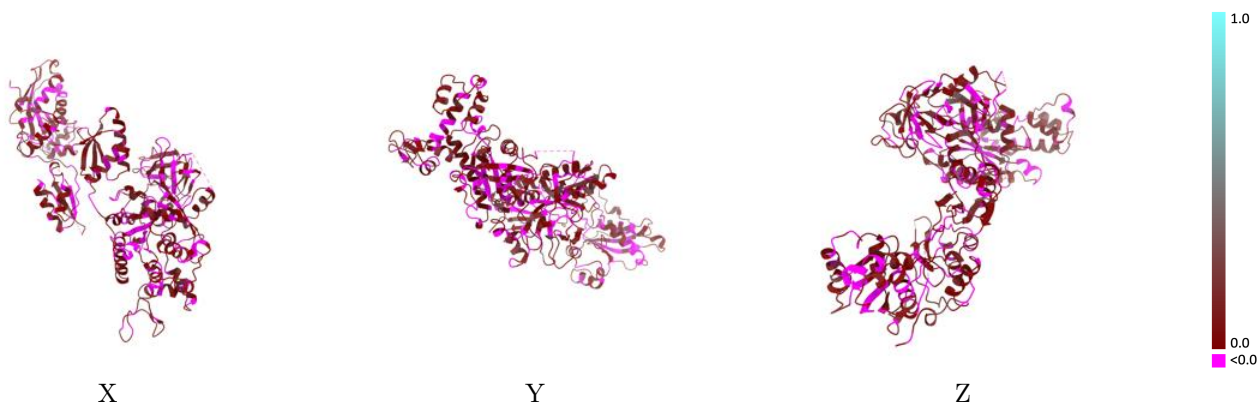
This section contains information regarding the fit between EMDB map EMD-1344 and PDB model 2P8Y. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



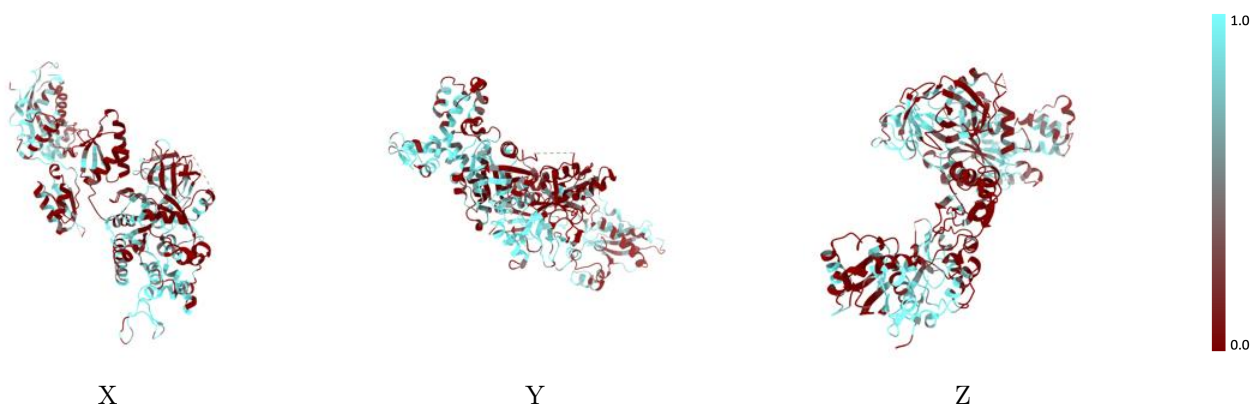
The images above show the 3D surface view of the map at the recommended contour level 66.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



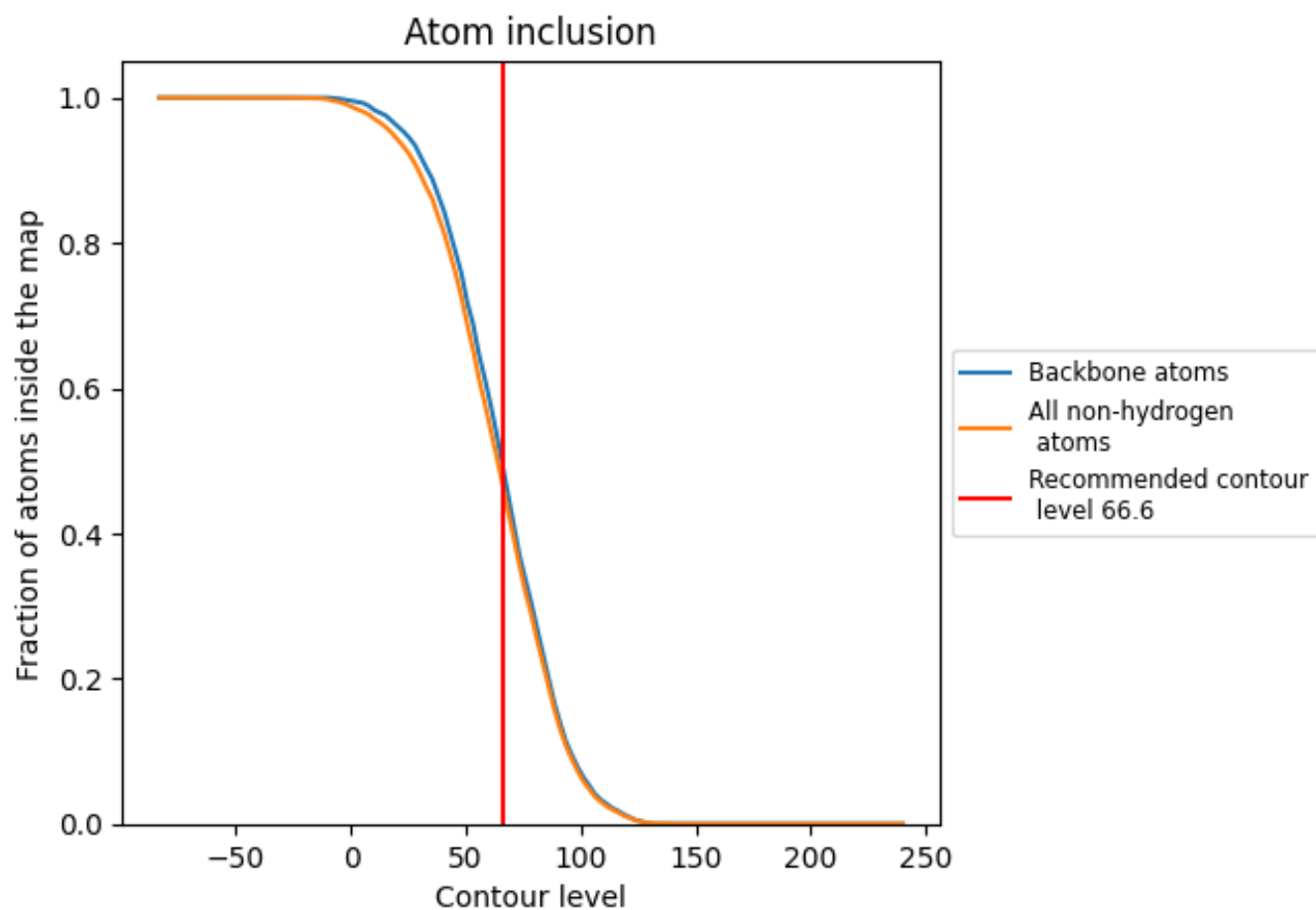
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (66.6).





9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (66.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4576	 0.0560
T	 0.4576	 0.0560

