



Full wwPDB EM Validation Report ⓘ

May 5, 2026 – 02:30 pm BST

PDB ID : 9RRQ / pdb_00009rrq
EMDB ID : EMD-54193
Title : Human TRPC5 in complex with (-) englerin A, partial occupancy (2EA:2LIP stoichiometry) state 1
Authors : Porav, A.S.; Bon, R.S.; Muench, S.
Deposited on : 2025-06-27
Resolution : 2.90 Å(reported)
Based on initial model : .

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.dev132
Mogul : 1.8.4, CSD as541be (2020)
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

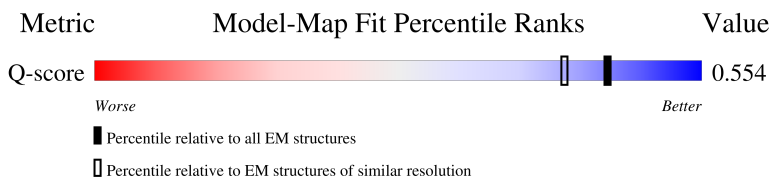
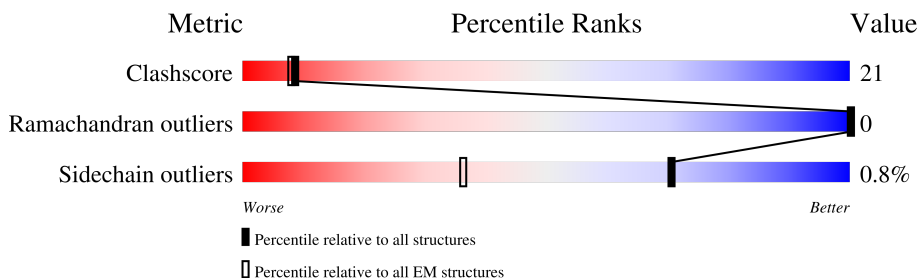
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	A	765	 60% 29% 10%
1	B	765	 56% 34% 10%
1	C	765	 57% 33% 10%
1	D	765	 57% 32% 11%

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
7	YZY	B	801	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 23555 atoms, of which 720 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Short transient receptor potential channel 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	686	Total	C	N	O	S	0	0
			5589	3633	927	999	30		
1	C	686	Total	C	N	O	S	0	0
			5592	3634	928	1000	30		
1	B	686	Total	C	N	O	S	0	0
			5588	3632	928	998	30		
1	D	683	Total	C	N	O	S	0	0
			5570	3622	922	996	30		

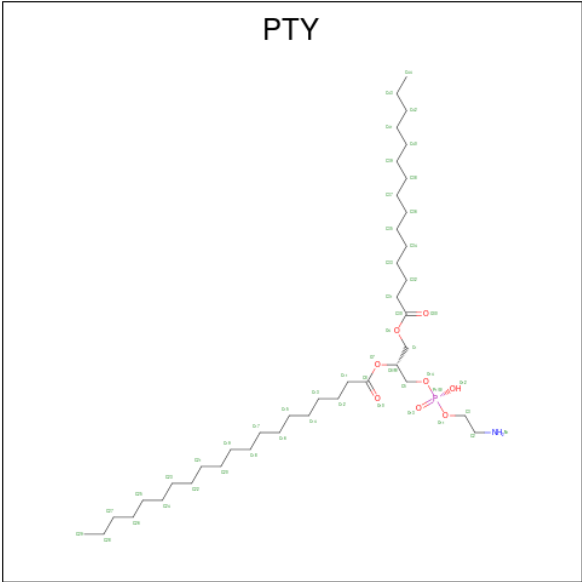
There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

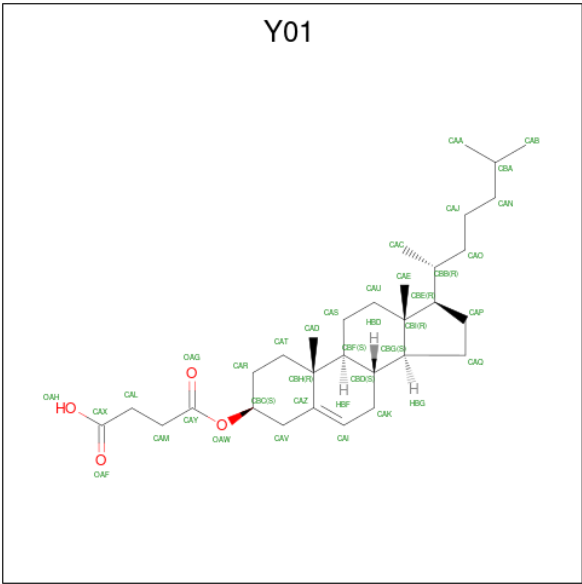
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Ca	0
			1	1	
2	C	1	Total	Ca	0
			1	1	
2	B	1	Total	Ca	0
			1	1	
2	D	1	Total	Ca	0
			1	1	

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



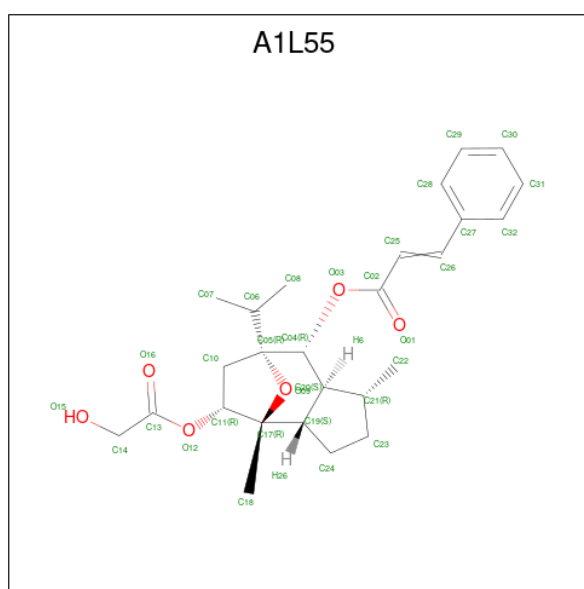
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total 129	C 40	H 79	N 1	O 8	P 1	0
3	C	1	Total 129	C 40	H 79	N 1	O 8	P 1	0
3	B	1	Total 129	C 40	H 79	N 1	O 8	P 1	0
3	D	1	Total 129	C 40	H 79	N 1	O 8	P 1	0

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			84	31	49	4	
4	C	1	Total	C	H	O	0
			84	31	49	4	
4	B	1	Total	C	H	O	0
			84	31	49	4	
4	D	1	Total	C	H	O	0
			84	31	49	4	

- Molecule 5 is (-)-englerin A (CCD ID: A1L55) (formula: C₂₆H₃₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	H	O	0
			66	26	34	6	
5	C	1	Total	C	H	O	0
			66	26	34	6	

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

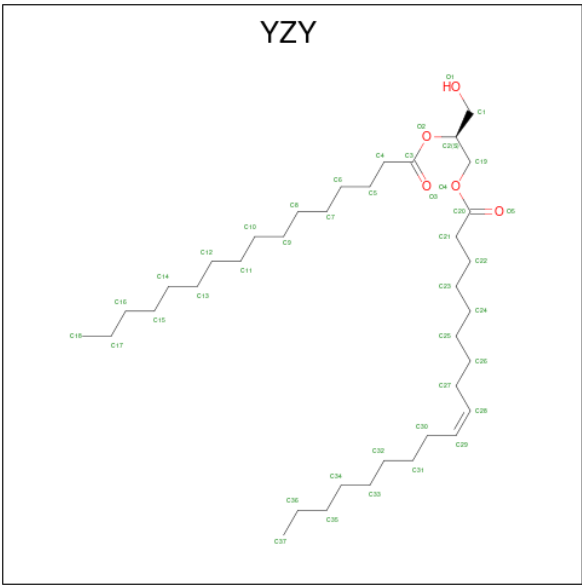
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	
6	C	1	Total	Zn	0
			1	1	
6	B	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Zn	0
			1	1	

- Molecule 7 is (2S)-2-(hexadecanoyloxy)-3-hydroxypropyl (9Z)-octadec-9-enoate (CCD ID: YZY) (formula: C₃₇H₇₀O₅).

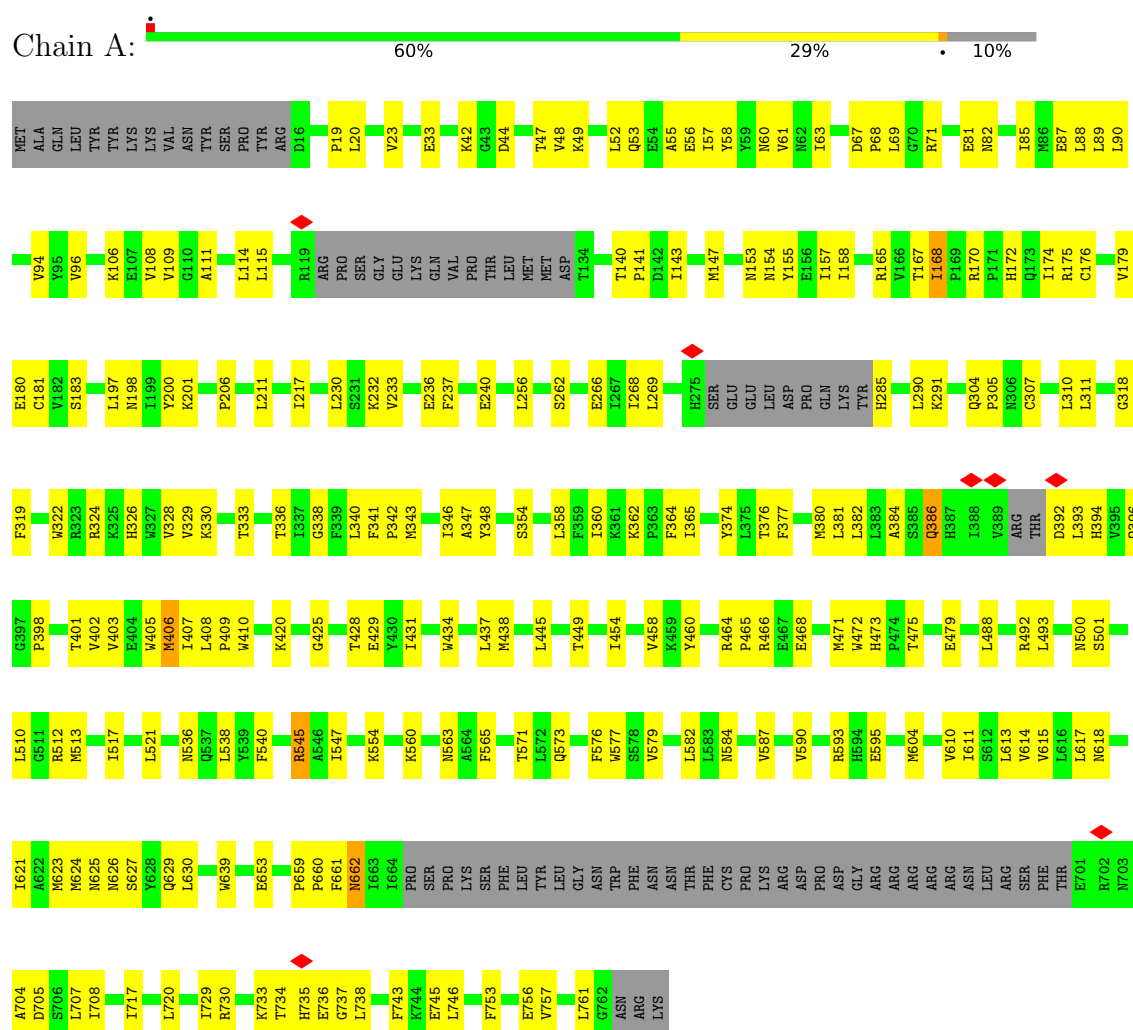


Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	H	O	0
			112	37	70	5	
7	D	1	Total	C	H	O	0
			112	37	70	5	

3 Residue-property plots

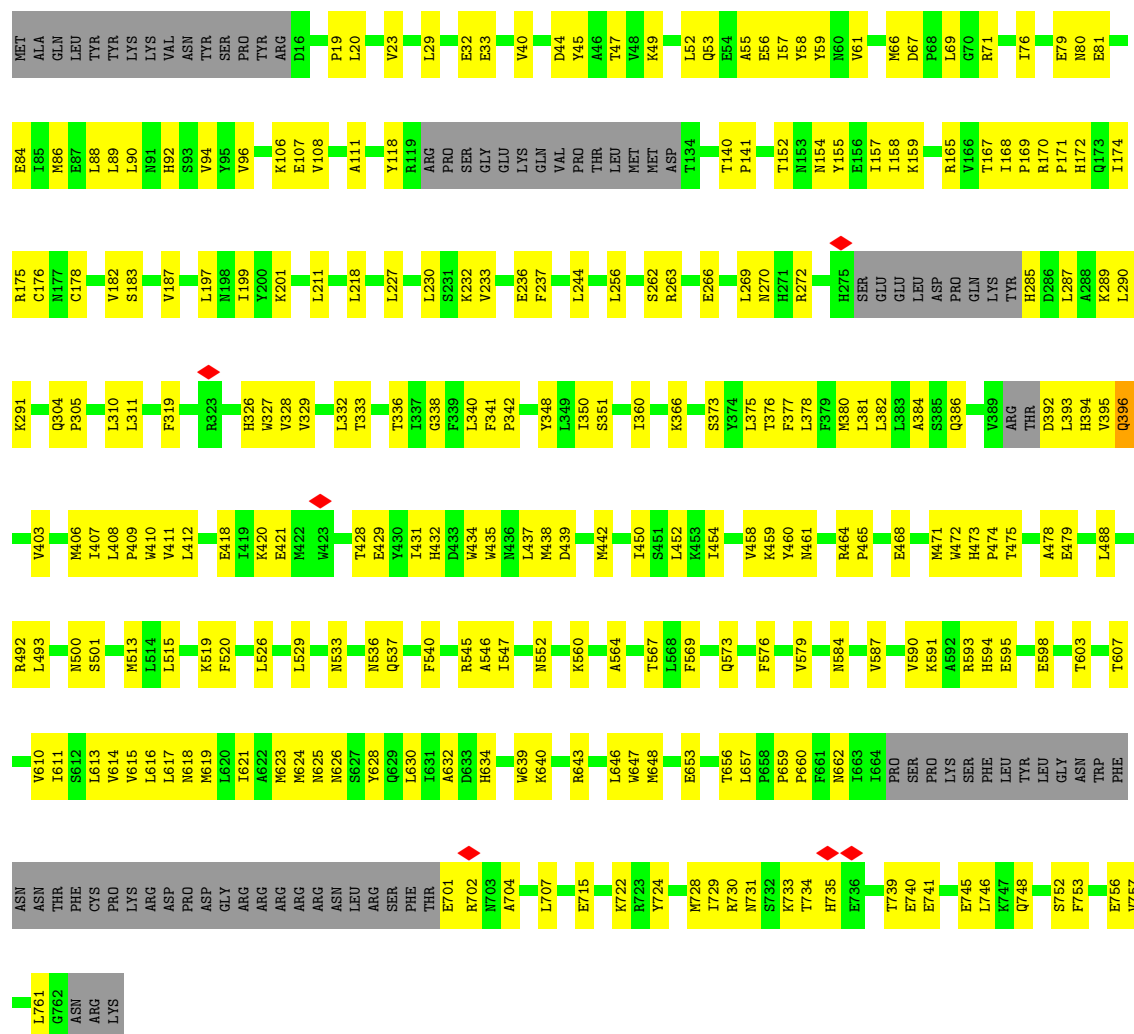
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Short transient receptor potential channel 5

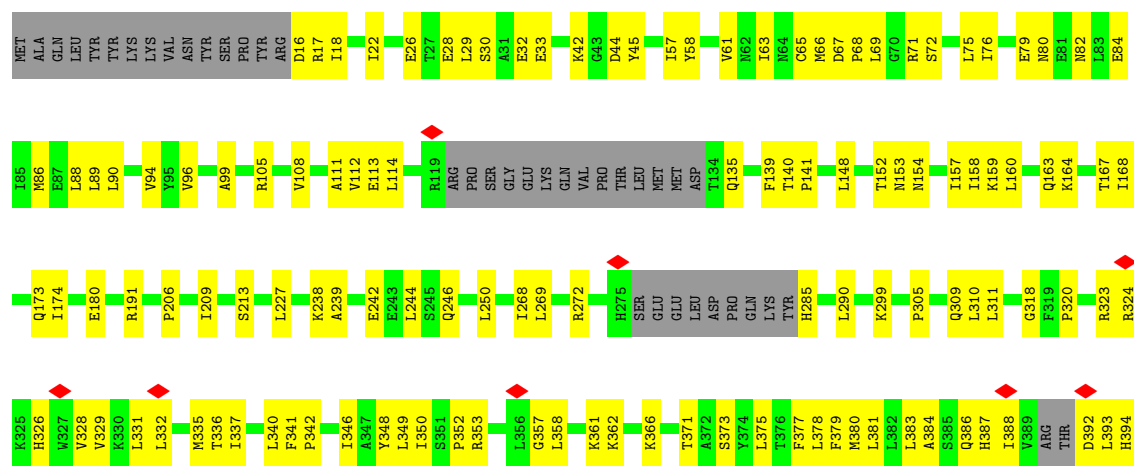


- Molecule 1: Short transient receptor potential channel 5





• Molecule 1: Short transient receptor potential channel 5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38365	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34.75	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	17.712	Depositor
Minimum map value	-9.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.333	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	368.256, 368.256, 368.256	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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: PTY, YZY, CA, ZN, Y01, A1L55

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	0.09	0/5721	0.22	0/7756
1	B	0.10	0/5720	0.24	0/7755
1	C	0.09	0/5724	0.20	0/7760
1	D	0.10	0/5702	0.23	0/7731
All	All	0.10	0/22867	0.22	0/31002

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5589	0	5608	242	0
1	B	5588	0	5608	276	0
1	C	5592	0	5611	262	0
1	D	5570	0	5588	271	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	50	79	79	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	50	79	79	3	0
3	C	50	79	79	3	0
3	D	50	79	79	5	0
4	A	35	49	49	1	0
4	B	35	49	49	7	0
4	C	35	49	49	5	0
4	D	35	49	49	5	0
5	A	32	34	0	2	0
5	C	32	34	0	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	B	42	70	69	4	0
7	D	42	70	70	4	0
All	All	22835	720	23066	971	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 21.

All (971) 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:D:67:ASP:OD1	1:D:68:PRO:HD2	1.56	1.05
1:B:513:MET:HE2	1:B:513:MET:HA	1.45	0.99
1:B:269:LEU:HD12	1:B:310:LEU:HD23	1.44	0.99
1:B:349:LEU:HD21	1:B:657:LEU:HD11	1.44	0.99
1:D:30:SER:HB3	1:D:33:GLU:HG3	1.47	0.97
1:D:349:LEU:HD21	1:D:657:LEU:HD11	1.47	0.94
1:D:326:HIS:HB3	1:D:329:VAL:HG23	1.48	0.93
1:D:629:GLN:HA	1:D:633:ASP:HB2	1.50	0.91
1:C:175:ARG:HG2	1:D:324:ARG:HG2	1.52	0.91
1:A:661:PHE:O	1:A:662:ASN:ND2	2.03	0.90
1:A:729:ILE:HD13	1:D:69:LEU:HD13	1.53	0.89
1:A:236:GLU:HB2	1:B:309:GLN:HE21	1.37	0.87
1:A:513:MET:HE3	1:A:624:MET:HE3	1.57	0.86
1:B:352:PRO:HB2	1:B:353:ARG:HD3	1.57	0.86
1:C:71:ARG:HH22	1:C:79:GLU:HG3	1.41	0.85
1:B:63:ILE:HG22	1:B:94:VAL:HG13	1.59	0.84
1:C:435:TRP:HB3	1:C:492:ARG:HH12	1.41	0.84
1:B:67:ASP:CG	1:B:68:PRO:HD2	2.04	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:HG2	1:B:191:ARG:HH11	1.44	0.82
1:D:191:ARG:HG2	1:D:191:ARG:HH11	1.45	0.81
1:B:547:ILE:HD12	1:B:547:ILE:H	1.45	0.81
1:B:326:HIS:HB3	1:B:329:VAL:HG23	1.61	0.81
1:A:236:GLU:HB2	1:B:309:GLN:NE2	1.95	0.81
1:B:342:PRO:O	1:B:346:ILE:HG13	1.81	0.81
1:A:393:LEU:HD12	1:A:394:HIS:N	1.96	0.80
1:D:411:VAL:O	1:D:415:ILE:HG13	1.81	0.80
1:B:628:TYR:O	1:B:633:ASP:HB2	1.81	0.80
1:C:178:CYS:O	1:C:182:VAL:HG22	1.81	0.80
1:B:82:ASN:HD22	1:B:748:GLN:HE22	1.30	0.79
1:D:341:PHE:CD1	1:D:342:PRO:HD3	2.17	0.79
1:D:740:GLU:HB3	1:D:744:LYS:NZ	1.99	0.78
1:A:108:VAL:HG23	1:A:111:ALA:HB3	1.66	0.78
1:D:547:ILE:H	1:D:547:ILE:HD12	1.49	0.78
1:C:540:PHE:HZ	1:D:388:ILE:HG13	1.48	0.77
1:A:393:LEU:HD12	1:A:394:HIS:H	1.48	0.77
1:C:464:ARG:HG2	1:C:465:PRO:HD2	1.67	0.77
1:A:346:ILE:HD12	1:A:347:ALA:N	1.99	0.77
1:D:629:GLN:HA	1:D:633:ASP:CB	2.14	0.77
1:B:624:MET:HG2	1:D:624:MET:HE1	1.67	0.76
1:A:236:GLU:HA	1:B:305:PRO:HB3	1.67	0.76
1:C:108:VAL:HG12	1:C:111:ALA:H	1.51	0.76
1:A:52:LEU:HD11	1:A:89:LEU:HD23	1.66	0.76
1:C:619:MET:O	1:C:623:MET:HG3	1.86	0.76
1:D:514:LEU:O	1:D:518:LEU:HD23	1.85	0.76
1:B:741:GLU:O	1:B:745:GLU:HG3	1.86	0.76
1:B:464:ARG:HG3	1:B:465:PRO:HD2	1.68	0.75
1:A:106:LYS:HG2	1:A:108:VAL:HG13	1.67	0.75
1:C:140:THR:HG22	1:C:141:PRO:HD2	1.68	0.75
1:B:331:LEU:O	1:B:335:MET:HG3	1.85	0.75
1:A:67:ASP:OD1	1:A:68:PRO:HD2	1.86	0.75
1:D:450:ILE:O	1:D:454:ILE:HG23	1.86	0.75
1:B:140:THR:HG22	1:B:141:PRO:HD2	1.68	0.75
1:C:540:PHE:CZ	1:D:388:ILE:HG13	2.21	0.75
1:D:82:ASN:OD1	1:D:84:GLU:HG3	1.86	0.75
1:A:82:ASN:OD1	1:A:85:ILE:HD12	1.87	0.74
1:A:445:LEU:O	1:A:449:THR:HG23	1.86	0.74
1:C:20:LEU:HD11	1:D:168:ILE:HG13	1.68	0.74
1:C:107:GLU:HG2	1:C:154:ASN:ND2	2.01	0.74
1:C:175:ARG:HG2	1:D:324:ARG:CG	2.17	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:PHE:HB2	1:B:410:TRP:CE3	2.23	0.74
1:C:576:PHE:O	1:C:579:VAL:HG12	1.87	0.74
1:D:380:MET:HE1	1:D:406:MET:O	1.88	0.74
1:D:172:HIS:HB3	1:D:176:CYS:SG	2.28	0.74
1:B:446:TYR:O	1:B:450:ILE:HG12	1.88	0.73
1:D:173:GLN:O	1:D:176:CYS:HB2	1.87	0.73
1:D:446:TYR:O	1:D:450:ILE:HG12	1.88	0.73
1:C:471:MET:SD	1:B:595:GLU:HB2	2.29	0.72
1:D:183:SER:O	1:D:186:GLU:HG3	1.90	0.72
1:D:333:THR:O	1:D:337:ILE:HD12	1.88	0.72
1:D:174:ILE:HG13	1:D:175:ARG:N	2.04	0.72
1:A:576:PHE:O	1:A:579:VAL:HG12	1.88	0.72
1:C:625:ASN:ND2	1:D:624:MET:HE3	2.04	0.72
1:A:464:ARG:HG3	1:A:465:PRO:HD2	1.70	0.72
1:B:326:HIS:ND1	1:B:328:VAL:HG22	2.04	0.72
1:D:708:ILE:HD12	1:D:709:GLN:N	2.05	0.72
1:D:740:GLU:HB3	1:D:744:LYS:HZ3	1.53	0.72
1:A:290:LEU:HD21	1:A:311:LEU:HD11	1.72	0.72
1:C:396:GLN:NE2	1:C:464:ARG:HD2	2.04	0.72
1:B:475:THR:O	1:B:479:GLU:HG3	1.90	0.72
1:A:471:MET:SD	1:D:595:GLU:HB2	2.30	0.72
1:B:67:ASP:HB2	1:B:71:ARG:O	1.90	0.72
1:B:381:LEU:HD23	1:B:407:ILE:HD13	1.70	0.72
1:B:173:GLN:OE1	1:B:174:ILE:HG22	1.89	0.72
1:B:108:VAL:HG13	1:B:111:ALA:HB3	1.71	0.71
1:B:473:HIS:ND1	1:B:475:THR:HG22	2.04	0.71
1:D:108:VAL:HG13	1:D:111:ALA:HB3	1.73	0.71
1:D:747:LYS:NZ	1:D:747:LYS:HB3	2.04	0.71
1:D:342:PRO:O	1:D:346:ILE:HG13	1.90	0.71
1:A:406:MET:O	1:A:409:PRO:HD2	1.91	0.71
1:B:513:MET:HE2	1:B:513:MET:CA	2.20	0.71
1:B:357:GLY:O	1:B:358:LEU:HG	1.91	0.70
1:C:332:LEU:O	1:C:336:THR:HG22	1.91	0.70
1:B:392:ASP:O	1:B:393:LEU:HG	1.91	0.70
1:A:233:VAL:O	1:B:323:ARG:HD2	1.92	0.70
1:D:349:LEU:CD2	1:D:657:LEU:HD11	2.22	0.70
1:C:175:ARG:HG2	1:D:324:ARG:HB3	1.74	0.70
1:B:396:GLN:CB	1:B:460:TYR:HB3	2.21	0.69
1:B:375:LEU:HD11	4:B:804:Y01:HAQ2	1.75	0.69
1:D:140:THR:HG22	1:D:141:PRO:HD2	1.72	0.69
1:B:341:PHE:CD2	1:B:342:PRO:HD3	2.28	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.58	0.69
1:B:396:GLN:HB2	1:B:460:TYR:HB3	1.73	0.69
1:A:396:GLN:HG2	1:A:473:HIS:HE2	1.57	0.69
1:A:471:MET:HE3	1:A:472:TRP:NE1	2.08	0.69
1:A:475:THR:O	1:A:479:GLU:HG3	1.92	0.69
1:A:618:ASN:HD21	1:B:623:MET:HG3	1.56	0.69
1:B:89:LEU:O	1:B:94:VAL:HG23	1.92	0.69
1:D:191:ARG:HG2	1:D:191:ARG:NH1	2.07	0.69
1:D:422:MET:HE2	1:D:422:MET:N	2.08	0.69
1:C:336:THR:O	1:C:340:LEU:HD13	1.93	0.68
1:B:428:THR:O	1:B:431:ILE:HG13	1.93	0.68
1:C:348:TYR:HB2	1:C:360:ILE:HG21	1.75	0.68
1:D:658:PRO:HB2	1:D:660:PRO:HD2	1.76	0.68
1:A:174:ILE:HG22	1:A:175:ARG:HG3	1.76	0.68
1:D:549:GLU:HB3	1:D:550:PRO:HD2	1.75	0.68
1:D:567:THR:O	1:D:571:THR:HG22	1.93	0.68
1:C:396:GLN:HG2	1:C:473:HIS:HE2	1.59	0.68
1:B:63:ILE:CG2	1:B:94:VAL:HG13	2.23	0.68
1:D:375:LEU:HD11	4:D:804:Y01:HAK1	1.76	0.68
1:B:513:MET:HA	1:B:513:MET:CE	2.23	0.67
1:C:19:PRO:HA	1:D:167:THR:HG22	1.76	0.67
1:B:380:MET:N	1:B:380:MET:HE2	2.09	0.67
1:D:154:ASN:OD1	1:D:157:ILE:HD13	1.94	0.67
1:C:89:LEU:O	1:C:94:VAL:HG23	1.93	0.67
1:A:614:VAL:HG23	1:A:615:VAL:HG23	1.76	0.67
1:C:471:MET:HE3	1:C:472:TRP:CE2	2.30	0.66
1:B:442:MET:HE1	1:B:492:ARG:HG3	1.75	0.66
1:C:611:ILE:O	1:C:615:VAL:HG22	1.94	0.66
1:B:191:ARG:HG2	1:B:191:ARG:NH1	2.10	0.66
1:A:593:ARG:HG3	1:A:593:ARG:HH11	1.60	0.66
1:C:593:ARG:HH11	1:C:593:ARG:HG3	1.60	0.66
1:C:460:TYR:HE1	1:C:474:PRO:HG2	1.60	0.66
1:B:75:LEU:O	1:B:79:GLU:HG2	1.96	0.66
1:D:475:THR:O	1:D:479:GLU:HG3	1.95	0.65
1:A:425:GLY:HA3	1:A:429:GLU:HG2	1.78	0.65
1:B:658:PRO:HB2	1:B:660:PRO:HD2	1.77	0.65
1:A:438:MET:HE1	3:A:802:PTY:H142	1.78	0.65
1:D:594:HIS:O	1:D:598:GLU:HG3	1.96	0.65
1:A:618:ASN:ND2	1:B:623:MET:HG3	2.10	0.65
1:C:392:ASP:O	1:C:393:LEU:HD13	1.96	0.65
1:D:401:THR:HB	1:D:404:GLU:HG2	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:GLY:O	1:D:360:ILE:HG22	1.96	0.65
1:B:415:ILE:HG12	1:B:443:ASN:HB3	1.79	0.65
1:D:376:THR:HG23	1:D:410:TRP:CZ3	2.32	0.65
1:A:20:LEU:HD11	1:B:168:ILE:HG13	1.79	0.64
1:A:736:GLU:HG2	1:A:737:GLY:H	1.60	0.64
1:A:167:THR:HG22	1:D:19:PRO:HA	1.79	0.64
1:C:435:TRP:HB3	1:C:492:ARG:NH1	2.11	0.64
1:B:348:TYR:CZ	1:B:656:THR:HG21	2.32	0.64
1:B:408:LEU:O	1:B:411:VAL:HG22	1.98	0.64
1:B:140:THR:CG2	1:B:141:PRO:HD2	2.27	0.64
1:B:509:SER:OG	1:B:631:ILE:HD13	1.97	0.64
1:A:143:ILE:HD13	1:A:147:MET:HE2	1.80	0.64
1:C:393:LEU:HB3	1:C:395:VAL:HG23	1.80	0.64
1:C:375:LEU:HD11	4:C:803:Y01:HAQ2	1.80	0.64
1:D:354:SER:O	1:D:358:LEU:HG	1.97	0.64
1:C:326:HIS:CE1	1:C:328:VAL:HG13	2.33	0.64
1:D:378:LEU:HD21	1:D:490:SER:HA	1.80	0.64
1:D:272:ARG:HB3	1:D:272:ARG:NH1	2.13	0.63
1:A:761:LEU:HD11	1:B:761:LEU:HD21	1.80	0.63
1:C:71:ARG:HH22	1:C:79:GLU:CG	2.10	0.63
1:D:49:LYS:O	1:D:53:GLN:HG2	1.98	0.63
1:B:29:LEU:HD11	1:B:67:ASP:HA	1.79	0.63
1:B:393:LEU:HD12	1:B:393:LEU:O	1.98	0.63
1:B:500:ASN:HB2	4:B:804:Y01:CAR	2.29	0.63
1:D:526:LEU:O	1:D:526:LEU:HD12	1.99	0.63
1:A:170:ARG:HB2	1:D:16:ASP:O	1.99	0.63
1:A:394:HIS:ND1	1:A:465:PRO:HA	2.13	0.63
1:A:19:PRO:HA	1:B:167:THR:HG22	1.80	0.63
1:A:729:ILE:CD1	1:D:69:LEU:HD13	2.26	0.63
1:C:52:LEU:HD23	1:C:92:HIS:ND1	2.14	0.63
1:D:174:ILE:HG13	1:D:175:ARG:H	1.62	0.63
1:D:75:LEU:O	1:D:79:GLU:HG2	1.99	0.63
1:A:197:LEU:HD12	1:A:197:LEU:O	1.98	0.63
1:A:626:ASN:O	1:A:630:LEU:HD22	1.98	0.63
1:A:67:ASP:OD1	1:A:68:PRO:CD	2.46	0.62
1:B:159:LYS:O	1:B:163:GLN:HG3	1.99	0.62
1:A:217:ILE:HD12	1:A:717:ILE:HD11	1.80	0.62
1:D:348:TYR:CZ	1:D:656:THR:HG21	2.34	0.62
1:C:81:GLU:HG2	1:C:108:VAL:HG21	1.80	0.62
1:C:459:LYS:HD2	1:C:460:TYR:CE1	2.35	0.62
1:B:659:PRO:HG2	1:B:660:PRO:HD3	1.79	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:724:TYR:CE1	1:D:728:MET:HE3	2.33	0.62
1:A:262:SER:O	1:A:266:GLU:HG3	2.00	0.62
1:C:526:LEU:HB2	4:D:804:Y01:HAC2	1.80	0.62
1:B:594:HIS:O	1:B:598:GLU:HG3	2.00	0.62
1:D:343:MET:HE3	1:D:356:LEU:HD21	1.80	0.62
1:B:290:LEU:CD2	1:B:311:LEU:HD21	2.30	0.61
1:B:318:GLY:HA3	1:B:362:LYS:HD3	1.80	0.61
1:D:377:PHE:HB2	1:D:410:TRP:HE3	1.65	0.61
1:A:434:TRP:HB2	3:A:802:PTY:O13	2.00	0.61
1:C:348:TYR:CZ	1:C:656:THR:HG21	2.35	0.61
1:C:640:LYS:HD3	1:C:643:ARG:HH21	1.65	0.61
1:B:526:LEU:HD12	1:B:526:LEU:O	2.00	0.61
1:B:67:ASP:OD1	1:B:68:PRO:HD2	2.00	0.61
1:A:340:LEU:HD23	1:A:343:MET:SD	2.41	0.61
1:D:563:ASN:O	1:D:570:GLU:HG2	1.99	0.61
1:C:57:ILE:HG22	1:C:58:TYR:CD2	2.36	0.61
1:D:376:THR:HG23	1:D:410:TRP:CH2	2.35	0.61
1:A:354:SER:O	1:A:358:LEU:HD23	2.01	0.61
1:B:624:MET:CG	1:D:624:MET:HE1	2.29	0.61
1:C:761:LEU:CD1	1:D:761:LEU:HD21	2.30	0.60
1:D:174:ILE:HG22	1:D:230:LEU:HD11	1.83	0.60
1:D:442:MET:HE1	1:D:492:ARG:HG3	1.82	0.60
1:A:736:GLU:HG2	1:A:737:GLY:N	2.15	0.60
1:C:57:ILE:HG22	1:C:58:TYR:HD2	1.64	0.60
1:A:381:LEU:HD23	1:A:407:ILE:CD1	2.32	0.60
1:A:438:MET:HE3	3:A:802:PTY:C31	2.31	0.60
1:C:659:PRO:N	1:C:660:PRO:HD2	2.17	0.60
1:B:45:TYR:OH	1:B:88:LEU:HD13	2.02	0.60
1:D:377:PHE:HB2	1:D:410:TRP:CE3	2.36	0.60
1:C:197:LEU:HD12	1:C:197:LEU:O	2.02	0.60
1:C:270:ASN:OD1	1:C:287:LEU:HD23	2.02	0.60
1:B:381:LEU:HD23	1:B:407:ILE:CD1	2.32	0.60
1:D:547:ILE:HD12	1:D:547:ILE:N	2.17	0.60
1:A:471:MET:HE3	1:A:472:TRP:CE2	2.36	0.60
1:D:464:ARG:HG2	1:D:465:PRO:HD2	1.84	0.60
1:A:595:GLU:CG	1:B:471:MET:HE2	2.30	0.60
1:C:262:SER:O	1:C:266:GLU:HG3	2.01	0.60
1:B:734:THR:HG23	1:B:735:HIS:ND1	2.17	0.60
1:D:659:PRO:HG2	1:D:660:PRO:HD3	1.84	0.60
1:A:236:GLU:HG3	1:B:305:PRO:HB2	1.82	0.60
1:C:272:ARG:HB2	1:C:272:ARG:NH1	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLU:HB3	1:B:65:CYS:SG	2.42	0.60
1:B:396:GLN:HG3	1:B:462:GLY:O	2.02	0.60
1:D:623:MET:HB2	1:D:630:LEU:HD11	1.83	0.60
1:C:376:THR:O	1:C:380:MET:HG2	2.02	0.59
1:C:761:LEU:HD11	1:D:761:LEU:HD21	1.84	0.59
1:B:401:THR:CG2	1:B:403:VAL:HG22	2.31	0.59
1:D:659:PRO:N	1:D:660:PRO:HD2	2.16	0.59
1:A:89:LEU:O	1:A:94:VAL:HG22	2.02	0.59
1:A:237:PHE:HB3	1:A:240:GLU:HB2	1.85	0.59
1:C:285:HIS:N	1:C:291:LYS:HZ1	1.99	0.59
1:C:396:GLN:HG2	1:C:473:HIS:NE2	2.17	0.59
1:A:346:ILE:HD12	1:A:346:ILE:C	2.28	0.59
1:A:348:TYR:HB2	1:A:360:ILE:HG21	1.84	0.59
1:A:705:ASP:O	1:A:708:ILE:HG13	2.02	0.59
1:C:175:ARG:HG2	1:D:324:ARG:CB	2.31	0.59
1:C:603:THR:HA	7:D:801:YZY:H192	1.84	0.59
1:B:154:ASN:O	1:B:158:ILE:HG13	2.02	0.59
1:B:375:LEU:HD21	4:B:804:Y01:HAP2	1.84	0.59
1:D:384:ALA:CB	1:D:403:VAL:HG11	2.33	0.59
1:C:471:MET:HE3	1:C:472:TRP:NE1	2.18	0.59
1:A:392:ASP:O	1:A:393:LEU:HG	2.03	0.59
1:A:393:LEU:CD1	1:A:394:HIS:H	2.15	0.59
1:A:513:MET:CE	1:A:624:MET:HE3	2.31	0.59
1:C:752:SER:O	1:C:756:GLU:HG3	2.03	0.59
1:D:422:MET:HE2	1:D:422:MET:CA	2.33	0.59
1:C:170:ARG:HB2	1:B:18:ILE:HG13	1.85	0.59
1:D:177:ASN:HA	1:D:182:VAL:CG2	2.33	0.59
1:A:396:GLN:HG2	1:A:473:HIS:NE2	2.17	0.58
1:D:513:MET:HG2	1:D:630:LEU:HD13	1.85	0.58
1:B:96:VAL:HG22	1:B:96:VAL:O	2.03	0.58
1:C:452:LEU:CB	1:C:478:ALA:HB2	2.33	0.58
1:B:411:VAL:O	1:B:415:ILE:HG13	2.03	0.58
1:D:438:MET:HE1	3:D:803:PTY:H151	1.85	0.58
1:D:174:ILE:HG13	1:D:175:ARG:HG2	1.84	0.58
1:D:442:MET:HE1	1:D:492:ARG:CD	2.33	0.58
1:B:164:LYS:HD3	1:B:164:LYS:N	2.17	0.58
1:B:547:ILE:HD12	1:B:547:ILE:N	2.17	0.58
1:B:89:LEU:HD12	1:B:94:VAL:HG21	1.83	0.58
1:D:304:GLN:OE1	1:D:306:ASN:HB2	2.04	0.58
1:D:379:PHE:CE1	1:D:383:LEU:HD11	2.38	0.58
1:A:108:VAL:CG2	1:A:111:ALA:HB3	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:PRO:N	1:B:660:PRO:HD2	2.18	0.58
1:D:616:LEU:HD11	7:D:801:YZY:H172	1.85	0.58
1:C:500:ASN:HB2	4:C:803:Y01:CAR	2.34	0.58
1:C:378:LEU:HD12	1:C:493:LEU:HD11	1.85	0.57
1:C:625:ASN:HD21	1:D:624:MET:HE3	1.69	0.57
1:B:378:LEU:HD12	1:B:493:LEU:HD11	1.85	0.57
1:D:414:PHE:CE1	1:D:659:PRO:HG3	2.38	0.57
1:D:430:TYR:OH	1:D:440:PHE:HB2	2.04	0.57
1:B:627:SER:HA	1:B:630:LEU:CB	2.34	0.57
1:A:729:ILE:HD13	1:D:69:LEU:CD1	2.30	0.57
1:C:421:GLU:O	1:C:421:GLU:HG2	2.05	0.57
1:D:372:ALA:O	1:D:376:THR:HG22	2.03	0.57
1:B:467:GLU:CD	1:B:467:GLU:H	2.13	0.57
1:B:543:GLU:HB2	1:B:566:SER:HB2	1.85	0.57
1:C:290:LEU:HD21	1:C:311:LEU:HD11	1.85	0.57
1:C:452:LEU:HB2	1:C:478:ALA:HB2	1.87	0.57
1:D:274:ASP:O	1:D:275:HIS:HB2	2.04	0.57
1:D:427:PHE:O	1:D:431:ILE:HG13	2.05	0.57
1:C:501:SER:HA	1:C:639:TRP:CZ2	2.39	0.56
1:D:663:ILE:O	1:D:664:ILE:HG12	2.05	0.56
1:B:153:ASN:ND2	1:B:206:PRO:HD2	2.19	0.56
1:C:52:LEU:HD21	1:C:89:LEU:HD23	1.85	0.56
1:C:79:GLU:O	1:C:106:LYS:HE3	2.05	0.56
1:C:341:PHE:CD2	1:C:342:PRO:HD3	2.40	0.56
1:B:552:ASN:O	1:B:552:ASN:OD1	2.24	0.56
1:D:190:LEU:HD12	1:D:190:LEU:O	2.05	0.56
1:A:438:MET:HE1	3:A:802:PTY:C14	2.35	0.56
1:A:513:MET:O	1:A:517:ILE:HD13	2.04	0.56
1:C:81:GLU:HG2	1:C:108:VAL:CG2	2.35	0.56
1:B:318:GLY:CA	1:B:362:LYS:HD3	2.34	0.56
1:D:393:LEU:HD12	1:D:393:LEU:O	2.05	0.56
1:D:401:THR:CB	1:D:404:GLU:HG2	2.35	0.56
1:C:465:PRO:HG2	1:C:468:GLU:CD	2.31	0.56
1:C:107:GLU:HG2	1:C:154:ASN:HD22	1.70	0.56
1:C:407:ILE:O	1:C:411:VAL:HG13	2.05	0.56
1:B:336:THR:O	1:B:340:LEU:HG	2.06	0.56
1:D:379:PHE:HE1	1:D:383:LEU:HD11	1.71	0.56
1:A:143:ILE:HD13	1:A:147:MET:CE	2.36	0.56
1:C:438:MET:HE1	3:C:802:PTY:H142	1.88	0.56
1:B:753:PHE:O	1:B:757:VAL:HG23	2.05	0.56
1:C:381:LEU:HD23	1:C:407:ILE:CD1	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:PHE:CE1	1:B:659:PRO:HG3	2.40	0.56
1:D:57:ILE:HD12	1:D:58:TYR:CD1	2.41	0.56
1:D:407:ILE:O	1:D:411:VAL:HG13	2.06	0.56
1:D:517:ILE:HD13	1:D:623:MET:HE1	1.87	0.56
1:A:109:VAL:HG22	1:A:157:ILE:HD11	1.88	0.56
1:C:408:LEU:O	1:C:411:VAL:HG22	2.06	0.56
1:A:55:ALA:HB2	1:A:61:VAL:HG12	1.87	0.56
1:A:590:VAL:O	1:A:593:ARG:HD2	2.06	0.56
1:C:71:ARG:HB3	1:C:71:ARG:HH11	1.71	0.56
1:C:724:TYR:CE1	1:C:728:MET:HE3	2.41	0.56
1:D:341:PHE:CZ	1:D:376:THR:HG21	2.41	0.56
1:A:172:HIS:HB3	1:A:176:CYS:SG	2.46	0.55
1:A:341:PHE:CD2	1:A:342:PRO:HD3	2.40	0.55
1:B:498:THR:OG1	1:B:646:LEU:HD12	2.06	0.55
1:A:237:PHE:HA	1:A:240:GLU:OE1	2.05	0.55
1:A:428:THR:O	1:A:431:ILE:HG13	2.07	0.55
1:D:422:MET:HE2	1:D:422:MET:HA	1.88	0.55
1:C:454:ILE:O	1:C:458:VAL:HG13	2.07	0.55
1:B:209:ILE:O	1:B:213:SER:HB2	2.06	0.55
1:D:384:ALA:HB2	1:D:403:VAL:HG11	1.89	0.55
1:D:452:LEU:HB3	1:D:478:ALA:HB2	1.87	0.55
1:A:269:LEU:HD12	1:A:310:LEU:HD23	1.88	0.55
1:A:285:HIS:HA	1:A:291:LYS:NZ	2.21	0.55
1:A:753:PHE:CD1	1:D:754:ARG:HG3	2.41	0.55
1:C:291:LYS:HG2	1:C:648:MET:HE1	1.88	0.55
1:C:429:GLU:HA	1:C:432:HIS:ND1	2.21	0.55
1:A:738:LEU:O	1:B:737:GLY:HA2	2.07	0.55
1:C:71:ARG:HB3	1:C:71:ARG:NH1	2.22	0.55
1:A:730:ARG:O	1:A:734:THR:HG23	2.07	0.55
1:B:349:LEU:CD2	1:B:657:LEU:HD11	2.25	0.55
1:A:53:GLN:O	1:A:56:GLU:HG2	2.07	0.55
1:A:304:GLN:NE2	1:A:305:PRO:HD2	2.22	0.55
1:B:82:ASN:OD1	1:B:84:GLU:HG3	2.07	0.55
1:A:154:ASN:O	1:A:158:ILE:HG13	2.07	0.55
1:B:547:ILE:H	1:B:547:ILE:CD1	2.18	0.55
1:D:28:GLU:OE2	1:D:28:GLU:HA	2.07	0.55
1:D:422:MET:HE1	1:D:430:TYR:CD1	2.42	0.55
1:C:152:THR:HG22	1:C:154:ASN:HB2	1.89	0.54
1:D:326:HIS:ND1	1:D:328:VAL:HG22	2.22	0.54
1:A:268:ILE:HD11	1:A:720:LEU:HD11	1.90	0.54
1:C:621:ILE:HG21	1:D:620:LEU:HD11	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:600:VAL:CG1	1:D:604:MET:HE3	2.38	0.54
1:A:554:LYS:HG3	1:A:563:ASN:HD22	1.73	0.54
1:A:610:VAL:O	1:A:614:VAL:HG22	2.08	0.54
1:A:734:THR:HG22	1:D:741:GLU:OE1	2.08	0.54
1:C:729:ILE:O	1:C:733:LYS:HB3	2.08	0.54
1:B:624:MET:SD	1:D:624:MET:HE1	2.47	0.54
1:B:627:SER:HA	1:B:630:LEU:HB2	1.88	0.54
1:A:147:MET:CE	1:A:198:ASN:HB3	2.38	0.54
1:C:154:ASN:O	1:C:158:ILE:HG13	2.07	0.54
1:C:350:ILE:HG22	1:C:351:SER:N	2.22	0.54
1:D:52:LEU:HD11	1:D:89:LEU:HD23	1.89	0.54
1:A:743:PHE:CD1	1:B:742:ASN:HB3	2.43	0.54
1:A:360:ILE:HG13	1:A:360:ILE:O	2.06	0.54
1:A:513:MET:HE1	1:D:618:ASN:HB2	1.89	0.54
1:D:109:VAL:HG22	1:D:157:ILE:CD1	2.38	0.54
1:A:438:MET:HE3	3:A:802:PTY:H311	1.90	0.54
1:B:373:SER:O	1:B:410:TRP:HZ3	1.91	0.54
1:B:600:VAL:CG1	1:B:604:MET:HE3	2.37	0.54
1:D:547:ILE:H	1:D:547:ILE:CD1	2.20	0.54
1:A:106:LYS:HG2	1:A:108:VAL:CG1	2.37	0.54
1:B:423:TRP:O	1:B:424:ASP:OD1	2.25	0.54
1:D:759:ASP:OD1	1:D:759:ASP:C	2.51	0.54
1:A:165:ARG:NH1	1:A:165:ARG:HB3	2.23	0.54
1:B:473:HIS:CE1	1:B:475:THR:HG22	2.43	0.54
1:C:326:HIS:CG	1:C:328:VAL:HG22	2.43	0.53
1:C:640:LYS:HD3	1:C:643:ARG:NH2	2.21	0.53
1:B:358:LEU:HA	1:B:361:LYS:HG3	1.90	0.53
1:B:402:VAL:O	1:B:406:MET:HG3	2.08	0.53
1:A:268:ILE:CD1	1:A:720:LEU:HD11	2.38	0.53
1:C:140:THR:HG22	1:C:141:PRO:CD	2.38	0.53
1:C:733:LYS:HG2	1:B:741:GLU:OE1	2.08	0.53
1:A:384:ALA:HA	1:A:403:VAL:HG11	1.91	0.53
1:A:420:LYS:NZ	1:A:420:LYS:HB3	2.23	0.53
1:A:704:ALA:HA	1:A:707:LEU:CD2	2.38	0.53
1:D:348:TYR:CE1	1:D:656:THR:HG21	2.43	0.53
1:A:746:LEU:O	1:A:746:LEU:HD12	2.09	0.53
1:B:510:LEU:HD11	7:B:801:YZY:H342	1.91	0.53
1:D:175:ARG:HH12	1:D:233:VAL:CG2	2.21	0.53
1:A:595:GLU:HG3	1:B:471:MET:HE2	1.88	0.53
1:A:708:ILE:C	1:A:708:ILE:HD12	2.34	0.53
1:C:360:ILE:HG13	1:C:360:ILE:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:THR:O	1:C:431:ILE:HG13	2.09	0.53
1:D:448:ALA:O	1:D:452:LEU:HD23	2.09	0.53
1:A:319:PHE:HE1	1:A:364:PHE:HD2	1.55	0.53
1:C:450:ILE:HG22	1:C:454:ILE:HD12	1.90	0.53
1:B:96:VAL:HG23	1:B:99:ALA:HB3	1.91	0.53
1:B:442:MET:HE1	1:B:492:ARG:CD	2.38	0.53
1:A:96:VAL:HG23	1:A:96:VAL:O	2.07	0.53
1:A:326:HIS:CD2	1:A:328:VAL:HB	2.44	0.53
1:A:376:THR:O	1:A:380:MET:HG2	2.09	0.53
1:A:425:GLY:HA3	1:A:429:GLU:CG	2.39	0.53
1:A:565:PHE:HD1	1:A:571:THR:HG23	1.73	0.53
1:B:375:LEU:HD11	4:B:804:Y01:CAQ	2.37	0.53
1:A:49:LYS:HB2	1:A:88:LEU:HD21	1.91	0.53
1:A:538:LEU:CD1	1:B:480:ALA:HA	2.38	0.53
1:B:28:GLU:OE1	1:B:28:GLU:C	2.52	0.53
1:D:269:LEU:HD12	1:D:310:LEU:HD23	1.89	0.53
1:D:387:HIS:O	1:D:387:HIS:CG	2.62	0.53
1:C:29:LEU:HD11	1:C:66:MET:O	2.08	0.53
1:B:17:ARG:HB3	1:B:17:ARG:NH1	2.24	0.52
1:B:238:LYS:HG3	1:B:239:ALA:N	2.24	0.52
1:C:174:ILE:HG13	1:C:230:LEU:CD2	2.39	0.52
1:C:464:ARG:CG	1:C:465:PRO:HD2	2.37	0.52
1:B:80:ASN:ND2	1:B:748:GLN:HG3	2.24	0.52
1:B:401:THR:HG23	1:B:403:VAL:HG22	1.89	0.52
1:A:165:ARG:HB3	1:A:165:ARG:HH11	1.75	0.52
1:A:393:LEU:HD13	1:A:466:ARG:HE	1.75	0.52
1:C:80:ASN:ND2	1:C:748:GLN:HG3	2.24	0.52
1:B:326:HIS:HB3	1:B:329:VAL:CG2	2.38	0.52
1:D:321:GLY:O	1:D:325:LYS:HG3	2.10	0.52
1:D:341:PHE:N	1:D:342:PRO:HD2	2.24	0.52
1:B:82:ASN:HB2	1:B:748:GLN:HE22	1.74	0.52
1:B:500:ASN:HB2	4:B:804:Y01:HAR2	1.92	0.52
1:D:175:ARG:HH12	1:D:233:VAL:HG22	1.73	0.52
1:D:465:PRO:HB2	1:D:468:GLU:HG3	1.92	0.52
1:A:69:LEU:HD12	1:A:69:LEU:N	2.25	0.52
1:C:236:GLU:OE1	1:C:236:GLU:N	2.39	0.52
1:D:327:TRP:CD1	1:D:328:VAL:HG13	2.44	0.52
1:C:52:LEU:HB3	1:C:92:HIS:CE1	2.45	0.52
1:D:405:TRP:O	1:D:406:MET:HB3	2.10	0.52
1:D:408:LEU:HD13	1:D:412:LEU:HD12	1.92	0.52
1:D:433:ASP:HB3	1:D:436:ASN:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ARG:HH21	1:A:547:ILE:HD11	1.75	0.52
1:C:326:HIS:ND1	1:C:328:VAL:HG22	2.25	0.52
1:D:380:MET:SD	1:D:406:MET:HG2	2.49	0.52
1:A:324:ARG:HG3	1:A:324:ARG:HH11	1.74	0.51
1:A:381:LEU:HD23	1:A:407:ILE:HD13	1.92	0.51
1:B:415:ILE:O	1:B:419:ILE:HG12	2.09	0.51
1:D:337:ILE:HD12	1:D:337:ILE:H	1.74	0.51
1:C:170:ARG:HB3	1:B:16:ASP:O	2.11	0.51
1:D:501:SER:HA	1:D:639:TRP:CZ2	2.45	0.51
1:C:573:GLN:HG2	5:C:804:A1L55:O16	2.10	0.51
1:C:341:PHE:N	1:C:342:PRO:HD2	2.24	0.51
1:C:408:LEU:HD23	1:C:412:LEU:HG	1.91	0.51
1:B:366:LYS:HD3	1:B:656:THR:HA	1.93	0.51
1:D:619:MET:HE1	7:D:801:YZY:H181	1.92	0.51
1:A:659:PRO:N	1:A:660:PRO:HD2	2.24	0.51
1:B:459:LYS:HD3	1:B:459:LYS:O	2.10	0.51
1:A:108:VAL:HG23	1:A:108:VAL:O	2.10	0.51
1:A:401:THR:HG22	1:A:402:VAL:H	1.75	0.51
1:A:554:LYS:HG3	1:A:563:ASN:ND2	2.24	0.51
1:B:470:GLU:HA	1:B:470:GLU:OE1	2.10	0.51
1:C:69:LEU:HD12	1:C:69:LEU:N	2.25	0.51
1:C:394:HIS:ND1	1:C:465:PRO:HA	2.24	0.51
1:B:421:GLU:OE1	1:B:421:GLU:HA	2.11	0.51
1:A:341:PHE:CG	1:A:342:PRO:HD3	2.46	0.51
1:C:594:HIS:O	1:C:598:GLU:HG3	2.11	0.51
1:D:272:ARG:HH12	1:D:275:HIS:C	2.19	0.51
1:A:465:PRO:HG2	1:A:468:GLU:CD	2.35	0.51
1:A:753:PHE:CZ	1:D:754:ARG:HA	2.46	0.51
1:C:96:VAL:O	1:C:96:VAL:HG22	2.11	0.51
1:C:154:ASN:HB3	1:C:157:ILE:HB	1.93	0.51
1:B:26:GLU:N	1:B:26:GLU:OE2	2.44	0.51
1:B:82:ASN:HD22	1:B:748:GLN:NE2	2.02	0.51
1:B:513:MET:O	1:B:517:ILE:HG12	2.11	0.51
1:D:69:LEU:HD23	1:D:69:LEU:N	2.26	0.51
1:D:148:LEU:O	1:D:152:THR:HG23	2.11	0.51
1:D:752:SER:O	1:D:756:GLU:HG3	2.10	0.51
1:A:49:LYS:CB	1:A:88:LEU:HD21	2.41	0.51
1:C:381:LEU:HD23	1:C:407:ILE:HD13	1.93	0.51
1:C:757:VAL:O	1:C:761:LEU:HD23	2.10	0.51
1:B:320:PRO:HD2	1:B:324:ARG:NH2	2.26	0.51
1:B:337:ILE:HA	1:B:340:LEU:HD11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:MET:HE1	1:B:492:ARG:CG	2.39	0.51
1:A:153:ASN:OD1	1:A:206:PRO:HD2	2.11	0.50
1:A:377:PHE:HB2	1:A:410:TRP:CD1	2.46	0.50
1:A:180:GLU:HG3	1:A:181:CYS:N	2.25	0.50
1:A:420:LYS:HB3	1:A:420:LYS:HZ2	1.75	0.50
1:A:736:GLU:CG	1:A:737:GLY:H	2.21	0.50
1:A:757:VAL:O	1:A:761:LEU:HD23	2.12	0.50
1:C:269:LEU:HD12	1:C:310:LEU:HD23	1.93	0.50
1:C:500:ASN:HB2	4:C:803:Y01:HAR2	1.92	0.50
1:B:630:LEU:HD22	1:B:631:ILE:CD1	2.41	0.50
1:D:349:LEU:HD21	1:D:657:LEU:CD1	2.31	0.50
1:A:743:PHE:HB2	1:B:738:LEU:HD11	1.92	0.50
1:C:740:GLU:OE1	1:D:733:LYS:HA	2.11	0.50
1:B:65:CYS:O	1:B:66:MET:HB2	2.11	0.50
1:D:274:ASP:OD1	1:D:274:ASP:C	2.53	0.50
1:D:747:LYS:HB3	1:D:747:LYS:HZ2	1.76	0.50
1:C:201:LYS:HG3	1:C:244:LEU:HD21	1.94	0.50
1:C:653:GLU:C	1:C:653:GLU:OE2	2.55	0.50
1:C:728:MET:HE2	1:C:728:MET:CA	2.41	0.50
1:D:66:MET:HE3	1:D:66:MET:HA	1.94	0.50
1:A:492:ARG:HH11	1:A:492:ARG:HG3	1.76	0.50
1:C:45:TYR:CD2	1:C:84:GLU:HG2	2.46	0.50
1:C:461:ASN:C	1:C:461:ASN:OD1	2.54	0.50
1:B:514:LEU:O	1:B:518:LEU:HG	2.11	0.50
1:B:734:THR:HG23	1:B:735:HIS:CE1	2.46	0.50
1:A:155:TYR:CE1	1:A:211:LEU:HG	2.47	0.50
1:A:595:GLU:HG3	1:B:471:MET:CE	2.42	0.50
1:C:172:HIS:HB3	1:C:176:CYS:HB2	1.94	0.50
1:C:396:GLN:HE21	1:C:464:ARG:HD2	1.76	0.50
1:A:584:ASN:O	1:A:587:VAL:HG22	2.12	0.50
1:C:287:LEU:O	1:C:291:LYS:HG3	2.11	0.50
1:B:400:PRO:HA	1:B:404:GLU:OE1	2.12	0.50
1:A:593:ARG:HG3	1:A:593:ARG:NH1	2.26	0.50
1:C:593:ARG:HG3	1:C:593:ARG:NH1	2.26	0.50
1:B:501:SER:HA	1:B:639:TRP:CZ2	2.47	0.50
1:D:319:PHE:CZ	1:D:365:ILE:HD11	2.46	0.50
1:A:623:MET:SD	1:B:506:LEU:HD11	2.52	0.49
1:D:272:ARG:HB3	1:D:272:ARG:HH11	1.77	0.49
1:A:71:ARG:HG3	1:A:71:ARG:NH1	2.23	0.49
1:C:464:ARG:HG2	1:C:465:PRO:CD	2.39	0.49
1:A:341:PHE:N	1:A:342:PRO:HD2	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:GLU:HG2	1:C:61:VAL:HG22	1.94	0.49
1:D:437:LEU:C	1:D:437:LEU:HD13	2.37	0.49
1:D:646:LEU:HD11	1:D:650:TYR:HE2	1.76	0.49
1:D:728:MET:HE2	1:D:728:MET:N	2.27	0.49
1:B:246:GLN:O	1:B:250:LEU:HD13	2.12	0.49
1:B:394:HIS:CD2	1:B:465:PRO:HA	2.47	0.49
1:C:333:THR:HA	1:C:336:THR:CG2	2.43	0.49
1:C:610:VAL:O	1:C:614:VAL:HB	2.12	0.49
1:D:17:ARG:NH1	1:D:17:ARG:HB3	2.28	0.49
1:D:164:LYS:HD3	1:D:164:LYS:N	2.27	0.49
1:D:421:GLU:C	1:D:422:MET:HE2	2.37	0.49
1:C:227:LEU:HD13	1:C:244:LEU:HB3	1.94	0.49
1:B:386:GLN:OE1	1:B:386:GLN:HA	2.12	0.49
1:B:629:GLN:OE1	1:B:629:GLN:N	2.43	0.49
1:D:410:TRP:CD1	1:D:410:TRP:N	2.79	0.49
1:A:322:TRP:CZ3	1:A:330:LYS:HE3	2.47	0.49
1:B:514:LEU:HG	7:B:801:YZY:H312	1.95	0.49
1:C:175:ARG:CG	1:D:324:ARG:HB3	2.40	0.49
1:C:338:GLY:O	1:C:341:PHE:HD2	1.95	0.49
1:C:729:ILE:HD12	1:B:69:LEU:HD13	1.94	0.49
1:B:396:GLN:HB3	1:B:460:TYR:HB3	1.94	0.49
1:A:761:LEU:HB3	1:B:760:LEU:HD13	1.95	0.49
1:C:730:ARG:O	1:C:734:THR:HG23	2.13	0.49
1:B:108:VAL:CG1	1:B:111:ALA:HB3	2.39	0.49
1:B:563:ASN:O	1:B:570:GLU:HG2	2.13	0.49
1:B:631:ILE:O	1:B:635:ALA:HB2	2.13	0.49
1:D:17:ARG:HB3	1:D:17:ARG:CZ	2.43	0.49
1:D:154:ASN:O	1:D:158:ILE:HG13	2.12	0.49
1:D:600:VAL:O	1:D:604:MET:HG3	2.13	0.49
1:C:584:ASN:O	1:C:587:VAL:HG22	2.12	0.48
1:B:180:GLU:OE1	1:B:180:GLU:HA	2.13	0.48
1:D:442:MET:HE1	1:D:492:ARG:CG	2.43	0.48
1:A:256:LEU:HD21	1:A:307:CYS:SG	2.53	0.48
1:A:573:GLN:HG2	5:A:804:A1L55:O16	2.12	0.48
1:C:628:TYR:O	1:C:632:ALA:HB2	2.14	0.48
1:B:396:GLN:HB2	1:B:460:TYR:O	2.13	0.48
1:B:626:ASN:OD1	1:B:626:ASN:C	2.56	0.48
1:D:340:LEU:C	1:D:342:PRO:HD2	2.37	0.48
4:D:804:Y01:HAU2	4:D:804:Y01:HAC1	1.96	0.48
1:C:159:LYS:HD3	1:C:211:LEU:HD21	1.96	0.48
1:C:408:LEU:CD2	1:C:412:LEU:HG	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:614:VAL:HG12	1:C:615:VAL:CG1	2.43	0.48
1:B:380:MET:HE2	1:B:380:MET:CA	2.43	0.48
1:D:719:ASN:O	1:D:723:ARG:HG3	2.13	0.48
1:B:112:VAL:HG21	1:B:157:ILE:HD13	1.95	0.48
1:A:733:LYS:HE3	1:D:741:GLU:HG3	1.96	0.48
1:C:429:GLU:HA	1:C:432:HIS:CE1	2.49	0.48
1:C:613:LEU:C	1:C:613:LEU:HD23	2.38	0.48
1:B:57:ILE:HG22	1:B:58:TYR:HD1	1.78	0.48
1:B:600:VAL:O	1:B:604:MET:HG3	2.13	0.48
1:D:326:HIS:O	1:D:330:LYS:HG3	2.12	0.48
1:A:33:GLU:CG	1:A:61:VAL:HG23	2.43	0.48
1:A:613:LEU:C	1:A:613:LEU:HD23	2.38	0.48
1:B:379:PHE:C	1:B:380:MET:HE2	2.38	0.48
1:C:465:PRO:HG2	1:C:468:GLU:OE1	2.14	0.48
1:C:501:SER:HA	1:C:639:TRP:CH2	2.49	0.48
1:C:536:ASN:O	1:C:540:PHE:HB3	2.14	0.48
1:B:44:ASP:OD2	1:B:44:ASP:C	2.56	0.48
1:D:401:THR:H	1:D:404:GLU:CG	2.27	0.48
1:A:33:GLU:HG3	1:A:61:VAL:HG23	1.95	0.48
1:C:237:PHE:CD1	1:C:237:PHE:N	2.82	0.48
1:C:590:VAL:O	1:C:593:ARG:HD2	2.14	0.48
1:B:473:HIS:ND1	1:B:474:PRO:HD2	2.29	0.48
1:C:168:ILE:HG13	1:C:169:PRO:HD2	1.96	0.47
1:C:341:PHE:CG	1:C:342:PRO:HD3	2.49	0.47
1:B:387:HIS:O	1:B:388:ILE:HD12	2.14	0.47
1:B:437:LEU:O	1:B:437:LEU:HD13	2.14	0.47
1:B:646:LEU:HD23	1:B:646:LEU:O	2.14	0.47
1:D:67:ASP:CG	1:D:68:PRO:HD2	2.35	0.47
1:D:397:GLY:HA3	1:D:456:ALA:O	2.13	0.47
1:D:452:LEU:CB	1:D:478:ALA:HB2	2.44	0.47
1:C:32:GLU:HG2	1:C:33:GLU:N	2.27	0.47
1:B:30:SER:HB3	1:B:33:GLU:HG3	1.96	0.47
1:B:448:ALA:O	1:B:452:LEU:HD23	2.15	0.47
1:C:272:ARG:NH1	1:C:272:ARG:CB	2.77	0.47
1:B:452:LEU:HB3	1:B:478:ALA:HB2	1.96	0.47
1:A:500:ASN:HB2	4:A:803:Y01:CAR	2.45	0.47
1:A:745:GLU:OE1	1:D:743:PHE:HZ	1.98	0.47
1:C:377:PHE:HB2	1:C:410:TRP:CD1	2.49	0.47
1:C:547:ILE:HD12	1:C:547:ILE:H	1.79	0.47
1:D:269:LEU:HD12	1:D:310:LEU:CD2	2.45	0.47
1:C:326:HIS:O	1:C:329:VAL:HG12	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:THR:O	1:C:479:GLU:HG3	2.14	0.47
1:C:701:GLU:CD	1:C:702:ARG:H	2.23	0.47
1:B:427:PHE:O	1:B:431:ILE:HG23	2.15	0.47
1:A:58:TYR:N	1:A:58:TYR:CD2	2.83	0.47
1:C:537:GLN:HE22	1:D:384:ALA:HB3	1.78	0.47
1:C:753:PHE:CZ	1:B:754:ARG:HA	2.50	0.47
1:D:89:LEU:O	1:D:94:VAL:HG22	2.14	0.47
1:D:414:PHE:HE1	1:D:659:PRO:HG3	1.80	0.47
1:D:728:MET:HE2	1:D:728:MET:CA	2.44	0.47
1:A:67:ASP:HB2	1:A:71:ARG:O	2.14	0.47
1:B:380:MET:HB3	1:B:407:ILE:CG1	2.44	0.47
1:B:519:LYS:HB3	1:B:519:LYS:HE2	1.74	0.47
1:D:327:TRP:NE1	1:D:328:VAL:HG13	2.30	0.47
1:D:513:MET:CG	1:D:630:LEU:HD13	2.45	0.47
1:A:147:MET:HE1	1:A:198:ASN:HB3	1.96	0.47
1:A:380:MET:HE3	1:A:406:MET:HB2	1.97	0.47
1:C:80:ASN:OD1	1:C:80:ASN:O	2.32	0.47
1:B:32:GLU:H	1:B:32:GLU:CD	2.22	0.47
1:D:216:PRO:HD2	1:D:717:ILE:HD12	1.95	0.47
1:C:646:LEU:HD23	1:C:647:TRP:HD1	1.80	0.47
1:C:707:LEU:HD22	1:C:707:LEU:H	1.80	0.47
1:A:285:HIS:HA	1:A:291:LYS:HZ1	1.79	0.46
1:A:330:LYS:O	1:A:333:THR:HG22	2.15	0.46
1:C:40:VAL:HG12	1:C:76:ILE:HG22	1.95	0.46
1:C:174:ILE:HG21	1:C:233:VAL:HG21	1.97	0.46
1:C:384:ALA:HA	1:C:403:VAL:HG11	1.95	0.46
1:B:58:TYR:N	1:B:58:TYR:CD1	2.83	0.46
1:D:644:THR:O	1:D:648:MET:HG3	2.15	0.46
1:D:660:PRO:HG2	1:D:661:PHE:HD2	1.80	0.46
1:C:174:ILE:HG13	1:C:230:LEU:HD23	1.97	0.46
1:D:108:VAL:CG1	1:D:111:ALA:HB3	2.42	0.46
1:A:625:ASN:HD22	1:B:624:MET:HG3	1.79	0.46
1:C:533:ASN:CG	1:D:382:LEU:HD23	2.40	0.46
1:C:560:LYS:O	1:C:560:LYS:HG3	2.15	0.46
1:B:405:TRP:HA	1:B:405:TRP:CE3	2.50	0.46
1:D:44:ASP:OD1	1:D:44:ASP:C	2.58	0.46
1:A:425:GLY:CA	1:A:429:GLU:HG2	2.44	0.46
1:A:545:ARG:NH2	1:A:547:ILE:HD11	2.30	0.46
1:A:653:GLU:C	1:A:653:GLU:OE2	2.58	0.46
1:C:175:ARG:CD	1:D:324:ARG:HB3	2.45	0.46
1:C:183:SER:O	1:C:187:VAL:HG22	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:595:GLU:HB2	1:D:471:MET:SD	2.56	0.46
1:C:746:LEU:HD12	1:C:746:LEU:O	2.16	0.46
1:D:715:GLU:OE1	1:D:715:GLU:HA	2.15	0.46
1:A:735:HIS:CG	1:A:736:GLU:H	2.33	0.46
1:B:332:LEU:HD12	1:B:332:LEU:O	2.15	0.46
1:A:401:THR:HG22	1:A:402:VAL:N	2.30	0.46
1:A:501:SER:HA	1:A:639:TRP:CH2	2.50	0.46
1:C:617:LEU:C	1:C:617:LEU:HD23	2.41	0.46
1:B:738:LEU:HD22	1:B:742:ASN:CG	2.40	0.46
1:A:319:PHE:CZ	1:A:365:ILE:HD11	2.50	0.46
1:A:326:HIS:NE2	1:A:328:VAL:HB	2.31	0.46
1:A:538:LEU:HD22	1:A:604:MET:HE2	1.97	0.46
1:C:171:PRO:HG3	1:C:199:ILE:HG21	1.98	0.46
1:C:513:MET:SD	1:C:624:MET:HE3	2.56	0.46
1:D:140:THR:HG22	1:D:141:PRO:CD	2.42	0.46
1:D:734:THR:HG23	1:D:735:HIS:ND1	2.30	0.46
1:A:175:ARG:CD	1:B:324:ARG:HA	2.46	0.46
1:D:415:ILE:O	1:D:419:ILE:HG13	2.16	0.46
1:D:290:LEU:HD21	1:D:311:LEU:HD11	1.98	0.45
1:D:467:GLU:H	1:D:467:GLU:CD	2.24	0.45
1:C:23:VAL:HG22	1:D:211:LEU:O	2.16	0.45
1:B:584:ASN:O	1:B:587:VAL:HG22	2.16	0.45
1:D:90:LEU:HD12	1:D:114:LEU:HD22	1.97	0.45
1:D:438:MET:HB2	3:D:803:PTY:H312	1.98	0.45
1:A:23:VAL:HG21	1:B:213:SER:O	2.16	0.45
1:A:336:THR:O	1:A:340:LEU:HD12	2.17	0.45
1:C:591:LYS:HB2	1:C:591:LYS:HE2	1.56	0.45
1:D:57:ILE:C	1:D:58:TYR:HD1	2.24	0.45
1:A:756:GLU:CD	1:D:754:ARG:HH21	2.25	0.45
1:C:49:LYS:CB	1:C:88:LEU:HD21	2.45	0.45
1:B:57:ILE:HG22	1:B:58:TYR:CD1	2.52	0.45
1:B:272:ARG:HH22	1:B:285:HIS:CE1	2.35	0.45
1:B:659:PRO:N	1:B:660:PRO:CD	2.79	0.45
1:C:174:ILE:N	1:C:174:ILE:HD12	2.32	0.45
1:C:373:SER:OG	1:C:660:PRO:HG3	2.16	0.45
1:C:728:MET:HE2	1:C:728:MET:N	2.31	0.45
1:B:140:THR:HG22	1:B:141:PRO:CD	2.43	0.45
1:B:268:ILE:HD11	1:B:720:LEU:HD11	1.98	0.45
1:B:371:THR:HG21	4:B:804:Y01:HAK2	1.99	0.45
1:D:659:PRO:N	1:D:660:PRO:CD	2.80	0.45
1:A:536:ASN:O	1:A:540:PHE:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ILE:O	1:D:621:ILE:HD11	2.16	0.45
1:B:397:GLY:HA3	1:B:456:ALA:O	2.16	0.45
1:D:387:HIS:O	1:D:388:ILE:C	2.60	0.45
1:C:567:THR:HG22	1:C:569:PHE:H	1.81	0.45
1:B:366:LYS:HG2	1:B:650:TYR:CD1	2.51	0.45
1:B:488:LEU:HD11	3:B:803:PTY:H381	1.97	0.45
1:D:405:TRP:HA	1:D:405:TRP:CE3	2.52	0.45
1:A:488:LEU:HD21	3:A:802:PTY:H202	1.99	0.45
1:C:107:GLU:HG3	1:C:152:THR:HG21	1.99	0.45
1:C:165:ARG:HH21	1:C:167:THR:HG22	1.82	0.45
1:C:564:ALA:HB2	1:C:587:VAL:HB	1.98	0.45
1:C:607:THR:HG23	7:D:801:YZY:H262	1.98	0.45
1:B:437:LEU:HD13	1:B:437:LEU:C	2.41	0.45
1:D:72:SER:HB3	1:D:75:LEU:HD23	1.98	0.45
1:D:388:ILE:O	1:D:389:VAL:C	2.59	0.45
1:D:459:LYS:HG2	1:D:460:TYR:CD2	2.52	0.45
1:A:304:GLN:HE21	1:A:305:PRO:HD2	1.82	0.45
1:A:577:TRP:CE3	1:A:582:LEU:HD12	2.52	0.45
1:C:529:LEU:HD12	1:C:529:LEU:HA	1.85	0.45
1:B:410:TRP:CD1	1:B:410:TRP:N	2.84	0.45
1:B:410:TRP:CD1	1:B:410:TRP:H	2.35	0.45
1:A:90:LEU:HD11	1:A:115:LEU:HD23	1.98	0.45
1:A:617:LEU:C	1:A:617:LEU:HD23	2.43	0.45
1:C:218:LEU:HD13	1:C:218:LEU:O	2.17	0.45
1:B:148:LEU:O	1:B:152:THR:HG23	2.16	0.45
1:B:268:ILE:CD1	1:B:720:LEU:HD11	2.46	0.45
1:B:513:MET:CE	1:B:630:LEU:HG	2.46	0.45
1:B:513:MET:HE3	1:B:630:LEU:HG	1.99	0.45
1:D:471:MET:HE3	1:D:471:MET:HB2	1.62	0.45
1:B:406:MET:O	1:B:409:PRO:HD2	2.17	0.44
1:B:408:LEU:O	1:B:408:LEU:HD22	2.16	0.44
1:A:384:ALA:CA	1:A:403:VAL:HG11	2.48	0.44
1:C:378:LEU:CD1	1:C:493:LEU:HD11	2.47	0.44
1:D:511:GLY:HA3	3:D:803:PTY:HC32	2.00	0.44
1:D:513:MET:O	1:D:517:ILE:HG12	2.18	0.44
1:C:533:ASN:OD1	1:D:382:LEU:HD23	2.17	0.44
1:B:44:ASP:OD2	1:B:44:ASP:O	2.36	0.44
1:B:108:VAL:HG13	1:B:108:VAL:O	2.17	0.44
1:B:501:SER:HA	1:B:639:TRP:CH2	2.52	0.44
1:D:340:LEU:O	1:D:344:LEU:HD12	2.16	0.44
1:D:438:MET:HE1	3:D:803:PTY:C15	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:641:PHE:O	1:D:645:LYS:HG3	2.17	0.44
1:D:708:ILE:HD12	1:D:709:GLN:H	1.81	0.44
1:A:613:LEU:HD23	1:A:614:VAL:N	2.32	0.44
1:B:516:ASP:C	1:B:623:MET:HE1	2.42	0.44
1:B:565:PHE:HD1	1:B:571:THR:HG23	1.82	0.44
1:D:434:TRP:HB3	3:D:803:PTY:C5	2.47	0.44
1:A:55:ALA:HB2	1:A:61:VAL:CG1	2.47	0.44
1:C:106:LYS:O	1:C:107:GLU:HB2	2.18	0.44
1:C:232:LYS:HE2	1:C:232:LYS:HB2	1.72	0.44
1:C:304:GLN:CD	1:C:305:PRO:HD2	2.43	0.44
1:C:702:ARG:HA	1:C:702:ARG:CZ	2.47	0.44
1:B:72:SER:O	1:B:76:ILE:HG13	2.16	0.44
1:D:44:ASP:OD1	1:D:44:ASP:O	2.35	0.44
1:D:403:VAL:O	1:D:407:ILE:HD12	2.18	0.44
1:D:623:MET:HE2	1:D:623:MET:HB3	1.80	0.44
1:A:318:GLY:HA2	1:A:362:LYS:HE3	2.00	0.44
1:C:155:TYR:CE1	1:C:211:LEU:HG	2.53	0.44
1:B:438:MET:HE3	3:B:803:PTY:H332	1.99	0.44
1:A:232:LYS:HE2	1:A:232:LYS:HB2	1.58	0.44
1:C:291:LYS:HG2	1:C:648:MET:CE	2.47	0.44
1:B:227:LEU:HD13	1:B:244:LEU:HB3	2.00	0.44
1:D:108:VAL:HG13	1:D:108:VAL:O	2.18	0.44
1:D:326:HIS:HB3	1:D:329:VAL:CG2	2.34	0.44
1:A:374:TYR:HD2	1:A:493:LEU:HD21	1.83	0.44
1:A:464:ARG:HG3	1:A:465:PRO:CD	2.45	0.44
1:C:626:ASN:O	1:C:630:LEU:HD13	2.17	0.44
1:C:746:LEU:HD21	1:B:746:LEU:HD13	1.99	0.44
4:C:803:Y01:HAB2	1:B:525:CYS:HB3	1.99	0.44
1:D:109:VAL:HG22	1:D:157:ILE:HD11	2.00	0.44
1:D:153:ASN:ND2	1:D:206:PRO:HD2	2.32	0.44
1:C:58:TYR:CD2	1:C:58:TYR:N	2.86	0.44
1:C:172:HIS:HB3	1:C:176:CYS:CB	2.47	0.44
1:C:452:LEU:HB3	1:C:478:ALA:HB2	1.99	0.44
1:D:57:ILE:HD12	1:D:58:TYR:HD1	1.83	0.44
1:A:538:LEU:HD22	1:A:604:MET:CE	2.48	0.43
1:B:311:LEU:HD13	1:B:644:THR:HG23	2.00	0.43
1:C:152:THR:CG2	1:C:154:ASN:HB2	2.48	0.43
1:C:272:ARG:CB	1:C:272:ARG:HH11	2.31	0.43
1:B:517:ILE:HG22	1:B:521:LEU:HG	2.00	0.43
1:B:524:TYR:OH	1:B:579:VAL:HG21	2.18	0.43
1:C:488:LEU:HD21	3:C:802:PTY:H202	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLN:O	1:B:135:GLN:HG3	2.18	0.43
1:B:526:LEU:HD12	1:B:526:LEU:C	2.43	0.43
1:B:556:ILE:O	1:B:561:GLN:HG2	2.18	0.43
1:D:348:TYR:O	1:D:352:PRO:HD3	2.17	0.43
1:A:81:GLU:HG3	1:A:745:GLU:HG3	1.99	0.43
1:A:501:SER:HA	1:A:639:TRP:CZ2	2.53	0.43
1:C:108:VAL:HG12	1:C:108:VAL:O	2.18	0.43
1:C:256:LEU:HD23	1:C:304:GLN:HG2	2.00	0.43
1:C:396:GLN:HE22	1:C:464:ARG:HD2	1.82	0.43
1:C:657:LEU:HD23	1:C:657:LEU:HA	1.77	0.43
1:D:631:ILE:O	1:D:635:ALA:HB2	2.19	0.43
1:A:233:VAL:O	1:A:233:VAL:CG1	2.67	0.43
1:A:381:LEU:HD23	1:A:407:ILE:HD11	1.99	0.43
1:C:289:LYS:HB2	1:C:289:LYS:HE2	1.70	0.43
1:C:615:VAL:HG23	1:C:616:LEU:N	2.33	0.43
1:C:659:PRO:N	1:C:660:PRO:CD	2.81	0.43
1:D:44:ASP:HB3	1:D:755:TYR:CD2	2.54	0.43
1:D:708:ILE:HD12	1:D:708:ILE:C	2.43	0.43
1:A:58:TYR:N	1:A:58:TYR:HD2	2.16	0.43
1:A:60:ASN:OD1	1:A:60:ASN:N	2.49	0.43
1:A:408:LEU:HB3	1:A:409:PRO:HD3	2.01	0.43
1:A:610:VAL:HG11	7:B:801:YZY:H252	2.01	0.43
1:C:715:GLU:OE1	1:C:715:GLU:HA	2.18	0.43
1:B:627:SER:HA	1:B:630:LEU:HB3	1.99	0.43
1:B:637:ILE:HD12	1:B:637:ILE:N	2.34	0.43
1:B:730:ARG:HD3	1:B:730:ARG:O	2.18	0.43
1:D:584:ASN:O	1:D:587:VAL:HG22	2.17	0.43
1:A:87:GLU:HG2	1:A:114:LEU:HD11	2.00	0.43
1:C:326:HIS:ND1	1:C:327:TRP:N	2.67	0.43
1:B:366:LYS:HG2	1:B:650:TYR:HD1	1.83	0.43
1:B:381:LEU:CD2	1:B:407:ILE:HD13	2.45	0.43
1:B:394:HIS:CD2	1:B:466:ARG:H	2.36	0.43
1:D:660:PRO:HG2	1:D:661:PHE:CD2	2.54	0.43
1:A:200:TYR:CE2	1:A:230:LEU:HD11	2.54	0.43
1:A:338:GLY:O	1:A:341:PHE:HD2	2.02	0.43
1:C:546:ALA:O	1:C:552:ASN:HA	2.18	0.43
1:D:593:ARG:HA	1:D:593:ARG:HD2	1.59	0.43
1:C:366:LYS:HD3	1:C:656:THR:HA	2.01	0.43
1:C:500:ASN:HB2	4:C:803:Y01:HAR1	2.01	0.43
1:C:659:PRO:HA	1:C:662:ASN:OD1	2.18	0.43
1:B:346:ILE:HG22	1:B:350:ILE:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:GLU:C	1:D:186:GLU:OE2	2.61	0.43
1:D:230:LEU:HD23	1:D:241:TYR:CE1	2.53	0.43
1:A:402:VAL:O	1:A:406:MET:HG3	2.18	0.43
1:D:375:LEU:HD21	4:D:804:Y01:HAQ2	2.01	0.43
1:D:396:GLN:HE21	1:D:460:TYR:HB3	1.84	0.43
1:D:746:LEU:HD12	1:D:746:LEU:HA	1.87	0.43
1:A:382:LEU:O	1:A:386:GLN:NE2	2.50	0.42
1:A:513:MET:HE1	1:D:618:ASN:CB	2.49	0.42
1:A:614:VAL:CG2	1:A:615:VAL:HG23	2.45	0.42
1:A:627:SER:HA	1:A:630:LEU:HD23	2.01	0.42
1:C:40:VAL:HG12	1:C:76:ILE:CG2	2.49	0.42
1:C:350:ILE:CG2	1:C:351:SER:N	2.82	0.42
1:C:438:MET:HE3	3:C:802:PTY:H312	2.00	0.42
1:B:409:PRO:HG2	1:B:410:TRP:HD1	1.84	0.42
1:B:500:ASN:HB2	4:B:804:Y01:HAR1	1.98	0.42
1:A:737:GLY:HA2	1:D:739:THR:HA	2.01	0.42
1:C:310:LEU:HD12	1:C:310:LEU:O	2.18	0.42
1:C:326:HIS:CE1	1:C:328:VAL:HG22	2.54	0.42
1:C:701:GLU:OE1	1:C:704:ALA:HB3	2.19	0.42
1:B:318:GLY:HA2	1:B:362:LYS:HE3	2.01	0.42
1:D:526:LEU:HD12	1:D:526:LEU:C	2.44	0.42
1:D:659:PRO:HG2	1:D:660:PRO:CD	2.48	0.42
1:A:560:LYS:O	1:A:560:LYS:HG3	2.20	0.42
1:C:263:ARG:HH11	1:C:263:ARG:HB3	1.84	0.42
1:C:393:LEU:N	1:C:393:LEU:HD22	2.34	0.42
1:C:734:THR:HG22	1:B:741:GLU:OE1	2.19	0.42
1:B:163:GLN:C	1:B:164:LYS:HD3	2.44	0.42
1:D:368:ILE:HD13	1:D:368:ILE:HA	1.88	0.42
1:D:740:GLU:HB3	1:D:744:LYS:HZ1	1.80	0.42
1:A:44:ASP:O	1:A:48:VAL:HG23	2.20	0.42
1:C:56:GLU:OE2	1:C:57:ILE:HG12	2.19	0.42
1:C:615:VAL:CG2	1:C:616:LEU:N	2.83	0.42
1:B:113:GLU:OE2	1:B:160:LEU:HD22	2.18	0.42
4:D:804:Y01:HAB1	4:D:804:Y01:HAC3	2.01	0.42
1:A:67:ASP:CB	1:A:71:ARG:HB2	2.49	0.42
1:A:454:ILE:O	1:A:458:VAL:HG13	2.20	0.42
1:A:595:GLU:HG2	1:B:471:MET:HE2	2.01	0.42
1:C:58:TYR:HD2	1:C:58:TYR:N	2.18	0.42
1:C:90:LEU:HD12	1:C:118:TYR:CE2	2.54	0.42
1:B:22:ILE:O	1:B:22:ILE:HG22	2.18	0.42
1:D:348:TYR:C	1:D:348:TYR:CD2	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:LEU:HA	1:D:571:THR:CG2	2.50	0.42
1:A:63:ILE:HD12	1:A:94:VAL:HG12	2.02	0.42
1:A:324:ARG:HH11	1:A:324:ARG:CG	2.32	0.42
1:A:348:TYR:HB2	1:A:360:ILE:CG2	2.49	0.42
1:C:333:THR:HA	1:C:336:THR:HG22	2.01	0.42
1:C:350:ILE:O	1:C:351:SER:C	2.62	0.42
1:D:174:ILE:HG22	1:D:230:LEU:CD1	2.48	0.42
1:D:196:ARG:HG3	1:D:196:ARG:HH11	1.83	0.42
1:D:536:ASN:O	1:D:540:PHE:HB3	2.20	0.42
1:D:663:ILE:O	1:D:663:ILE:HG22	2.18	0.42
1:A:147:MET:HE3	1:A:198:ASN:HB3	2.02	0.42
1:C:420:LYS:HB2	1:C:420:LYS:HE2	1.74	0.42
1:B:384:ALA:HA	1:B:403:VAL:HG21	2.02	0.42
1:B:513:MET:HE1	1:B:630:LEU:CD1	2.50	0.42
1:A:611:ILE:O	1:A:615:VAL:HB	2.19	0.42
1:A:736:GLU:HG2	1:D:740:GLU:OE2	2.20	0.42
1:C:406:MET:O	1:C:409:PRO:HD2	2.20	0.42
1:B:656:THR:HG23	1:B:657:LEU:N	2.35	0.42
1:D:78:ILE:HG13	1:D:86:MET:SD	2.60	0.42
1:A:168:ILE:HG13	1:D:20:LEU:HD11	2.00	0.42
1:C:96:VAL:O	1:C:96:VAL:CG2	2.67	0.42
1:A:437:LEU:HD23	3:A:802:PTY:H322	2.02	0.42
1:A:625:ASN:N	1:D:621:ILE:HD13	2.34	0.42
1:C:174:ILE:N	1:C:174:ILE:CD1	2.83	0.42
1:B:33:GLU:HG2	1:B:61:VAL:HG13	2.01	0.42
1:B:58:TYR:HD1	1:B:58:TYR:N	2.17	0.42
1:B:383:LEU:O	1:B:387:HIS:HB2	2.19	0.42
1:D:659:PRO:CD	1:D:660:PRO:HD2	2.50	0.42
1:A:140:THR:HB	1:A:141:PRO:HD2	2.01	0.41
1:A:512:ARG:NH1	1:A:512:ARG:HG2	2.35	0.41
1:A:659:PRO:N	1:A:660:PRO:CD	2.83	0.41
1:C:86:MET:HE2	1:C:86:MET:HB2	1.87	0.41
1:C:621:ILE:HD12	1:D:620:LEU:HD13	2.02	0.41
1:C:745:GLU:OE1	1:B:743:PHE:HZ	2.03	0.41
1:B:513:MET:HE1	1:B:630:LEU:HD11	2.01	0.41
1:A:44:ASP:CG	1:A:47:THR:HB	2.45	0.41
1:A:69:LEU:HD23	1:B:729:ILE:CD1	2.50	0.41
1:A:197:LEU:HD12	1:A:197:LEU:C	2.45	0.41
1:A:374:TYR:CD2	1:A:493:LEU:HD21	2.56	0.41
1:C:408:LEU:N	1:C:409:PRO:HD2	2.34	0.41
1:C:434:TRP:O	1:C:437:LEU:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:ASN:O	1:C:735:HIS:HB2	2.19	0.41
1:B:90:LEU:HD12	1:B:114:LEU:HD22	2.02	0.41
1:D:96:VAL:O	1:D:96:VAL:HG12	2.20	0.41
1:D:197:LEU:HD21	1:D:240:GLU:HG2	2.02	0.41
1:A:438:MET:HE3	3:A:802:PTY:H312	2.01	0.41
1:A:625:ASN:O	1:A:629:GLN:HG2	2.20	0.41
1:C:236:GLU:HG2	1:D:309:GLN:HB2	2.02	0.41
1:C:439:ASP:HA	1:C:442:MET:HE3	2.01	0.41
1:C:545:ARG:HB3	1:C:547:ILE:HD12	2.03	0.41
1:B:409:PRO:HG2	1:B:410:TRP:CD1	2.55	0.41
1:B:438:MET:HE1	3:B:803:PTY:H142	2.01	0.41
1:B:659:PRO:HG2	1:B:660:PRO:CD	2.49	0.41
1:D:328:VAL:HA	1:D:331:LEU:HD12	2.01	0.41
1:A:326:HIS:O	1:A:329:VAL:HG12	2.21	0.41
1:C:519:LYS:HE2	1:C:519:LYS:HB2	1.81	0.41
1:B:82:ASN:ND2	1:B:748:GLN:HE22	2.08	0.41
1:B:113:GLU:OE1	1:B:113:GLU:HA	2.20	0.41
1:D:190:LEU:HD12	1:D:190:LEU:C	2.45	0.41
1:D:327:TRP:CD1	1:D:328:VAL:H	2.38	0.41
1:D:408:LEU:O	1:D:411:VAL:HG22	2.20	0.41
1:D:416:TRP:CB	1:D:663:ILE:HD11	2.50	0.41
1:A:42:LYS:HA	1:A:42:LYS:HD3	1.85	0.41
1:A:57:ILE:HG22	1:A:58:TYR:HD2	1.84	0.41
1:A:396:GLN:O	1:A:398:PRO:HD3	2.21	0.41
1:A:707:LEU:HD22	1:A:707:LEU:H	1.85	0.41
1:C:613:LEU:HD23	1:C:614:VAL:N	2.36	0.41
1:B:86:MET:HE2	1:B:86:MET:HB3	1.85	0.41
1:B:421:GLU:OE1	1:B:421:GLU:CA	2.69	0.41
1:B:464:ARG:HG3	1:B:465:PRO:CD	2.43	0.41
1:B:591:LYS:HE2	1:B:591:LYS:HB2	1.56	0.41
1:D:227:LEU:HD13	1:D:244:LEU:HB3	2.03	0.41
1:D:341:PHE:N	1:D:342:PRO:CD	2.83	0.41
1:A:322:TRP:O	1:A:330:LYS:HD2	2.21	0.41
1:A:405:TRP:CE3	1:A:405:TRP:HA	2.56	0.41
1:C:618:ASN:OD1	1:D:623:MET:SD	2.79	0.41
1:B:744:LYS:O	1:B:747:LYS:HG2	2.21	0.41
1:B:759:ASP:OD1	1:B:759:ASP:C	2.63	0.41
1:A:154:ASN:OD1	1:A:157:ILE:HG12	2.20	0.41
1:A:625:ASN:HD22	1:B:624:MET:CG	2.33	0.41
1:C:69:LEU:HD23	1:D:729:ILE:HD12	2.02	0.41
1:B:377:PHE:HB2	1:B:410:TRP:HE3	1.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:THR:HG21	1:D:482:PHE:HB2	2.03	0.41
1:A:179:VAL:O	1:A:183:SER:HB3	2.21	0.41
1:C:44:ASP:CG	1:C:47:THR:HB	2.46	0.41
1:C:67:ASP:HB2	1:C:71:ARG:HG3	2.02	0.41
1:C:108:VAL:CG1	1:C:111:ALA:H	2.29	0.41
1:C:515:LEU:HD13	1:C:515:LEU:HA	1.92	0.41
1:C:520:PHE:HE2	5:C:804:A1L55:C31	2.34	0.41
1:C:722:LYS:HB2	1:C:722:LYS:HE2	1.89	0.41
1:B:353:ARG:HD3	1:B:353:ARG:N	2.36	0.41
1:B:630:LEU:HD22	1:B:631:ILE:HD11	2.02	0.41
1:B:646:LEU:HD23	1:B:646:LEU:C	2.46	0.41
1:B:725:VAL:O	1:B:729:ILE:HG13	2.21	0.41
1:D:49:LYS:HB2	1:D:88:LEU:HD21	2.02	0.41
1:D:180:GLU:O	1:D:180:GLU:CD	2.63	0.41
1:D:402:VAL:O	1:D:405:TRP:O	2.39	0.41
1:A:201:LYS:HE3	1:A:201:LYS:HB2	1.77	0.41
1:A:396:GLN:HB3	1:A:460:TYR:CG	2.55	0.41
1:C:79:GLU:OE1	1:C:79:GLU:HA	2.21	0.41
1:C:648:MET:HE3	1:C:648:MET:HB3	1.84	0.41
1:B:105:ARG:HD3	1:B:139:PHE:HE1	1.86	0.41
1:B:658:PRO:C	1:B:660:PRO:HD2	2.46	0.41
1:A:510:LEU:CD2	1:D:618:ASN:HD22	2.34	0.40
1:A:615:VAL:HG11	7:B:801:YZY:H351	2.03	0.40
1:C:392:ASP:C	1:C:393:LEU:HD13	2.46	0.40
1:B:17:ARG:HB3	1:B:17:ARG:HH11	1.86	0.40
1:B:299:LYS:HG3	1:B:641:PHE:CG	2.56	0.40
1:A:319:PHE:HE1	1:A:364:PHE:CD2	2.38	0.40
1:A:517:ILE:O	1:A:521:LEU:HB2	2.22	0.40
1:C:55:ALA:O	1:C:59:TYR:HA	2.20	0.40
1:C:479:GLU:OE1	1:B:541:TYR:CE2	2.75	0.40
1:C:492:ARG:O	1:C:492:ARG:HG3	2.19	0.40
1:B:89:LEU:HB3	1:B:94:VAL:HG21	2.04	0.40
1:B:353:ARG:HG2	1:B:353:ARG:HH11	1.86	0.40
1:A:319:PHE:CE1	1:A:364:PHE:HD2	2.37	0.40
5:A:804:A1L55:C18	5:A:804:A1L55:C13	3.00	0.40
1:C:67:ASP:HB2	1:C:71:ARG:CG	2.51	0.40
1:B:44:ASP:HB3	1:B:755:TYR:CD2	2.57	0.40
1:B:408:LEU:N	1:B:409:PRO:HD2	2.36	0.40
1:B:593:ARG:HD2	1:B:593:ARG:HA	1.55	0.40
1:D:568:LEU:HA	1:D:571:THR:HG22	2.04	0.40
1:C:272:ARG:HB2	1:C:272:ARG:CZ	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ILE:HG22	1:C:351:SER:H	1.84	0.40
1:C:739:THR:OG1	1:C:741:GLU:HG2	2.22	0.40
1:D:179:VAL:CG1	1:D:180:GLU:N	2.83	0.40
1:A:517:ILE:CD1	1:A:517:ILE:N	2.84	0.40
1:C:326:HIS:HB3	1:C:329:VAL:HG12	2.02	0.40
1:B:42:LYS:HA	1:B:42:LYS:HD2	1.83	0.40
1:B:380:MET:HE2	1:B:380:MET:HA	2.03	0.40
1:B:619:MET:O	1:B:623:MET:HG2	2.21	0.40
1:B:707:LEU:H	1:B:707:LEU:HD22	1.85	0.40
1:D:401:THR:HG22	1:D:402:VAL:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	676/765 (88%)	658 (97%)	18 (3%)	0	100	100
1	B	676/765 (88%)	662 (98%)	14 (2%)	0	100	100
1	C	676/765 (88%)	659 (98%)	17 (2%)	0	100	100
1	D	673/765 (88%)	659 (98%)	14 (2%)	0	100	100
All	All	2701/3060 (88%)	2638 (98%)	63 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	611/687 (89%)	606 (99%)	5 (1%)	73	90
1	B	611/687 (89%)	608 (100%)	3 (0%)	81	93
1	C	612/687 (89%)	605 (99%)	7 (1%)	65	88
1	D	610/687 (89%)	605 (99%)	5 (1%)	73	90
All	All	2444/2748 (89%)	2424 (99%)	20 (1%)	70	90

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	ILE
1	A	386	GLN
1	A	406	MET
1	A	545	ARG
1	A	662	ASN
1	C	53	GLN
1	C	319	PHE
1	C	382	LEU
1	C	386	GLN
1	C	396	GLN
1	C	418	GLU
1	C	634	HIS
1	B	242	GLU
1	B	591	LYS
1	B	709	GLN
1	D	69	LEU
1	D	388	ILE
1	D	389	VAL
1	D	393	LEU
1	D	470	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	192	HIS
1	A	563	ASN
1	A	584	ASN
1	C	80	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	154	ASN
1	C	308	GLN
1	C	396	GLN
1	C	609	ASN
1	B	62	ASN
1	B	92	HIS
1	B	247	GLN
1	B	298	GLN
1	B	309	GLN
1	B	394	HIS
1	B	507	GLN
1	B	552	ASN
1	B	711	GLN
1	B	714	GLN
1	B	731	ASN
1	B	748	GLN
1	D	154	ASN
1	D	247	GLN
1	D	298	GLN
1	D	308	GLN
1	D	394	HIS
1	D	396	GLN
1	D	536	ASN
1	D	742	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PTY	C	802	-	49,49,49	0.46	0	52,54,54	0.47	0
3	PTY	B	803	-	49,49,49	0.46	0	52,54,54	0.43	0
5	A1L55	C	804	-	33,35,35	0.32	0	37,53,53	0.67	1 (2%)
4	Y01	D	804	-	38,38,38	0.54	0	57,57,57	0.94	1 (1%)
4	Y01	A	803	-	38,38,38	0.55	0	57,57,57	0.98	3 (5%)
7	YZY	D	801	-	41,41,41	0.35	0	43,43,43	0.44	1 (2%)
3	PTY	D	803	-	49,49,49	0.47	0	52,54,54	0.40	0
3	PTY	A	802	-	49,49,49	0.47	0	52,54,54	0.41	0
4	Y01	B	804	-	38,38,38	0.55	0	57,57,57	1.06	3 (5%)
7	YZY	B	801	-	41,41,41	0.35	0	43,43,43	1.04	2 (4%)
5	A1L55	A	804	-	33,35,35	0.35	0	37,53,53	0.67	2 (5%)
4	Y01	C	803	-	38,38,38	0.55	0	57,57,57	0.98	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PTY	C	802	-	-	27/53/53/53	-
3	PTY	B	803	-	-	30/53/53/53	-
5	A1L55	C	804	-	-	2/21/67/67	0/5/4/4
4	Y01	D	804	-	-	4/19/77/77	0/4/4/4
4	Y01	A	803	-	-	5/19/77/77	0/4/4/4
7	YZY	D	801	-	-	18/43/43/43	-
3	PTY	D	803	-	-	24/53/53/53	-
7	YZY	B	801	-	1/1/5/5	19/43/43/43	-
3	PTY	A	802	-	-	28/53/53/53	-
4	Y01	B	804	-	-	5/19/77/77	0/4/4/4
5	A1L55	A	804	-	-	2/21/67/67	0/5/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Y01	C	803	-	-	4/19/77/77	0/4/4/4

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	801	YZY	C19-C2-C1	5.64	125.01	111.80
7	B	801	YZY	O2-C2-C1	2.75	118.24	108.36
4	B	804	Y01	CAR-CBC-CAV	2.59	114.85	110.99
4	A	803	Y01	CBH-CBF-CBD	-2.48	109.01	112.73
4	B	804	Y01	CBH-CBF-CBD	-2.32	109.25	112.73
5	C	804	A1L55	O12-C11-C10	-2.27	105.95	111.32
4	B	804	Y01	CAU-CBI-CBG	-2.27	103.75	107.27
4	A	803	Y01	CBF-CBD-CBG	2.22	112.06	109.09
5	A	804	A1L55	C18-C17-C19	-2.17	109.59	113.12
4	C	803	Y01	CAR-CBC-CAV	2.16	114.20	110.99
4	C	803	Y01	CBH-CBF-CBD	-2.16	109.50	112.73
4	D	804	Y01	CAR-CBC-CAV	2.08	114.09	110.99
4	A	803	Y01	CAR-CBC-CAV	2.02	114.00	110.99
5	A	804	A1L55	O03-C04-C05	2.02	113.28	108.97
7	D	801	YZY	C19-C2-C1	2.01	116.52	111.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	801	YZY	C2

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	PTY	O30-C30-O4-C1
3	A	802	PTY	C5-O14-P1-O13
3	C	802	PTY	C3-O11-P1-O12
3	C	802	PTY	C3-O11-P1-O13
3	C	802	PTY	C3-O11-P1-O14
3	B	803	PTY	C3-O11-P1-O12
3	B	803	PTY	C3-O11-P1-O13
3	D	803	PTY	O10-C8-O7-C6
3	D	803	PTY	C5-O14-P1-O12
5	A	804	A1L55	O12-C13-C14-O15
5	A	804	A1L55	O16-C13-C14-O15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	801	YZY	O1-C1-C2-C19
7	D	801	YZY	O1-C1-C2-O2
7	D	801	YZY	O1-C1-C2-C19
3	A	802	PTY	C31-C30-O4-C1
3	A	802	PTY	O10-C8-O7-C6
3	A	802	PTY	C11-C8-O7-C6
3	D	803	PTY	C11-C8-O7-C6
3	B	803	PTY	O30-C30-O4-C1
3	B	803	PTY	C31-C30-O4-C1
3	D	803	PTY	C31-C30-O4-C1
7	B	801	YZY	C21-C20-O4-C19
4	A	803	Y01	CAM-CAY-OAW-CBC
7	B	801	YZY	O5-C20-O4-C19
3	C	802	PTY	C31-C30-O4-C1
3	D	803	PTY	O30-C30-O4-C1
3	B	803	PTY	C11-C8-O7-C6
3	C	802	PTY	O30-C30-O4-C1
3	C	802	PTY	C11-C8-O7-C6
7	B	801	YZY	C20-C21-C22-C23
3	C	802	PTY	C8-C11-C12-C13
4	A	803	Y01	OAG-CAY-OAW-CBC
3	B	803	PTY	C8-C11-C12-C13
3	C	802	PTY	O10-C8-O7-C6
3	B	803	PTY	O10-C8-O7-C6
3	A	802	PTY	C5-O14-P1-O11
3	B	803	PTY	C3-O11-P1-O14
3	D	803	PTY	C5-O14-P1-O11
7	D	801	YZY	C21-C20-O4-C19
3	B	803	PTY	C18-C19-C20-C21
7	B	801	YZY	C13-C14-C15-C16
3	A	802	PTY	C18-C19-C20-C21
3	D	803	PTY	C15-C16-C17-C18
7	D	801	YZY	C10-C11-C12-C13
3	C	802	PTY	C39-C40-C41-C42
7	B	801	YZY	C9-C10-C11-C12
3	B	803	PTY	C22-C23-C24-C25
7	B	801	YZY	C23-C24-C25-C26
4	D	804	Y01	CAO-CAJ-CAN-CBA
7	B	801	YZY	C10-C11-C12-C13
7	D	801	YZY	C29-C30-C31-C32
3	C	802	PTY	C22-C23-C24-C25
3	D	803	PTY	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	802	PTY	C15-C16-C17-C18
7	D	801	YZY	O5-C20-O4-C19
3	B	803	PTY	C15-C16-C17-C18
7	D	801	YZY	C11-C10-C9-C8
3	B	803	PTY	C34-C35-C36-C37
3	D	803	PTY	C37-C38-C39-C40
3	B	803	PTY	C32-C33-C34-C35
7	D	801	YZY	C23-C24-C25-C26
3	C	802	PTY	C15-C16-C17-C18
3	D	803	PTY	C19-C20-C21-C22
7	D	801	YZY	C12-C13-C14-C15
3	C	802	PTY	C38-C39-C40-C41
3	C	802	PTY	C12-C13-C14-C15
7	D	801	YZY	C5-C6-C7-C8
3	A	802	PTY	C11-C12-C13-C14
3	A	802	PTY	C12-C13-C14-C15
4	C	803	Y01	CAM-CAY-OAW-CBC
4	B	804	Y01	CAM-CAY-OAW-CBC
5	C	804	A1L55	C25-C26-C27-C32
7	D	801	YZY	O4-C19-C2-O2
4	B	804	Y01	OAG-CAY-OAW-CBC
3	D	803	PTY	C6-C5-O14-P1
7	B	801	YZY	C5-C6-C7-C8
5	C	804	A1L55	C25-C26-C27-C28
7	B	801	YZY	C11-C10-C9-C8
3	B	803	PTY	C19-C20-C21-C22
3	D	803	PTY	C32-C33-C34-C35
3	A	802	PTY	C37-C38-C39-C40
3	B	803	PTY	C23-C24-C25-C26
3	D	803	PTY	C12-C13-C14-C15
7	D	801	YZY	C4-C5-C6-C7
3	D	803	PTY	C8-C11-C12-C13
3	C	802	PTY	C19-C20-C21-C22
3	C	802	PTY	C11-C12-C13-C14
3	C	802	PTY	C23-C24-C25-C26
3	D	803	PTY	O14-C5-C6-O7
3	D	803	PTY	O4-C1-C6-O7
3	C	802	PTY	C18-C19-C20-C21
3	B	803	PTY	C39-C40-C41-C42
3	A	802	PTY	C39-C40-C41-C42
3	D	803	PTY	O14-C5-C6-C1
3	A	802	PTY	N1-C2-C3-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	803	PTY	C11-C12-C13-C14
4	C	803	Y01	OAG-CAY-OAW-CBC
7	B	801	YZY	C15-C16-C17-C18
3	A	802	PTY	C6-C5-O14-P1
7	D	801	YZY	O4-C19-C2-C1
3	D	803	PTY	C18-C19-C20-C21
7	B	801	YZY	O4-C19-C2-O2
3	B	803	PTY	C35-C36-C37-C38
7	B	801	YZY	C34-C35-C36-C37
3	A	802	PTY	C22-C23-C24-C25
3	A	802	PTY	C35-C36-C37-C38
3	B	803	PTY	C38-C39-C40-C41
3	C	802	PTY	C35-C36-C37-C38
3	C	802	PTY	C5-C6-O7-C8
7	B	801	YZY	C29-C30-C31-C32
3	D	803	PTY	O4-C1-C6-C5
3	A	802	PTY	C23-C24-C25-C26
3	B	803	PTY	O14-C5-C6-O7
3	A	802	PTY	C14-C15-C16-C17
7	B	801	YZY	C11-C12-C13-C14
7	B	801	YZY	C33-C34-C35-C36
3	C	802	PTY	C37-C38-C39-C40
3	A	802	PTY	C5-O14-P1-O12
3	D	803	PTY	C3-O11-P1-O12
3	A	802	PTY	C8-C11-C12-C13
3	B	803	PTY	O14-C5-C6-C1
3	A	802	PTY	C19-C20-C21-C22
3	A	802	PTY	C38-C39-C40-C41
3	A	802	PTY	C5-C6-O7-C8
7	B	801	YZY	C21-C22-C23-C24
3	D	803	PTY	C22-C23-C24-C25
7	D	801	YZY	C26-C27-C28-C29
3	A	802	PTY	C34-C35-C36-C37
4	A	803	Y01	CAM-CAL-CAX-OAF
4	B	804	Y01	CAM-CAL-CAX-OAF
3	C	802	PTY	C16-C17-C18-C19
3	B	803	PTY	C5-C6-O7-C8
4	A	803	Y01	CAM-CAL-CAX-OAH
4	C	803	Y01	CAM-CAL-CAX-OAF
4	B	804	Y01	CAM-CAL-CAX-OAH
4	A	803	Y01	CAO-CAJ-CAN-CBA
3	D	803	PTY	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	D	801	YZY	C3-C4-C5-C6
3	A	802	PTY	C24-C25-C26-C27
7	D	801	YZY	C14-C15-C16-C17
3	B	803	PTY	N1-C2-C3-O11
3	B	803	PTY	C12-C13-C14-C15
3	B	803	PTY	C14-C15-C16-C17
3	B	803	PTY	C12-C11-C8-O7
3	A	802	PTY	C3-O11-P1-O14
3	C	802	PTY	C5-O14-P1-O11
3	C	802	PTY	C24-C25-C26-C27
4	D	804	Y01	CAV-CBC-OAW-CAY
7	D	801	YZY	C33-C34-C35-C36
3	C	802	PTY	C12-C11-C8-O7
7	B	801	YZY	O2-C3-C4-C5
4	C	803	Y01	CAM-CAL-CAX-OAH
3	B	803	PTY	C20-C21-C22-C23
4	B	804	Y01	CAJ-CAO-CBB-CAC
4	D	804	Y01	CAM-CAL-CAX-OAF
3	D	803	PTY	C34-C35-C36-C37
3	B	803	PTY	C37-C38-C39-C40
3	B	803	PTY	C12-C11-C8-O10
7	B	801	YZY	O3-C3-C4-C5
3	C	802	PTY	C32-C33-C34-C35
3	B	803	PTY	C16-C17-C18-C19
3	C	802	PTY	C12-C11-C8-O10
4	D	804	Y01	CAM-CAL-CAX-OAH
3	A	802	PTY	C3-O11-P1-O13
3	C	802	PTY	C5-O14-P1-O13
3	B	803	PTY	C11-C12-C13-C14
7	D	801	YZY	C15-C16-C17-C18
3	A	802	PTY	C12-C11-C8-O7

There are no ring outliers.

12 monomers are involved in 49 short contacts:

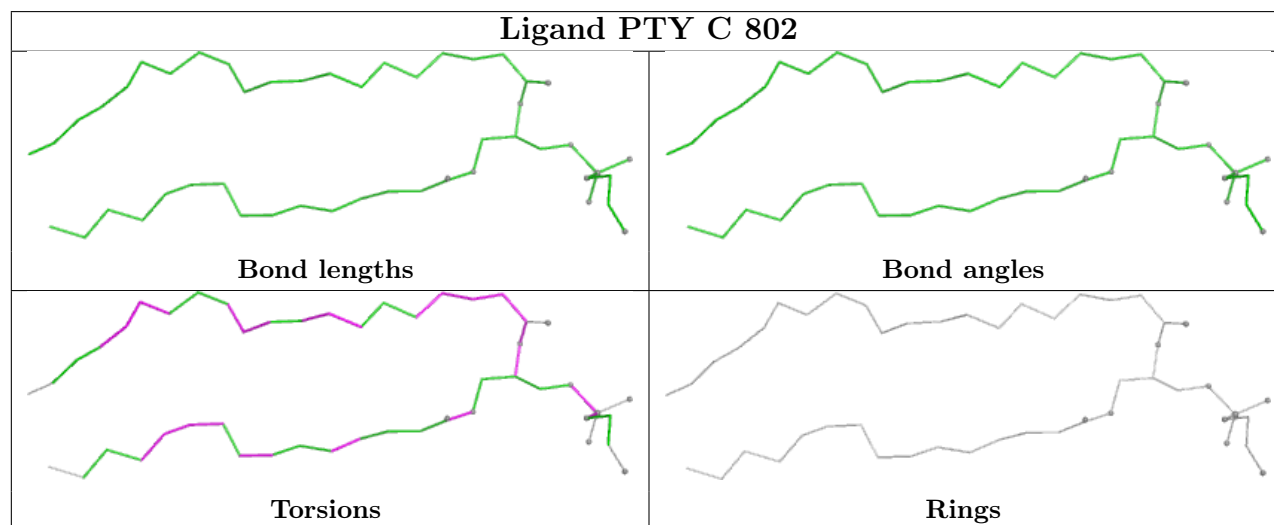
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	802	PTY	3	0
3	B	803	PTY	3	0
5	C	804	A1L55	2	0
4	D	804	Y01	5	0
4	A	803	Y01	1	0
7	D	801	YZY	4	0

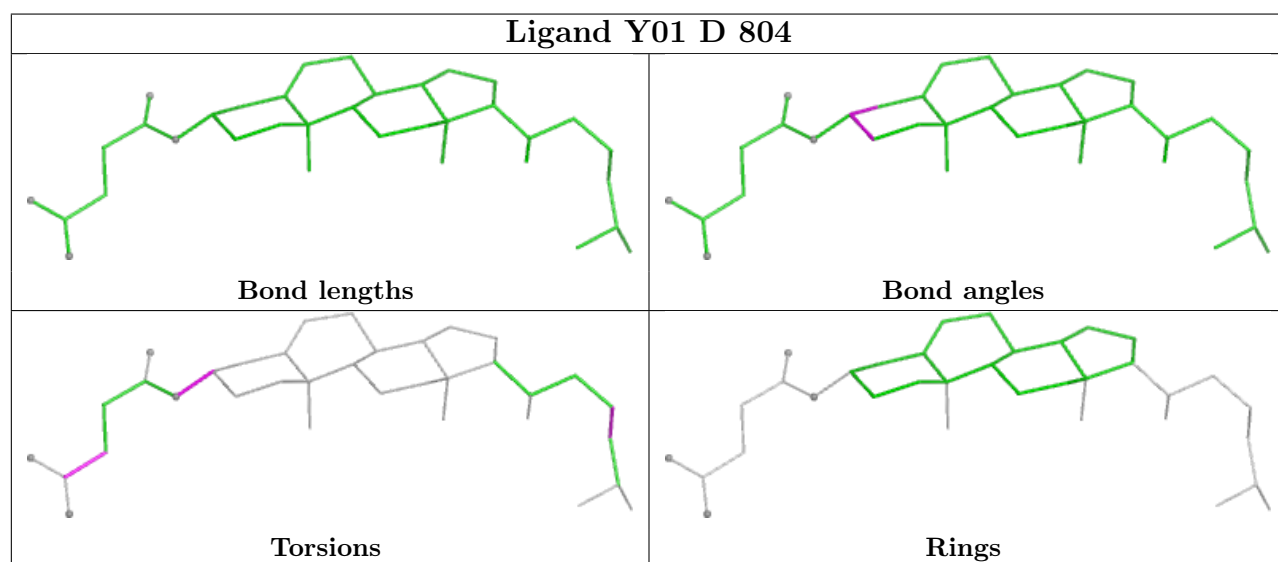
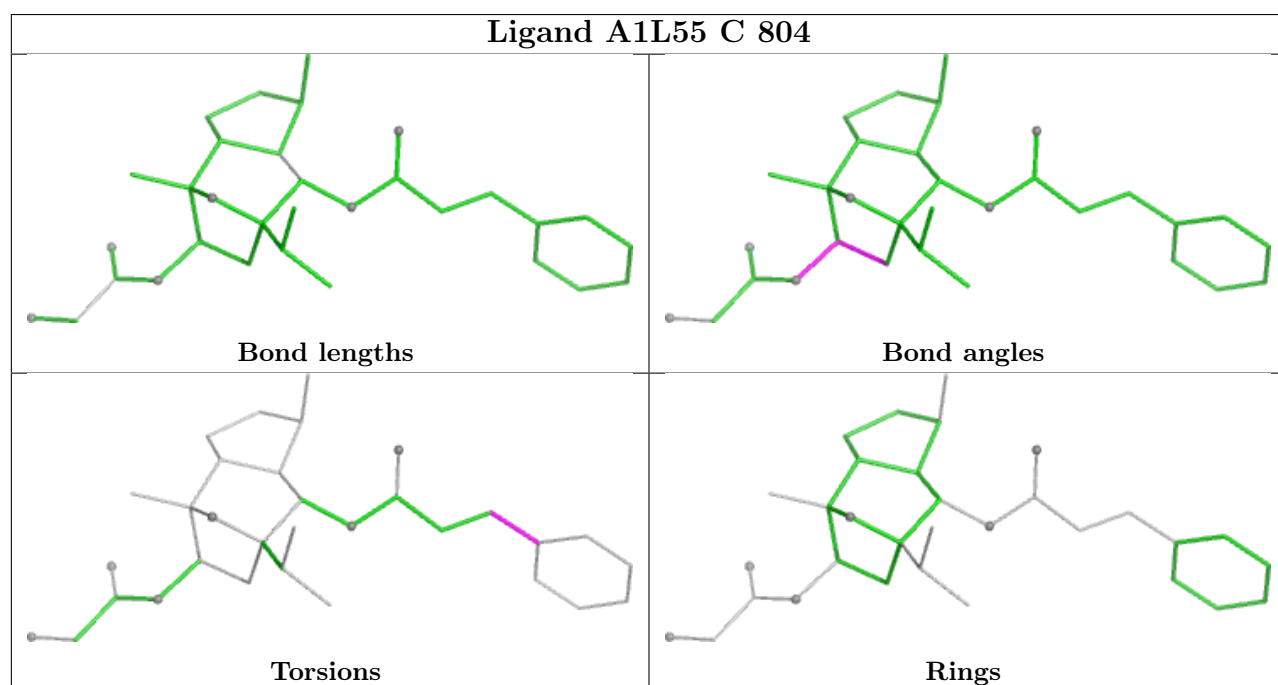
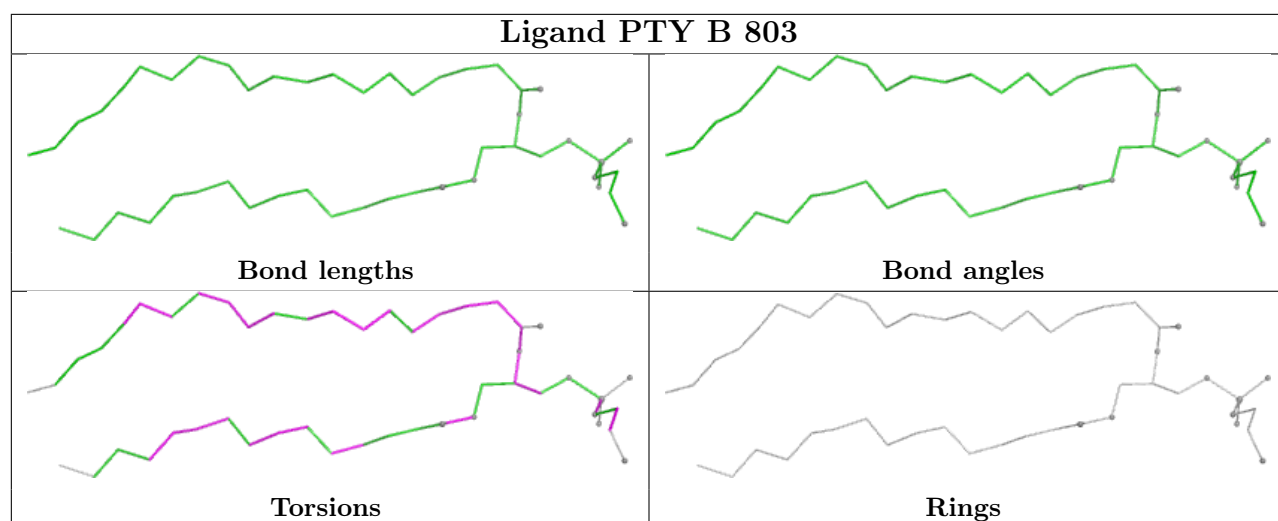
Continued on next page...

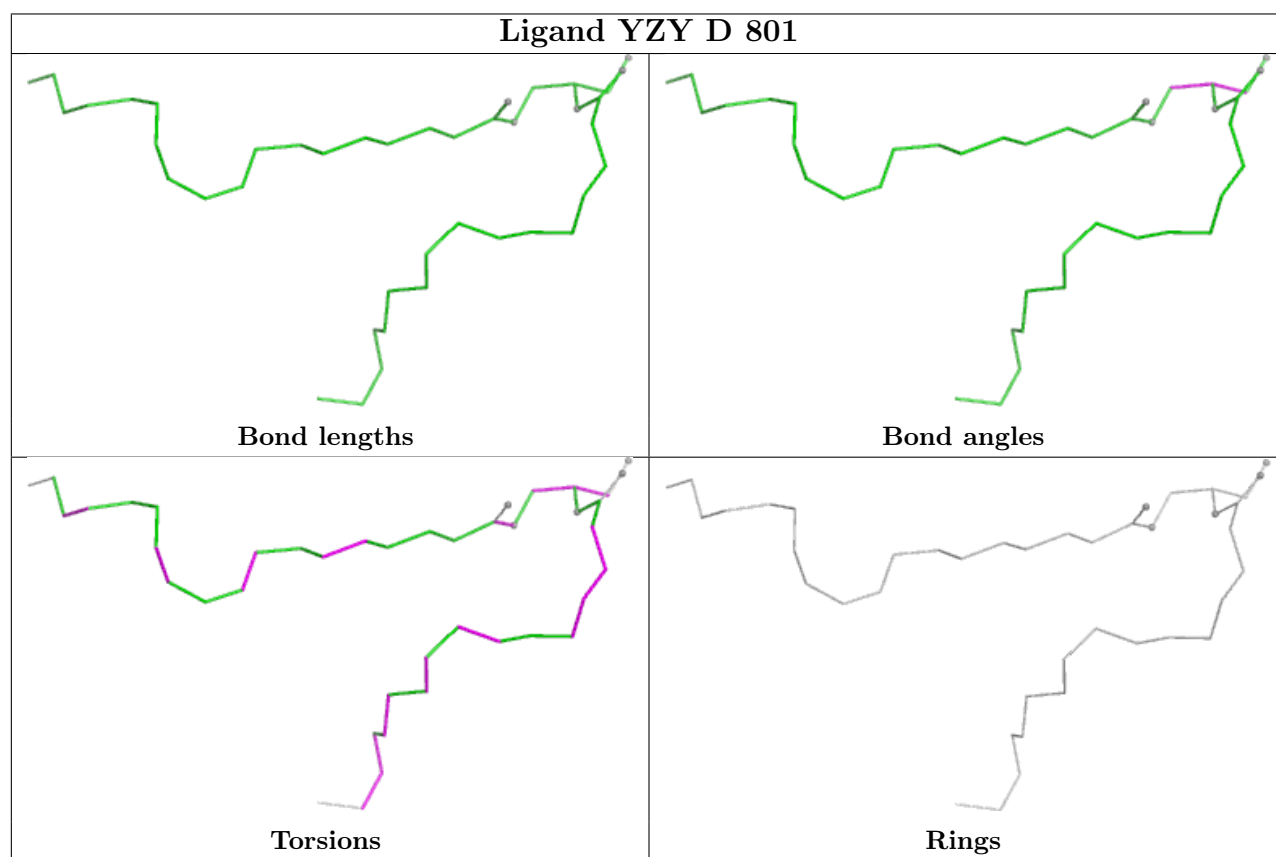
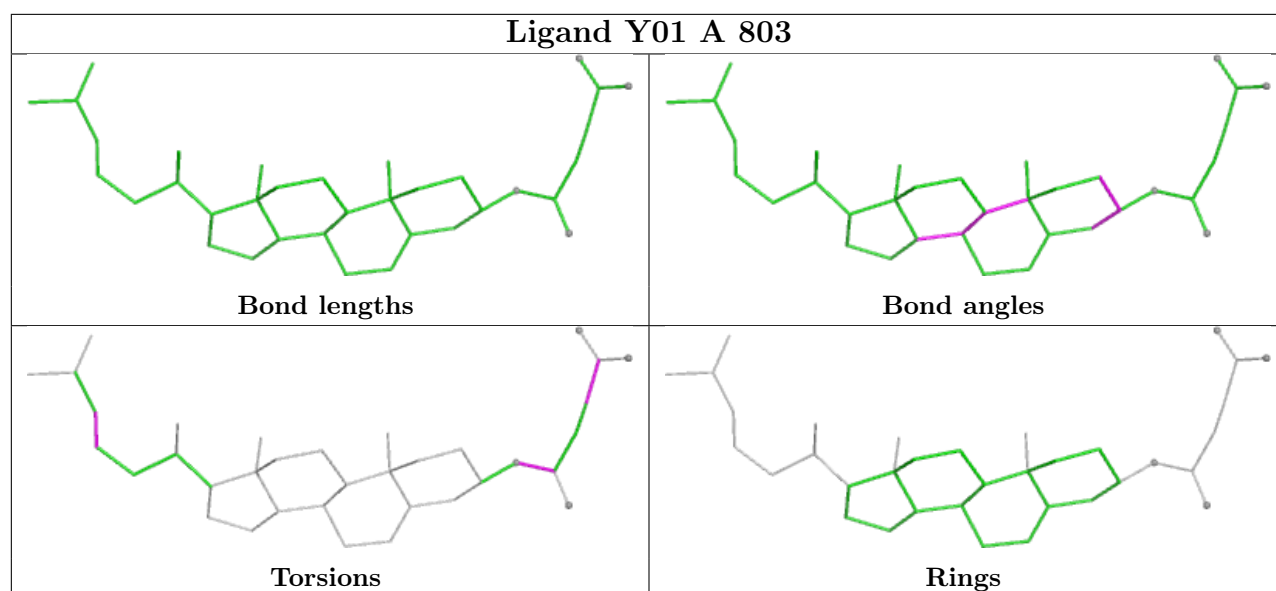
Continued from previous page...

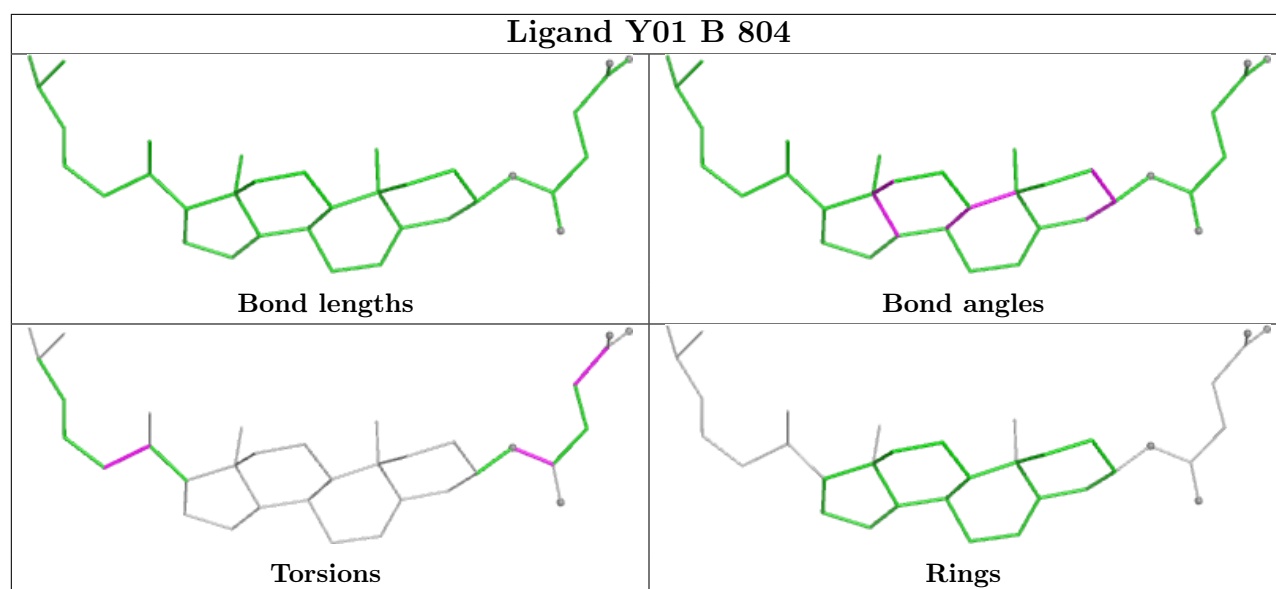
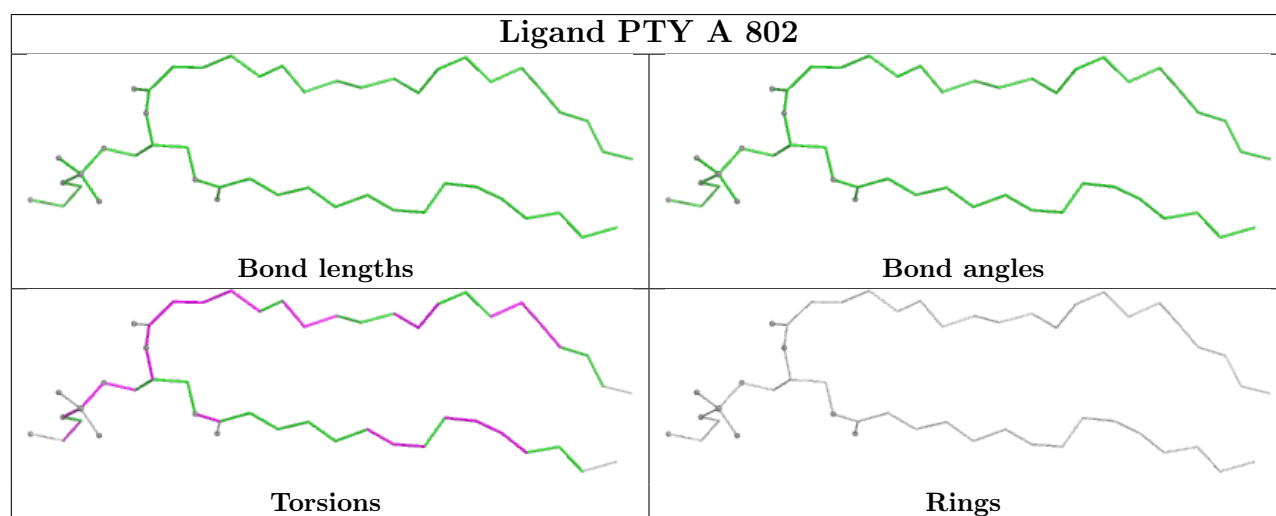
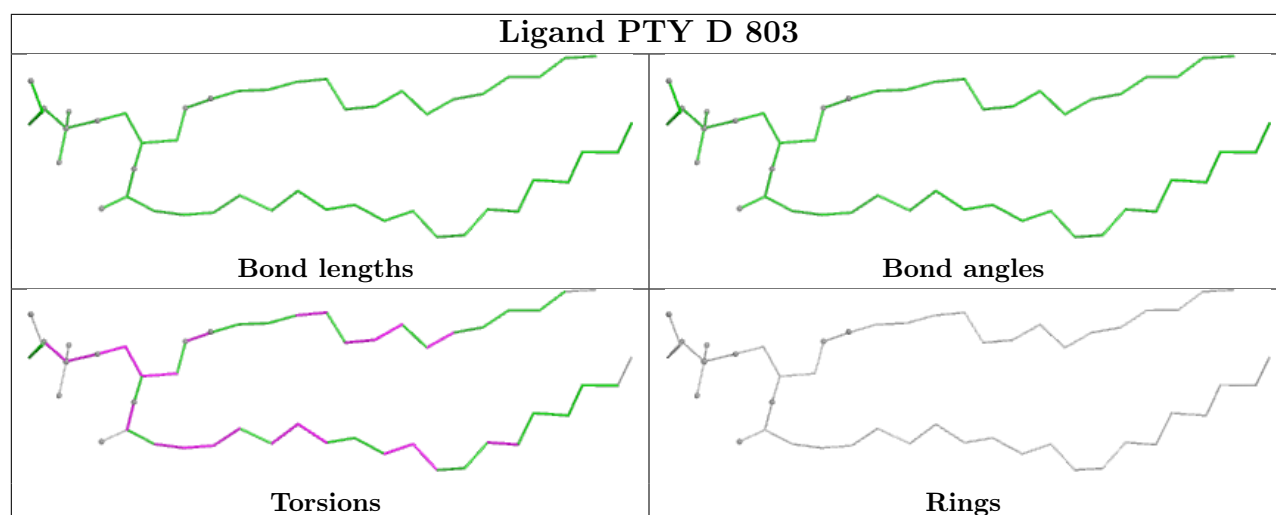
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	803	PTY	5	0
3	A	802	PTY	8	0
4	B	804	Y01	7	0
7	B	801	YZY	4	0
5	A	804	A1L55	2	0
4	C	803	Y01	5	0

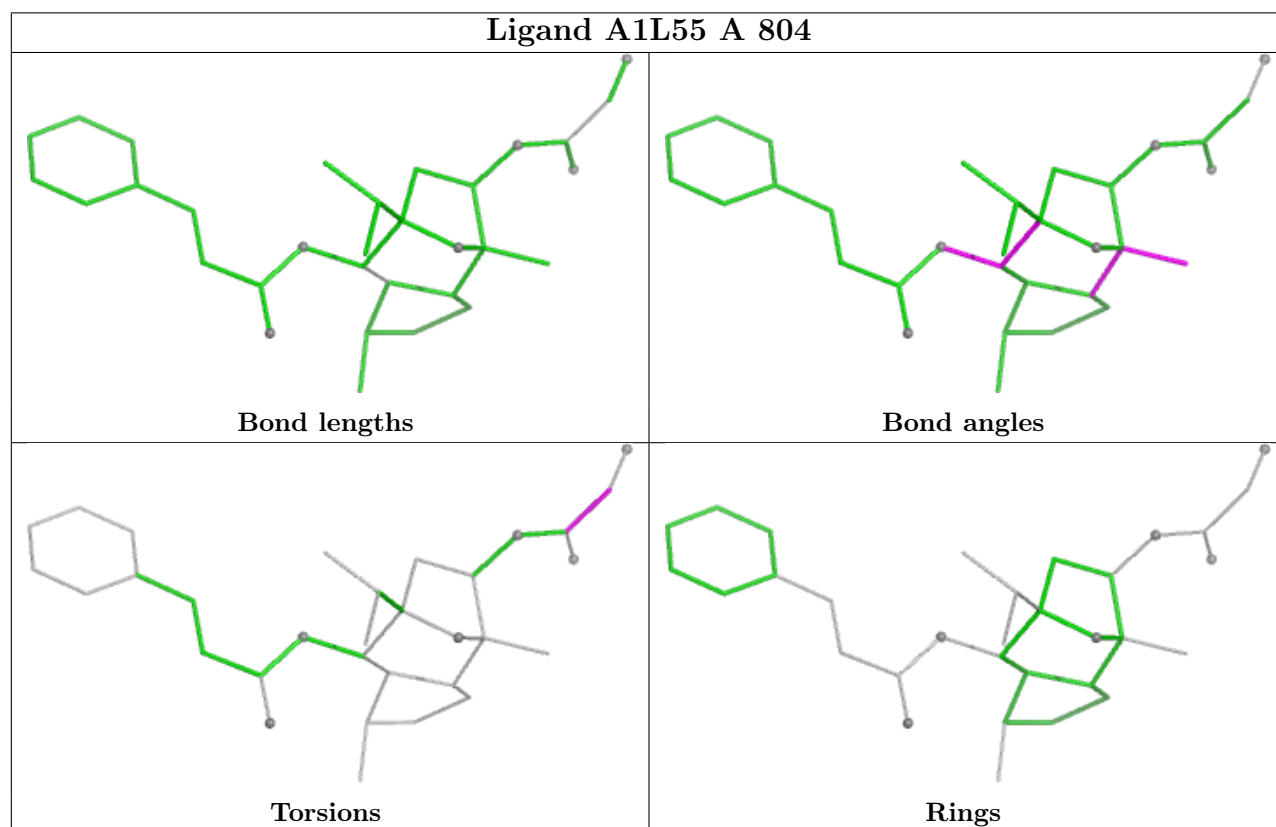
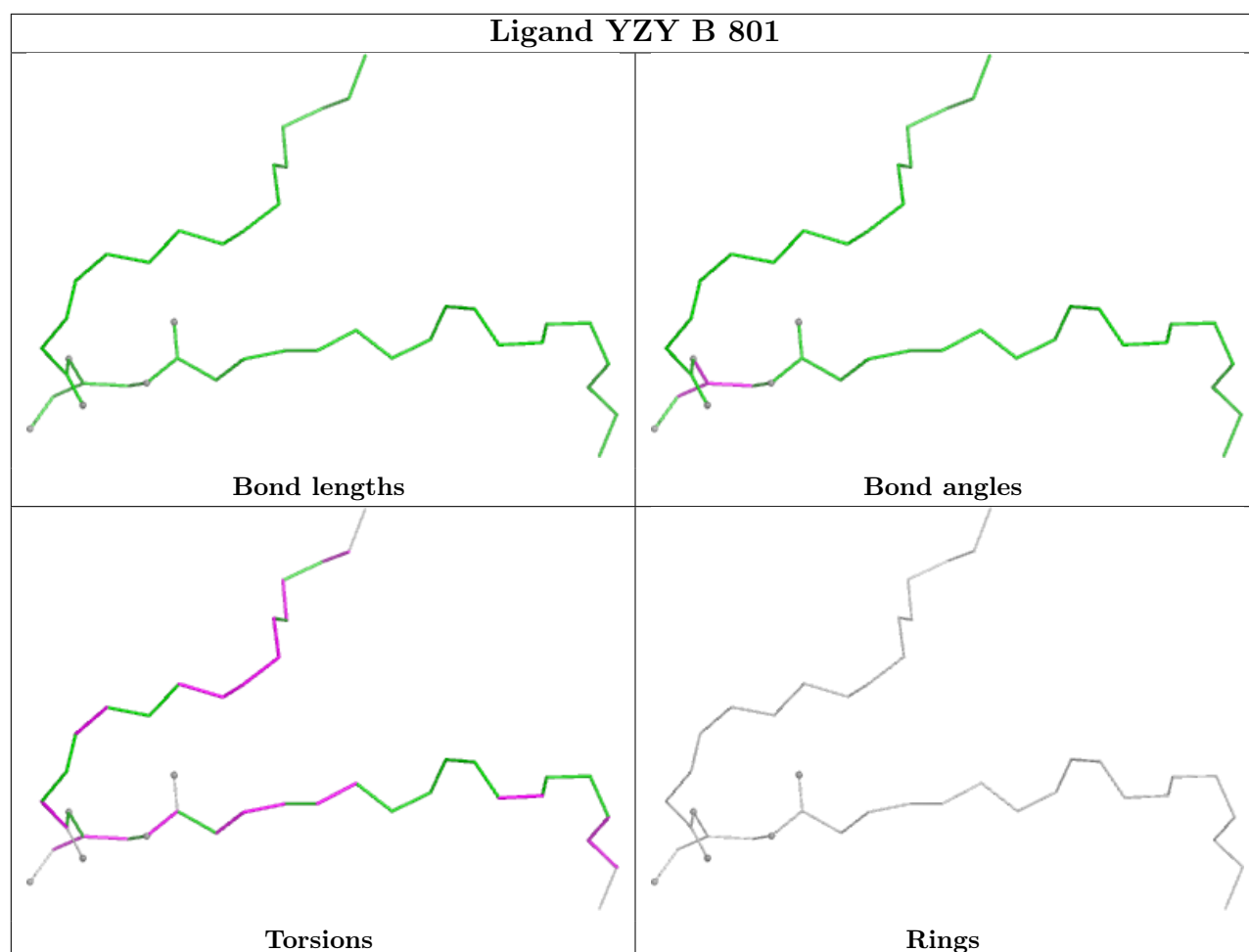
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

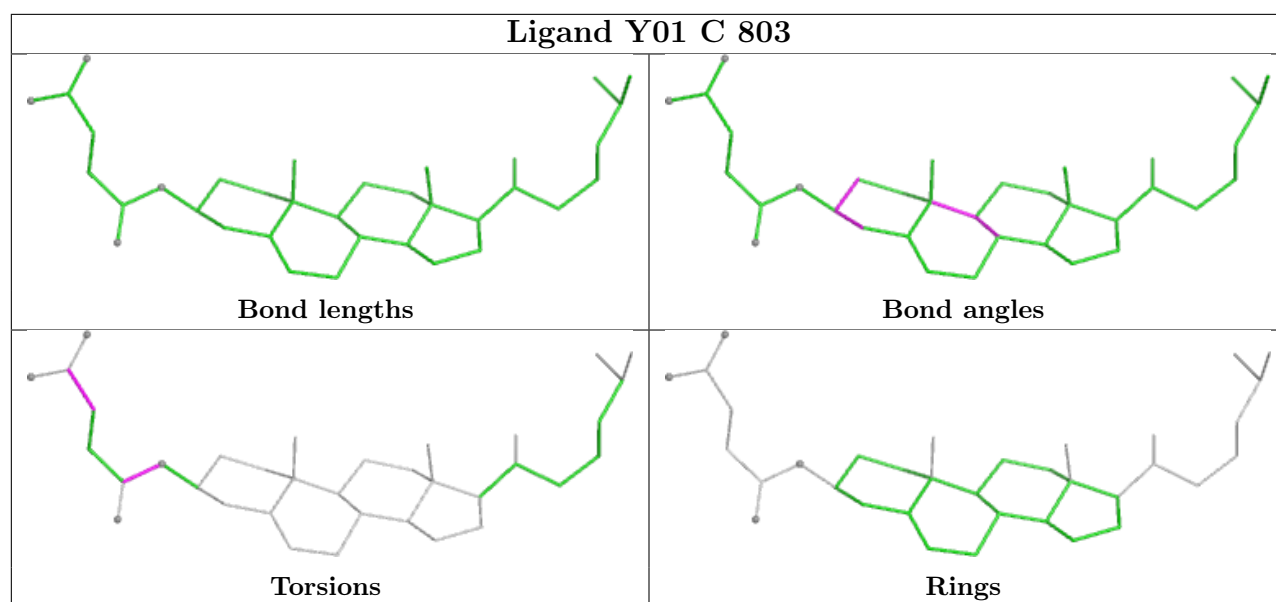












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

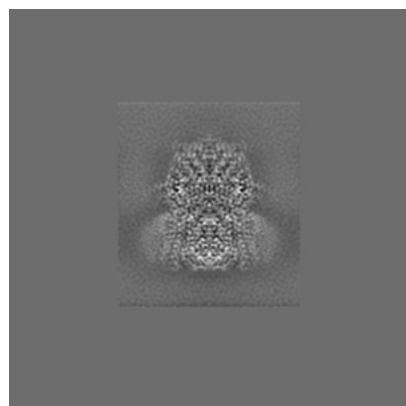
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54193. These allow visual inspection of the internal detail of the map and identification of artifacts.

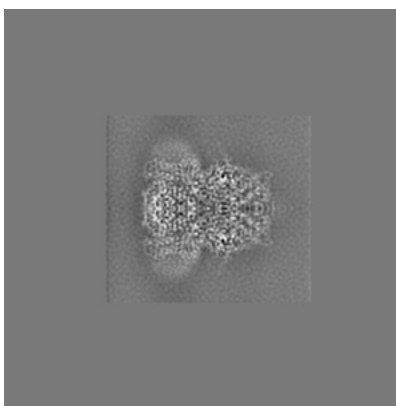
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

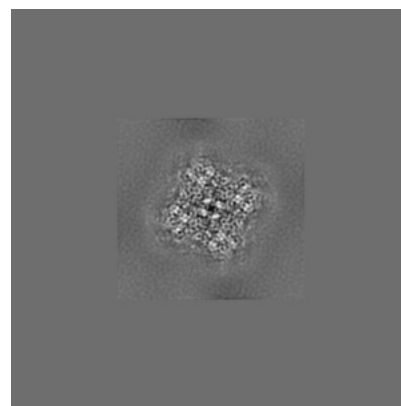
6.1.1 Primary map



X

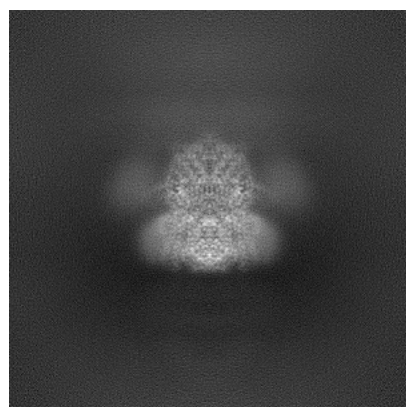


Y

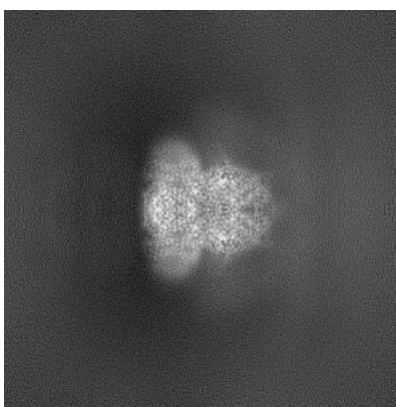


Z

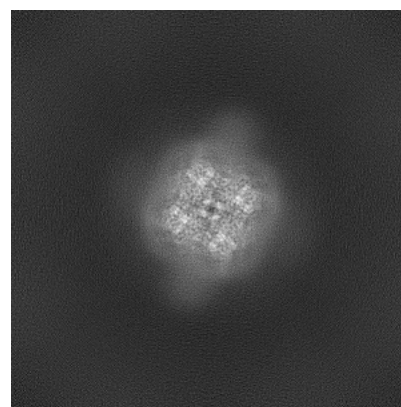
6.1.2 Raw map



X



Y

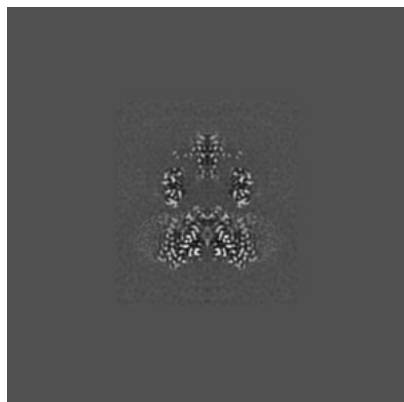


Z

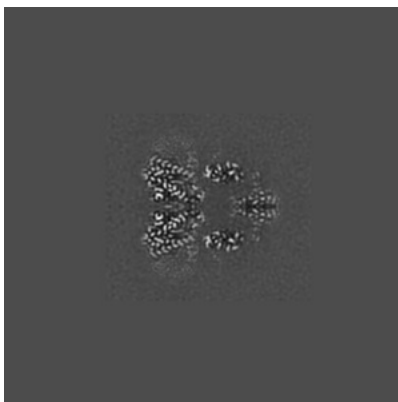
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

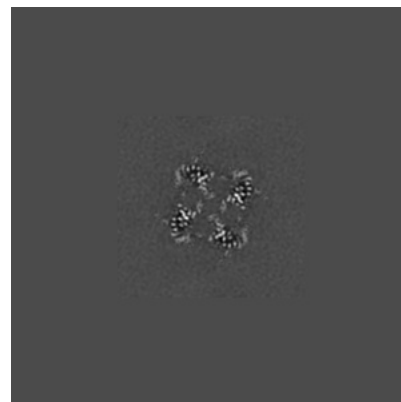
6.2.1 Primary map



X Index: 224

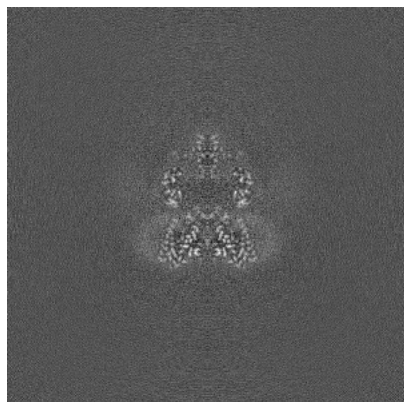


Y Index: 224

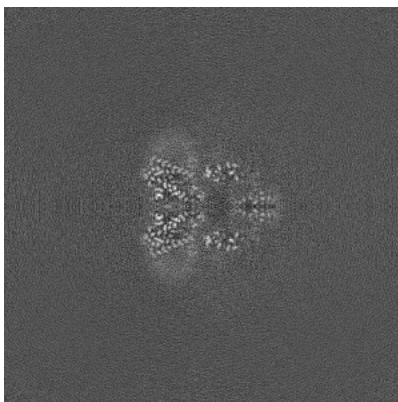


Z Index: 224

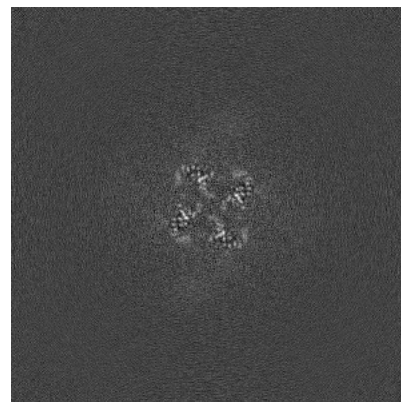
6.2.2 Raw map



X Index: 224



Y Index: 224

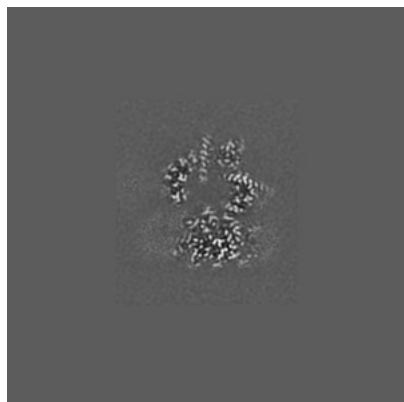


Z Index: 224

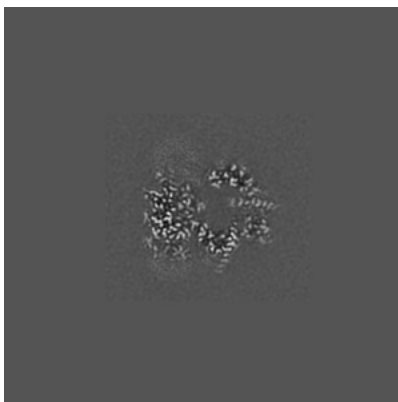
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

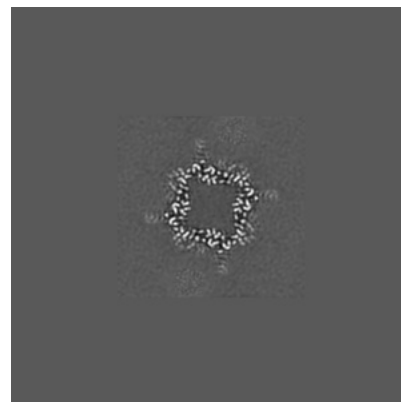
6.3.1 Primary map



X Index: 213

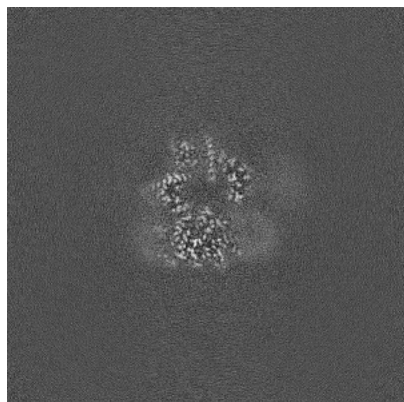


Y Index: 213

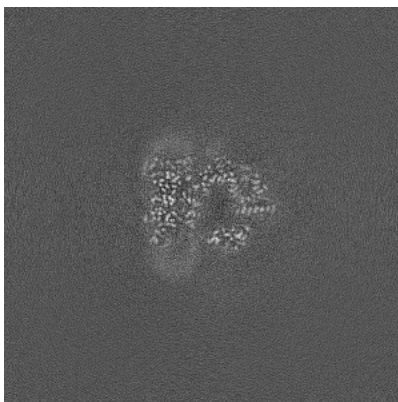


Z Index: 242

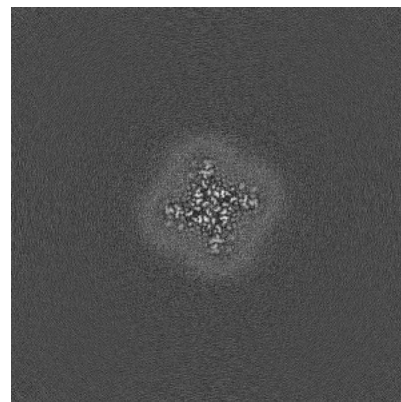
6.3.2 Raw map



X Index: 235



Y Index: 231

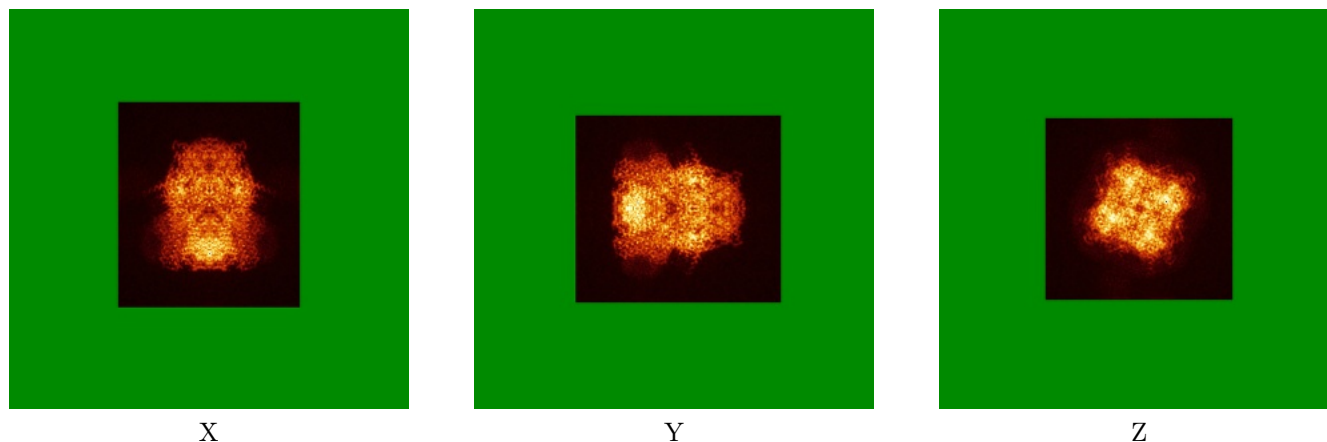


Z Index: 182

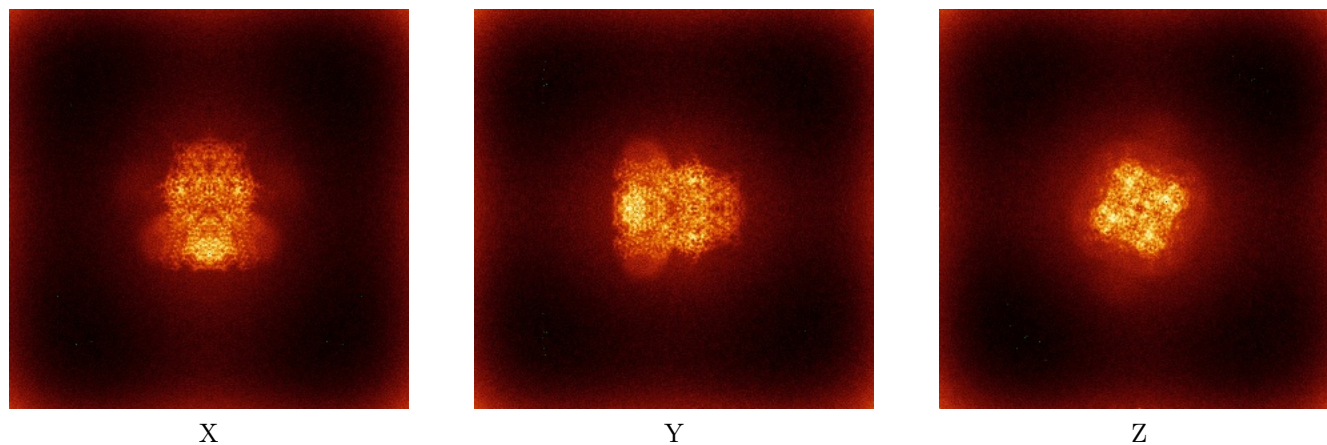
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



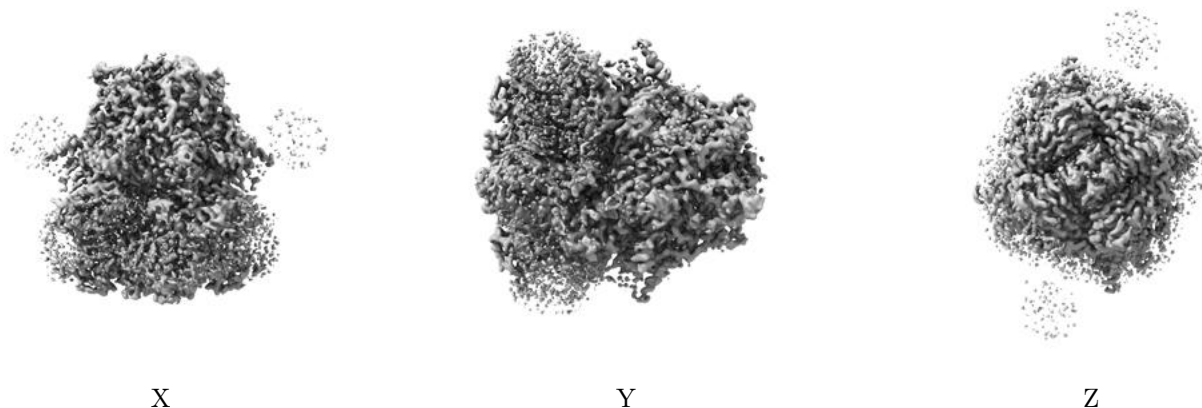
6.4.2 Raw map



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

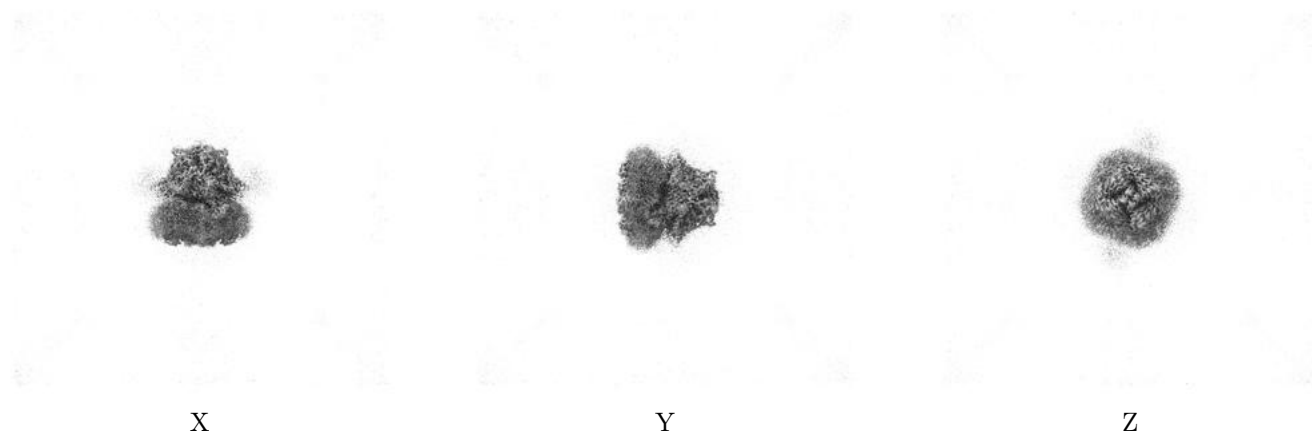
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

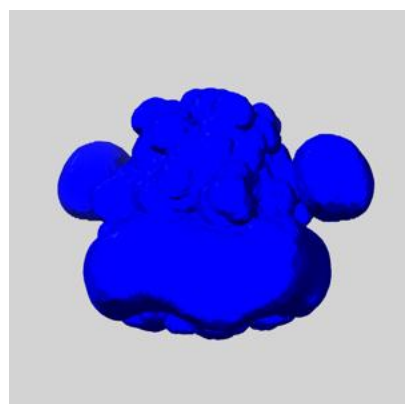
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

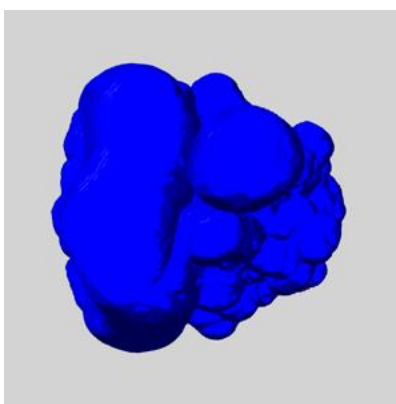
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

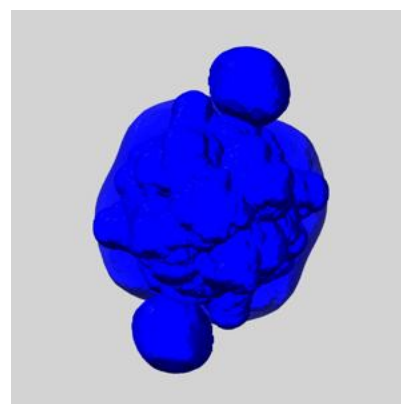
6.6.1 emd_54193_msk_1.map [i](#)



X

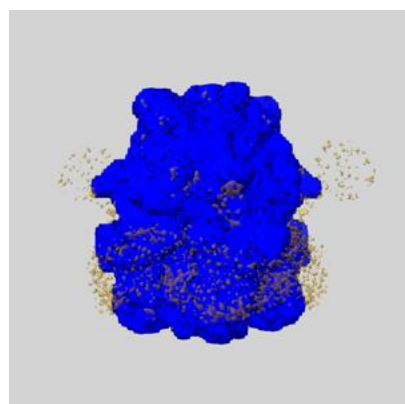


Y

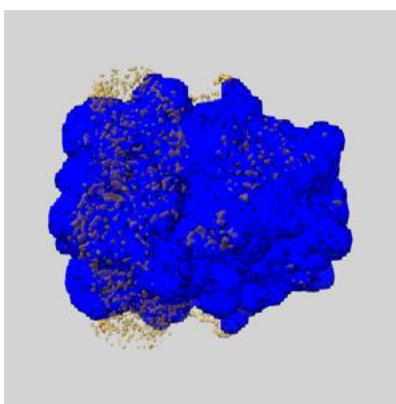


Z

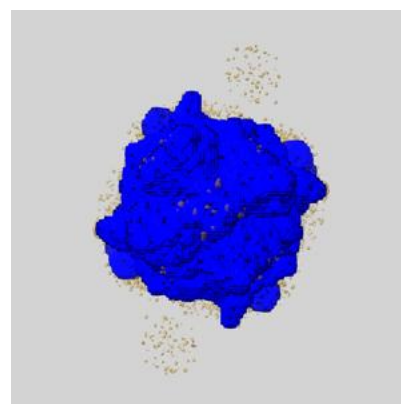
6.6.2 emd_54193_msk_2.map [i](#)



X



Y

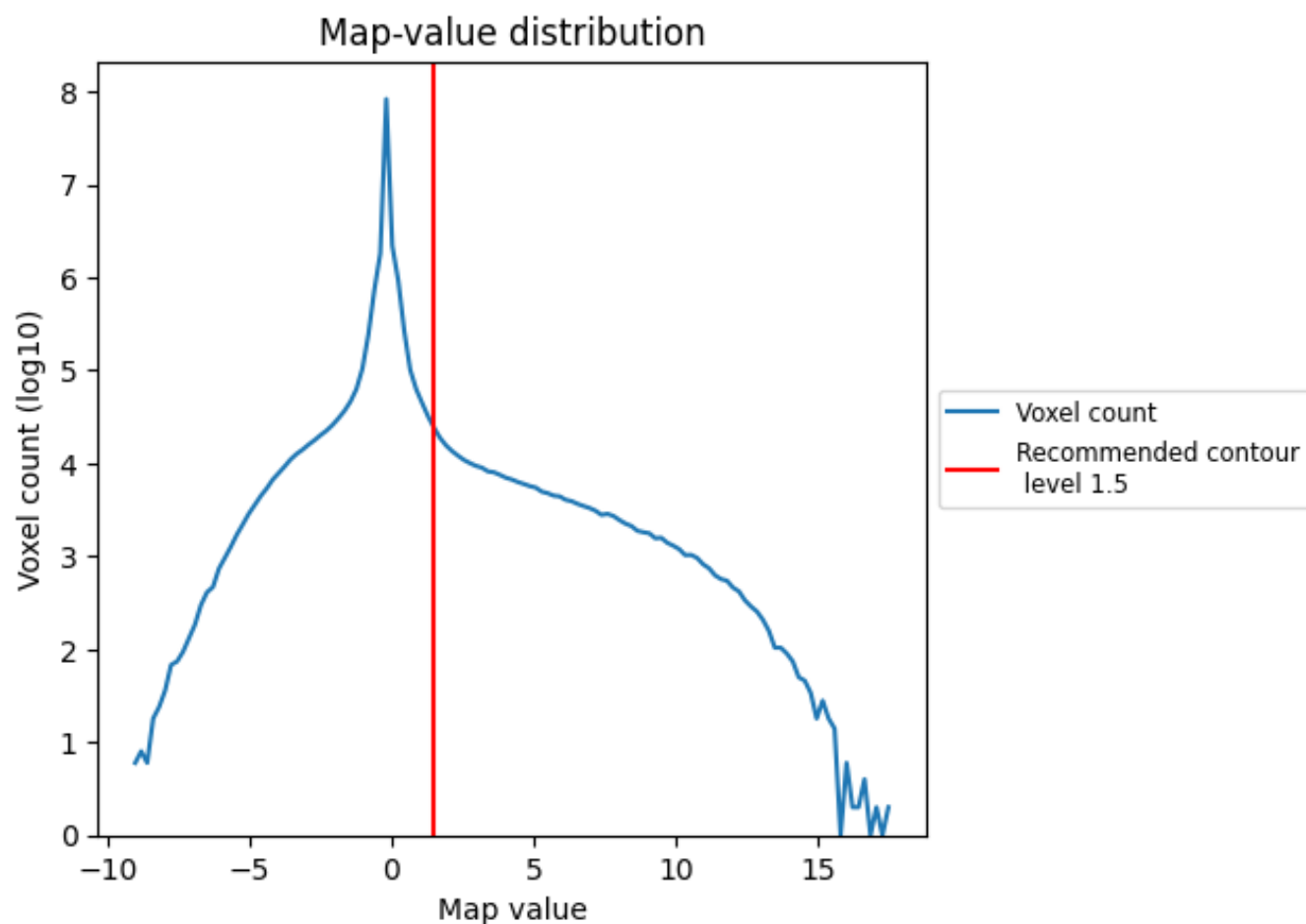


Z

7 Map analysis [i](#)

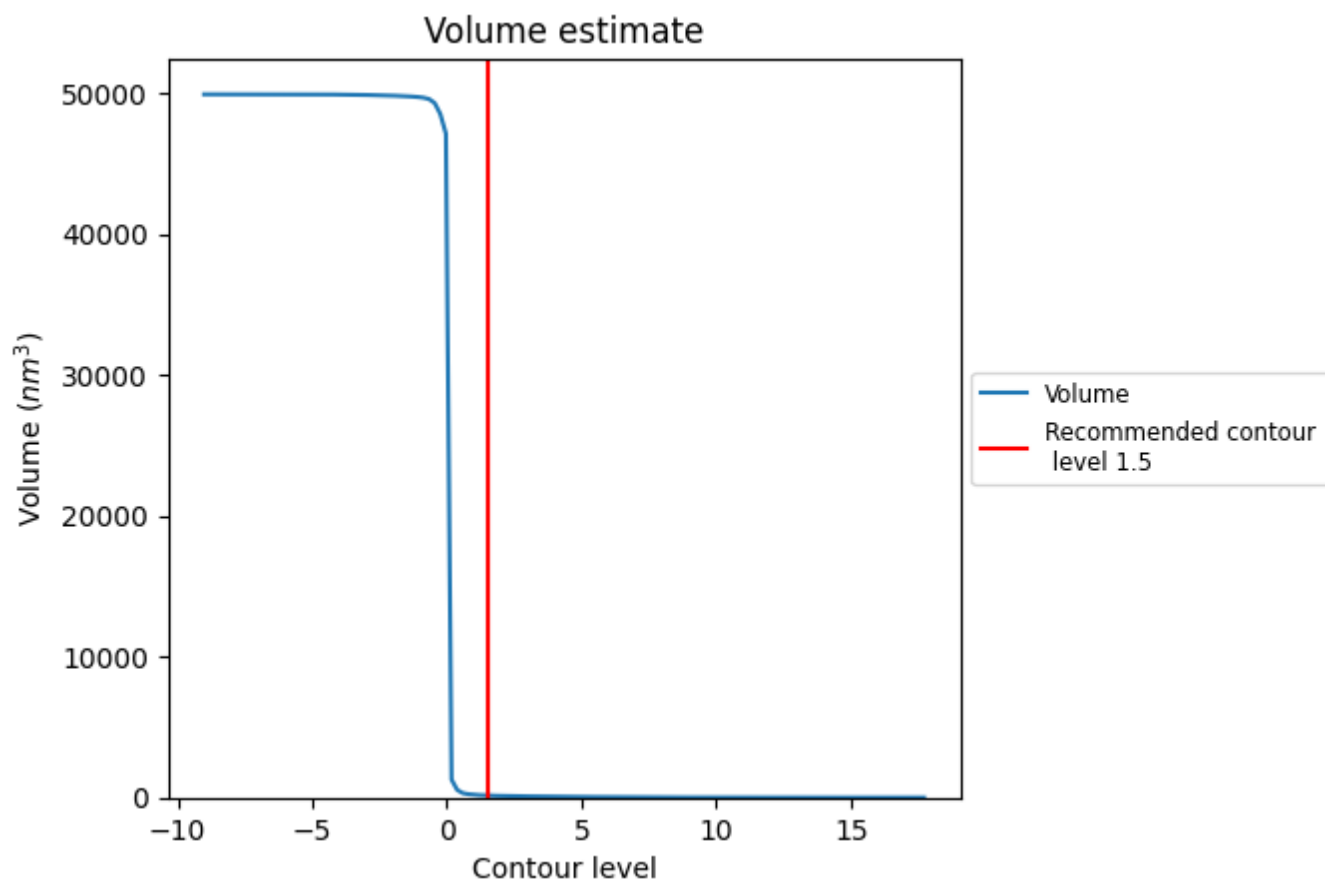
This section contains the results of statistical analysis of the map.

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.

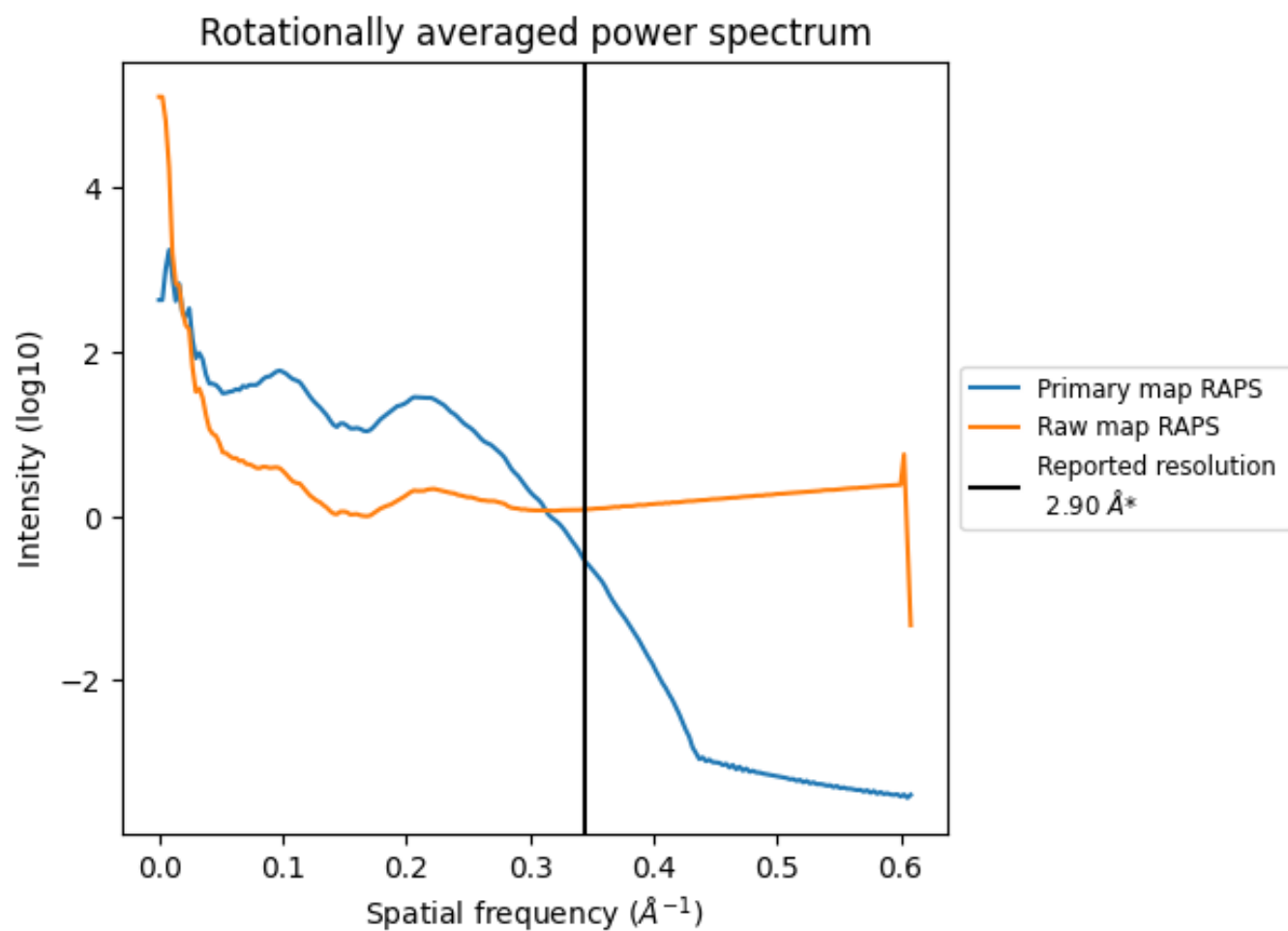
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm^3 ; this corresponds to an approximate mass of 132 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 ⓘ

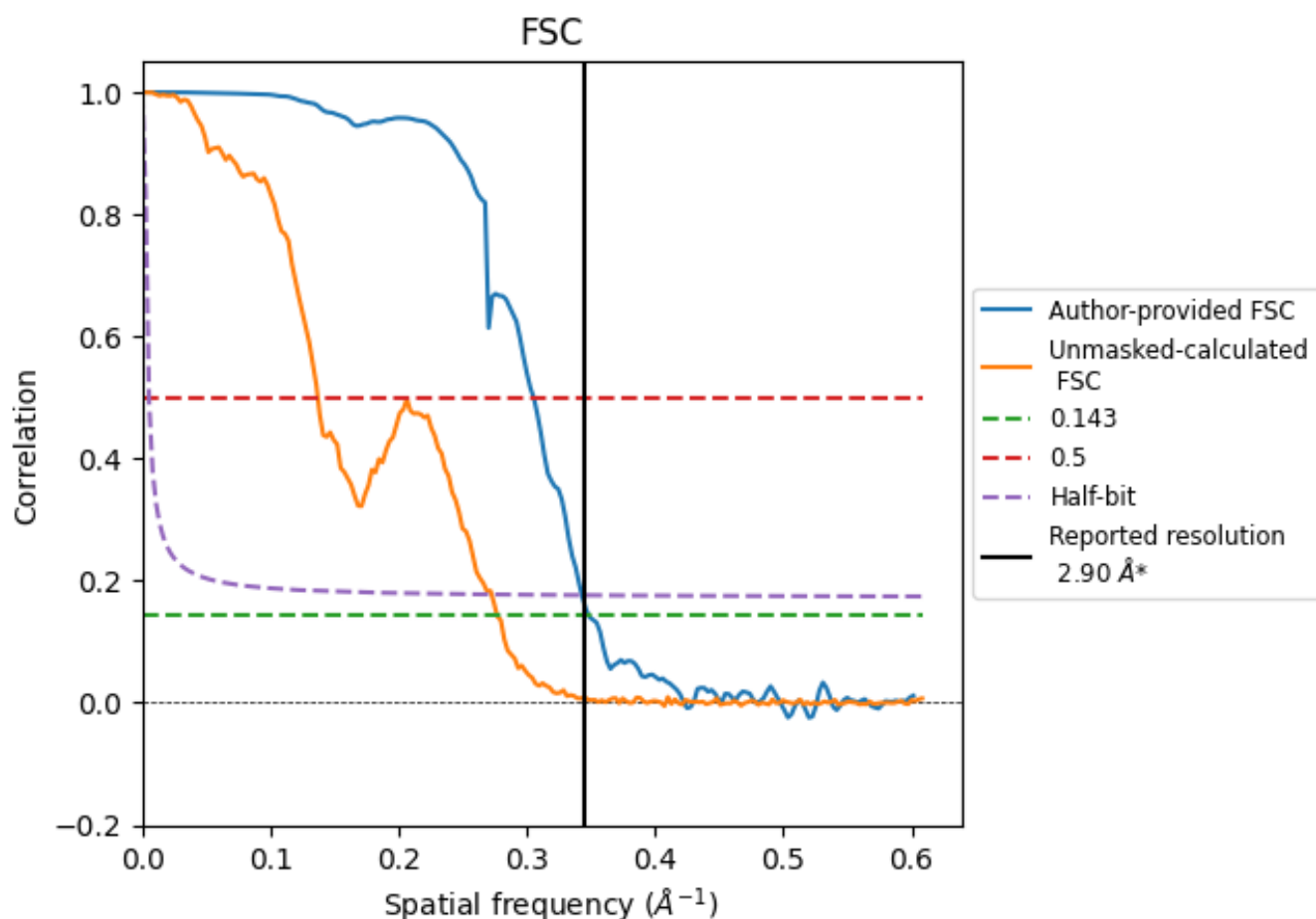


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

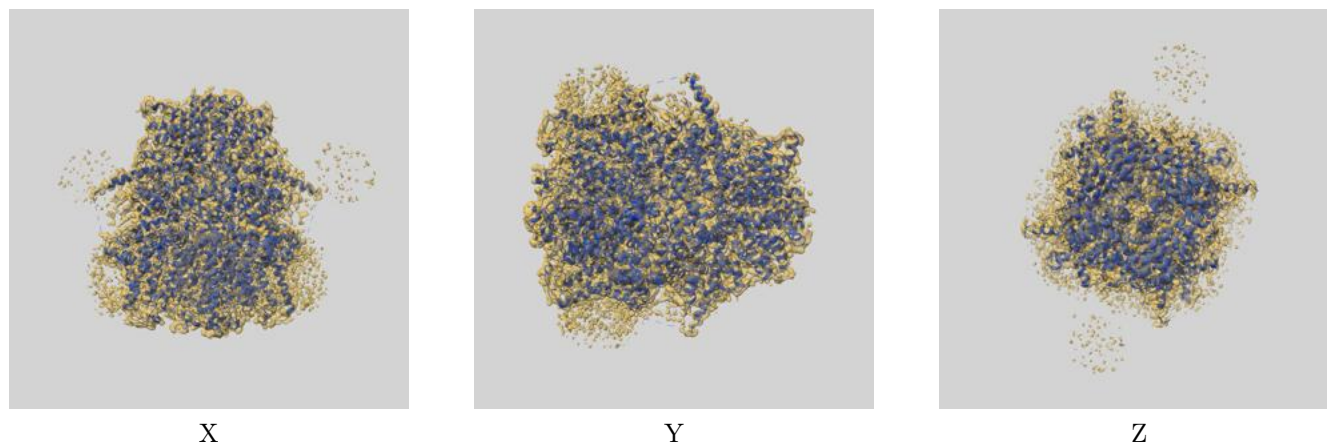
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.28	2.92
Unmasked-calculated*	3.61	7.30	3.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.61 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

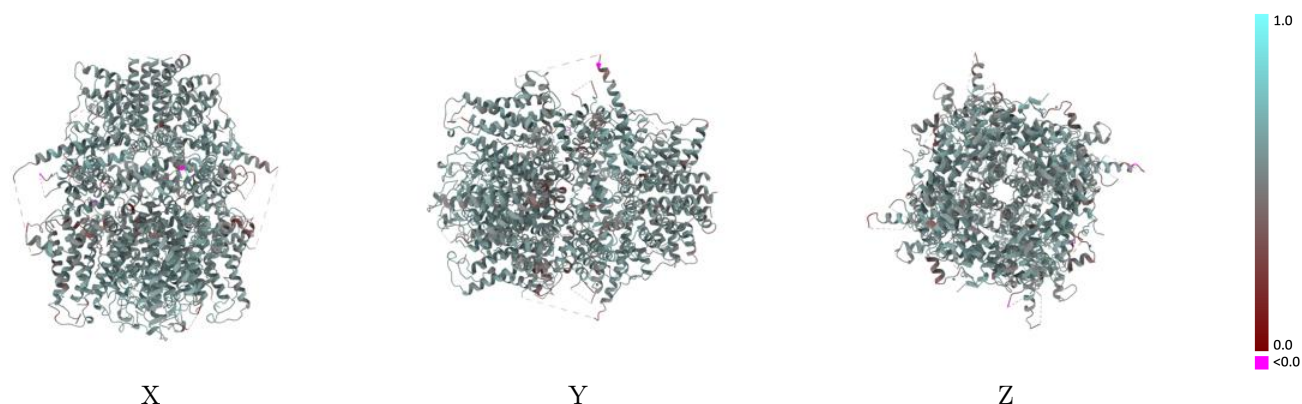
This section contains information regarding the fit between EMDB map EMD-54193 and PDB model 9RRQ. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



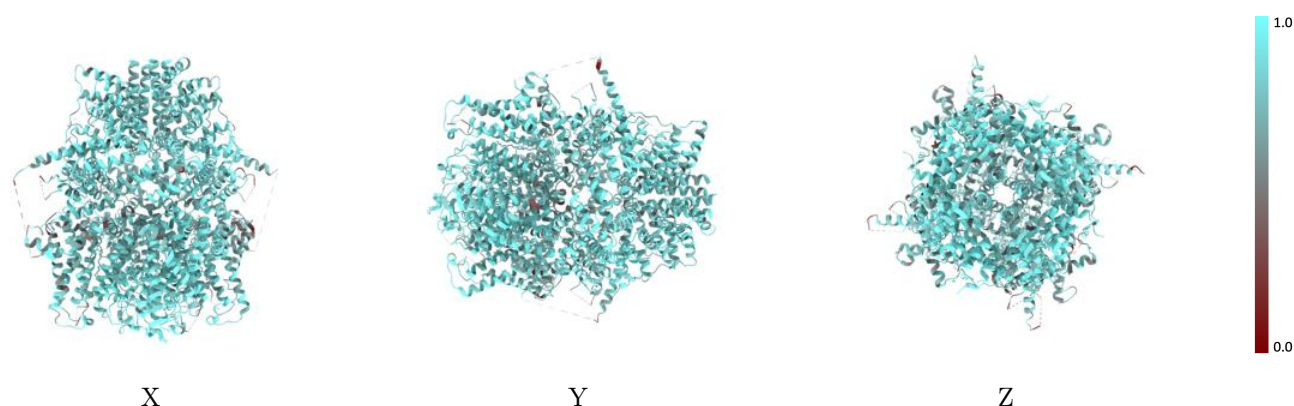
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



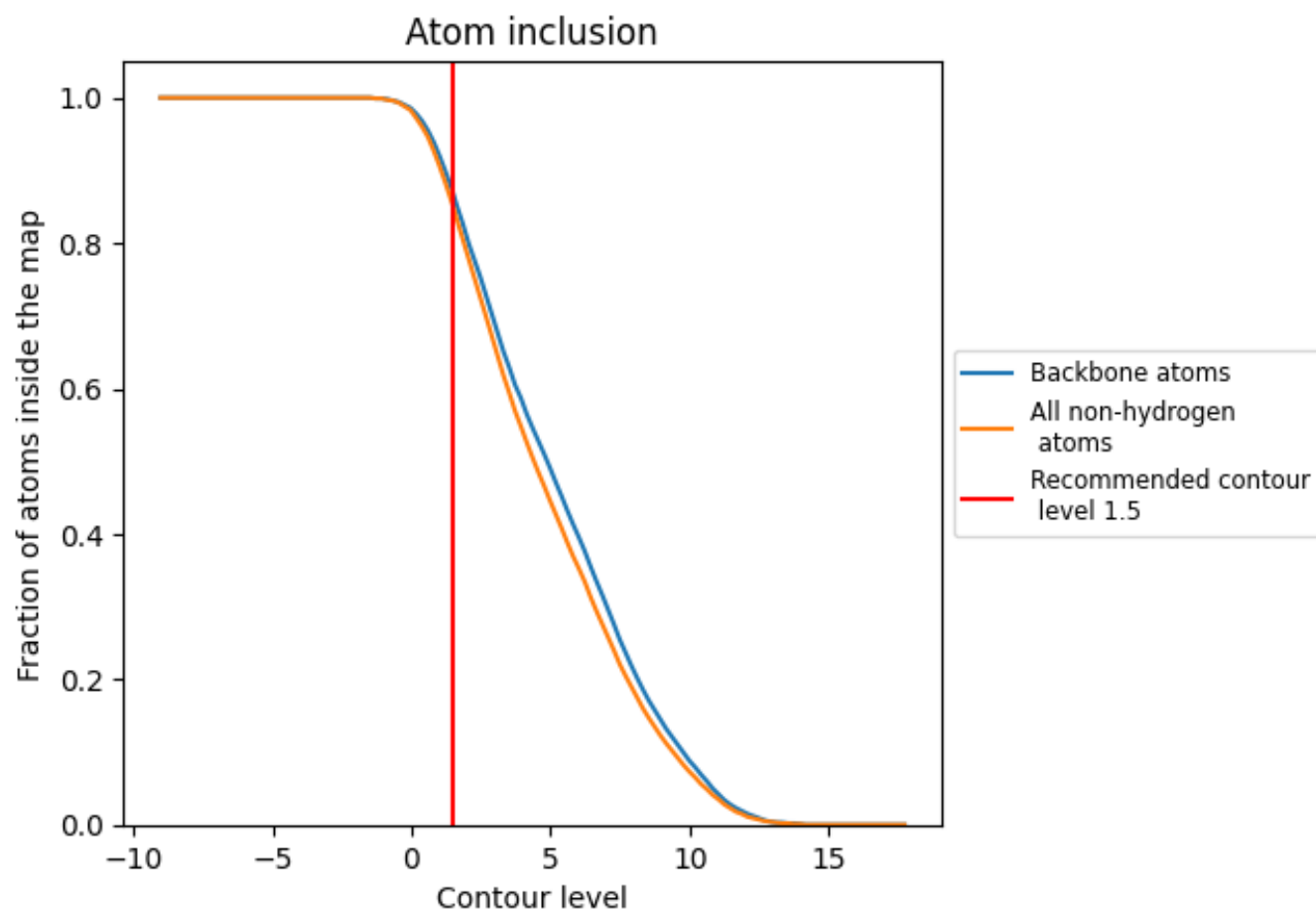
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8500	<div><div></div></div> 0.5540
A	<div><div></div></div> 0.8650	<div><div></div></div> 0.5600
B	<div><div></div></div> 0.8380	<div><div></div></div> 0.5460
C	<div><div></div></div> 0.8670	<div><div></div></div> 0.5600
D	<div><div></div></div> 0.8430	<div><div></div></div> 0.5490

