



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 12:50 AM UTC

PDB ID : 6P2P / pdb_00006p2p
EMDB ID : EMD-20239
Title : Tetrameric structure of ACAT1
Authors : Yan, N.; Qian, H.W.
Deposited on : 2019-05-21
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

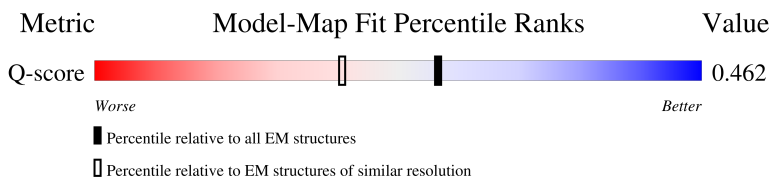
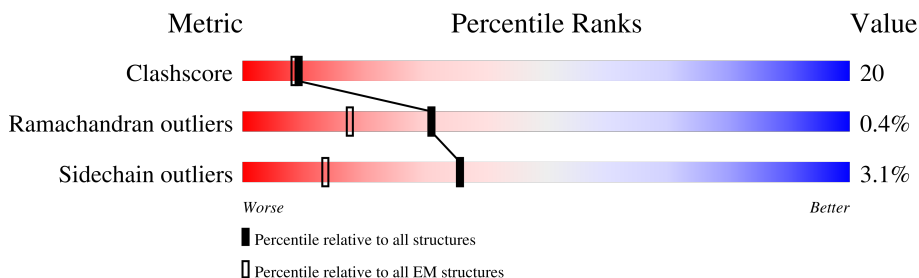
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	594	 7% 43% 25% 31%
1	B	594	 7% 42% 24% 31%
1	C	594	 7% 43% 25% 31%
1	D	594	 7% 43% 24% 31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13952 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 Sterol O-acyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	408	Total	C	N	O	S	0	0
			3427	2331	537	541	18		
1	B	407	Total	C	N	O	S	0	0
			3415	2323	536	538	18		
1	C	408	Total	C	N	O	S	0	0
			3427	2331	537	541	18		
1	D	407	Total	C	N	O	S	0	0
			3415	2323	536	538	18		

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P35610
A	-19	ALA	-	expression tag	UNP P35610
A	-18	ASP	-	expression tag	UNP P35610
A	-17	TYR	-	expression tag	UNP P35610
A	-16	LYS	-	expression tag	UNP P35610
A	-15	ASP	-	expression tag	UNP P35610
A	-14	ASP	-	expression tag	UNP P35610
A	-13	ASP	-	expression tag	UNP P35610
A	-12	ASP	-	expression tag	UNP P35610
A	-11	LYS	-	expression tag	UNP P35610
A	-10	SER	-	expression tag	UNP P35610
A	-9	GLY	-	expression tag	UNP P35610
A	-8	PRO	-	expression tag	UNP P35610
A	-7	ASP	-	expression tag	UNP P35610
A	-6	GLU	-	expression tag	UNP P35610
A	-5	VAL	-	expression tag	UNP P35610
A	-4	ASP	-	expression tag	UNP P35610
A	-3	ALA	-	expression tag	UNP P35610
A	-2	SER	-	expression tag	UNP P35610
A	-1	GLY	-	expression tag	UNP P35610
A	0	ARG	-	expression tag	UNP P35610
A	551	LEU	-	expression tag	UNP P35610

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	GLU	-	expression tag	UNP P35610
A	553	GLY	-	expression tag	UNP P35610
A	554	SER	-	expression tag	UNP P35610
A	555	ASP	-	expression tag	UNP P35610
A	556	GLU	-	expression tag	UNP P35610
A	557	VAL	-	expression tag	UNP P35610
A	558	ASP	-	expression tag	UNP P35610
A	559	ALA	-	expression tag	UNP P35610
A	560	VAL	-	expression tag	UNP P35610
A	561	GLU	-	expression tag	UNP P35610
A	562	GLY	-	expression tag	UNP P35610
A	563	SER	-	expression tag	UNP P35610
A	564	HIS	-	expression tag	UNP P35610
A	565	HIS	-	expression tag	UNP P35610
A	566	HIS	-	expression tag	UNP P35610
A	567	HIS	-	expression tag	UNP P35610
A	568	HIS	-	expression tag	UNP P35610
A	569	HIS	-	expression tag	UNP P35610
A	570	HIS	-	expression tag	UNP P35610
A	571	HIS	-	expression tag	UNP P35610
A	572	HIS	-	expression tag	UNP P35610
A	573	HIS	-	expression tag	UNP P35610
B	-20	MET	-	initiating methionine	UNP P35610
B	-19	ALA	-	expression tag	UNP P35610
B	-18	ASP	-	expression tag	UNP P35610
B	-17	TYR	-	expression tag	UNP P35610
B	-16	LYS	-	expression tag	UNP P35610
B	-15	ASP	-	expression tag	UNP P35610
B	-14	ASP	-	expression tag	UNP P35610
B	-13	ASP	-	expression tag	UNP P35610
B	-12	ASP	-	expression tag	UNP P35610
B	-11	LYS	-	expression tag	UNP P35610
B	-10	SER	-	expression tag	UNP P35610
B	-9	GLY	-	expression tag	UNP P35610
B	-8	PRO	-	expression tag	UNP P35610
B	-7	ASP	-	expression tag	UNP P35610
B	-6	GLU	-	expression tag	UNP P35610
B	-5	VAL	-	expression tag	UNP P35610
B	-4	ASP	-	expression tag	UNP P35610
B	-3	ALA	-	expression tag	UNP P35610
B	-2	SER	-	expression tag	UNP P35610
B	-1	GLY	-	expression tag	UNP P35610

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ARG	-	expression tag	UNP P35610
B	551	LEU	-	expression tag	UNP P35610
B	552	GLU	-	expression tag	UNP P35610
B	553	GLY	-	expression tag	UNP P35610
B	554	SER	-	expression tag	UNP P35610
B	555	ASP	-	expression tag	UNP P35610
B	556	GLU	-	expression tag	UNP P35610
B	557	VAL	-	expression tag	UNP P35610
B	558	ASP	-	expression tag	UNP P35610
B	559	ALA	-	expression tag	UNP P35610
B	560	VAL	-	expression tag	UNP P35610
B	561	GLU	-	expression tag	UNP P35610
B	562	GLY	-	expression tag	UNP P35610
B	563	SER	-	expression tag	UNP P35610
B	564	HIS	-	expression tag	UNP P35610
B	565	HIS	-	expression tag	UNP P35610
B	566	HIS	-	expression tag	UNP P35610
B	567	HIS	-	expression tag	UNP P35610
B	568	HIS	-	expression tag	UNP P35610
B	569	HIS	-	expression tag	UNP P35610
B	570	HIS	-	expression tag	UNP P35610
B	571	HIS	-	expression tag	UNP P35610
B	572	HIS	-	expression tag	UNP P35610
B	573	HIS	-	expression tag	UNP P35610
C	-20	MET	-	initiating methionine	UNP P35610
C	-19	ALA	-	expression tag	UNP P35610
C	-18	ASP	-	expression tag	UNP P35610
C	-17	TYR	-	expression tag	UNP P35610
C	-16	LYS	-	expression tag	UNP P35610
C	-15	ASP	-	expression tag	UNP P35610
C	-14	ASP	-	expression tag	UNP P35610
C	-13	ASP	-	expression tag	UNP P35610
C	-12	ASP	-	expression tag	UNP P35610
C	-11	LYS	-	expression tag	UNP P35610
C	-10	SER	-	expression tag	UNP P35610
C	-9	GLY	-	expression tag	UNP P35610
C	-8	PRO	-	expression tag	UNP P35610
C	-7	ASP	-	expression tag	UNP P35610
C	-6	GLU	-	expression tag	UNP P35610
C	-5	VAL	-	expression tag	UNP P35610
C	-4	ASP	-	expression tag	UNP P35610
C	-3	ALA	-	expression tag	UNP P35610

Continued on next page...

Continued from previous page...

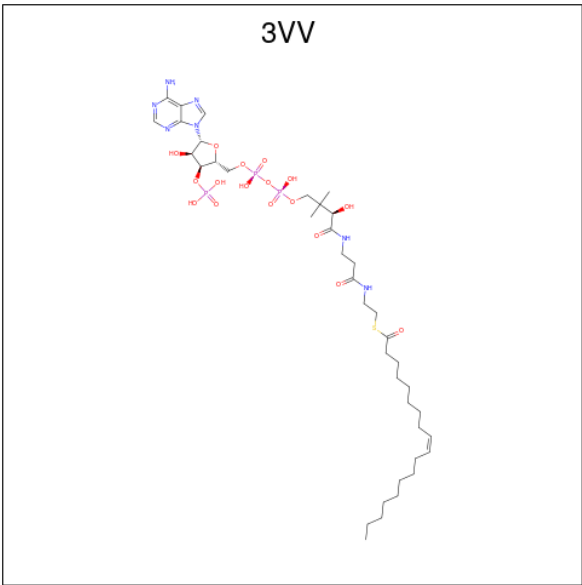
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP P35610
C	-1	GLY	-	expression tag	UNP P35610
C	0	ARG	-	expression tag	UNP P35610
C	551	LEU	-	expression tag	UNP P35610
C	552	GLU	-	expression tag	UNP P35610
C	553	GLY	-	expression tag	UNP P35610
C	554	SER	-	expression tag	UNP P35610
C	555	ASP	-	expression tag	UNP P35610
C	556	GLU	-	expression tag	UNP P35610
C	557	VAL	-	expression tag	UNP P35610
C	558	ASP	-	expression tag	UNP P35610
C	559	ALA	-	expression tag	UNP P35610
C	560	VAL	-	expression tag	UNP P35610
C	561	GLU	-	expression tag	UNP P35610
C	562	GLY	-	expression tag	UNP P35610
C	563	SER	-	expression tag	UNP P35610
C	564	HIS	-	expression tag	UNP P35610
C	565	HIS	-	expression tag	UNP P35610
C	566	HIS	-	expression tag	UNP P35610
C	567	HIS	-	expression tag	UNP P35610
C	568	HIS	-	expression tag	UNP P35610
C	569	HIS	-	expression tag	UNP P35610
C	570	HIS	-	expression tag	UNP P35610
C	571	HIS	-	expression tag	UNP P35610
C	572	HIS	-	expression tag	UNP P35610
C	573	HIS	-	expression tag	UNP P35610
D	-20	MET	-	initiating methionine	UNP P35610
D	-19	ALA	-	expression tag	UNP P35610
D	-18	ASP	-	expression tag	UNP P35610
D	-17	TYR	-	expression tag	UNP P35610
D	-16	LYS	-	expression tag	UNP P35610
D	-15	ASP	-	expression tag	UNP P35610
D	-14	ASP	-	expression tag	UNP P35610
D	-13	ASP	-	expression tag	UNP P35610
D	-12	ASP	-	expression tag	UNP P35610
D	-11	LYS	-	expression tag	UNP P35610
D	-10	SER	-	expression tag	UNP P35610
D	-9	GLY	-	expression tag	UNP P35610
D	-8	PRO	-	expression tag	UNP P35610
D	-7	ASP	-	expression tag	UNP P35610
D	-6	GLU	-	expression tag	UNP P35610
D	-5	VAL	-	expression tag	UNP P35610

Continued on next page...

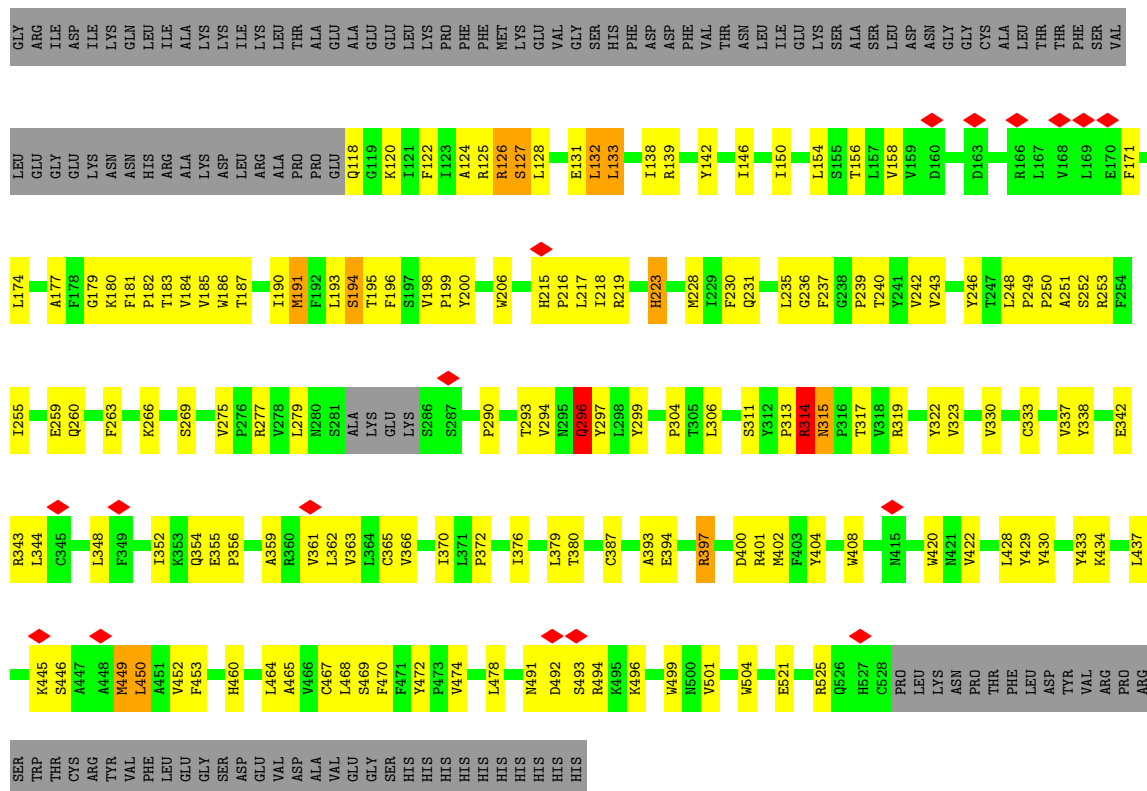
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ASP	-	expression tag	UNP P35610
D	-3	ALA	-	expression tag	UNP P35610
D	-2	SER	-	expression tag	UNP P35610
D	-1	GLY	-	expression tag	UNP P35610
D	0	ARG	-	expression tag	UNP P35610
D	551	LEU	-	expression tag	UNP P35610
D	552	GLU	-	expression tag	UNP P35610
D	553	GLY	-	expression tag	UNP P35610
D	554	SER	-	expression tag	UNP P35610
D	555	ASP	-	expression tag	UNP P35610
D	556	GLU	-	expression tag	UNP P35610
D	557	VAL	-	expression tag	UNP P35610
D	558	ASP	-	expression tag	UNP P35610
D	559	ALA	-	expression tag	UNP P35610
D	560	VAL	-	expression tag	UNP P35610
D	561	GLU	-	expression tag	UNP P35610
D	562	GLY	-	expression tag	UNP P35610
D	563	SER	-	expression tag	UNP P35610
D	564	HIS	-	expression tag	UNP P35610
D	565	HIS	-	expression tag	UNP P35610
D	566	HIS	-	expression tag	UNP P35610
D	567	HIS	-	expression tag	UNP P35610
D	568	HIS	-	expression tag	UNP P35610
D	569	HIS	-	expression tag	UNP P35610
D	570	HIS	-	expression tag	UNP P35610
D	571	HIS	-	expression tag	UNP P35610
D	572	HIS	-	expression tag	UNP P35610
D	573	HIS	-	expression tag	UNP P35610

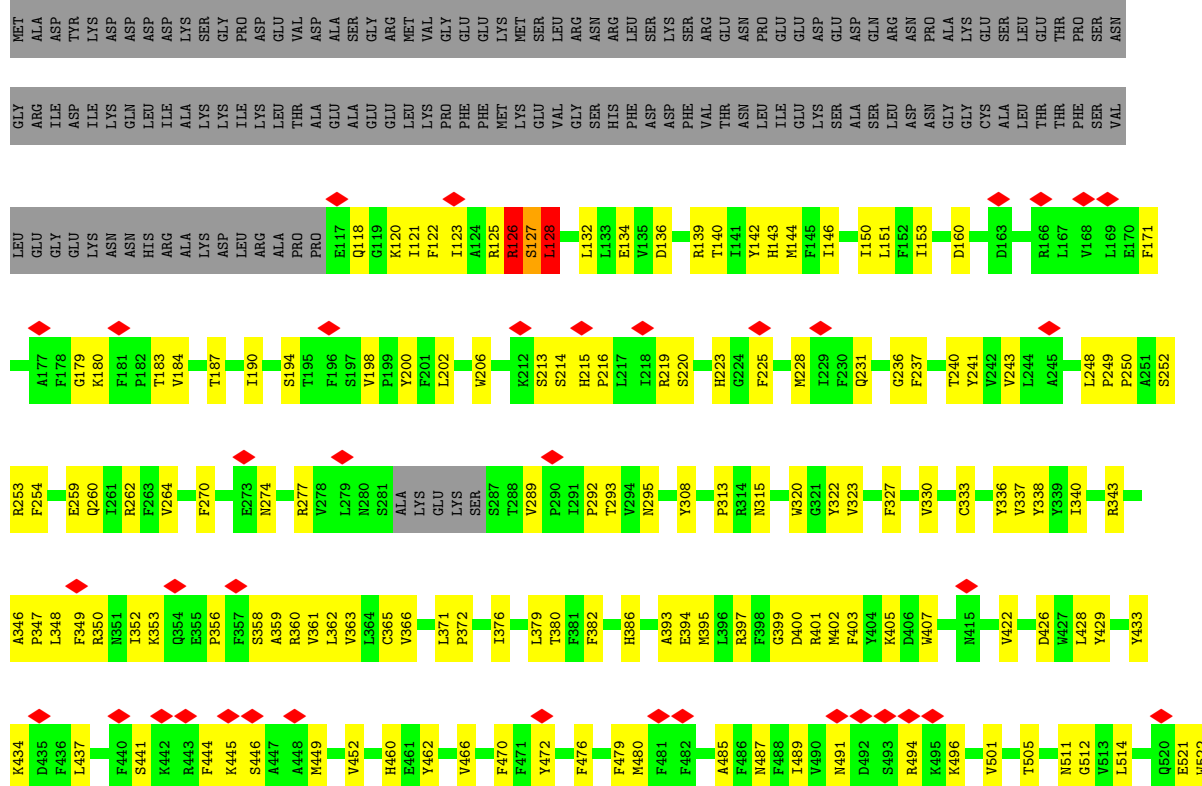
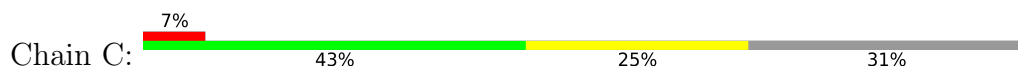
- Molecule 2 is S-{(3R,5R,9R)-1-[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonooxy)tetrahydrofuran-2-yl]-3,5,9-trihydroxy-8,8-dimethyl-3,5-dioxido-10,14-dioxo-2,4,6-trioxa-11,15-diaza-3lambda 5 ,5lambda 5 -diphosphaheptadecan-17-yl} (9Z)-octadec-9-enethioate (non-preferred name) (CCD ID: 3VV) (formula: C₃₉H₆₈N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



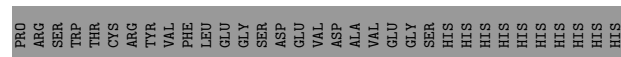
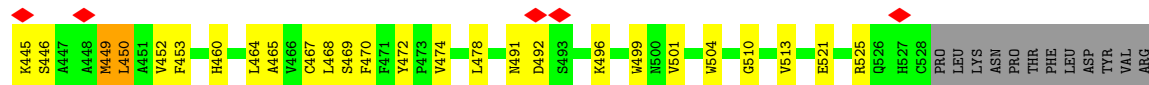
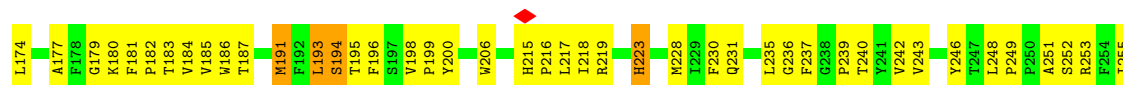
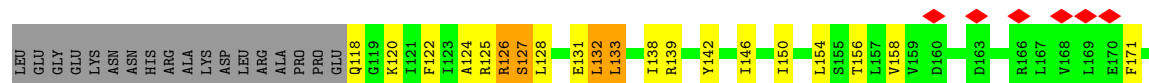
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			67	39	7	17	3	1	
2	B	1	Total	C	N	O	P	S	0
			67	39	7	17	3	1	
2	C	1	Total	C	N	O	P	S	0
			67	39	7	17	3	1	
2	D	1	Total	C	N	O	P	S	0
			67	39	7	17	3	1	



• Molecule 1: Sterol O-acyltransferase 1



- Molecule 1: Sterol O-acyltransferase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183794	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.123	Depositor
Minimum map value	-0.069	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	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: 3VV

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	0.24	0/3559	0.48	1/4849 (0.0%)
1	B	0.29	0/3546	0.55	2/4830 (0.0%)
1	C	0.24	0/3559	0.48	1/4849 (0.0%)
1	D	0.29	0/3546	0.55	2/4830 (0.0%)
All	All	0.26	0/14210	0.52	6/19358 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	ARG	N-CA-C	5.91	120.03	107.67
1	D	314	ARG	N-CA-C	5.91	120.03	107.67
1	A	128	LEU	N-CA-C	-5.77	105.88	114.64
1	C	128	LEU	N-CA-C	-5.77	105.88	114.64
1	B	296	GLN	N-CA-C	-5.41	106.36	113.12
1	D	296	GLN	N-CA-C	-5.41	106.36	113.12

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	3427	0	3358	124	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3415	0	3336	151	0
1	C	3427	0	3358	120	0
1	D	3415	0	3336	152	0
2	A	67	0	64	5	0
2	B	67	0	64	14	0
2	C	67	0	64	5	0
2	D	67	0	64	15	0
All	All	13952	0	13644	564	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (564) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:THR:HA	1:B:397:ARG:NH2	1.67	1.09
1:D:317:THR:HA	1:D:397:ARG:NH2	1.67	1.08
2:D:700:3VV:H26	2:D:700:3VV:C11	1.91	1.00
2:B:700:3VV:H26	2:B:700:3VV:H32	1.02	1.00
2:D:700:3VV:H26	2:D:700:3VV:H32	1.02	1.00
1:A:126:ARG:O	1:A:401:ARG:HB3	1.62	1.00
2:B:700:3VV:H26	2:B:700:3VV:C11	1.91	0.99
1:C:126:ARG:O	1:C:401:ARG:HB3	1.62	0.98
1:D:317:THR:HA	1:D:397:ARG:HH21	1.25	0.97
2:D:700:3VV:H32	2:D:700:3VV:C06	1.95	0.95
1:B:460:HIS:NE2	2:B:700:3VV:H39	1.81	0.95
1:D:460:HIS:NE2	2:D:700:3VV:H39	1.81	0.95
2:B:700:3VV:H32	2:B:700:3VV:C06	1.95	0.93
1:B:449:MET:HE1	1:B:453:PHE:CE2	2.04	0.92
1:B:317:THR:HA	1:B:397:ARG:HH21	1.25	0.91
1:D:449:MET:HE1	1:D:453:PHE:CE2	2.04	0.91
1:B:179:GLY:HA3	1:B:249:PRO:HG2	1.54	0.90
1:D:449:MET:SD	1:D:453:PHE:CE2	2.65	0.90
1:B:449:MET:SD	1:B:453:PHE:CE2	2.65	0.89
1:D:179:GLY:HA3	1:D:249:PRO:HG2	1.53	0.89
1:B:133:LEU:CD1	1:B:139:ARG:HA	2.03	0.89
1:D:133:LEU:CD1	1:D:139:ARG:HA	2.03	0.86
1:B:120:LYS:HB2	1:B:430:TYR:HE2	1.40	0.85
1:D:120:LYS:HB2	1:D:430:TYR:HE2	1.40	0.84
1:D:124:ALA:O	1:D:125:ARG:HG3	1.78	0.83
1:B:124:ALA:O	1:B:125:ARG:HG3	1.78	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:MET:HE1	1:B:453:PHE:HE2	1.45	0.82
1:B:449:MET:CE	1:B:453:PHE:HE2	1.93	0.82
1:D:449:MET:CE	1:D:453:PHE:HE2	1.93	0.82
1:B:133:LEU:HD12	1:B:139:ARG:HA	1.59	0.81
2:B:700:3VV:H49	2:B:700:3VV:O39	1.81	0.81
1:D:449:MET:HE1	1:D:453:PHE:HE2	1.45	0.80
1:D:133:LEU:HD12	1:D:139:ARG:HA	1.59	0.80
1:D:317:THR:CA	1:D:397:ARG:HH21	1.94	0.80
1:B:317:THR:CA	1:B:397:ARG:HH21	1.94	0.80
1:D:449:MET:CE	1:D:453:PHE:CE2	2.65	0.79
1:B:206:TRP:CZ3	1:B:219:ARG:HG2	2.17	0.79
2:D:700:3VV:O39	2:D:700:3VV:H49	1.81	0.79
1:D:206:TRP:CZ3	1:D:219:ARG:HG2	2.17	0.79
1:B:449:MET:CE	1:B:453:PHE:CE2	2.65	0.78
1:D:215:HIS:HD2	1:D:216:PRO:HD2	1.52	0.75
1:A:293:THR:HG22	1:A:295:ASN:H	1.52	0.74
1:B:206:TRP:HZ3	1:B:219:ARG:HG2	1.53	0.74
1:C:293:THR:HG22	1:C:295:ASN:H	1.52	0.74
1:D:206:TRP:HZ3	1:D:219:ARG:HG2	1.53	0.73
1:A:120:LYS:NZ	1:A:426:ASP:OD2	2.20	0.73
1:C:337:VAL:HG13	1:C:376:ILE:HD12	1.71	0.72
1:D:314:ARG:O	1:D:315:ASN:C	2.31	0.72
1:A:179:GLY:HA3	1:A:249:PRO:HG3	1.71	0.72
1:A:337:VAL:HG13	1:A:376:ILE:HD12	1.71	0.72
1:A:429:TYR:CE1	1:A:433:TYR:HD2	2.08	0.72
1:B:215:HIS:HD2	1:B:216:PRO:HD2	1.52	0.72
1:C:429:TYR:CE1	1:C:433:TYR:HD2	2.08	0.71
1:C:179:GLY:HA3	1:C:249:PRO:HG3	1.71	0.71
1:C:120:LYS:NZ	1:C:426:ASP:OD2	2.20	0.71
1:D:195:THR:HG21	1:D:263:PHE:CD1	2.26	0.70
1:B:314:ARG:O	1:B:315:ASN:C	2.31	0.70
1:B:348:LEU:HD21	1:B:365:CYS:HB2	1.74	0.70
1:B:195:THR:HG21	1:B:263:PHE:CD1	2.26	0.70
1:D:449:MET:SD	1:D:453:PHE:CD2	2.85	0.69
1:D:348:LEU:HD21	1:D:365:CYS:HB2	1.74	0.69
1:D:253:ARG:HD3	1:D:467:CYS:HA	1.74	0.69
1:A:126:ARG:O	1:A:401:ARG:CB	2.40	0.69
1:B:449:MET:SD	1:B:453:PHE:CD2	2.85	0.68
1:C:126:ARG:O	1:C:401:ARG:CB	2.40	0.68
1:A:393:ALA:O	1:A:397:ARG:N	2.27	0.68
2:B:700:3VV:H41	2:B:700:3VV:O32	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ARG:HD3	1:B:467:CYS:HA	1.74	0.68
1:C:393:ALA:O	1:C:397:ARG:N	2.27	0.68
2:B:700:3VV:H46	2:B:700:3VV:O40	1.94	0.67
1:B:122:PHE:HB2	1:B:400:ASP:HB2	1.76	0.67
1:D:255:ILE:O	1:D:259:GLU:HG2	1.95	0.67
1:B:255:ILE:O	1:B:259:GLU:HG2	1.95	0.66
1:B:314:ARG:HH11	1:B:314:ARG:HG2	1.60	0.66
1:D:314:ARG:HG2	1:D:314:ARG:HH11	1.60	0.66
1:D:122:PHE:HB2	1:D:400:ASP:HB2	1.76	0.66
2:D:700:3VV:O32	2:D:700:3VV:H41	1.94	0.66
1:C:353:LYS:HG3	1:C:523:TYR:OH	1.96	0.66
2:D:700:3VV:H46	2:D:700:3VV:O40	1.94	0.66
1:B:348:LEU:HD11	1:B:365:CYS:HA	1.78	0.66
1:A:121:ILE:HG22	1:A:122:PHE:H	1.60	0.66
1:B:200:TYR:CZ	1:B:294:VAL:HB	2.31	0.65
1:C:363:VAL:HA	1:C:366:VAL:HG22	1.79	0.65
1:B:429:TYR:HE1	1:B:433:TYR:HD2	1.44	0.65
1:B:243:VAL:HA	1:B:248:LEU:HD13	1.78	0.65
1:C:121:ILE:HG22	1:C:122:PHE:H	1.60	0.65
1:D:200:TYR:CZ	1:D:294:VAL:HB	2.31	0.65
1:C:489:ILE:HA	1:C:494:ARG:HH21	1.61	0.65
1:A:353:LYS:HG3	1:A:523:TYR:OH	1.96	0.65
1:D:429:TYR:HE1	1:D:433:TYR:HD2	1.44	0.65
1:D:243:VAL:HA	1:D:248:LEU:HD13	1.78	0.64
1:D:237:PHE:HA	1:D:240:THR:HG22	1.80	0.64
1:A:489:ILE:HA	1:A:494:ARG:HH21	1.61	0.64
1:B:237:PHE:HA	1:B:240:THR:HG22	1.80	0.64
1:A:363:VAL:HA	1:A:366:VAL:HG22	1.79	0.64
1:D:348:LEU:HD11	1:D:365:CYS:HA	1.78	0.64
1:D:215:HIS:CD2	1:D:216:PRO:HD2	2.33	0.64
1:D:133:LEU:HD11	1:D:139:ARG:HA	1.80	0.63
1:C:125:ARG:O	1:C:126:ARG:HB2	1.98	0.63
1:B:194:SER:O	1:B:198:VAL:HG12	1.99	0.63
1:B:127:SER:HA	1:B:401:ARG:O	1.99	0.62
1:D:433:TYR:CZ	2:D:700:3VV:O43	2.52	0.62
1:D:127:SER:HA	1:D:401:ARG:O	1.99	0.62
1:A:125:ARG:O	1:A:126:ARG:HB2	1.98	0.62
1:C:277:ARG:HB3	1:C:289:VAL:HG21	1.82	0.62
1:B:215:HIS:CD2	1:B:216:PRO:HD2	2.33	0.62
1:A:206:TRP:CH2	1:A:219:ARG:HG3	2.35	0.62
1:B:433:TYR:CZ	2:B:700:3VV:O43	2.52	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:SER:O	1:D:198:VAL:HG12	1.99	0.62
1:A:277:ARG:HB3	1:A:289:VAL:HG21	1.82	0.62
1:C:225:PHE:O	1:C:228:MET:HG3	2.00	0.61
1:A:460:HIS:NE2	2:A:700:3VV:S20	2.73	0.61
1:B:133:LEU:HD11	1:B:139:ARG:HA	1.80	0.61
1:A:206:TRP:CZ3	1:A:219:ARG:HG3	2.36	0.61
1:B:184:VAL:HG11	1:B:252:SER:HB2	1.83	0.61
1:D:184:VAL:HG11	1:D:252:SER:HB2	1.83	0.61
1:A:225:PHE:O	1:A:228:MET:HG3	2.00	0.61
1:B:184:VAL:HA	1:B:187:THR:HG22	1.83	0.60
1:D:184:VAL:HA	1:D:187:THR:HG22	1.83	0.60
1:D:314:ARG:HH11	1:D:314:ARG:CG	2.14	0.60
1:A:394:GLU:OE2	1:A:401:ARG:NH1	2.34	0.60
1:A:429:TYR:CE1	1:A:433:TYR:CD2	2.90	0.60
1:B:304:PRO:HG2	1:B:393:ALA:HB2	1.83	0.60
1:C:206:TRP:CH2	1:C:219:ARG:HG3	2.35	0.60
1:C:206:TRP:CZ3	1:C:219:ARG:HG3	2.36	0.60
1:C:460:HIS:NE2	2:C:700:3VV:S20	2.73	0.60
1:C:429:TYR:CE1	1:C:433:TYR:CD2	2.90	0.60
1:D:304:PRO:HG2	1:D:393:ALA:HB2	1.83	0.60
1:C:250:PRO:O	1:C:254:PHE:N	2.33	0.59
1:D:124:ALA:C	1:D:125:ARG:HG3	2.28	0.59
1:C:125:ARG:O	1:C:126:ARG:CB	2.50	0.59
1:C:206:TRP:CH2	1:C:220:SER:HA	2.38	0.59
1:C:394:GLU:OE2	1:C:401:ARG:NH1	2.34	0.59
1:A:206:TRP:CH2	1:A:220:SER:HA	2.38	0.59
2:B:700:3VV:H49	2:B:700:3VV:P38	2.43	0.58
1:B:124:ALA:C	1:B:125:ARG:HG3	2.28	0.58
1:B:314:ARG:HH11	1:B:314:ARG:CG	2.14	0.58
1:A:125:ARG:O	1:A:126:ARG:CB	2.50	0.58
1:A:128:LEU:O	1:A:128:LEU:HD22	2.04	0.57
2:D:700:3VV:H49	2:D:700:3VV:P38	2.43	0.57
1:D:314:ARG:O	1:D:315:ASN:O	2.22	0.57
1:B:314:ARG:O	1:B:315:ASN:O	2.22	0.57
1:A:487:ASN:O	1:A:491:ASN:HB2	2.05	0.57
1:C:128:LEU:O	1:C:128:LEU:HD22	2.04	0.57
1:C:476:PHE:O	1:C:480:MET:HG2	2.05	0.57
1:A:160:ASP:OD2	1:A:343:ARG:NH2	2.38	0.57
1:C:487:ASN:O	1:C:491:ASN:HB2	2.05	0.56
1:B:215:HIS:HB3	1:B:218:ILE:HG12	1.86	0.56
1:C:160:ASP:OD2	1:C:343:ARG:NH2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:TYR:O	1:D:342:GLU:HG2	2.05	0.56
1:B:126:ARG:O	1:B:127:SER:C	2.48	0.56
1:D:133:LEU:HD12	1:D:133:LEU:O	2.05	0.56
1:A:501:VAL:O	1:A:505:THR:HG23	2.06	0.56
1:B:133:LEU:HD12	1:B:133:LEU:O	2.05	0.56
1:A:250:PRO:O	1:A:254:PHE:N	2.33	0.56
1:A:352:ILE:O	1:A:356:PRO:HB3	2.06	0.56
1:C:470:PHE:HB2	1:C:522:TRP:HD1	1.71	0.56
1:D:215:HIS:HB3	1:D:218:ILE:HG12	1.86	0.56
1:A:476:PHE:O	1:A:480:MET:HG2	2.05	0.55
1:B:183:THR:HA	1:B:186:TRP:CD1	2.41	0.55
1:B:338:TYR:O	1:B:342:GLU:HG2	2.05	0.55
1:B:182:PRO:HA	1:B:185:VAL:HG22	1.89	0.55
1:C:352:ILE:O	1:C:356:PRO:HB3	2.06	0.55
1:D:183:THR:HA	1:D:186:TRP:CD1	2.41	0.55
1:B:343:ARG:HG2	1:B:344:LEU:HD22	1.89	0.55
1:A:470:PHE:HB2	1:A:522:TRP:HD1	1.71	0.55
1:C:356:PRO:HB2	1:C:524:ALA:HB2	1.89	0.55
1:D:322:TYR:HD2	1:D:394:GLU:HG2	1.71	0.55
1:C:184:VAL:HA	1:C:187:THR:HG22	1.89	0.55
1:C:501:VAL:O	1:C:505:THR:HG23	2.06	0.55
1:B:133:LEU:O	1:B:139:ARG:HB2	2.06	0.55
1:A:184:VAL:HA	1:A:187:THR:HG22	1.89	0.55
1:B:322:TYR:HD2	1:B:394:GLU:HG2	1.71	0.55
1:D:133:LEU:O	1:D:139:ARG:HB2	2.06	0.55
1:D:126:ARG:O	1:D:127:SER:C	2.48	0.55
1:D:128:LEU:O	1:D:132:LEU:HB2	2.06	0.55
1:B:133:LEU:HD13	1:B:138:ILE:HG22	1.89	0.54
1:C:243:VAL:HA	1:C:248:LEU:HD23	1.88	0.54
1:C:353:LYS:HA	1:C:523:TYR:CE2	2.43	0.54
1:D:317:THR:HA	1:D:397:ARG:HH22	1.69	0.54
1:A:243:VAL:HA	1:A:248:LEU:HD23	1.88	0.54
1:D:182:PRO:HA	1:D:185:VAL:HG22	1.89	0.54
1:D:343:ARG:HG2	1:D:344:LEU:HD22	1.89	0.54
1:D:133:LEU:HD13	1:D:138:ILE:HG22	1.89	0.53
1:A:353:LYS:HA	1:A:523:TYR:CE2	2.43	0.53
1:A:356:PRO:HB2	1:A:524:ALA:HB2	1.89	0.53
1:A:171:PHE:HA	1:A:338:TYR:OH	2.08	0.53
1:B:196:PHE:HE1	1:B:294:VAL:CG2	2.21	0.53
1:B:128:LEU:O	1:B:132:LEU:HB2	2.06	0.53
1:B:429:TYR:HE1	1:B:433:TYR:CD2	2.25	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LEU:HD12	1:D:139:ARG:CA	2.35	0.53
1:D:199:PRO:HG3	1:D:230:PHE:CE2	2.44	0.53
1:B:181:PHE:O	1:B:184:VAL:HG22	2.09	0.53
1:A:127:SER:HA	1:A:401:ARG:O	2.09	0.53
1:C:171:PHE:HA	1:C:338:TYR:OH	2.08	0.53
1:C:127:SER:HA	1:C:401:ARG:O	2.09	0.52
1:D:181:PHE:O	1:D:184:VAL:HG22	2.09	0.52
1:D:196:PHE:HE1	1:D:294:VAL:CG2	2.21	0.52
1:A:259:GLU:OE1	1:A:262:ARG:NH1	2.43	0.52
1:B:199:PRO:HG3	1:B:230:PHE:CE2	2.44	0.52
1:C:194:SER:O	1:C:198:VAL:HG12	2.09	0.52
1:D:240:THR:HA	1:D:243:VAL:HG12	1.92	0.52
1:D:429:TYR:HE1	1:D:433:TYR:CD2	2.25	0.52
1:A:253:ARG:HD3	1:A:466:VAL:O	2.10	0.52
1:B:434:LYS:HA	1:B:437:LEU:HD12	1.91	0.52
1:D:449:MET:SD	1:D:453:PHE:HE2	2.22	0.52
1:A:194:SER:O	1:A:198:VAL:HG12	2.09	0.52
2:B:700:3VV:O30	2:B:700:3VV:H51	2.09	0.52
1:C:253:ARG:HD3	1:C:466:VAL:O	2.10	0.52
1:C:259:GLU:OE1	1:C:262:ARG:NH1	2.43	0.52
1:A:237:PHE:O	1:A:241:TYR:N	2.33	0.52
1:B:352:ILE:O	1:B:356:PRO:HB3	2.10	0.52
1:D:352:ILE:O	1:D:356:PRO:HB3	2.10	0.52
2:D:700:3VV:H46	2:D:700:3VV:P38	2.51	0.52
1:B:133:LEU:HD12	1:B:139:ARG:CA	2.35	0.51
1:B:180:LYS:HD3	1:B:249:PRO:HD3	1.93	0.51
1:D:180:LYS:HD3	1:D:249:PRO:HD3	1.93	0.51
1:B:191:MET:SD	1:B:239:PRO:HG3	2.50	0.51
1:B:449:MET:SD	1:B:449:MET:C	2.94	0.51
1:C:228:MET:SD	1:C:228:MET:C	2.94	0.51
1:A:315:ASN:HD21	1:A:399:GLY:HA2	1.74	0.51
1:D:191:MET:SD	1:D:239:PRO:HG3	2.50	0.51
1:A:228:MET:SD	1:A:228:MET:C	2.94	0.51
1:C:315:ASN:HD21	1:C:399:GLY:HA2	1.74	0.51
1:D:449:MET:SD	1:D:449:MET:C	2.94	0.51
1:B:240:THR:HA	1:B:243:VAL:HG12	1.92	0.51
2:B:700:3VV:H46	2:B:700:3VV:P38	2.50	0.51
2:D:700:3VV:O30	2:D:700:3VV:H51	2.09	0.51
1:D:434:LYS:HA	1:D:437:LEU:HD12	1.91	0.51
1:A:184:VAL:HG11	1:A:252:SER:HB3	1.93	0.50
1:B:449:MET:HE1	1:B:453:PHE:CZ	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ASP:N	1:C:136:ASP:OD1	2.44	0.50
1:B:127:SER:HB3	1:B:404:TYR:CE1	2.46	0.50
1:D:120:LYS:HB2	1:D:430:TYR:CE2	2.33	0.50
1:D:127:SER:HB3	1:D:404:TYR:CE1	2.46	0.50
1:C:446:SER:O	1:C:449:MET:HG3	2.12	0.50
1:B:323:VAL:HG13	1:B:394:GLU:HG2	1.93	0.50
1:C:184:VAL:HG11	1:C:252:SER:HB3	1.93	0.50
1:D:402:MET:O	1:D:422:VAL:HG21	2.12	0.50
1:B:118:GLN:OE1	1:B:118:GLN:N	2.45	0.50
1:B:314:ARG:CG	1:B:314:ARG:NH1	2.73	0.50
1:D:118:GLN:N	1:D:118:GLN:OE1	2.45	0.50
1:B:496:LYS:HB2	1:B:499:TRP:HD1	1.77	0.50
1:B:133:LEU:HD21	1:B:142:TYR:CG	2.47	0.50
1:D:133:LEU:HD21	1:D:142:TYR:CG	2.47	0.50
1:D:496:LYS:HB2	1:D:499:TRP:HD1	1.77	0.50
2:D:700:3VV:O30	2:D:700:3VV:H47	2.12	0.50
1:C:376:ILE:O	1:C:380:THR:HG22	2.12	0.50
1:A:277:ARG:HE	1:A:289:VAL:HG21	1.77	0.50
1:A:462:TYR:O	1:A:466:VAL:HG12	2.11	0.50
1:D:314:ARG:CG	1:D:314:ARG:NH1	2.73	0.50
1:B:402:MET:O	1:B:422:VAL:HG21	2.12	0.49
1:C:470:PHE:HB2	1:C:522:TRP:CD1	2.47	0.49
1:B:474:VAL:HB	1:B:478:LEU:HD23	1.94	0.49
1:D:171:PHE:HD1	1:D:338:TYR:HE2	1.60	0.49
1:A:270:PHE:O	1:A:274:ASN:ND2	2.45	0.49
1:A:470:PHE:HB2	1:A:522:TRP:CD1	2.47	0.49
1:D:323:VAL:HG13	1:D:394:GLU:HG2	1.93	0.49
1:A:136:ASP:N	1:A:136:ASP:OD1	2.44	0.49
2:B:700:3VV:O30	2:B:700:3VV:H47	2.12	0.49
1:D:491:ASN:CG	1:D:492:ASP:H	2.20	0.49
1:A:362:LEU:O	1:A:366:VAL:HG13	2.13	0.49
1:A:376:ILE:O	1:A:380:THR:HG22	2.12	0.49
1:C:270:PHE:O	1:C:274:ASN:ND2	2.45	0.49
1:D:354:GLN:O	1:D:356:PRO:HD3	2.13	0.49
1:A:446:SER:O	1:A:449:MET:HG3	2.11	0.49
1:C:348:LEU:HD13	1:C:365:CYS:CB	2.42	0.49
1:C:401:ARG:HA	1:C:403:PHE:CZ	2.48	0.49
1:D:154:LEU:O	1:D:158:VAL:HG23	2.13	0.49
1:A:348:LEU:HD13	1:A:365:CYS:CB	2.42	0.49
1:B:354:GLN:O	1:B:356:PRO:HD3	2.13	0.49
1:B:376:ILE:O	1:B:380:THR:HG22	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:PHE:HB2	1:D:400:ASP:CB	2.43	0.49
1:D:215:HIS:ND1	1:D:218:ILE:HG23	2.28	0.49
1:D:277:ARG:NE	1:D:290:PRO:HG2	2.28	0.49
2:A:700:3VV:H5	2:A:700:3VV:H10	1.95	0.49
1:B:277:ARG:NE	1:B:290:PRO:HG2	2.28	0.49
1:C:462:TYR:O	1:C:466:VAL:HG12	2.11	0.49
1:A:401:ARG:HA	1:A:403:PHE:CZ	2.48	0.49
1:B:215:HIS:ND1	1:B:218:ILE:HG23	2.28	0.49
1:C:323:VAL:HG21	1:C:395:MET:HG3	1.95	0.49
1:A:213:SER:OG	1:A:214:SER:N	2.46	0.48
1:B:317:THR:HA	1:B:397:ARG:HH22	1.69	0.48
1:C:118:GLN:CD	1:C:118:GLN:H	2.21	0.48
1:C:277:ARG:HE	1:C:289:VAL:HG21	1.77	0.48
1:A:118:GLN:H	1:A:118:GLN:CD	2.21	0.48
2:C:700:3VV:H5	2:C:700:3VV:H10	1.95	0.48
1:B:359:ALA:O	1:B:363:VAL:HG23	2.14	0.48
1:C:358:SER:O	1:C:360:ARG:NH1	2.46	0.48
1:D:449:MET:HE1	1:D:453:PHE:CZ	2.46	0.48
1:B:171:PHE:HD1	1:B:338:TYR:HE2	1.60	0.48
1:C:132:LEU:O	1:C:134:GLU:N	2.47	0.48
1:D:474:VAL:HB	1:D:478:LEU:HD23	1.94	0.48
1:A:350:ARG:O	1:A:353:LYS:HB3	2.14	0.48
2:A:700:3VV:H1	2:A:700:3VV:H26	1.96	0.48
1:B:122:PHE:HB2	1:B:400:ASP:CB	2.43	0.48
1:B:491:ASN:CG	1:B:492:ASP:H	2.20	0.48
1:C:213:SER:OG	1:C:214:SER:N	2.46	0.48
1:D:317:THR:C	1:D:397:ARG:HH21	2.21	0.48
1:D:359:ALA:O	1:D:363:VAL:HG23	2.14	0.48
1:A:323:VAL:HG21	1:A:395:MET:HG3	1.95	0.48
1:C:362:LEU:O	1:C:366:VAL:HG13	2.13	0.48
1:D:376:ILE:O	1:D:380:THR:HG22	2.13	0.48
1:A:433:TYR:HE2	2:A:700:3VV:H57	1.79	0.48
1:B:317:THR:C	1:B:397:ARG:HH21	2.21	0.48
1:C:200:TYR:OH	1:C:292:PRO:O	2.29	0.48
1:C:402:MET:O	1:C:422:VAL:HG21	2.14	0.48
1:A:231:GLN:HE21	1:A:264:VAL:HG13	1.79	0.48
1:B:177:ALA:O	1:B:249:PRO:HB2	2.14	0.48
1:C:237:PHE:O	1:C:241:TYR:N	2.33	0.48
1:C:433:TYR:HE2	2:C:700:3VV:H57	1.79	0.48
2:C:700:3VV:H1	2:C:700:3VV:H26	1.96	0.48
1:A:292:PRO:HG3	1:A:308:TYR:OH	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:SER:O	1:A:360:ARG:NH1	2.46	0.47
1:C:485:ALA:O	1:C:489:ILE:HG23	2.14	0.47
1:C:206:TRP:CZ2	1:C:220:SER:HA	2.49	0.47
1:C:277:ARG:HB3	1:C:289:VAL:CG2	2.44	0.47
1:A:402:MET:O	1:A:422:VAL:HG21	2.14	0.47
1:A:206:TRP:CZ2	1:A:220:SER:HA	2.49	0.47
1:A:277:ARG:HB3	1:A:289:VAL:CG2	2.44	0.47
1:B:154:LEU:O	1:B:158:VAL:HG23	2.13	0.47
1:C:125:ARG:HG2	1:C:399:GLY:O	2.15	0.47
1:C:231:GLN:HE21	1:C:264:VAL:HG13	1.79	0.47
1:D:428:LEU:HA	1:D:428:LEU:HD23	1.69	0.47
1:A:125:ARG:HG2	1:A:399:GLY:O	2.15	0.47
1:A:132:LEU:O	1:A:134:GLU:N	2.47	0.47
1:A:434:LYS:O	1:A:437:LEU:HG	2.15	0.47
1:C:143:HIS:HD2	1:D:501:VAL:HG23	1.80	0.47
1:C:292:PRO:HG3	1:C:308:TYR:OH	2.13	0.47
1:C:327:PHE:HA	1:C:330:VAL:HG12	1.96	0.47
1:C:350:ARG:O	1:C:353:LYS:HB3	2.14	0.47
1:C:429:TYR:HD1	1:C:433:TYR:HB3	1.80	0.47
1:D:177:ALA:O	1:D:249:PRO:HB2	2.14	0.47
1:D:239:PRO:HA	1:D:242:VAL:HG12	1.97	0.47
1:D:311:SER:O	1:D:311:SER:OG	2.33	0.47
1:C:434:LYS:O	1:C:437:LEU:HG	2.15	0.47
1:A:200:TYR:OH	1:A:292:PRO:O	2.29	0.47
1:A:123:ILE:HD12	1:A:123:ILE:H	1.80	0.47
1:A:143:HIS:HD2	1:B:501:VAL:HG23	1.80	0.47
1:A:485:ALA:O	1:A:489:ILE:HG23	2.14	0.47
1:B:314:ARG:NE	1:B:397:ARG:HE	2.13	0.47
1:C:123:ILE:HD12	1:C:123:ILE:H	1.80	0.47
1:D:314:ARG:C	1:D:315:ASN:O	2.58	0.47
1:A:359:ALA:HB1	1:A:361:VAL:HG22	1.97	0.46
1:A:327:PHE:HA	1:A:330:VAL:HG12	1.96	0.46
1:A:511:ASN:OD1	1:A:512:GLY:N	2.49	0.46
1:B:174:LEU:HB2	1:B:338:TYR:CZ	2.51	0.46
1:D:133:LEU:HD11	1:D:142:TYR:CB	2.46	0.46
1:C:125:ARG:HA	1:C:400:ASP:O	2.16	0.46
1:A:429:TYR:HD1	1:A:433:TYR:HB3	1.80	0.46
1:A:441:SER:OG	1:A:444:PHE:HB2	2.16	0.46
1:C:511:ASN:OD1	1:C:512:GLY:N	2.49	0.46
1:A:125:ARG:HA	1:A:400:ASP:O	2.16	0.46
1:B:239:PRO:HA	1:B:242:VAL:HG12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ARG:HG2	1:C:143:HIS:CE1	2.51	0.46
1:C:441:SER:OG	1:C:444:PHE:HB2	2.16	0.46
1:A:139:ARG:HG2	1:A:143:HIS:CE1	2.51	0.46
1:A:333:CYS:O	1:A:337:VAL:HG23	2.16	0.46
1:B:133:LEU:HD11	1:B:142:TYR:CB	2.46	0.46
1:C:359:ALA:HB1	1:C:361:VAL:HG22	1.97	0.46
1:B:191:MET:HG2	1:B:235:LEU:HD21	1.98	0.45
1:B:299:TYR:CD1	1:B:299:TYR:C	2.94	0.45
1:D:174:LEU:HB2	1:D:338:TYR:CZ	2.50	0.45
1:D:314:ARG:NE	1:D:397:ARG:HE	2.13	0.45
1:D:348:LEU:O	1:D:352:ILE:HG22	2.17	0.45
1:A:521:GLU:OE1	1:A:525:ARG:HB3	2.17	0.45
1:B:294:VAL:O	1:B:297:TYR:N	2.49	0.45
1:C:348:LEU:HD13	1:C:365:CYS:HB3	1.98	0.45
1:D:430:TYR:CD1	1:D:434:LYS:HE2	2.52	0.45
1:B:124:ALA:O	1:B:400:ASP:HA	2.17	0.45
1:B:450:LEU:O	1:B:453:PHE:HB2	2.16	0.45
1:D:450:LEU:HD13	1:D:450:LEU:HA	1.81	0.45
1:C:151:LEU:HD23	1:C:151:LEU:HA	1.82	0.45
1:B:127:SER:H	1:B:401:ARG:HB3	1.81	0.45
1:B:430:TYR:CD1	1:B:434:LYS:HE2	2.52	0.45
1:D:193:LEU:HD13	1:D:193:LEU:HA	1.77	0.45
1:D:299:TYR:CD1	1:D:299:TYR:C	2.94	0.45
1:B:465:ALA:O	1:B:469:SER:N	2.50	0.45
1:C:382:PHE:O	1:C:386:HIS:HB3	2.17	0.45
1:B:196:PHE:O	1:B:196:PHE:CD1	2.70	0.45
1:D:124:ALA:O	1:D:400:ASP:HA	2.17	0.45
1:D:191:MET:HG2	1:D:235:LEU:HD21	1.98	0.45
1:B:314:ARG:C	1:B:315:ASN:O	2.58	0.45
1:B:333:CYS:O	1:B:337:VAL:HG23	2.17	0.45
1:D:127:SER:H	1:D:401:ARG:HB3	1.81	0.45
1:A:153:ILE:HG12	1:A:336:TYR:HE2	1.82	0.45
1:A:180:LYS:O	1:A:183:THR:HG22	2.17	0.45
1:B:429:TYR:CE1	1:B:433:TYR:HD2	2.31	0.45
1:C:449:MET:O	1:C:452:VAL:HG12	2.17	0.45
1:D:294:VAL:O	1:D:297:TYR:N	2.49	0.45
1:D:465:ALA:O	1:D:469:SER:N	2.50	0.45
1:B:239:PRO:HB2	1:B:260:GLN:NE2	2.32	0.44
1:B:359:ALA:O	1:B:362:LEU:HG	2.17	0.44
1:C:153:ILE:HG12	1:C:336:TYR:HE2	1.82	0.44
1:D:196:PHE:O	1:D:196:PHE:CD1	2.70	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:HD13	1:A:365:CYS:HB3	1.98	0.44
1:C:333:CYS:O	1:C:337:VAL:HG23	2.16	0.44
1:C:521:GLU:OE1	1:C:525:ARG:HB3	2.16	0.44
1:D:195:THR:O	1:D:199:PRO:HD2	2.17	0.44
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.82	0.44
1:C:346:ALA:HB3	1:C:347:PRO:HD3	1.99	0.44
1:D:132:LEU:HD22	1:D:132:LEU:O	2.17	0.44
1:D:365:CYS:SG	1:D:366:VAL:N	2.91	0.44
1:D:450:LEU:O	1:D:453:PHE:HB2	2.16	0.44
1:A:346:ALA:HB3	1:A:347:PRO:HD3	1.99	0.44
1:B:311:SER:O	1:B:311:SER:OG	2.33	0.44
1:C:180:LYS:O	1:C:183:THR:HG22	2.17	0.44
1:A:464:LEU:HD12	1:A:464:LEU:HA	1.83	0.44
1:B:348:LEU:O	1:B:352:ILE:HG22	2.17	0.44
1:B:365:CYS:SG	1:B:366:VAL:N	2.91	0.44
1:C:127:SER:HB3	1:C:128:LEU:H	1.56	0.44
1:D:470:PHE:CE2	1:D:472:TYR:HB2	2.53	0.44
1:A:382:PHE:O	1:A:386:HIS:HB3	2.17	0.44
1:B:449:MET:O	1:B:452:VAL:HG12	2.18	0.44
1:D:239:PRO:HB2	1:D:260:GLN:NE2	2.32	0.44
1:D:359:ALA:O	1:D:362:LEU:HG	2.17	0.44
1:C:348:LEU:HD13	1:C:365:CYS:SG	2.58	0.44
1:B:218:ILE:HG13	1:B:219:ARG:N	2.33	0.44
1:D:333:CYS:O	1:D:337:VAL:HG23	2.17	0.44
1:B:428:LEU:HD23	1:B:428:LEU:HA	1.69	0.44
1:B:464:LEU:HD12	1:B:464:LEU:HA	1.79	0.44
1:B:470:PHE:CE2	1:B:472:TYR:HB2	2.53	0.44
1:D:218:ILE:HG13	1:D:219:ARG:N	2.33	0.44
1:B:120:LYS:HB2	1:B:430:TYR:CE2	2.33	0.43
1:D:314:ARG:HD3	1:D:397:ARG:CD	2.48	0.43
1:A:348:LEU:HD13	1:A:365:CYS:SG	2.58	0.43
1:B:433:TYR:CE2	2:B:700:3VV:O43	2.71	0.43
1:D:433:TYR:CE2	2:D:700:3VV:O43	2.71	0.43
1:A:336:TYR:CE1	1:A:340:ILE:HG13	2.54	0.43
1:C:240:THR:HA	1:C:243:VAL:HG12	2.01	0.43
1:D:449:MET:O	1:D:452:VAL:HG12	2.18	0.43
1:B:177:ALA:O	1:B:251:ALA:HB3	2.18	0.43
1:B:314:ARG:HD3	1:B:397:ARG:CD	2.48	0.43
1:B:379:LEU:HD23	1:B:379:LEU:HA	1.84	0.43
1:C:470:PHE:CE1	1:C:526:GLN:HG3	2.54	0.43
1:A:449:MET:O	1:A:452:VAL:HG12	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:THR:O	1:B:199:PRO:HD2	2.17	0.43
1:C:215:HIS:CG	1:C:216:PRO:HD3	2.54	0.43
1:D:177:ALA:O	1:D:251:ALA:HB3	2.18	0.43
1:D:235:LEU:HD23	1:D:235:LEU:HA	1.82	0.43
1:D:429:TYR:CE1	1:D:433:TYR:HD2	2.31	0.43
1:C:336:TYR:CE1	1:C:340:ILE:HG13	2.54	0.43
1:C:348:LEU:HD12	1:C:348:LEU:O	2.19	0.43
1:A:122:PHE:CE2	1:A:313:PRO:HD3	2.54	0.43
1:A:236:GLY:HA2	1:A:260:GLN:HE21	1.84	0.43
1:A:470:PHE:CE1	1:A:526:GLN:HG3	2.54	0.43
1:A:479:PHE:CZ	1:A:514:LEU:HD11	2.54	0.43
1:D:405:LYS:HE3	1:D:405:LYS:HB2	1.93	0.43
1:A:240:THR:HA	1:A:243:VAL:HG12	2.01	0.43
1:A:348:LEU:HD12	1:A:348:LEU:O	2.19	0.43
1:B:275:VAL:O	1:B:279:LEU:HG	2.19	0.43
1:C:379:LEU:HD23	1:C:379:LEU:HA	1.84	0.43
1:D:275:VAL:O	1:D:279:LEU:HG	2.19	0.43
1:A:349:PHE:HA	1:A:352:ILE:HG12	2.01	0.42
1:B:127:SER:HB3	1:B:404:TYR:CZ	2.54	0.42
1:B:249:PRO:HA	1:B:250:PRO:HD3	1.86	0.42
1:C:479:PHE:CZ	1:C:514:LEU:HD11	2.54	0.42
1:D:330:VAL:HG23	1:D:387:CYS:HB3	2.01	0.42
1:A:215:HIS:CG	1:A:216:PRO:HD3	2.54	0.42
2:D:700:3VV:H13	2:D:700:3VV:H10	1.70	0.42
1:D:294:VAL:C	1:D:296:GLN:H	2.26	0.42
1:A:153:ILE:HD13	1:A:153:ILE:HA	1.85	0.42
1:A:206:TRP:CZ3	1:A:223:HIS:HB3	2.54	0.42
1:B:132:LEU:HD22	1:B:132:LEU:O	2.19	0.42
1:B:294:VAL:C	1:B:296:GLN:H	2.26	0.42
1:D:196:PHE:CD1	1:D:196:PHE:C	2.97	0.42
1:D:293:THR:HG23	1:D:296:GLN:HB2	2.00	0.42
1:B:183:THR:HA	1:B:186:TRP:NE1	2.35	0.42
1:B:293:THR:HG23	1:B:296:GLN:HB2	2.00	0.42
1:D:468:LEU:O	1:D:469:SER:C	2.62	0.42
1:D:127:SER:HB3	1:D:404:TYR:CZ	2.54	0.42
1:D:183:THR:HA	1:D:186:TRP:NE1	2.35	0.42
1:D:434:LYS:O	1:D:437:LEU:HB2	2.20	0.42
1:B:468:LEU:O	1:B:469:SER:C	2.62	0.42
1:B:494:ARG:C	1:B:496:LYS:H	2.28	0.42
1:C:142:TYR:CZ	1:C:146:ILE:HD11	2.55	0.42
1:C:320:TRP:HA	1:C:323:VAL:HG12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:GLU:O	1:D:361:VAL:HG11	2.20	0.42
1:B:355:GLU:O	1:B:361:VAL:HG11	2.20	0.42
1:C:151:LEU:HD13	1:D:370:ILE:HG21	2.02	0.42
1:C:433:TYR:CE2	2:C:700:3VV:H57	2.54	0.42
1:D:122:PHE:CZ	1:D:313:PRO:HD3	2.55	0.42
1:A:146:ILE:O	1:A:150:ILE:HG22	2.20	0.41
1:A:202:LEU:HG	1:A:223:HIS:CE1	2.55	0.41
1:B:294:VAL:C	1:B:296:GLN:N	2.78	0.41
1:B:420:TRP:CH2	2:B:700:3VV:H7	2.55	0.41
1:C:206:TRP:CZ3	1:C:223:HIS:HB3	2.54	0.41
1:D:420:TRP:CH2	2:D:700:3VV:H7	2.55	0.41
1:D:521:GLU:OE1	1:D:525:ARG:NH2	2.53	0.41
1:C:146:ILE:O	1:C:150:ILE:HG22	2.20	0.41
1:C:202:LEU:HG	1:C:223:HIS:CE1	2.55	0.41
1:C:236:GLY:HA2	1:C:260:GLN:HE21	1.84	0.41
1:D:319:ARG:HB2	1:D:322:TYR:HB3	2.02	0.41
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.88	0.41
1:A:433:TYR:CE2	2:A:700:3VV:H57	2.54	0.41
1:D:219:ARG:O	1:D:223:HIS:HB2	2.21	0.41
1:A:215:HIS:CE1	1:A:216:PRO:HD3	2.55	0.41
1:A:470:PHE:CZ	1:A:472:TYR:HB2	2.55	0.41
1:B:128:LEU:HB2	1:B:404:TYR:CE2	2.56	0.41
1:B:190:ILE:HD13	1:B:190:ILE:HA	1.93	0.41
1:B:217:LEU:HD23	1:B:217:LEU:H	1.85	0.41
1:B:330:VAL:HG23	1:B:387:CYS:HB3	2.01	0.41
1:C:405:LYS:O	1:C:407:TRP:N	2.52	0.41
1:C:428:LEU:HD23	1:C:428:LEU:HA	1.87	0.41
1:D:294:VAL:C	1:D:296:GLN:N	2.78	0.41
1:A:187:THR:HA	1:A:190:ILE:HG12	2.02	0.41
1:B:122:PHE:CZ	1:B:313:PRO:HD3	2.55	0.41
1:B:319:ARG:HB2	1:B:322:TYR:HB3	2.02	0.41
1:C:470:PHE:CZ	1:C:472:TYR:HB2	2.55	0.41
1:D:146:ILE:O	1:D:150:ILE:HG22	2.21	0.41
1:A:151:LEU:HD13	1:B:370:ILE:HG21	2.02	0.41
1:A:405:LYS:O	1:A:407:TRP:N	2.52	0.41
1:C:122:PHE:CE2	1:C:313:PRO:HD3	2.54	0.41
1:C:144:MET:HE2	1:D:504:TRP:CZ2	2.56	0.41
1:C:187:THR:HA	1:C:190:ILE:HG12	2.02	0.41
1:C:349:PHE:HA	1:C:352:ILE:HG12	2.01	0.41
1:B:246:TYR:HB2	1:B:248:LEU:HD12	2.03	0.41
1:C:215:HIS:CE1	1:C:216:PRO:HD3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:TYR:HB2	1:D:248:LEU:HD12	2.03	0.41
1:A:371:LEU:HB3	1:A:372:PRO:HD3	2.02	0.41
1:A:429:TYR:HE1	1:A:433:TYR:CD2	2.38	0.41
1:C:371:LEU:HB3	1:C:372:PRO:HD3	2.02	0.41
1:C:496:LYS:HE2	1:C:496:LYS:HB3	1.88	0.41
1:D:128:LEU:HB2	1:D:404:TYR:CE2	2.56	0.41
1:D:217:LEU:H	1:D:217:LEU:HD23	1.85	0.41
1:D:464:LEU:HA	1:D:464:LEU:HD12	1.79	0.41
1:A:140:THR:HG21	1:B:408:TRP:HB2	2.03	0.41
1:B:434:LYS:O	1:B:437:LEU:HB2	2.20	0.41
1:C:206:TRP:HH2	1:C:219:ARG:C	2.29	0.41
1:D:191:MET:SD	1:D:239:PRO:CG	3.09	0.41
1:D:266:LYS:HG3	1:D:306:LEU:HD23	2.02	0.41
1:D:510:GLY:HA2	1:D:513:VAL:HG12	2.03	0.41
1:A:126:ARG:HB2	1:A:127:SER:H	1.71	0.41
1:B:521:GLU:OE1	1:B:525:ARG:NH2	2.53	0.41
1:D:231:GLN:O	1:D:236:GLY:N	2.54	0.41
1:D:240:THR:O	1:D:243:VAL:HG12	2.21	0.41
1:A:215:HIS:ND1	1:A:216:PRO:HD3	2.37	0.40
1:B:231:GLN:O	1:B:236:GLY:N	2.54	0.40
1:B:266:LYS:HG3	1:B:306:LEU:HD23	2.02	0.40
1:B:468:LEU:HD23	1:B:468:LEU:HA	1.93	0.40
1:C:322:TYR:CD1	1:C:394:GLU:HG2	2.57	0.40
1:D:423:VAL:HG23	1:D:424:VAL:H	1.87	0.40
1:A:320:TRP:HA	1:A:323:VAL:HG12	2.02	0.40
1:A:496:LYS:HB3	1:A:496:LYS:HE2	1.88	0.40
1:B:146:ILE:O	1:B:150:ILE:HG22	2.21	0.40
1:B:177:ALA:HB1	1:B:251:ALA:HB2	2.04	0.40
1:C:153:ILE:HD13	1:C:153:ILE:HA	1.85	0.40
1:A:127:SER:HB3	1:A:128:LEU:H	1.56	0.40
1:A:183:THR:O	1:A:187:THR:HG22	2.21	0.40
1:A:198:VAL:O	1:A:202:LEU:HB2	2.21	0.40
1:B:493:SER:O	1:B:493:SER:OG	2.33	0.40
1:A:142:TYR:CZ	1:A:146:ILE:HD11	2.55	0.40
1:A:144:MET:HE2	1:B:504:TRP:CZ2	2.56	0.40
1:A:322:TYR:CD1	1:A:394:GLU:HG2	2.57	0.40
1:B:372:PRO:O	1:B:376:ILE:HG12	2.22	0.40
1:C:293:THR:HG22	1:C:295:ASN:N	2.30	0.40
1:D:122:PHE:CE1	1:D:313:PRO:HG3	2.56	0.40
1:A:128:LEU:HA	1:A:128:LEU:HD23	1.77	0.40
1:A:429:TYR:CD1	1:A:433:TYR:HD2	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:PHE:CE1	1:B:313:PRO:HG3	2.56	0.40
1:B:219:ARG:O	1:B:223:HIS:HB2	2.20	0.40
1:B:240:THR:O	1:B:243:VAL:HG12	2.21	0.40
1:C:140:THR:HG21	1:D:408:TRP:HB2	2.03	0.40
1:C:183:THR:O	1:C:187:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	404/594 (68%)	369 (91%)	33 (8%)	2 (0%)	24	57
1	B	403/594 (68%)	372 (92%)	30 (7%)	1 (0%)	43	73
1	C	404/594 (68%)	369 (91%)	33 (8%)	2 (0%)	24	57
1	D	403/594 (68%)	372 (92%)	30 (7%)	1 (0%)	43	73
All	All	1614/2376 (68%)	1482 (92%)	126 (8%)	6 (0%)	31	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	ARG
1	C	126	ARG
1	A	127	SER
1	C	127	SER
1	B	315	ASN
1	D	315	ASN

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	361/532 (68%)	358 (99%)	3 (1%)	73	81
1	B	357/532 (67%)	338 (95%)	19 (5%)	20	51
1	C	361/532 (68%)	358 (99%)	3 (1%)	73	81
1	D	357/532 (67%)	338 (95%)	19 (5%)	20	51
All	All	1436/2128 (68%)	1392 (97%)	44 (3%)	36	64

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	ARG
1	A	128	LEU
1	A	445	LYS
1	B	126	ARG
1	B	127	SER
1	B	131	GLU
1	B	132	LEU
1	B	133	LEU
1	B	156	THR
1	B	191	MET
1	B	193	LEU
1	B	194	SER
1	B	223	HIS
1	B	228	MET
1	B	269	SER
1	B	296	GLN
1	B	314	ARG
1	B	397	ARG
1	B	445	LYS
1	B	446	SER
1	B	449	MET
1	B	450	LEU
1	C	126	ARG
1	C	128	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	445	LYS
1	D	126	ARG
1	D	127	SER
1	D	131	GLU
1	D	132	LEU
1	D	133	LEU
1	D	156	THR
1	D	191	MET
1	D	193	LEU
1	D	194	SER
1	D	223	HIS
1	D	228	MET
1	D	269	SER
1	D	296	GLN
1	D	314	ARG
1	D	397	ARG
1	D	445	LYS
1	D	446	SER
1	D	449	MET
1	D	450	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	231	GLN
1	A	280	ASN
1	A	295	ASN
1	A	315	ASN
1	A	351	ASN
1	B	118	GLN
1	B	231	GLN
1	B	260	GLN
1	B	315	ASN
1	B	386	HIS
1	B	409	ASN
1	B	425	HIS
1	C	204	GLN
1	C	231	GLN
1	C	280	ASN
1	C	295	ASN
1	C	315	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	351	ASN
1	D	118	GLN
1	D	231	GLN
1	D	260	GLN
1	D	315	ASN
1	D	409	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	3VV	C	700	-	67,69,69	0.40	0	89,95,95	2.01	8 (8%)
2	3VV	A	700	-	67,69,69	0.40	0	89,95,95	2.01	8 (8%)
2	3VV	D	700	-	67,69,69	0.43	0	89,95,95	0.53	0
2	3VV	B	700	-	67,69,69	0.43	0	89,95,95	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3VV	C	700	-	-	17/68/84/84	0/3/3/3
2	3VV	A	700	-	-	17/68/84/84	0/3/3/3
2	3VV	D	700	-	-	34/68/84/84	0/3/3/3
2	3VV	B	700	-	-	34/68/84/84	0/3/3/3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	3VV	O41-P42-O44	-8.31	85.71	110.70
2	C	700	3VV	O41-P42-O44	-8.31	85.71	110.70
2	A	700	3VV	O37-P38-O40	-8.05	77.03	108.94
2	C	700	3VV	O37-P38-O40	-8.04	77.06	108.94
2	A	700	3VV	O43-P42-O41	7.67	128.02	107.27
2	C	700	3VV	O43-P42-O41	7.66	127.98	107.27
2	C	700	3VV	O41-P38-O40	-6.69	90.56	110.70
2	A	700	3VV	O41-P38-O40	-6.69	90.57	110.70
2	C	700	3VV	O43-P42-O44	-4.51	91.47	112.44
2	A	700	3VV	O43-P42-O44	-4.50	91.49	112.44
2	A	700	3VV	O39-P38-O41	4.37	119.09	107.27
2	C	700	3VV	O39-P38-O41	4.36	119.06	107.27
2	C	700	3VV	O39-P38-O40	-4.15	93.13	112.44
2	A	700	3VV	O39-P38-O40	-4.15	93.14	112.44
2	A	700	3VV	O39-P38-O37	4.06	125.97	107.57
2	C	700	3VV	O39-P38-O37	4.06	125.97	107.57

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	3VV	C24-C26-C27-N28
2	A	700	3VV	C46-O45-P42-O41
2	A	700	3VV	C17-C18-S20-C21
2	A	700	3VV	O19-C18-S20-C21
2	A	700	3VV	C31-C29-N28-C27
2	A	700	3VV	N28-C29-C31-O32
2	B	700	3VV	C15-C16-C17-C18
2	B	700	3VV	C22-C21-S20-C18
2	B	700	3VV	C36-O37-P38-O39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	700	3VV	C36-O37-P38-O41
2	B	700	3VV	C17-C18-S20-C21
2	B	700	3VV	O19-C18-S20-C21
2	B	700	3VV	O30-C29-N28-C27
2	B	700	3VV	C31-C29-N28-C27
2	B	700	3VV	N28-C29-C31-O32
2	B	700	3VV	O30-C29-C31-C33
2	B	700	3VV	C31-C33-C36-O37
2	B	700	3VV	C34-C33-C36-O37
2	B	700	3VV	C35-C33-C36-O37
2	B	700	3VV	C33-C36-O37-P38
2	B	700	3VV	O45-C46-C47-C52
2	B	700	3VV	O48-C49-N58-C59
2	B	700	3VV	O48-C49-N58-C67
2	C	700	3VV	C24-C26-C27-N28
2	C	700	3VV	C46-O45-P42-O41
2	C	700	3VV	C17-C18-S20-C21
2	C	700	3VV	O19-C18-S20-C21
2	C	700	3VV	C31-C29-N28-C27
2	C	700	3VV	N28-C29-C31-O32
2	D	700	3VV	C15-C16-C17-C18
2	D	700	3VV	C22-C21-S20-C18
2	D	700	3VV	C36-O37-P38-O39
2	D	700	3VV	C36-O37-P38-O41
2	D	700	3VV	C17-C18-S20-C21
2	D	700	3VV	O19-C18-S20-C21
2	D	700	3VV	O30-C29-N28-C27
2	D	700	3VV	C31-C29-N28-C27
2	D	700	3VV	N28-C29-C31-O32
2	D	700	3VV	O30-C29-C31-C33
2	D	700	3VV	C31-C33-C36-O37
2	D	700	3VV	C34-C33-C36-O37
2	D	700	3VV	C35-C33-C36-O37
2	D	700	3VV	C33-C36-O37-P38
2	D	700	3VV	O45-C46-C47-C52
2	D	700	3VV	O48-C49-N58-C59
2	D	700	3VV	O48-C49-N58-C67
2	B	700	3VV	C26-C24-N23-C22
2	D	700	3VV	C26-C24-N23-C22
2	B	700	3VV	O25-C24-N23-C22
2	D	700	3VV	O25-C24-N23-C22
2	B	700	3VV	O45-C46-C47-O48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	700	3VV	O45-C46-C47-O48
2	D	700	3VV	C03-C04-C05-C06
2	B	700	3VV	C03-C04-C05-C06
2	B	700	3VV	C13-C14-C15-C16
2	D	700	3VV	C13-C14-C15-C16
2	B	700	3VV	C12-C13-C14-C15
2	D	700	3VV	C12-C13-C14-C15
2	A	700	3VV	O30-C29-C31-O32
2	B	700	3VV	O30-C29-C31-O32
2	C	700	3VV	O30-C29-C31-O32
2	D	700	3VV	O30-C29-C31-O32
2	B	700	3VV	C08-C09-C10-C11
2	D	700	3VV	C08-C09-C10-C11
2	A	700	3VV	O30-C29-C31-C33
2	C	700	3VV	O30-C29-C31-C33
2	B	700	3VV	S20-C21-C22-N23
2	D	700	3VV	S20-C21-C22-N23
2	B	700	3VV	N28-C29-C31-C33
2	D	700	3VV	N28-C29-C31-C33
2	B	700	3VV	C01-C02-C03-C04
2	D	700	3VV	C01-C02-C03-C04
2	A	700	3VV	C47-C46-O45-P42
2	C	700	3VV	C47-C46-O45-P42
2	A	700	3VV	C16-C17-C18-O19
2	A	700	3VV	C16-C17-C18-S20
2	B	700	3VV	C16-C17-C18-O19
2	B	700	3VV	C16-C17-C18-S20
2	C	700	3VV	C16-C17-C18-O19
2	C	700	3VV	C16-C17-C18-S20
2	D	700	3VV	C16-C17-C18-O19
2	D	700	3VV	C16-C17-C18-S20
2	B	700	3VV	C04-C05-C06-C07
2	D	700	3VV	C04-C05-C06-C07
2	B	700	3VV	C52-O53-P54-O56
2	D	700	3VV	C52-O53-P54-O56
2	A	700	3VV	C36-O37-P38-O40
2	C	700	3VV	C36-O37-P38-O40
2	A	700	3VV	C26-C27-N28-C29
2	C	700	3VV	C26-C27-N28-C29
2	B	700	3VV	C05-C06-C07-C08
2	D	700	3VV	C05-C06-C07-C08
2	A	700	3VV	C07-C08-C09-C10

Continued on next page...

Continued from previous page...

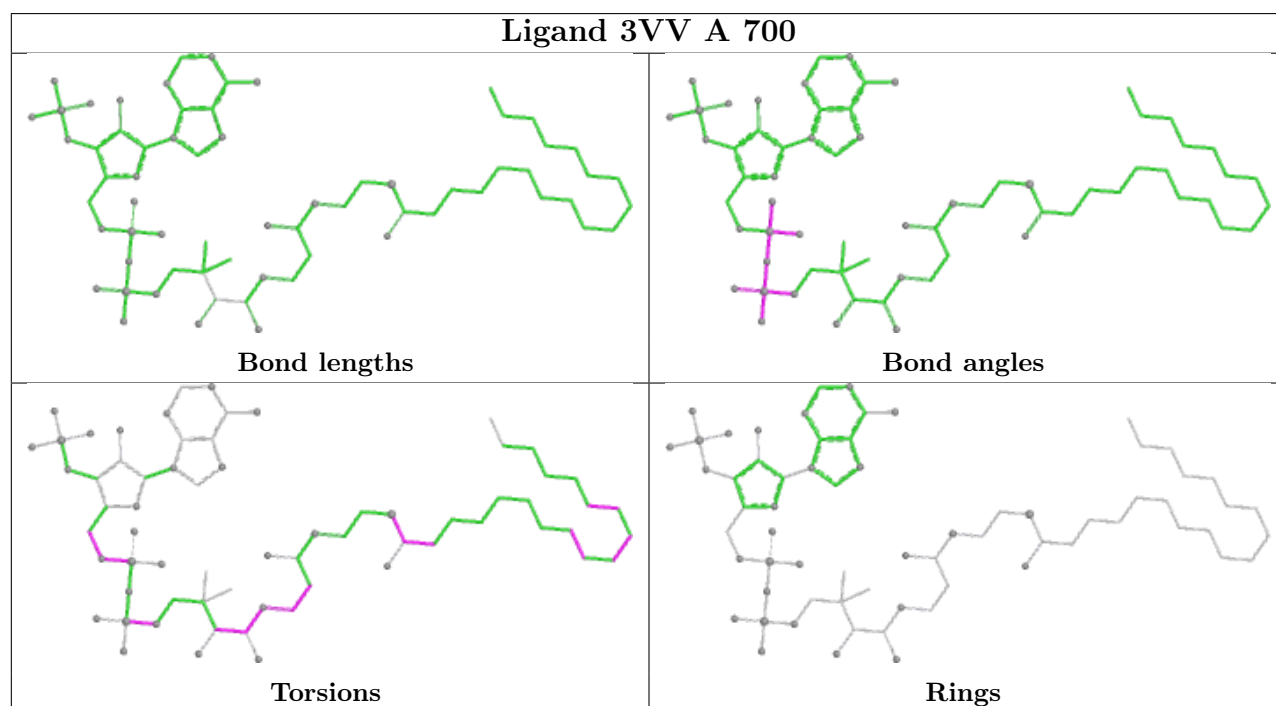
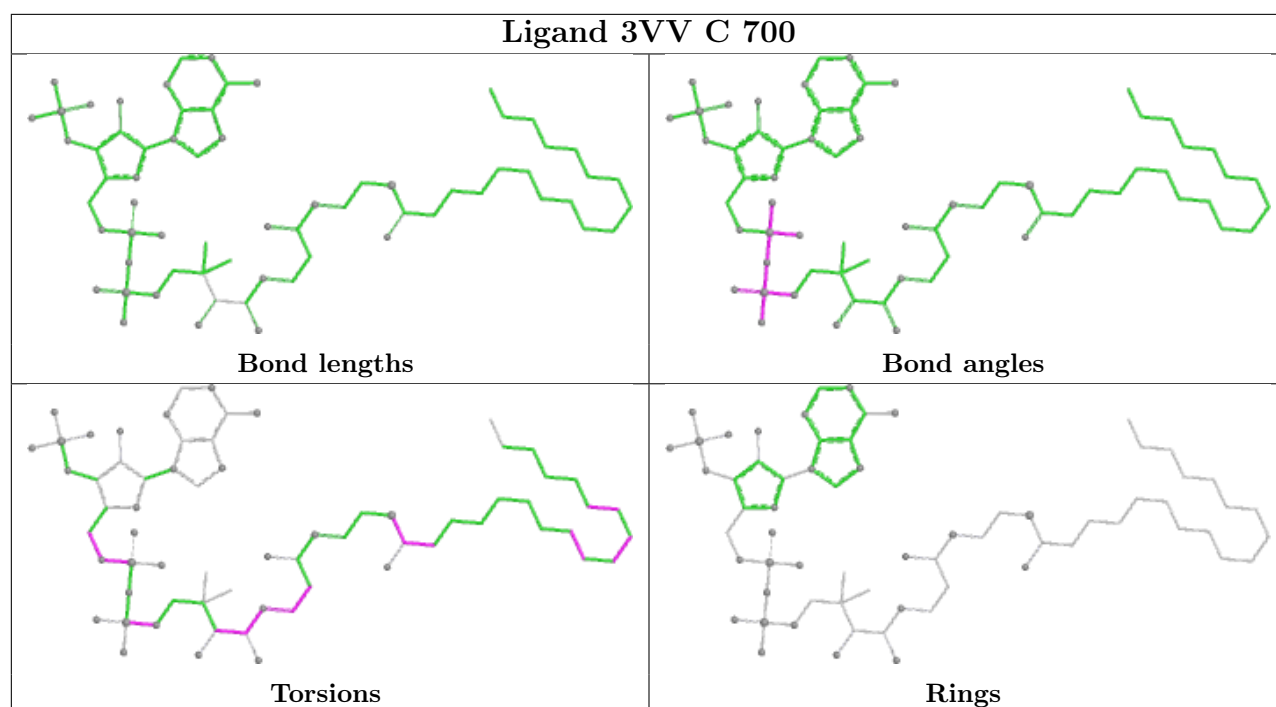
Mol	Chain	Res	Type	Atoms
2	C	700	3VV	C07-C08-C09-C10
2	B	700	3VV	C11-C12-C13-C14
2	D	700	3VV	C11-C12-C13-C14
2	A	700	3VV	O30-C29-N28-C27
2	C	700	3VV	O30-C29-N28-C27
2	A	700	3VV	C09-C10-C11-C12
2	C	700	3VV	C09-C10-C11-C12
2	A	700	3VV	C05-C06-C07-C08
2	C	700	3VV	C05-C06-C07-C08

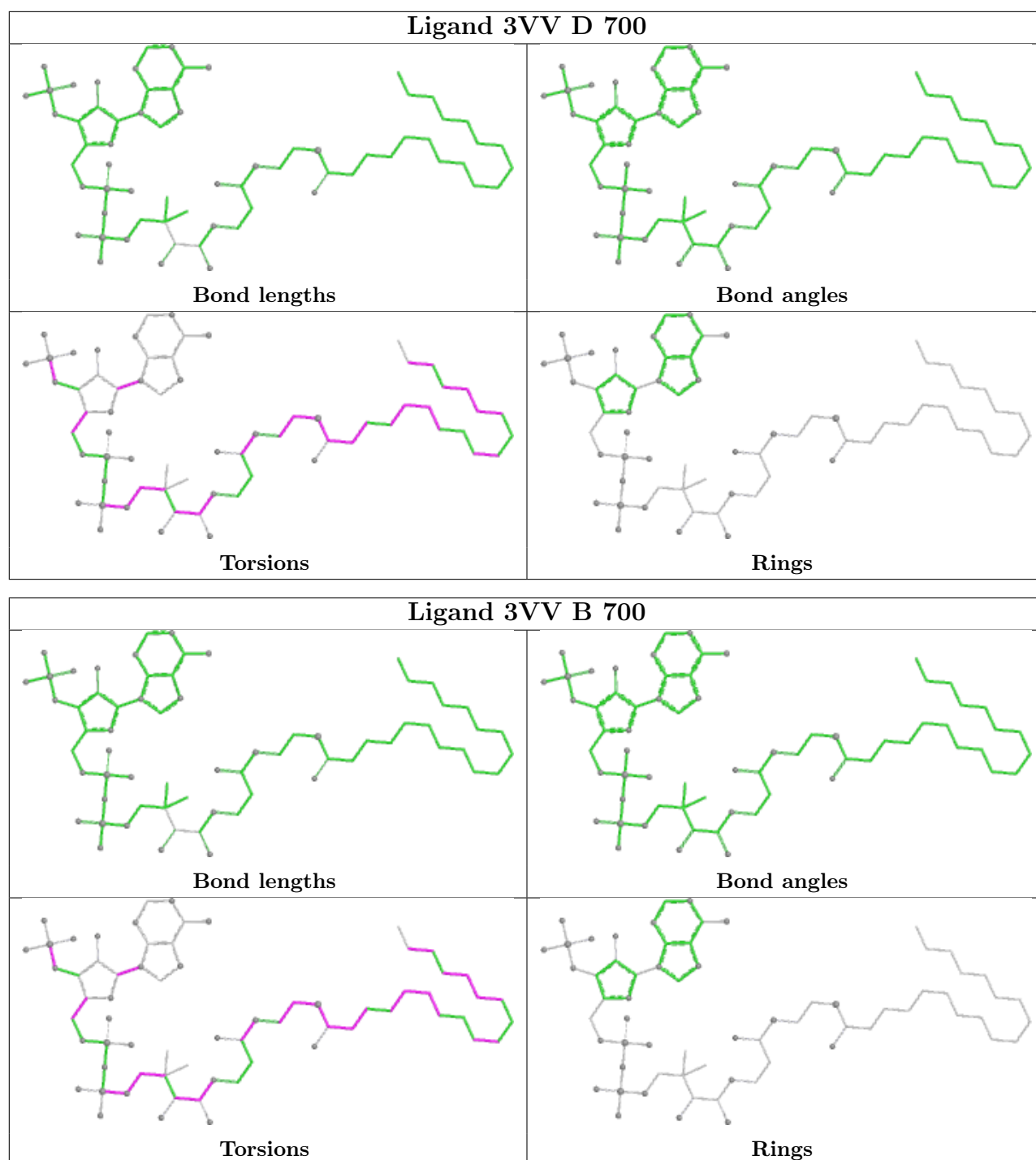
There are no ring outliers.

4 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	700	3VV	5	0
2	A	700	3VV	5	0
2	D	700	3VV	15	0
2	B	700	3VV	14	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.

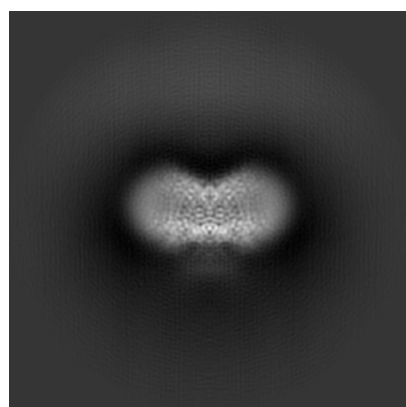
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20239. These allow visual inspection of the internal detail of the map and identification of artifacts.

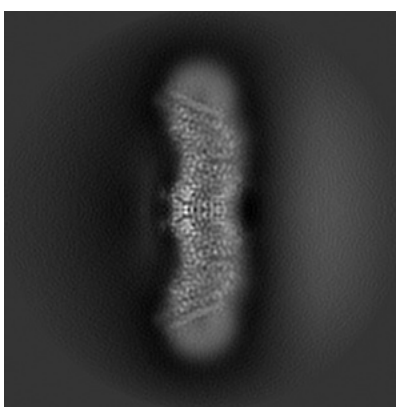
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

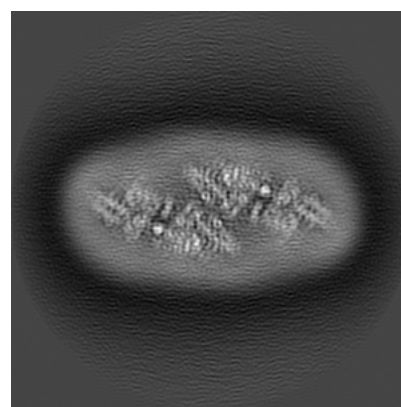
6.1.1 Primary map



X



Y

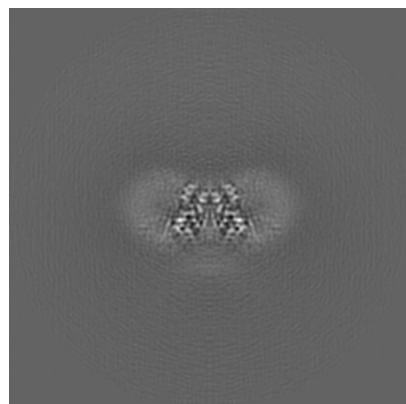


Z

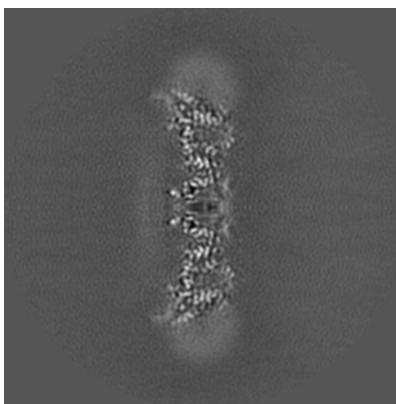
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

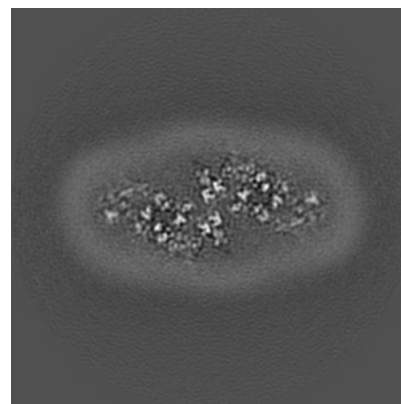
6.2.1 Primary map



X Index: 140



Y Index: 140

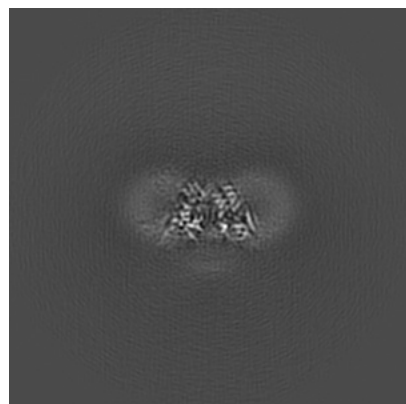


Z Index: 140

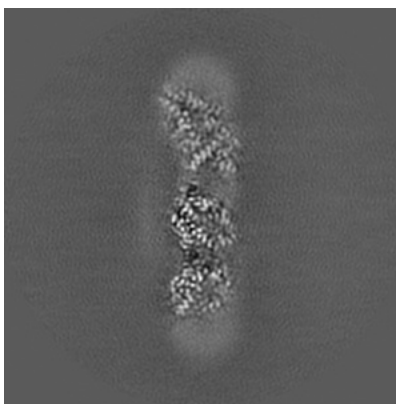
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

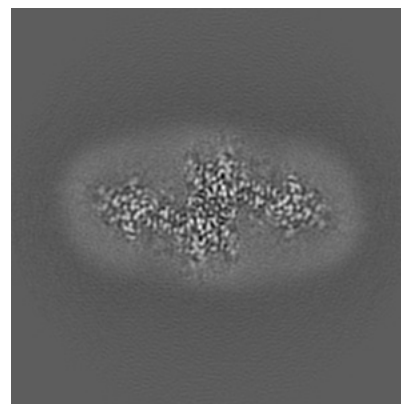
6.3.1 Primary map



X Index: 138



Y Index: 132

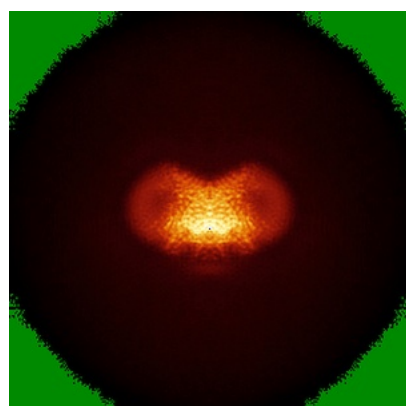


Z Index: 128

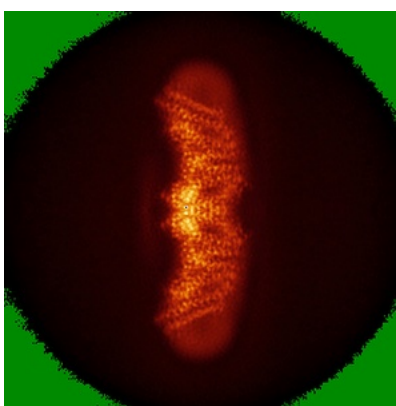
The images above show the largest variance slices of the map in three orthogonal directions.

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

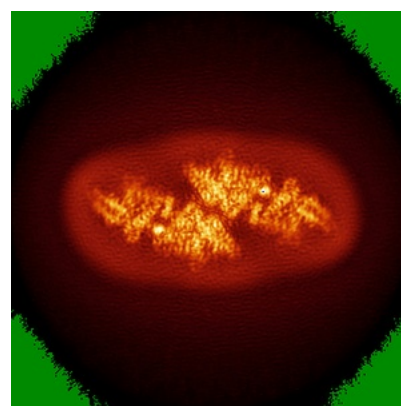
6.4.1 Primary map



X



Y

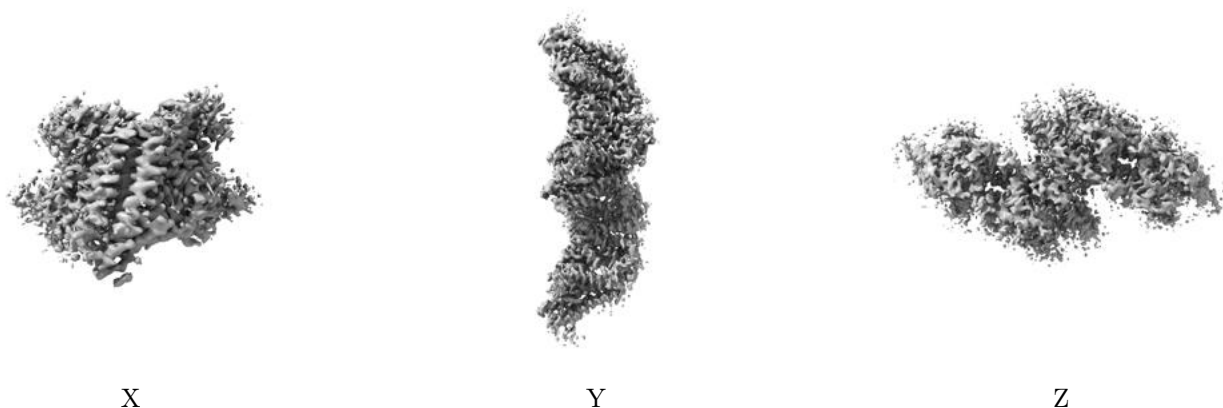


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

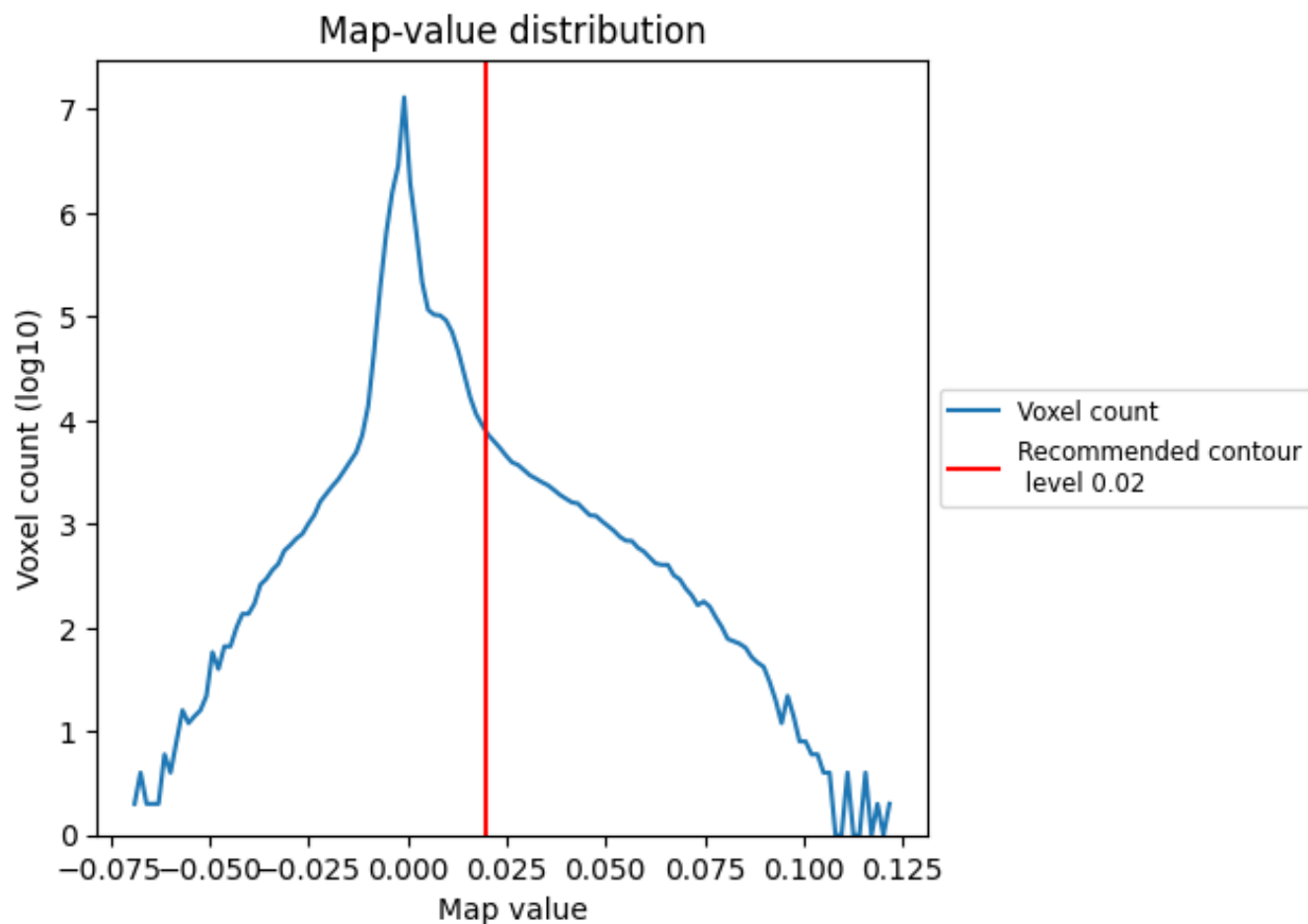
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

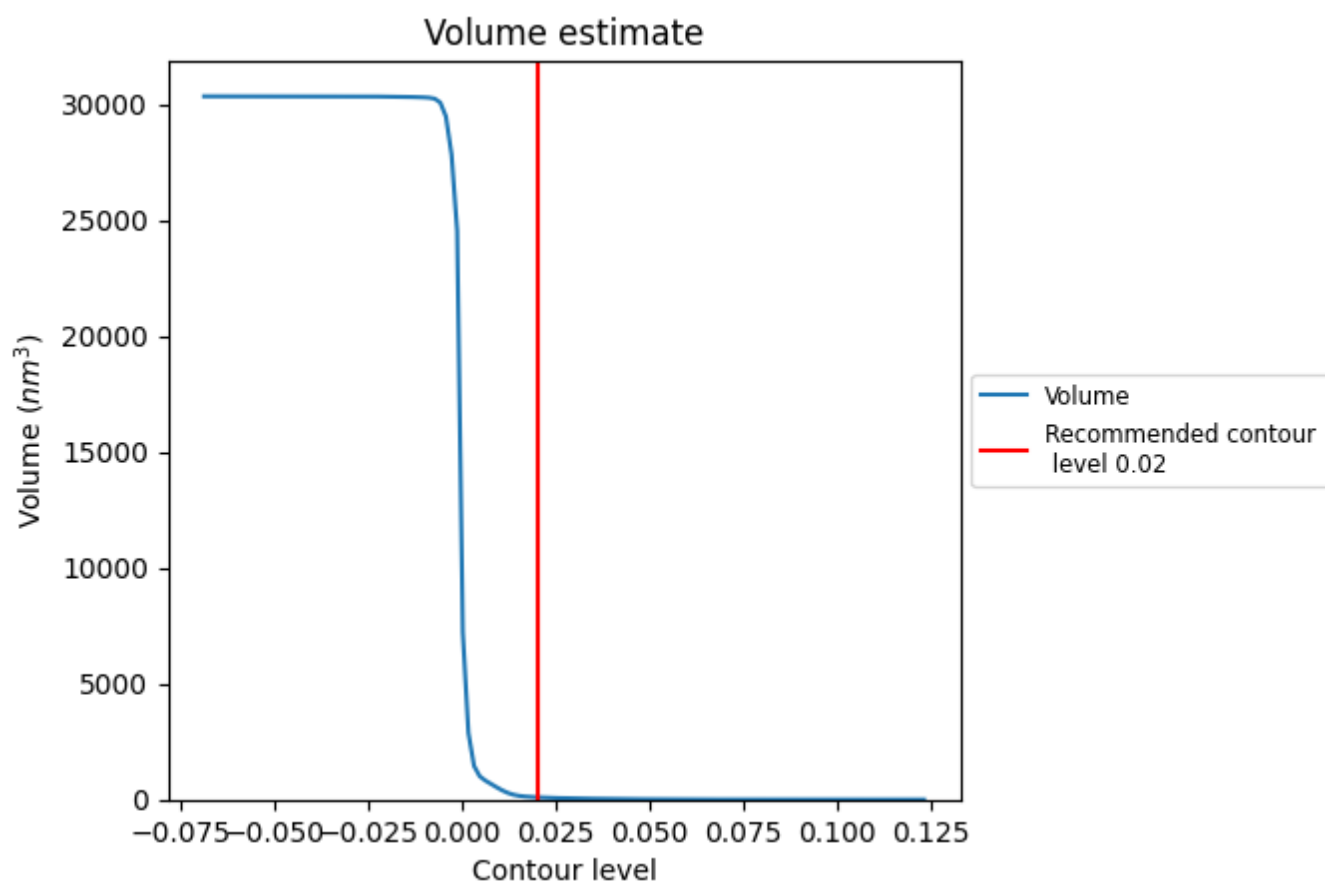
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

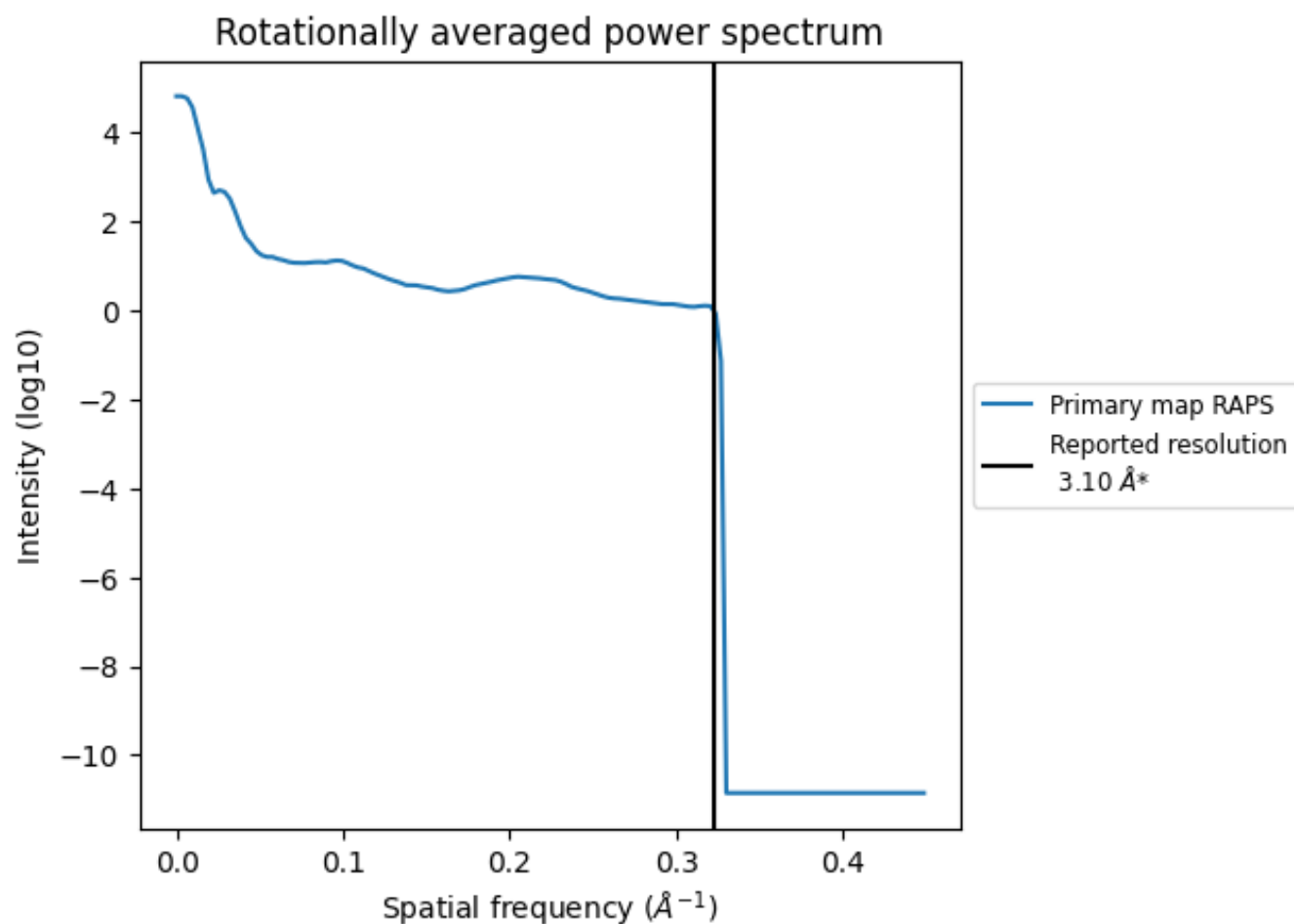
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm^3 ; this corresponds to an approximate mass of 88 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 0.323 $\text{\AA}^{-1}$

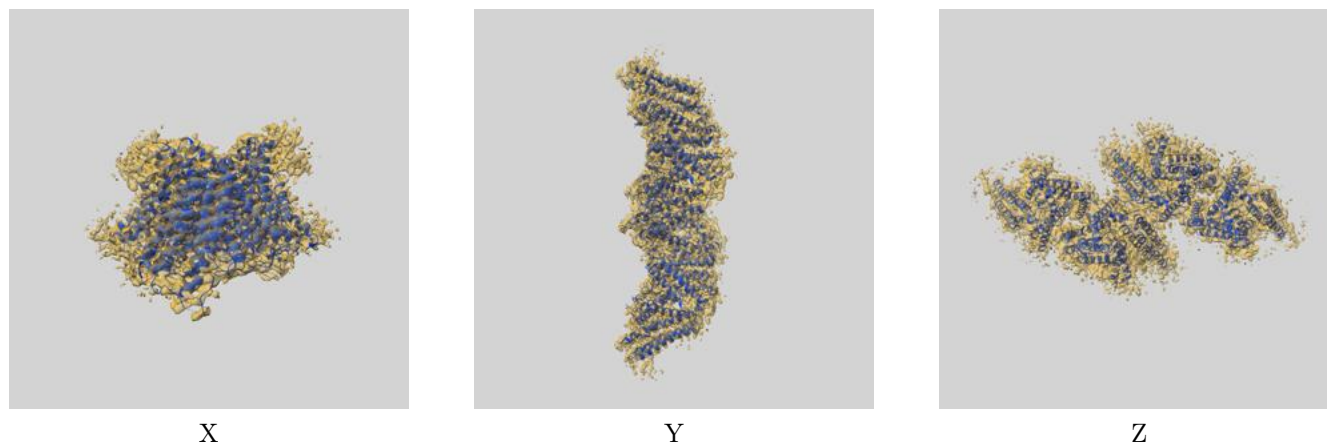
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

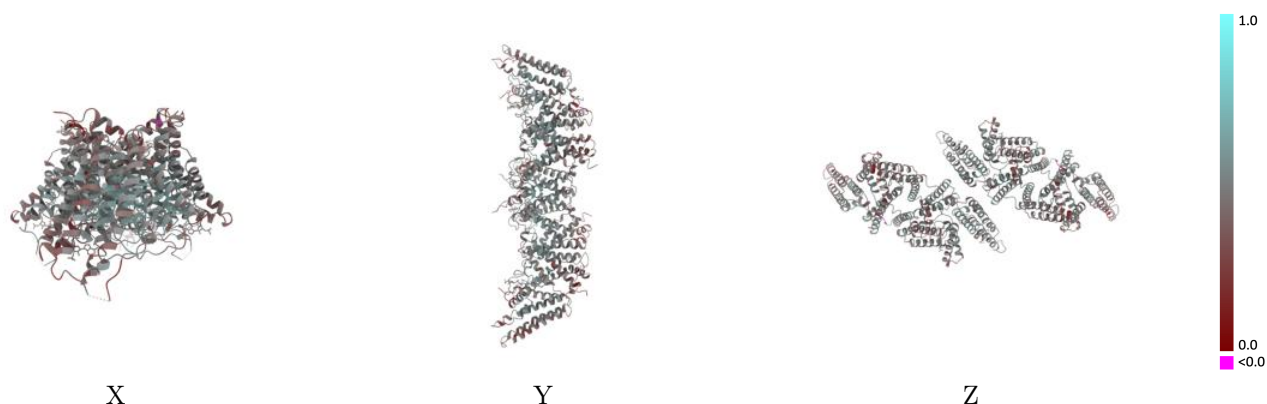
This section contains information regarding the fit between EMDB map EMD-20239 and PDB model 6P2P. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



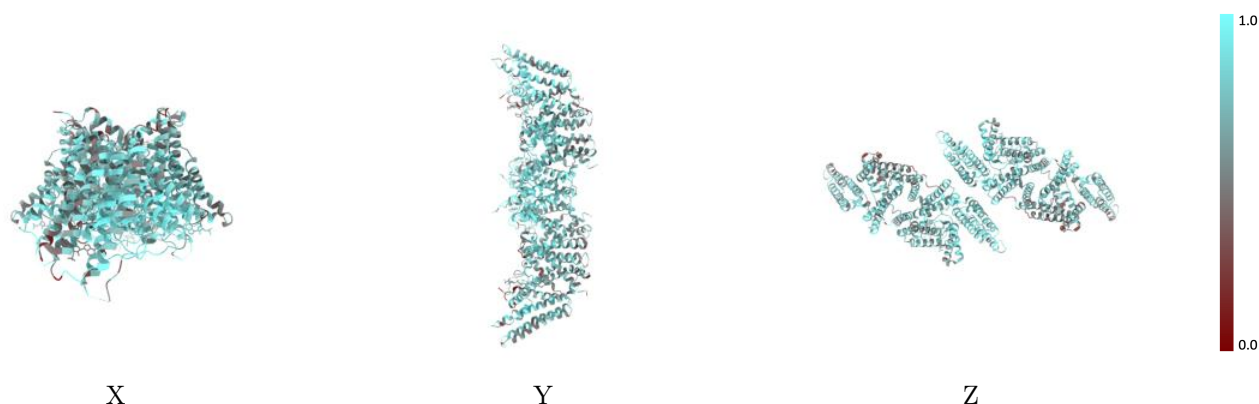
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



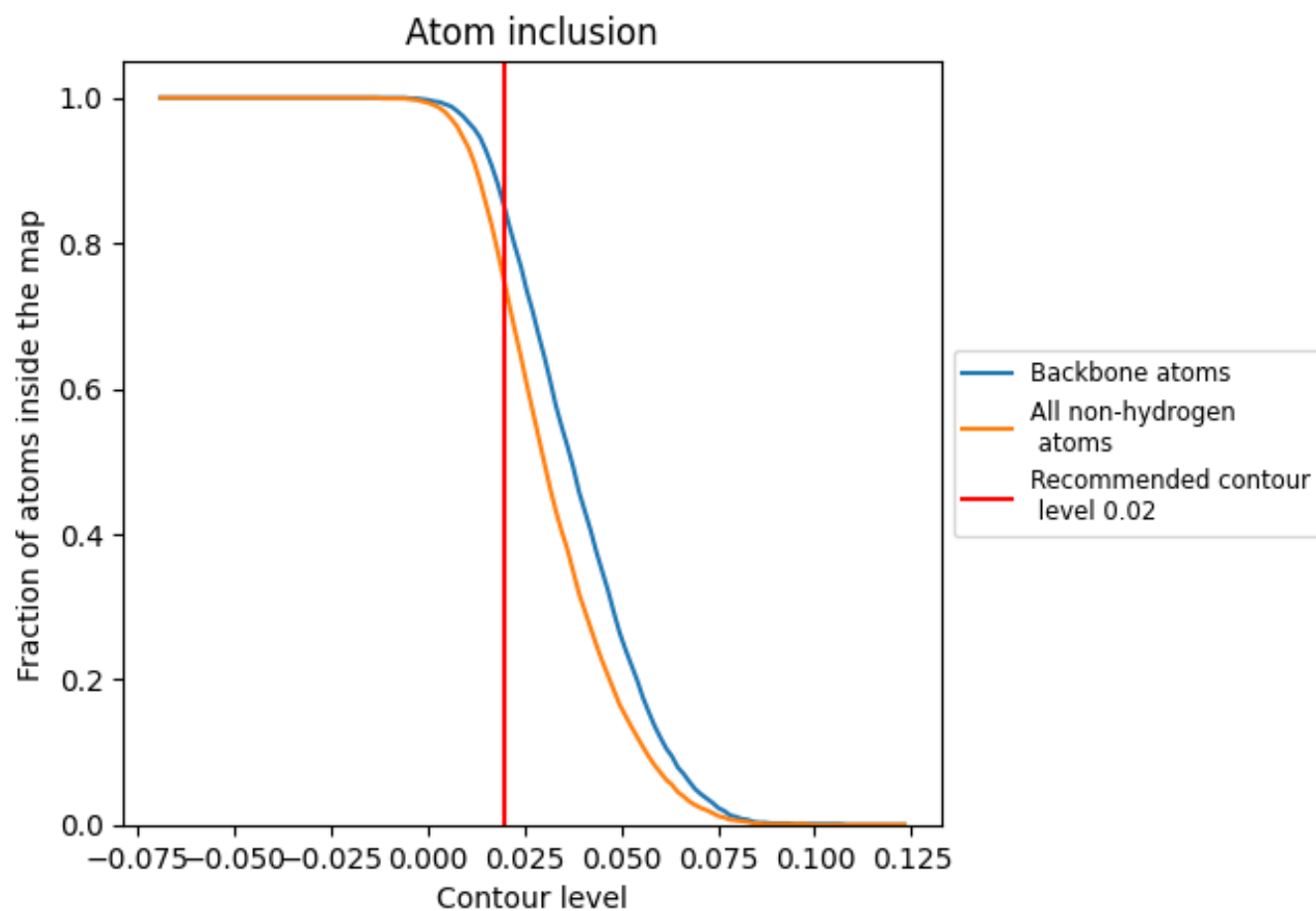
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7440	0.4620
A	0.7080	0.4480
B	0.7810	0.4770
C	0.7080	0.4480
D	0.7810	0.4750

