



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 07:29 PM JST

PDB ID : 7XJ0
EMDB ID : EMD-33214
Title : Structure of human TRPV3 in complex with Trpvicin
Authors : Fan, J.; Yue, Z.; Jiang, D.; Lei, X.
Deposited on : 2022-04-14
Resolution : 2.53 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

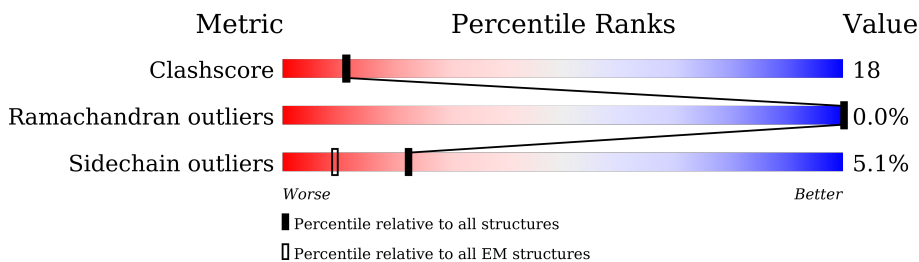
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	1061	
1	B	1061	
1	C	1061	
1	D	1061	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18791 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.

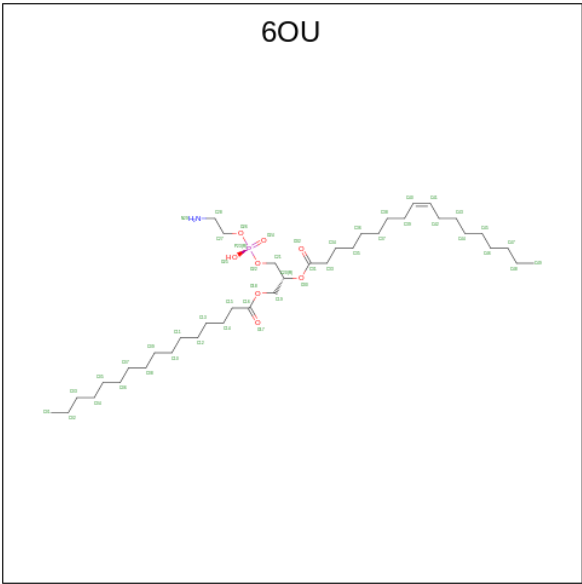
- Molecule 1 is a protein called Fusion protein of Transient receptor potential cation channel subfamily V member 3 and 3C-GFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	608	Total	C	N	O	S	0	0
			4591	3019	761	783	28		
1	C	608	Total	C	N	O	S	0	0
			4583	3016	760	779	28		
1	A	606	Total	C	N	O	S	0	0
			4575	3011	761	775	28		
1	D	606	Total	C	N	O	S	0	0
			4572	3009	759	776	28		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ILE	VAL	conflict	UNP B2KYM6
B	117	ARG	GLY	conflict	UNP B2KYM6
B	246	LYS	ARG	conflict	UNP B2KYM6
B	247	GLY	GLU	conflict	UNP B2KYM6
B	772	ASN	ASP	conflict	UNP B2KYM6
C	25	ILE	VAL	conflict	UNP B2KYM6
C	117	ARG	GLY	conflict	UNP B2KYM6
C	246	LYS	ARG	conflict	UNP B2KYM6
C	247	GLY	GLU	conflict	UNP B2KYM6
C	772	ASN	ASP	conflict	UNP B2KYM6
A	25	ILE	VAL	conflict	UNP B2KYM6
A	117	ARG	GLY	conflict	UNP B2KYM6
A	246	LYS	ARG	conflict	UNP B2KYM6
A	247	GLY	GLU	conflict	UNP B2KYM6
A	772	ASN	ASP	conflict	UNP B2KYM6
D	25	ILE	VAL	conflict	UNP B2KYM6
D	117	ARG	GLY	conflict	UNP B2KYM6
D	246	LYS	ARG	conflict	UNP B2KYM6
D	247	GLY	GLU	conflict	UNP B2KYM6
D	772	ASN	ASP	conflict	UNP B2KYM6

- Molecule 2 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: C₃₉H₇₆NO₈P).



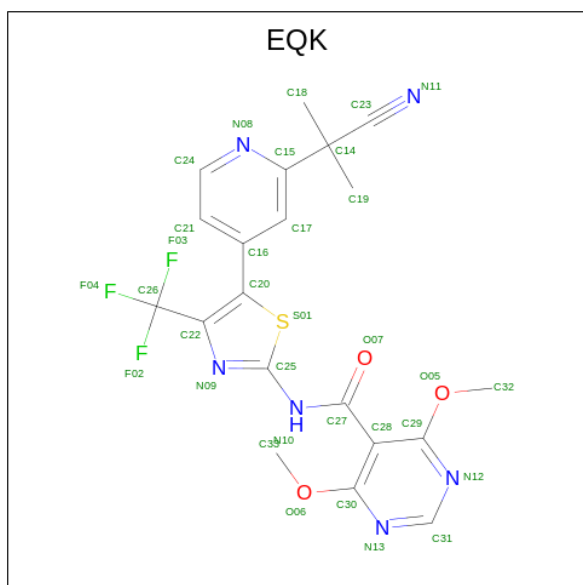
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total C 14 14					0
2	B	1	Total C 14 14					0
2	B	1	Total C 14 14					0
2	B	1	Total C 12 12					0
2	B	1	Total 30	C 22	N 1	O 6	P 1	0
2	C	1	Total 30	C 22	N 1	O 6	P 1	0
2	C	1	Total C 13 13					0
2	C	1	Total C 13 13					0
2	C	1	Total C 14 14					0
2	C	1	Total C 14 14					0
2	A	1	Total C 14 14					0
2	A	1	Total C 14 14					0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C				0
			14	14				
2	A	1	Total	C				0
			14	14				
2	A	1	Total	C	N	O	P	0
			30	22	1	6	1	
2	A	1	Total	C				0
			12	12				
2	D	1	Total	C				0
			14	14				
2	D	1	Total	C				0
			14	14				
2	D	1	Total	C				0
			14	14				
2	D	1	Total	C	N	O	P	0
			30	22	1	6	1	

- Molecule 3 is N-[5-[2-(2-cyanopropan-2-yl)pyridin-4-yl]-4-(trifluoromethyl)-1,3-thiazol-2-yl]-4,6-dimethoxy-pyrimidine-5-carboxamide (three-letter code: EQK) (formula: C₂₀H₁₇F₃N₆O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	B	1	Total	C	F	N	O	S	0
			33	20	3	6	3	1	
3	C	1	Total	C	F	N	O	S	0
			33	20	3	6	3	1	

Continued on next page...

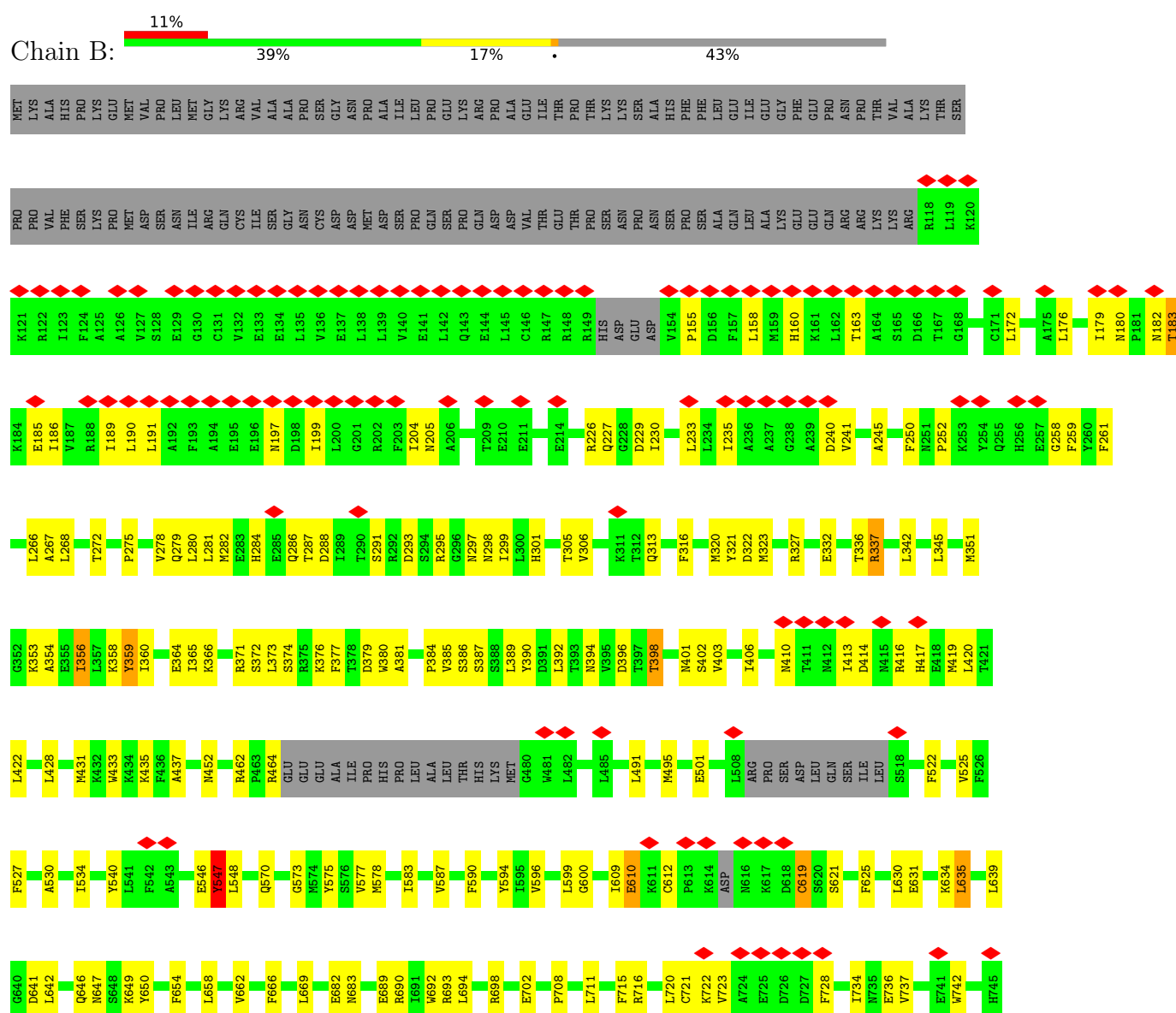
Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	F	N	O	S	0
			33	20	3	6	3	1	
3	D	1	Total	C	F	N	O	S	0
			33	20	3	6	3	1	

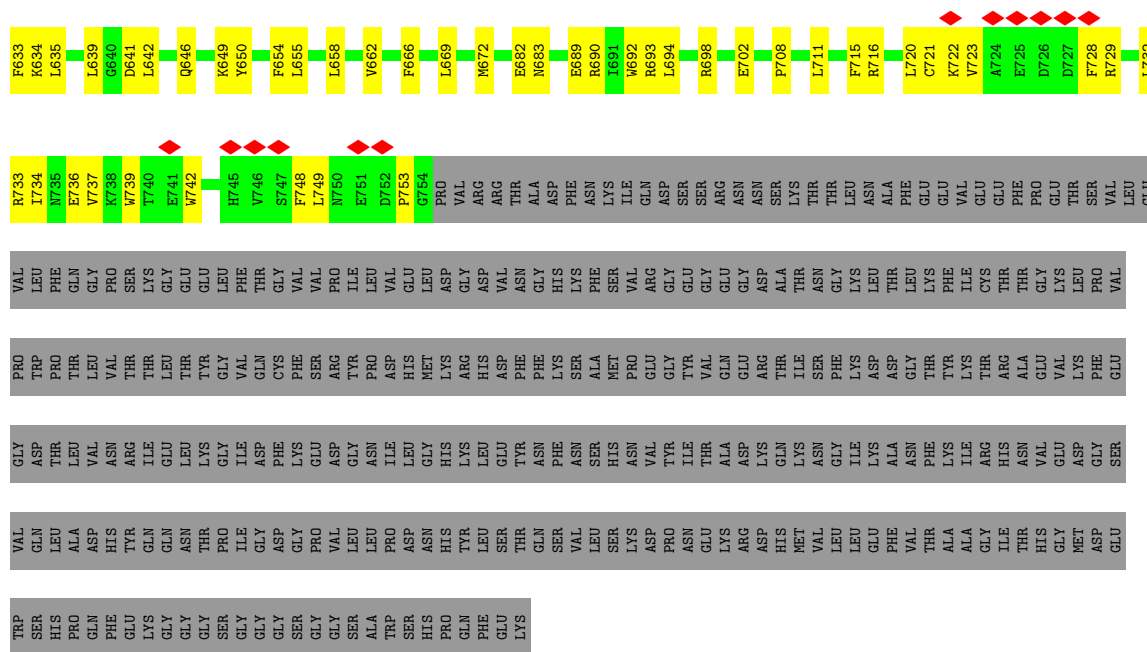
3 Residue-property plots

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.

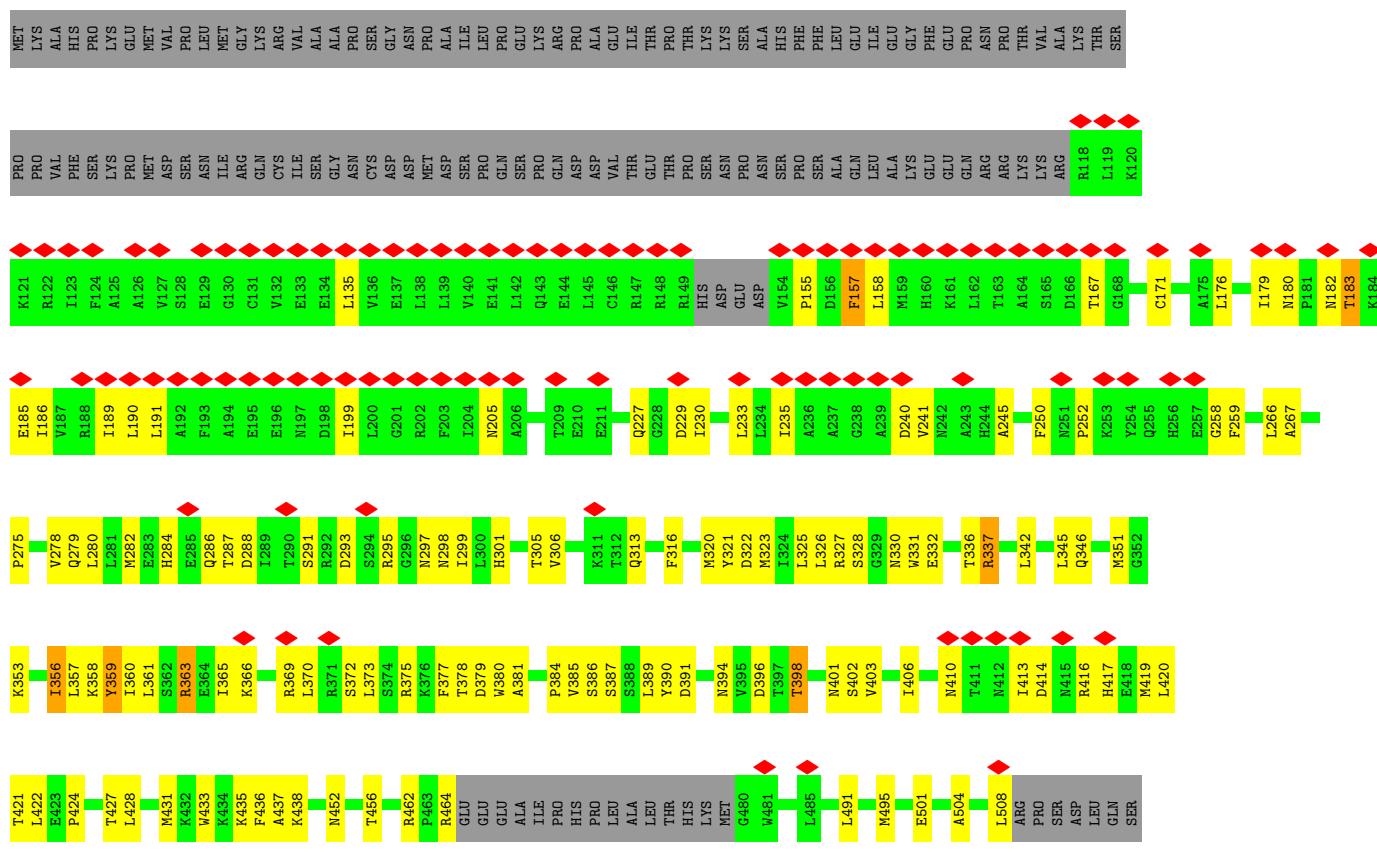
- Molecule 1: Fusion protein of Transient receptor potential cation channel subfamily V member 3 and 3C-GFP

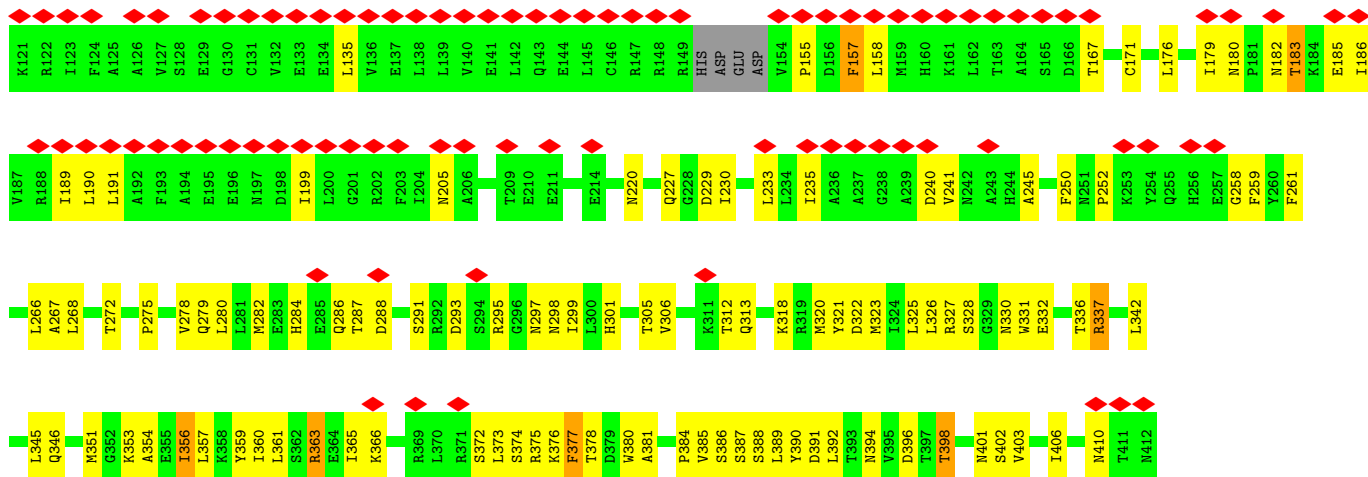






- Molecule 1: Fusion protein of Transient receptor potential cation channel subfamily V member 3 and 3C-GFP







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	503757	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	13.181	Depositor
Minimum map value	-7.967	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.172	Depositor
Recommended contour level	0.85	Depositor
Map size (\AA)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	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: 6OU, EQK

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	0.68	0/4673	0.60	0/6358
1	B	0.69	0/4689	0.60	0/6381
1	C	0.69	0/4681	0.63	0/6370
1	D	0.68	0/4670	0.59	0/6355
All	All	0.69	0/18713	0.60	0/25464

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	4575	0	4419	169	0
1	B	4591	0	4427	171	0
1	C	4583	0	4416	163	0
1	D	4572	0	4412	178	0
2	A	98	0	0	2	0
2	B	84	0	0	0	0
2	C	84	0	0	2	0
2	D	72	0	0	0	0
3	A	33	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	0	5	0
3	C	33	0	0	5	0
3	D	33	0	0	5	0
All	All	18791	0	17674	645	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (645) 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:406:ILE:HG23	1:B:410:ASN:ND2	1.29	1.48
1:D:406:ILE:HG23	1:D:410:ASN:ND2	1.29	1.47
1:A:406:ILE:HG23	1:A:410:ASN:ND2	1.29	1.40
1:C:406:ILE:HG23	1:C:410:ASN:ND2	1.29	1.40
1:A:420:LEU:HD11	1:A:694:LEU:CD1	1.68	1.22
1:A:420:LEU:CD1	1:A:694:LEU:HD13	1.75	1.17
1:B:186:ILE:O	1:B:190:LEU:HD13	1.62	0.99
1:A:384:PRO:O	1:A:737:VAL:HA	1.62	0.99
1:C:406:ILE:CG2	1:C:410:ASN:ND2	2.26	0.99
1:B:406:ILE:CG2	1:B:410:ASN:ND2	2.25	0.99
1:A:438:LYS:HE3	2:A:1505:6OU:N29	1.76	0.99
1:D:384:PRO:O	1:D:737:VAL:HA	1.63	0.99
1:D:406:ILE:CG2	1:D:410:ASN:ND2	2.25	0.98
1:A:406:ILE:CG2	1:A:410:ASN:ND2	2.25	0.98
1:B:406:ILE:CG2	1:B:410:ASN:HD22	1.79	0.96
1:D:406:ILE:CG2	1:D:410:ASN:HD22	1.79	0.96
1:C:406:ILE:CG2	1:C:410:ASN:HD22	1.79	0.95
1:C:358:LYS:HG3	1:C:422:LEU:HD22	1.48	0.95
1:A:406:ILE:CG2	1:A:410:ASN:HD22	1.79	0.93
1:D:420:LEU:HD11	1:D:429:LEU:CD1	2.00	0.92
1:A:612:CYS:CB	1:A:619:CYS:SG	2.58	0.91
1:B:721:CYS:O	1:B:723:VAL:HG23	1.70	0.90
1:B:540:TYR:HB2	1:B:547:TYR:CD2	2.08	0.89
1:D:596:VAL:O	3:D:1101:EQK:C31	2.21	0.88
1:B:384:PRO:O	1:B:737:VAL:HA	1.71	0.87
1:B:610:GLU:HG3	1:B:647:ASN:O	1.75	0.86
1:B:172:LEU:CD1	1:B:191:LEU:CD1	2.53	0.86
1:B:596:VAL:O	3:B:1406:EQK:C31	2.24	0.85
1:A:630:LEU:HG	1:A:634:LYS:HE3	1.60	0.84
1:A:649:LYS:HG3	1:A:650:TYR:CD2	2.13	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:649:LYS:HG3	1:D:650:TYR:CD2	2.13	0.84
1:B:172:LEU:HD11	1:B:191:LEU:CD1	2.08	0.83
1:D:176:LEU:HD21	1:D:230:ILE:HG21	1.61	0.81
1:A:176:LEU:HD21	1:A:230:ILE:HG21	1.61	0.81
1:B:630:LEU:HG	1:B:634:LYS:HE3	1.61	0.81
1:C:176:LEU:HD21	1:C:230:ILE:HG21	1.61	0.81
1:A:406:ILE:HG23	1:A:410:ASN:HD21	1.46	0.81
1:B:406:ILE:HG23	1:B:410:ASN:HD22	0.98	0.81
1:A:406:ILE:HG23	1:A:410:ASN:HD22	0.97	0.81
1:B:619:CYS:O	1:B:619:CYS:SG	2.39	0.80
1:B:172:LEU:CD1	1:B:191:LEU:HD11	2.11	0.80
1:C:630:LEU:HG	1:C:634:LYS:HE3	1.61	0.80
1:D:721:CYS:O	1:D:723:VAL:HG13	1.81	0.80
1:C:721:CYS:O	1:C:723:VAL:HG13	1.81	0.80
1:D:406:ILE:HG23	1:D:410:ASN:HD22	0.98	0.80
1:C:406:ILE:HG23	1:C:410:ASN:HD22	0.98	0.80
1:B:176:LEU:HD21	1:B:230:ILE:HG21	1.61	0.79
1:B:590:PHE:CE1	1:B:669:LEU:HG	2.17	0.79
1:C:590:PHE:CE1	1:C:669:LEU:HG	2.17	0.79
1:C:649:LYS:HG3	1:C:650:TYR:CD2	2.16	0.79
1:A:721:CYS:O	1:A:723:VAL:HG13	1.81	0.79
1:A:590:PHE:CE1	1:A:669:LEU:HG	2.18	0.79
1:D:406:ILE:HG23	1:D:410:ASN:HD21	1.46	0.79
1:B:610:GLU:HG2	1:B:649:LYS:HG3	1.64	0.78
1:D:590:PHE:CE1	1:D:669:LEU:HG	2.17	0.78
1:A:259:PHE:CE1	1:D:384:PRO:HG2	2.19	0.78
1:B:384:PRO:HG2	1:C:259:PHE:CE1	2.19	0.77
1:A:596:VAL:O	3:A:1506:EQK:C31	2.33	0.77
1:B:172:LEU:HD13	1:B:191:LEU:CD1	2.15	0.76
1:C:427:THR:HG22	1:C:732:LEU:HD21	1.68	0.76
1:C:406:ILE:HG23	1:C:410:ASN:HD21	1.46	0.76
1:B:186:ILE:O	1:B:190:LEU:CD1	2.34	0.76
1:B:379:ASP:O	1:B:748:PHE:HB2	1.84	0.76
1:B:406:ILE:HG23	1:B:410:ASN:HD21	1.46	0.76
1:D:387:SER:OG	1:D:733:ARG:HD3	1.86	0.75
1:C:639:LEU:HD11	1:D:635:LEU:HD23	1.68	0.75
1:B:259:PHE:CE1	1:A:384:PRO:HG2	2.23	0.74
1:A:612:CYS:HB3	1:A:619:CYS:SG	2.26	0.74
1:D:649:LYS:HG3	1:D:650:TYR:CE2	2.22	0.74
1:B:172:LEU:HD11	1:B:191:LEU:HD11	1.66	0.74
1:A:649:LYS:HG3	1:A:650:TYR:CE2	2.22	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:PRO:O	1:C:737:VAL:HA	1.86	0.74
1:C:621:SER:H	1:C:646:GLN:HE22	1.36	0.73
1:D:360:ILE:HG23	1:D:363:ARG:HH21	1.54	0.73
1:A:297:ASN:HB3	1:A:301:HIS:HB2	1.71	0.72
1:C:596:VAL:HG12	3:C:1101:EQK:N12	2.04	0.72
1:A:420:LEU:HD11	1:A:694:LEU:HD13	0.83	0.72
1:D:297:ASN:HB3	1:D:301:HIS:HB2	1.71	0.72
1:B:297:ASN:HB3	1:B:301:HIS:HB2	1.71	0.72
1:D:621:SER:H	1:D:646:GLN:HE22	1.37	0.72
1:A:621:SER:H	1:A:646:GLN:HE22	1.37	0.71
1:A:345:LEU:HD13	1:A:360:ILE:CG2	2.21	0.71
1:A:361:LEU:HD13	1:A:424:PRO:HG2	1.72	0.71
1:B:414:ASP:HA	1:B:416:ARG:HH21	1.56	0.71
1:C:297:ASN:HB3	1:C:301:HIS:HB2	1.71	0.71
1:D:414:ASP:HA	1:D:416:ARG:HH21	1.56	0.71
1:A:298:ASN:ND2	1:A:336:THR:OG1	2.24	0.71
1:D:298:ASN:ND2	1:D:336:THR:OG1	2.24	0.71
1:B:172:LEU:HD13	1:B:191:LEU:HD12	1.73	0.71
1:C:360:ILE:HG23	1:C:363:ARG:HH21	1.56	0.71
1:C:414:ASP:HA	1:C:416:ARG:HH21	1.56	0.71
1:C:298:ASN:ND2	1:C:336:THR:OG1	2.24	0.70
1:B:365:ILE:HD12	1:B:373:LEU:O	1.91	0.70
1:A:414:ASP:HA	1:A:416:ARG:HH21	1.55	0.70
1:D:384:PRO:CB	1:D:737:VAL:HG13	2.22	0.70
1:B:298:ASN:ND2	1:B:336:THR:OG1	2.24	0.70
1:A:384:PRO:CB	1:A:737:VAL:HG13	2.22	0.69
1:B:345:LEU:HD13	1:B:360:ILE:CG2	2.22	0.69
1:C:387:SER:OG	1:C:733:ARG:HD3	1.92	0.69
1:C:337:ARG:HH12	1:C:346:GLN:HE22	1.40	0.69
1:A:396:ASP:OD1	1:A:428:LEU:HD22	1.91	0.69
1:C:384:PRO:HG2	1:D:259:PHE:CE1	2.27	0.68
1:A:385:VAL:HA	1:A:736:GLU:O	1.92	0.68
1:D:337:ARG:HH12	1:D:346:GLN:HE22	1.40	0.68
1:D:612:CYS:CB	1:D:619:CYS:SG	2.81	0.68
1:A:337:ARG:HH12	1:A:346:GLN:HE22	1.40	0.67
1:A:427:THR:HG22	1:A:732:LEU:HD21	1.76	0.67
1:C:155:PRO:HB3	1:C:199:ILE:HD12	1.75	0.67
1:B:752:ASP:OD1	1:C:169:LYS:NZ	2.25	0.67
1:D:420:LEU:HD11	1:D:429:LEU:HD11	1.77	0.67
1:D:612:CYS:HB3	1:D:619:CYS:SG	2.34	0.67
1:B:155:PRO:HB3	1:B:199:ILE:HD12	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:PRO:HB3	1:D:199:ILE:HD12	1.75	0.67
1:C:723:VAL:HG21	1:C:729:ARG:HG2	1.77	0.66
1:A:155:PRO:HB3	1:A:199:ILE:HD12	1.75	0.66
1:C:252:PRO:HB3	1:C:258:GLY:HA3	1.78	0.66
1:C:626:SER:OG	2:C:1104:6OU:C37	2.43	0.66
1:A:252:PRO:HB3	1:A:258:GLY:HA3	1.78	0.66
1:D:252:PRO:HB3	1:D:258:GLY:HA3	1.77	0.66
1:B:252:PRO:HB3	1:B:258:GLY:HA3	1.77	0.66
1:D:723:VAL:HG21	1:D:729:ARG:HG2	1.78	0.66
1:A:723:VAL:HG21	1:A:729:ARG:HG2	1.78	0.66
1:A:433:TRP:HA	1:A:437:ALA:HB3	1.79	0.65
1:A:360:ILE:HG23	1:A:363:ARG:HH21	1.61	0.65
1:C:655:LEU:HD23	2:C:1105:6OU:C38	2.27	0.64
1:B:293:ASP:OD1	1:B:295:ARG:N	2.30	0.64
1:C:293:ASP:OD1	1:C:295:ARG:N	2.30	0.64
1:C:621:SER:H	1:C:646:GLN:NE2	1.95	0.64
1:D:433:TRP:HA	1:D:437:ALA:HB3	1.79	0.64
1:D:293:ASP:OD1	1:D:295:ARG:N	2.30	0.64
1:A:345:LEU:HD13	1:A:360:ILE:HG21	1.79	0.64
1:C:433:TRP:HA	1:C:437:ALA:HB3	1.79	0.63
1:A:353:LYS:HB3	1:A:356:ILE:HG22	1.81	0.63
1:A:293:ASP:OD1	1:A:295:ARG:N	2.30	0.63
1:B:433:TRP:HA	1:B:437:ALA:HB3	1.79	0.63
1:D:322:ASP:HA	1:D:359:TYR:OH	1.99	0.63
1:A:708:PRO:HD2	1:A:711:LEU:HB2	1.81	0.62
1:B:546:GLU:N	1:B:546:GLU:OE1	2.31	0.62
1:D:622:TYR:CD1	1:D:631:GLU:OE2	2.52	0.62
1:D:330:ASN:CA	1:D:373:LEU:HD11	2.30	0.62
1:C:708:PRO:HD2	1:C:711:LEU:HB2	1.81	0.62
1:A:621:SER:H	1:A:646:GLN:NE2	1.97	0.62
1:D:708:PRO:HD2	1:D:711:LEU:HB2	1.81	0.62
1:B:708:PRO:HD2	1:B:711:LEU:HB2	1.81	0.61
1:D:621:SER:H	1:D:646:GLN:NE2	1.97	0.61
1:B:298:ASN:H	1:B:301:HIS:HD2	1.47	0.61
1:D:298:ASN:H	1:D:301:HIS:HD2	1.47	0.61
1:D:321:TYR:CD1	1:D:359:TYR:HE2	2.19	0.61
1:D:570:GLN:HG3	1:D:692:TRP:CZ3	2.36	0.61
1:A:298:ASN:H	1:A:301:HIS:HD2	1.47	0.61
1:C:739:TRP:HB2	1:D:312:THR:O	2.01	0.61
1:D:380:TRP:HE3	1:D:380:TRP:O	1.84	0.61
1:A:298:ASN:H	1:A:301:HIS:CD2	2.19	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:TRP:HE3	1:B:380:TRP:O	1.84	0.61
1:B:462:ARG:HD3	1:B:548:LEU:HD13	1.83	0.61
1:B:384:PRO:CB	1:B:737:VAL:HG13	2.31	0.60
1:A:380:TRP:O	1:A:380:TRP:HE3	1.84	0.60
1:A:570:GLN:HG3	1:A:692:TRP:CZ3	2.36	0.60
1:B:621:SER:H	1:B:646:GLN:HE22	1.47	0.60
1:C:301:HIS:O	1:C:305:THR:HG23	2.01	0.60
1:C:380:TRP:HE3	1:C:380:TRP:O	1.83	0.60
1:D:298:ASN:H	1:D:301:HIS:CD2	2.19	0.60
1:B:345:LEU:HD13	1:B:360:ILE:HG21	1.83	0.60
1:C:298:ASN:H	1:C:301:HIS:HD2	1.47	0.60
1:C:722:LYS:HA	1:C:728:PHE:HD1	1.66	0.60
1:D:462:ARG:HD3	1:D:548:LEU:HD13	1.83	0.60
1:B:298:ASN:H	1:B:301:HIS:CD2	2.19	0.60
1:B:594:TYR:HB2	1:B:669:LEU:HD21	1.83	0.60
1:C:570:GLN:HG3	1:C:692:TRP:CZ3	2.36	0.60
1:A:462:ARG:HD3	1:A:548:LEU:HD13	1.83	0.60
1:B:570:GLN:HG3	1:B:692:TRP:CZ3	2.36	0.60
1:C:245:ALA:HB1	1:C:250:PHE:CD2	2.37	0.60
1:C:330:ASN:CA	1:C:373:LEU:HD11	2.32	0.60
1:A:330:ASN:CA	1:A:373:LEU:HD11	2.32	0.60
1:D:245:ALA:HB1	1:D:250:PHE:CD2	2.37	0.60
1:D:301:HIS:O	1:D:305:THR:HG23	2.01	0.60
1:D:722:LYS:HA	1:D:728:PHE:HD1	1.66	0.60
1:A:722:LYS:HA	1:A:728:PHE:HD1	1.66	0.60
1:B:301:HIS:O	1:B:305:THR:HG23	2.01	0.59
1:B:722:LYS:HA	1:B:728:PHE:HD1	1.66	0.59
1:A:301:HIS:O	1:A:305:THR:HG23	2.01	0.59
1:A:384:PRO:HB2	1:A:737:VAL:HG13	1.83	0.59
1:D:594:TYR:HB2	1:D:669:LEU:HD21	1.84	0.59
1:C:382:TYR:OH	1:D:220:ASN:OD1	2.21	0.59
1:D:322:ASP:CA	1:D:359:TYR:OH	2.50	0.59
1:B:245:ALA:HB1	1:B:250:PHE:CD2	2.37	0.59
1:A:245:ALA:HB1	1:A:250:PHE:CD2	2.37	0.59
1:C:298:ASN:H	1:C:301:HIS:CD2	2.19	0.59
1:A:594:TYR:HB2	1:A:669:LEU:HD21	1.83	0.59
1:D:612:CYS:SG	1:D:617:LYS:O	2.47	0.59
1:A:672:MET:HE1	1:D:578:MET:HG2	1.83	0.59
1:D:621:SER:HB3	1:D:631:GLU:CD	2.23	0.59
1:B:385:VAL:HA	1:B:736:GLU:O	2.03	0.59
1:B:610:GLU:CG	1:B:649:LYS:HG3	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:ARG:HD3	1:C:548:LEU:HD13	1.83	0.58
1:C:594:TYR:HB2	1:C:669:LEU:HD21	1.83	0.58
1:D:621:SER:HB3	1:D:631:GLU:OE1	2.03	0.58
1:B:609:ILE:O	1:A:464:ARG:NH2	2.35	0.58
1:D:375:ARG:O	1:D:391:ASP:N	2.30	0.58
1:C:345:LEU:HD13	1:C:360:ILE:CG2	2.34	0.58
1:C:464:ARG:NH2	1:D:609:ILE:O	2.37	0.58
1:A:282:MET:HA	1:A:287:THR:HG21	1.86	0.58
1:A:416:ARG:HA	1:A:419:MET:HE2	1.85	0.58
1:C:288:ASP:HB3	1:C:291:SER:OG	2.04	0.58
1:D:282:MET:HA	1:D:287:THR:HG21	1.86	0.58
1:B:377:PHE:CE2	1:B:723:VAL:CG1	2.87	0.57
1:A:438:LYS:CE	2:A:1505:6OU:N29	2.61	0.57
1:D:288:ASP:HB3	1:D:291:SER:OG	2.04	0.57
1:B:158:LEU:HD22	1:B:197:ASN:OD1	2.04	0.57
1:B:191:LEU:HG	1:B:204:ILE:CG2	2.35	0.57
1:B:621:SER:H	1:B:646:GLN:NE2	2.03	0.57
1:C:431:MET:O	1:C:435:LYS:HB2	2.04	0.57
1:A:288:ASP:HB3	1:A:291:SER:OG	2.04	0.57
1:A:612:CYS:HB2	1:A:619:CYS:SG	2.44	0.57
1:C:282:MET:HE3	1:C:327:ARG:HG2	1.87	0.57
1:B:282:MET:HA	1:B:287:THR:HG21	1.86	0.57
1:D:288:ASP:HB3	1:D:291:SER:HG	1.70	0.57
1:C:282:MET:HA	1:C:287:THR:HG21	1.86	0.57
1:A:593:VAL:HG21	1:D:575:TYR:HE2	1.69	0.57
1:A:600:GLY:HA3	3:A:1506:EQK:N13	2.20	0.57
1:B:650:TYR:OH	1:A:546:GLU:HA	2.05	0.56
1:B:282:MET:HE3	1:B:327:ARG:HG2	1.87	0.56
1:A:384:PRO:HA	1:A:738:LYS:O	2.05	0.56
1:B:288:ASP:HB3	1:B:291:SER:OG	2.04	0.56
1:B:698:ARG:O	1:B:702:GLU:HG3	2.05	0.56
1:A:630:LEU:CG	1:A:634:LYS:HE3	2.34	0.56
1:A:672:MET:CE	1:D:578:MET:HG2	2.36	0.56
1:A:698:ARG:O	1:A:702:GLU:HG3	2.06	0.56
1:D:698:ARG:O	1:D:702:GLU:HG3	2.05	0.56
1:C:698:ARG:O	1:C:702:GLU:HG3	2.05	0.56
1:A:321:TYR:CD2	1:A:356:ILE:HD11	2.41	0.56
1:D:282:MET:HE3	1:D:327:ARG:HG2	1.88	0.56
1:A:396:ASP:O	1:A:398:THR:N	2.39	0.56
1:D:621:SER:HB3	1:D:631:GLU:OE2	2.05	0.56
1:D:396:ASP:O	1:D:398:THR:N	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:MET:HE3	1:A:327:ARG:HG2	1.87	0.55
1:C:578:MET:HG2	1:D:672:MET:HE1	1.89	0.55
1:B:377:PHE:CZ	1:B:723:VAL:CG1	2.89	0.55
1:C:722:LYS:HA	1:C:728:PHE:CD1	2.42	0.55
1:A:379:ASP:O	1:A:748:PHE:HB2	2.06	0.55
1:A:387:SER:OG	1:A:733:ARG:HD3	2.06	0.55
1:D:376:LYS:HD2	1:D:390:TYR:CE2	2.42	0.55
1:C:396:ASP:O	1:C:398:THR:N	2.39	0.55
1:D:722:LYS:HA	1:D:728:PHE:CD1	2.42	0.55
1:C:384:PRO:CB	1:C:737:VAL:HG13	2.37	0.55
1:D:377:PHE:N	1:D:377:PHE:CD1	2.74	0.55
1:D:385:VAL:HA	1:D:736:GLU:O	2.06	0.55
1:B:158:LEU:CD2	1:B:197:ASN:OD1	2.55	0.54
1:B:396:ASP:O	1:B:398:THR:N	2.39	0.54
1:B:722:LYS:HA	1:B:728:PHE:CD1	2.42	0.54
1:C:599:LEU:HD22	1:C:625:PHE:HZ	1.73	0.54
1:A:722:LYS:HA	1:A:728:PHE:CD1	2.42	0.54
1:B:365:ILE:CD1	1:B:373:LEU:O	2.56	0.54
1:B:377:PHE:CE2	1:B:723:VAL:HG12	2.43	0.54
1:A:321:TYR:CZ	1:A:360:ILE:HD11	2.43	0.54
1:A:332:GLU:O	1:A:336:THR:HG23	2.08	0.54
1:D:332:GLU:O	1:D:336:THR:HG23	2.08	0.54
1:D:392:LEU:HD22	1:D:428:LEU:HD11	1.90	0.54
1:B:377:PHE:CE1	1:B:723:VAL:HG11	2.43	0.53
1:C:385:VAL:HA	1:C:736:GLU:O	2.08	0.53
1:C:392:LEU:HD22	1:C:428:LEU:HD11	1.90	0.53
1:C:609:ILE:HD11	1:C:654:PHE:CE2	2.43	0.53
1:D:530:ALA:O	1:D:534:ILE:HG22	2.08	0.53
1:B:530:ALA:O	1:B:534:ILE:HG22	2.08	0.53
1:B:694:LEU:O	1:B:698:ARG:HG3	2.08	0.53
1:C:332:GLU:O	1:C:336:THR:HG23	2.08	0.53
1:C:694:LEU:O	1:C:698:ARG:HG3	2.08	0.53
1:B:573:GLY:O	1:B:577:VAL:HG13	2.09	0.53
1:A:288:ASP:HB3	1:A:291:SER:HG	1.73	0.53
1:C:530:ALA:O	1:C:534:ILE:HG22	2.08	0.53
1:C:573:GLY:O	1:C:577:VAL:HG13	2.09	0.53
1:D:384:PRO:HB3	1:D:737:VAL:CG1	2.39	0.53
1:A:530:ALA:O	1:A:534:ILE:HG22	2.08	0.53
1:D:694:LEU:O	1:D:698:ARG:HG3	2.08	0.53
1:A:381:ALA:HA	1:A:386:SER:HA	1.91	0.53
1:B:332:GLU:O	1:B:336:THR:HG23	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:LEU:O	1:A:698:ARG:HG3	2.08	0.53
1:C:630:LEU:CG	1:C:634:LYS:HE3	2.35	0.52
1:A:345:LEU:HD13	1:A:360:ILE:HG22	1.92	0.52
1:D:573:GLY:O	1:D:577:VAL:HG13	2.09	0.52
1:A:182:ASN:O	1:A:186:ILE:HG13	2.10	0.52
1:C:361:LEU:HD13	1:C:424:PRO:HG2	1.91	0.52
1:B:381:ALA:HA	1:B:386:SER:HA	1.91	0.52
1:B:630:LEU:CG	1:B:634:LYS:HE3	2.35	0.52
1:C:578:MET:HG2	1:D:672:MET:CE	2.39	0.52
1:B:392:LEU:HD22	1:B:428:LEU:HD11	1.90	0.52
1:D:384:PRO:HB2	1:D:737:VAL:HG13	1.91	0.52
1:D:182:ASN:O	1:D:186:ILE:HG13	2.10	0.52
1:A:573:GLY:O	1:A:577:VAL:HG13	2.09	0.52
1:A:689:GLU:OE1	1:A:693:ARG:NH1	2.43	0.52
1:D:689:GLU:OE1	1:D:693:ARG:NH1	2.43	0.52
1:B:182:ASN:O	1:B:186:ILE:HG13	2.10	0.52
1:C:345:LEU:HG	1:C:403:VAL:HG21	1.92	0.52
1:D:374:SER:HB2	1:D:377:PHE:CE2	2.45	0.52
1:D:345:LEU:HG	1:D:403:VAL:HG21	1.92	0.51
1:B:345:LEU:HG	1:B:403:VAL:HG21	1.92	0.51
1:D:330:ASN:N	1:D:373:LEU:HD11	2.25	0.51
1:D:331:TRP:NE1	1:D:372:SER:O	2.42	0.51
1:D:354:ALA:HB2	1:D:419:MET:HG2	1.90	0.51
1:B:546:GLU:HA	1:C:650:TYR:OH	2.10	0.51
1:B:689:GLU:OE1	1:B:693:ARG:NH1	2.43	0.51
1:C:384:PRO:HD2	1:D:259:PHE:CZ	2.46	0.51
1:A:345:LEU:HG	1:A:403:VAL:HG21	1.92	0.51
1:D:622:TYR:CE1	1:D:631:GLU:OE2	2.64	0.51
1:C:182:ASN:O	1:C:186:ILE:HG13	2.10	0.51
1:B:322:ASP:HA	1:B:359:TYR:OH	2.11	0.51
1:C:689:GLU:OE1	1:C:693:ARG:NH1	2.43	0.51
1:C:326:LEU:CD2	1:C:365:ILE:HD13	2.41	0.51
1:D:621:SER:CB	1:D:631:GLU:OE2	2.59	0.51
1:C:326:LEU:HD21	1:C:365:ILE:HD13	1.93	0.50
1:C:413:ILE:HD11	1:C:416:ARG:HG3	1.93	0.50
1:A:322:ASP:HA	1:A:359:TYR:OH	2.11	0.50
1:B:345:LEU:HD13	1:B:360:ILE:HG22	1.93	0.50
1:B:431:MET:O	1:B:435:LYS:HB2	2.10	0.50
1:D:375:ARG:O	1:D:391:ASP:CB	2.60	0.50
1:C:600:GLY:HA3	3:C:1101:EQK:N13	2.27	0.50
1:A:330:ASN:N	1:A:373:LEU:HD11	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:PRO:HB3	1:A:737:VAL:CG1	2.41	0.50
1:B:711:LEU:HD22	1:B:715:PHE:CE2	2.47	0.50
1:C:390:TYR:CD1	1:C:734:ILE:HD12	2.47	0.50
1:C:711:LEU:HD22	1:C:715:PHE:CE2	2.47	0.50
1:B:191:LEU:CD2	1:B:204:ILE:HG21	2.42	0.49
1:A:351:MET:O	1:A:353:LYS:N	2.43	0.49
1:B:413:ILE:HD11	1:B:416:ARG:HG3	1.93	0.49
1:C:278:VAL:HG21	1:C:320:MET:HE1	1.94	0.49
1:A:345:LEU:HD12	1:A:357:LEU:HD12	1.94	0.49
1:D:711:LEU:HD22	1:D:715:PHE:CE2	2.47	0.49
1:C:379:ASP:O	1:C:748:PHE:HB2	2.12	0.49
1:C:575:TYR:HE2	1:D:593:VAL:HG21	1.77	0.49
1:A:306:VAL:O	1:A:313:GLN:NE2	2.45	0.49
1:A:390:TYR:CD1	1:A:734:ILE:HD12	2.47	0.49
1:D:278:VAL:HG21	1:D:320:MET:HE1	1.95	0.49
1:D:590:PHE:HE1	1:D:669:LEU:HG	1.71	0.49
1:C:306:VAL:O	1:C:313:GLN:NE2	2.45	0.49
1:A:431:MET:O	1:A:435:LYS:HB2	2.13	0.49
1:D:306:VAL:O	1:D:313:GLN:NE2	2.45	0.49
1:D:420:LEU:CD1	1:D:429:LEU:CD1	2.83	0.49
1:B:390:TYR:CD1	1:B:734:ILE:HD12	2.47	0.49
1:C:345:LEU:HD12	1:C:357:LEU:HD12	1.95	0.49
1:C:649:LYS:HG3	1:C:650:TYR:HD2	1.75	0.49
1:D:413:ILE:HD11	1:D:416:ARG:HG3	1.93	0.49
1:D:596:VAL:HG12	3:D:1101:EQK:C31	2.42	0.49
1:B:306:VAL:O	1:B:313:GLN:NE2	2.45	0.49
1:A:711:LEU:HD22	1:A:715:PHE:CE2	2.47	0.49
1:B:275:PRO:HB3	1:B:323:MET:HE1	1.95	0.49
1:D:390:TYR:CD1	1:D:734:ILE:HD12	2.47	0.49
1:B:364:GLU:HG3	1:B:376:LYS:O	2.13	0.48
3:B:1406:EQK:C26	3:B:1406:EQK:C21	2.91	0.48
1:A:326:LEU:HD21	1:A:365:ILE:HD13	1.95	0.48
1:A:413:ILE:HD11	1:A:416:ARG:HG3	1.93	0.48
1:D:351:MET:O	1:D:353:LYS:N	2.43	0.48
1:A:326:LEU:CD2	1:A:365:ILE:HD13	2.43	0.48
1:B:186:ILE:C	1:B:190:LEU:HD13	2.29	0.48
3:C:1101:EQK:C26	3:C:1101:EQK:C21	2.91	0.48
1:D:381:ALA:HB2	1:D:386:SER:HB2	1.94	0.48
1:D:384:PRO:HB3	1:D:737:VAL:HG13	1.94	0.48
1:C:288:ASP:HB3	1:C:291:SER:HG	1.77	0.48
1:C:590:PHE:HE1	1:C:669:LEU:HG	1.71	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:LEU:HD13	1:D:360:ILE:CG2	2.43	0.48
1:D:612:CYS:CB	1:D:619:CYS:HG	2.24	0.48
1:B:742:TRP:CH2	1:C:272:THR:HA	2.48	0.48
1:A:275:PRO:HB3	1:A:323:MET:HE1	1.95	0.48
1:D:330:ASN:HA	1:D:373:LEU:HD11	1.96	0.48
1:A:331:TRP:NE1	1:A:372:SER:O	2.46	0.48
1:D:345:LEU:HD12	1:D:357:LEU:HD12	1.95	0.48
1:B:288:ASP:HB3	1:B:291:SER:HG	1.77	0.48
1:C:381:ALA:HB2	1:C:386:SER:HB2	1.95	0.48
1:B:259:PHE:CZ	1:A:384:PRO:HD2	2.48	0.48
1:C:401:ASN:OD1	1:C:401:ASN:N	2.47	0.48
1:A:583:ILE:HA	1:A:587:VAL:HB	1.96	0.48
1:B:583:ILE:HA	1:B:587:VAL:HB	1.96	0.47
1:C:330:ASN:HA	1:C:373:LEU:HD11	1.96	0.47
1:A:401:ASN:OD1	1:A:401:ASN:N	2.47	0.47
1:A:640:GLY:O	1:D:639:LEU:O	2.32	0.47
1:A:321:TYR:CD1	1:A:359:TYR:HE2	2.31	0.47
1:D:229:ASP:O	1:D:233:LEU:HG	2.14	0.47
1:D:318:LYS:HG3	1:D:359:TYR:CG	2.49	0.47
1:C:266:LEU:HD11	1:C:278:VAL:HG13	1.97	0.47
1:C:380:TRP:CE3	1:C:753:PRO:HB3	2.50	0.47
1:A:229:ASP:O	1:A:233:LEU:HG	2.14	0.47
1:B:229:ASP:O	1:B:233:LEU:HG	2.14	0.47
1:B:351:MET:O	1:B:353:LYS:N	2.43	0.47
1:B:590:PHE:HE1	1:B:669:LEU:HG	1.71	0.47
1:A:590:PHE:HE1	1:A:669:LEU:HG	1.72	0.47
1:D:297:ASN:N	1:D:297:ASN:OD1	2.47	0.47
1:D:401:ASN:OD1	1:D:401:ASN:N	2.47	0.47
1:B:278:VAL:HG21	1:B:320:MET:HE1	1.96	0.47
1:B:297:ASN:OD1	1:B:297:ASN:N	2.47	0.47
1:B:321:TYR:CD1	1:B:359:TYR:HE2	2.31	0.47
1:B:401:ASN:N	1:B:401:ASN:OD1	2.47	0.47
1:C:229:ASP:O	1:C:233:LEU:HG	2.14	0.47
1:C:330:ASN:N	1:C:373:LEU:HD11	2.29	0.47
1:A:266:LEU:HD11	1:A:278:VAL:HG13	1.97	0.47
1:D:275:PRO:HB3	1:D:323:MET:HE1	1.95	0.47
1:B:241:VAL:CG1	1:B:281:LEU:HD22	2.44	0.47
1:B:266:LEU:HD11	1:B:278:VAL:HG13	1.97	0.47
1:C:380:TRP:O	1:C:380:TRP:CE3	2.67	0.47
1:C:275:PRO:HB3	1:C:323:MET:HE1	1.95	0.47
1:A:278:VAL:HG21	1:A:320:MET:HE1	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:SER:O	1:D:733:ARG:HA	2.14	0.47
1:D:627:ASP:OD1	1:D:627:ASP:N	2.48	0.47
1:D:613:PRO:C	1:D:617:LYS:N	2.68	0.47
1:B:377:PHE:CD2	1:B:723:VAL:HG13	2.51	0.46
1:A:639:LEU:HD23	1:A:639:LEU:HA	1.71	0.46
1:D:266:LEU:HD11	1:D:278:VAL:HG13	1.97	0.46
1:B:377:PHE:CZ	1:B:723:VAL:HG11	2.49	0.46
1:D:596:VAL:HG12	3:D:1101:EQK:N12	2.31	0.46
1:A:185:GLU:O	1:A:189:ILE:HG13	2.16	0.46
1:C:345:LEU:HD13	1:C:360:ILE:HG21	1.97	0.46
1:C:633:PHE:CZ	1:D:659:ILE:HD12	2.51	0.46
1:A:157:PHE:N	1:A:157:PHE:CD1	2.84	0.46
1:D:157:PHE:CD1	1:D:157:PHE:N	2.84	0.46
1:D:583:ILE:HA	1:D:587:VAL:HB	1.96	0.46
1:D:682:GLU:HG3	1:D:683:ASN:N	2.31	0.46
1:B:284:HIS:HD2	1:B:286:GLN:H	1.63	0.46
1:D:326:LEU:HD21	1:D:365:ILE:HD13	1.97	0.46
1:B:389:LEU:HD12	1:B:389:LEU:HA	1.76	0.46
1:C:185:GLU:O	1:C:189:ILE:HG13	2.16	0.46
1:C:583:ILE:HA	1:C:587:VAL:HB	1.96	0.46
1:A:330:ASN:HA	1:A:373:LEU:HD11	1.97	0.46
1:B:185:GLU:O	1:B:189:ILE:HG13	2.16	0.46
1:B:321:TYR:CD2	1:B:356:ILE:HD11	2.51	0.46
1:B:380:TRP:O	1:B:380:TRP:CE3	2.67	0.46
1:C:381:ALA:HA	1:C:386:SER:HA	1.96	0.46
1:A:284:HIS:HD2	1:A:286:GLN:H	1.63	0.46
1:A:358:LYS:HG3	1:A:422:LEU:HD22	1.97	0.46
1:C:395:VAL:HG13	1:C:425:LEU:HD21	1.97	0.46
1:D:321:TYR:CD2	1:D:356:ILE:HD11	2.51	0.46
1:B:354:ALA:HB2	1:B:419:MET:HG2	1.97	0.46
1:C:235:ILE:HD11	1:C:280:LEU:HD21	1.98	0.46
1:A:297:ASN:N	1:A:297:ASN:OD1	2.47	0.46
1:D:185:GLU:O	1:D:189:ILE:HG13	2.16	0.46
1:D:384:PRO:CB	1:D:737:VAL:CG1	2.94	0.46
1:B:358:LYS:HG3	1:B:422:LEU:HD22	1.98	0.45
1:B:600:GLY:HA3	3:B:1406:EQK:N13	2.31	0.45
1:C:351:MET:O	1:C:353:LYS:N	2.43	0.45
1:D:284:HIS:HD2	1:D:286:GLN:H	1.63	0.45
1:B:235:ILE:HD11	1:B:280:LEU:HD21	1.98	0.45
1:B:716:ARG:HA	1:B:716:ARG:HD3	1.73	0.45
1:C:297:ASN:OD1	1:C:297:ASN:N	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:600:GLY:HA3	3:D:1101:EQK:N13	2.31	0.45
1:C:157:PHE:CD1	1:C:157:PHE:N	2.84	0.45
1:C:639:LEU:HD11	1:D:635:LEU:CD2	2.42	0.45
1:D:381:ALA:HA	1:D:386:SER:HA	1.97	0.45
1:C:284:HIS:HD2	1:C:286:GLN:H	1.63	0.45
1:A:375:ARG:O	1:A:391:ASP:N	2.38	0.45
1:D:337:ARG:NH1	1:D:346:GLN:HE22	2.10	0.45
1:B:284:HIS:CD2	1:B:286:GLN:H	2.35	0.45
1:A:235:ILE:HD11	1:A:280:LEU:HD21	1.98	0.45
1:A:284:HIS:CD2	1:A:286:GLN:H	2.35	0.45
1:A:380:TRP:O	1:A:380:TRP:CE3	2.67	0.45
1:B:599:LEU:HD22	1:B:625:PHE:HZ	1.82	0.45
1:C:590:PHE:CD1	1:C:669:LEU:HG	2.52	0.45
1:D:389:LEU:HD12	1:D:389:LEU:HA	1.76	0.45
1:D:436:PHE:CZ	1:D:704:GLU:HG3	2.52	0.45
1:C:337:ARG:NH1	1:C:346:GLN:HE22	2.10	0.45
1:C:739:TRP:HB3	1:D:313:GLN:HG2	1.98	0.45
1:A:205:ASN:OD1	1:A:240:ASP:N	2.45	0.45
1:A:384:PRO:CB	1:A:737:VAL:CG1	2.92	0.45
1:D:235:ILE:HD11	1:D:280:LEU:HD21	1.98	0.45
1:D:326:LEU:CD2	1:D:365:ILE:HD13	2.47	0.45
1:C:284:HIS:CD2	1:C:286:GLN:H	2.35	0.45
1:C:682:GLU:HG3	1:C:683:ASN:N	2.31	0.45
1:C:321:TYR:CD2	1:C:356:ILE:HD11	2.51	0.45
1:C:630:LEU:O	1:C:634:LYS:HG3	2.17	0.45
1:A:259:PHE:CZ	1:D:384:PRO:HD2	2.52	0.45
1:D:590:PHE:CD1	1:D:669:LEU:HG	2.52	0.45
1:C:720:LEU:HD21	1:C:728:PHE:HB3	2.00	0.44
1:B:380:TRP:CZ2	1:B:387:SER:OG	2.62	0.44
1:B:682:GLU:HG3	1:B:683:ASN:N	2.31	0.44
1:B:720:LEU:HD21	1:B:728:PHE:HB3	1.99	0.44
1:C:179:ILE:H	1:C:179:ILE:HG13	1.61	0.44
1:C:326:LEU:HD21	1:C:365:ILE:CD1	2.47	0.44
1:A:337:ARG:NH1	1:A:346:GLN:HE22	2.10	0.44
1:A:384:PRO:O	1:A:738:LYS:N	2.49	0.44
1:A:609:ILE:HD11	1:A:654:PHE:CE2	2.53	0.44
1:A:642:LEU:HB2	1:D:639:LEU:HD12	1.99	0.44
1:A:682:GLU:HG3	1:A:683:ASN:N	2.31	0.44
1:D:284:HIS:CD2	1:D:286:GLN:H	2.35	0.44
1:D:609:ILE:HD11	1:D:654:PHE:CE2	2.53	0.44
1:B:267:ALA:HA	1:B:299:ILE:HD13	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LYS:HG2	1:B:747:SER:HB3	1.98	0.44
1:A:267:ALA:HA	1:A:299:ILE:HD13	2.00	0.44
1:D:720:LEU:HD21	1:D:728:PHE:HB3	2.00	0.44
1:B:609:ILE:HD11	1:B:654:PHE:CE2	2.53	0.44
1:B:630:LEU:O	1:B:634:LYS:HG3	2.18	0.44
1:C:183:THR:HA	1:C:186:ILE:HD12	2.00	0.44
1:C:491:LEU:O	1:C:495:MET:HG3	2.18	0.44
1:A:389:LEU:HD12	1:A:389:LEU:HA	1.78	0.44
1:A:720:LEU:HD21	1:A:728:PHE:HB3	2.00	0.44
1:A:361:LEU:HD13	1:A:424:PRO:CG	2.46	0.43
1:A:381:ALA:HB2	1:A:386:SER:HB2	1.99	0.43
1:A:573:GLY:HA3	1:A:692:TRP:CD1	2.53	0.43
1:A:630:LEU:O	1:A:634:LYS:HG3	2.17	0.43
1:D:267:ALA:HA	1:D:299:ILE:HD13	2.00	0.43
1:D:600:GLY:C	3:D:1101:EQK:C33	2.86	0.43
1:C:573:GLY:HA3	1:C:692:TRP:CD1	2.53	0.43
1:A:452:ASN:HD22	1:A:452:ASN:HA	1.66	0.43
1:A:621:SER:HB3	1:A:631:GLU:CG	2.48	0.43
1:B:384:PRO:HB2	1:B:737:VAL:HG13	1.99	0.43
1:B:578:MET:HG2	1:C:672:MET:CE	2.48	0.43
1:D:573:GLY:HA3	1:D:692:TRP:CD1	2.53	0.43
1:B:573:GLY:HA3	1:B:692:TRP:CD1	2.53	0.43
1:B:272:THR:HA	1:A:742:TRP:CH2	2.53	0.43
1:B:491:LEU:O	1:B:495:MET:HG3	2.18	0.43
1:C:267:ALA:HA	1:C:299:ILE:HD13	2.00	0.43
1:C:331:TRP:NE1	1:C:372:SER:O	2.47	0.43
1:A:326:LEU:HD21	1:A:365:ILE:CD1	2.49	0.43
1:B:384:PRO:HB3	1:B:737:VAL:CG1	2.49	0.43
1:C:389:LEU:HD12	1:C:389:LEU:HA	1.77	0.43
1:C:642:LEU:HD11	1:C:658:LEU:HD21	2.01	0.43
1:A:180:ASN:HD21	1:A:186:ILE:HD11	1.84	0.43
1:D:205:ASN:OD1	1:D:240:ASP:N	2.45	0.43
1:D:634:LYS:HB3	1:D:634:LYS:HE2	1.74	0.43
1:B:205:ASN:OD1	1:B:240:ASP:N	2.45	0.43
1:B:420:LEU:HD22	1:B:694:LEU:HD13	2.01	0.43
1:A:183:THR:HA	1:A:186:ILE:HD12	2.00	0.43
1:A:522:PHE:HA	1:A:525:VAL:HG22	2.01	0.43
1:D:183:THR:HA	1:D:186:ILE:HD12	1.99	0.43
1:B:180:ASN:HD21	1:B:186:ILE:HD11	1.84	0.43
1:C:179:ILE:HG21	1:C:227:GLN:HG3	2.01	0.43
1:C:716:ARG:HA	1:C:716:ARG:HD3	1.73	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:MET:O	1:D:435:LYS:HB2	2.19	0.43
1:D:522:PHE:HA	1:D:525:VAL:HG22	2.01	0.43
1:B:380:TRP:CE3	1:B:753:PRO:HB3	2.54	0.43
1:B:452:ASN:HD22	1:B:452:ASN:HA	1.66	0.43
1:B:578:MET:HG2	1:C:672:MET:HE1	1.99	0.43
1:B:635:LEU:HD23	1:A:639:LEU:HD11	2.01	0.43
1:A:662:VAL:O	1:A:666:PHE:HB3	2.19	0.43
1:B:183:THR:HA	1:B:186:ILE:HD12	2.00	0.42
1:C:566:THR:HG1	1:C:576:SER:CB	2.29	0.42
1:C:596:VAL:HG12	3:C:1101:EQK:C31	2.48	0.42
1:C:621:SER:HB3	1:C:631:GLU:HG2	2.01	0.42
1:D:491:LEU:O	1:D:495:MET:HG3	2.18	0.42
1:C:180:ASN:HD21	1:C:186:ILE:HD11	1.84	0.42
1:D:376:LYS:HD2	1:D:390:TYR:CZ	2.54	0.42
1:B:261:PHE:CE1	1:B:268:LEU:HB2	2.54	0.42
1:D:179:ILE:HG21	1:D:227:GLN:HG3	2.01	0.42
1:D:180:ASN:HD21	1:D:186:ILE:HD11	1.84	0.42
1:D:649:LYS:CG	1:D:650:TYR:CE2	2.97	0.42
1:B:464:ARG:NH2	1:C:609:ILE:O	2.51	0.42
1:B:546:GLU:N	1:B:546:GLU:CD	2.72	0.42
1:B:191:LEU:HG	1:B:204:ILE:HG21	2.01	0.42
1:B:642:LEU:HD11	1:B:658:LEU:HD21	2.01	0.42
1:B:711:LEU:HD23	1:B:711:LEU:HA	1.91	0.42
1:C:321:TYR:CD1	1:C:359:TYR:HE2	2.37	0.42
1:C:462:ARG:HH12	1:D:649:LYS:NZ	2.18	0.42
1:A:377:PHE:CD1	1:A:377:PHE:N	2.87	0.42
1:A:642:LEU:HD11	1:A:658:LEU:HD21	2.01	0.42
1:D:380:TRP:O	1:D:380:TRP:CE3	2.67	0.42
1:B:179:ILE:HD12	1:B:179:ILE:O	2.20	0.42
1:B:337:ARG:HA	1:B:342:LEU:O	2.19	0.42
1:B:639:LEU:HA	1:B:639:LEU:HD23	1.71	0.42
1:D:261:PHE:CE1	1:D:268:LEU:HB2	2.55	0.42
1:D:387:SER:HA	1:D:735:ASN:HA	2.00	0.42
1:B:279:GLN:HG2	1:B:327:ARG:HH12	1.85	0.42
1:B:522:PHE:HA	1:B:525:VAL:HG22	2.01	0.42
1:C:548:LEU:HD23	1:D:650:TYR:HE2	1.84	0.42
1:C:662:VAL:O	1:C:666:PHE:HB3	2.19	0.42
1:D:376:LYS:HB2	1:D:390:TYR:CD2	2.55	0.42
1:D:642:LEU:HD11	1:D:658:LEU:HD21	2.01	0.42
1:D:722:LYS:O	1:D:749:LEU:HD22	2.20	0.42
1:B:662:VAL:O	1:B:666:PHE:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:ASN:HD22	1:C:452:ASN:HA	1.66	0.42
1:A:722:LYS:O	1:A:749:LEU:HD22	2.20	0.42
1:A:279:GLN:HG2	1:A:327:ARG:HH12	1.85	0.42
1:A:491:LEU:O	1:A:495:MET:HG3	2.18	0.42
1:A:635:LEU:HD23	1:D:639:LEU:HD11	2.02	0.42
1:B:179:ILE:HG21	1:B:227:GLN:HG3	2.01	0.42
1:B:377:PHE:CG	1:B:723:VAL:HG13	2.55	0.41
1:C:179:ILE:O	1:C:179:ILE:HD12	2.20	0.41
1:A:179:ILE:HG21	1:A:227:GLN:HG3	2.01	0.41
1:A:711:LEU:HD23	1:A:711:LEU:HA	1.91	0.41
1:B:259:PHE:HE1	1:A:739:TRP:CH2	2.38	0.41
1:B:420:LEU:HD12	1:B:420:LEU:HA	1.66	0.41
1:A:301:HIS:HE1	1:A:342:LEU:O	2.03	0.41
1:B:384:PRO:HD2	1:C:259:PHE:CZ	2.55	0.41
1:B:742:TRP:HB3	1:C:226:ARG:CZ	2.51	0.41
3:B:1406:EQK:O07	3:B:1406:EQK:S01	2.79	0.41
1:A:179:ILE:O	1:A:179:ILE:HD12	2.20	0.41
1:A:649:LYS:CG	1:A:650:TYR:CE2	2.97	0.41
1:B:575:TYR:HE2	1:C:593:VAL:HG21	1.85	0.41
1:B:722:LYS:O	1:B:749:LEU:HD22	2.20	0.41
1:C:279:GLN:HG2	1:C:327:ARG:HH12	1.85	0.41
1:C:380:TRP:CE3	1:C:753:PRO:CB	3.03	0.41
1:C:522:PHE:HA	1:C:525:VAL:HG22	2.01	0.41
1:C:592:PHE:O	1:C:596:VAL:HG23	2.20	0.41
1:C:742:TRP:CH2	1:D:272:THR:HA	2.54	0.41
1:A:716:ARG:HA	1:A:716:ARG:HD3	1.73	0.41
1:D:711:LEU:HD23	1:D:711:LEU:HA	1.91	0.41
1:A:176:LEU:HD21	1:A:230:ILE:CG2	2.43	0.41
1:D:179:ILE:HD12	1:D:179:ILE:O	2.20	0.41
1:D:279:GLN:HG2	1:D:327:ARG:HH12	1.85	0.41
1:B:377:PHE:CD2	1:B:723:VAL:CG1	3.03	0.41
1:C:301:HIS:HE1	1:C:342:LEU:O	2.03	0.41
3:C:1101:EQK:O07	3:C:1101:EQK:S01	2.79	0.41
1:A:369:ARG:HG3	1:A:370:LEU:HG	2.03	0.41
1:D:631:GLU:HA	1:D:634:LYS:HB2	2.02	0.41
1:B:179:ILE:H	1:B:179:ILE:HG13	1.61	0.41
1:B:301:HIS:HE1	1:B:342:LEU:O	2.03	0.41
1:C:384:PRO:HB2	1:C:737:VAL:HG13	2.02	0.41
1:B:160:HIS:HA	1:B:163:THR:HG22	2.03	0.41
1:B:381:ALA:HB2	1:B:386:SER:HB2	2.01	0.41
1:C:322:ASP:HA	1:C:359:TYR:OH	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:PHE:CZ	1:A:704:GLU:HG3	2.56	0.41
1:D:301:HIS:HE1	1:D:342:LEU:O	2.03	0.41
1:B:417:HIS:CB	1:B:690:ARG:HD2	2.51	0.41
1:B:501:GLU:HB2	1:B:527:PHE:HB2	2.03	0.41
1:C:160:HIS:HA	1:C:163:THR:HG22	2.03	0.41
1:C:384:PRO:HB3	1:C:737:VAL:HG13	2.02	0.41
1:C:620:SER:OG	1:C:646:GLN:O	2.24	0.41
1:C:649:LYS:HG3	1:C:650:TYR:CE2	2.55	0.41
1:C:722:LYS:O	1:C:749:LEU:HD22	2.20	0.41
1:A:501:GLU:HB2	1:A:527:PHE:HB2	2.03	0.41
1:A:590:PHE:CD1	1:A:669:LEU:HG	2.52	0.41
1:D:501:GLU:HB2	1:D:527:PHE:HB2	2.03	0.41
1:D:662:VAL:O	1:D:666:PHE:HB3	2.19	0.41
1:B:316:PHE:O	1:B:320:MET:HG2	2.20	0.41
1:B:384:PRO:HB3	1:B:737:VAL:HG13	2.00	0.41
1:B:385:VAL:O	1:B:385:VAL:HG13	2.21	0.41
1:C:417:HIS:CB	1:C:690:ARG:HD2	2.51	0.41
1:C:501:GLU:HB2	1:C:527:PHE:HB2	2.03	0.41
1:D:176:LEU:HD21	1:D:230:ILE:CG2	2.43	0.41
1:B:226:ARG:CZ	1:A:742:TRP:HB3	2.52	0.40
1:C:448:TYR:HD2	1:C:562:MET:SD	2.44	0.40
1:A:316:PHE:O	1:A:320:MET:HG2	2.20	0.40
1:A:417:HIS:CB	1:A:690:ARG:HD2	2.51	0.40
1:A:456:THR:HA	1:A:555:MET:HG3	2.03	0.40
1:D:387:SER:OG	1:D:733:ARG:CD	2.65	0.40
1:C:385:VAL:HG13	1:C:385:VAL:O	2.21	0.40
1:C:613:PRO:HD2	1:C:619:CYS:SG	2.61	0.40
1:A:605:LEU:O	1:A:609:ILE:HG12	2.22	0.40
3:A:1506:EQK:O07	3:A:1506:EQK:S01	2.78	0.40
1:D:361:LEU:HD23	1:D:361:LEU:HA	1.86	0.40
1:D:417:HIS:CB	1:D:690:ARG:HD2	2.51	0.40
1:B:596:VAL:HG12	3:B:1406:EQK:N12	2.36	0.40
1:A:387:SER:HA	1:A:735:ASN:HA	2.04	0.40
1:A:504:ALA:O	1:A:508:LEU:HG	2.21	0.40
1:A:621:SER:HB3	1:A:631:GLU:HG3	2.03	0.40
1:D:325:LEU:HD21	1:D:363:ARG:NH1	2.36	0.40
1:D:420:LEU:HD21	1:D:693:ARG:HG2	2.03	0.40
1:D:504:ALA:O	1:D:508:LEU:HG	2.21	0.40
1:C:316:PHE:O	1:C:320:MET:HG2	2.21	0.40
1:A:325:LEU:HG	1:A:373:LEU:HD23	2.04	0.40
1:D:420:LEU:CD1	1:D:429:LEU:HD11	2.46	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	596/1061 (56%)	554 (93%)	42 (7%)	0	100	100
1	B	598/1061 (56%)	555 (93%)	42 (7%)	1 (0%)	44	62
1	C	598/1061 (56%)	557 (93%)	41 (7%)	0	100	100
1	D	596/1061 (56%)	555 (93%)	41 (7%)	0	100	100
All	All	2388/4244 (56%)	2221 (93%)	166 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	547	TYR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	434/933 (46%)	412 (95%)	22 (5%)	20	38
1	B	437/933 (47%)	420 (96%)	17 (4%)	27	50
1	C	434/933 (46%)	407 (94%)	27 (6%)	15	29
1	D	434/933 (46%)	411 (95%)	23 (5%)	19	36
All	All	1739/3732 (47%)	1650 (95%)	89 (5%)	22	38

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	183	THR
1	B	337	ARG
1	B	356	ILE
1	B	359	TYR
1	B	371	ARG
1	B	372	SER
1	B	374	SER
1	B	394	ASN
1	B	398	THR
1	B	402	SER
1	B	547	TYR
1	B	610	GLU
1	B	612	CYS
1	B	619	CYS
1	B	631	GLU
1	B	635	LEU
1	B	641	ASP
1	C	135	LEU
1	C	157	PHE
1	C	158	LEU
1	C	167	THR
1	C	171	CYS
1	C	183	THR
1	C	190	LEU
1	C	191	LEU
1	C	241	VAL
1	C	328	SER
1	C	337	ARG
1	C	356	ILE
1	C	359	TYR
1	C	363	ARG
1	C	366	LYS
1	C	378	THR
1	C	380	TRP
1	C	394	ASN
1	C	398	THR
1	C	402	SER
1	C	421	THR
1	C	435	LYS
1	C	612	CYS
1	C	620	SER
1	C	631	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	635	LEU
1	C	641	ASP
1	A	135	LEU
1	A	157	PHE
1	A	158	LEU
1	A	167	THR
1	A	171	CYS
1	A	183	THR
1	A	190	LEU
1	A	191	LEU
1	A	241	VAL
1	A	328	SER
1	A	337	ARG
1	A	356	ILE
1	A	359	TYR
1	A	363	ARG
1	A	366	LYS
1	A	378	THR
1	A	394	ASN
1	A	398	THR
1	A	402	SER
1	A	421	THR
1	A	635	LEU
1	A	641	ASP
1	D	135	LEU
1	D	157	PHE
1	D	158	LEU
1	D	167	THR
1	D	171	CYS
1	D	183	THR
1	D	190	LEU
1	D	191	LEU
1	D	241	VAL
1	D	328	SER
1	D	337	ARG
1	D	356	ILE
1	D	363	ARG
1	D	366	LYS
1	D	377	PHE
1	D	378	THR
1	D	394	ASN
1	D	398	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	402	SER
1	D	421	THR
1	D	627	ASP
1	D	635	LEU
1	D	641	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	178	ASN
1	B	284	HIS
1	B	298	ASN
1	B	301	HIS
1	B	339	ASN
1	B	346	GLN
1	B	394	ASN
1	B	410	ASN
1	B	452	ASN
1	B	580	GLN
1	B	646	GLN
1	C	178	ASN
1	C	197	ASN
1	C	284	HIS
1	C	298	ASN
1	C	301	HIS
1	C	339	ASN
1	C	346	GLN
1	C	394	ASN
1	C	410	ASN
1	C	452	ASN
1	C	580	GLN
1	C	646	GLN
1	C	647	ASN
1	A	178	ASN
1	A	197	ASN
1	A	284	HIS
1	A	298	ASN
1	A	301	HIS
1	A	339	ASN
1	A	346	GLN
1	A	394	ASN
1	A	410	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	452	ASN
1	A	580	GLN
1	A	646	GLN
1	A	647	ASN
1	D	178	ASN
1	D	197	ASN
1	D	284	HIS
1	D	298	ASN
1	D	301	HIS
1	D	339	ASN
1	D	346	GLN
1	D	394	ASN
1	D	410	ASN
1	D	452	ASN
1	D	580	GLN
1	D	646	GLN
1	D	647	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](#)

24 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	6OU	A	1501	-	13,13,48	0.26	0	12,12,53	0.87	0
2	6OU	D	1103	-	13,13,48	0.22	0	12,12,53	0.95	0
2	6OU	A	1504	-	13,13,48	0.22	0	12,12,53	0.94	0
2	6OU	B	1401	-	13,13,48	0.31	0	12,12,53	0.69	0
3	EQK	B	1406	-	29,35,35	4.37	19 (65%)	33,52,52	2.00	11 (33%)
2	6OU	B	1405	-	29,29,48	0.82	1 (3%)	31,32,53	1.00	1 (3%)
2	6OU	D	1105	-	29,29,48	0.85	1 (3%)	31,32,53	0.89	1 (3%)
2	6OU	B	1404	-	11,11,48	0.23	0	10,10,53	0.93	0
2	6OU	C	1103	-	12,12,48	0.26	0	11,11,53	0.80	0
2	6OU	C	1104	-	12,12,48	0.26	0	11,11,53	0.71	0
2	6OU	C	1106	-	13,13,48	0.29	0	12,12,53	0.78	0
2	6OU	B	1403	-	13,13,48	0.26	0	12,12,53	0.88	0
2	6OU	A	1503	-	13,13,48	0.20	0	12,12,53	0.65	0
2	6OU	A	1505	-	29,29,48	0.85	1 (3%)	31,32,53	0.99	1 (3%)
2	6OU	D	1102	-	13,13,48	0.25	0	12,12,53	0.84	0
2	6OU	D	1104	-	13,13,48	0.23	0	12,12,53	0.98	0
3	EQK	D	1101	-	29,35,35	4.87	19 (65%)	33,52,52	2.31	13 (39%)
2	6OU	B	1402	-	13,13,48	1.02	1 (7%)	12,12,53	0.84	0
2	6OU	A	1502	-	13,13,48	1.04	1 (7%)	12,12,53	0.98	0
2	6OU	C	1105	-	13,13,48	0.26	0	12,12,53	0.85	0
3	EQK	A	1506	-	29,35,35	3.35	16 (55%)	33,52,52	2.71	14 (42%)
2	6OU	A	1507	-	11,11,48	0.30	0	9,10,53	0.93	0
2	6OU	C	1102	-	29,29,48	0.83	1 (3%)	31,32,53	0.96	1 (3%)
3	EQK	C	1101	-	29,35,35	4.37	19 (65%)	33,52,52	1.99	10 (30%)

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	6OU	A	1501	-	-	6/11/11/52	-
2	6OU	D	1103	-	-	6/11/11/52	-
2	6OU	A	1504	-	-	8/11/11/52	-
2	6OU	B	1401	-	-	6/11/11/52	-
3	EQK	B	1406	-	-	11/26/31/31	0/3/3/3
2	6OU	B	1405	-	-	6/30/30/52	-
2	6OU	D	1105	-	-	13/30/30/52	-
2	6OU	B	1404	-	-	6/9/9/52	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6OU	C	1103	-	-	6/10/10/52	-
2	6OU	C	1104	-	-	4/10/10/52	-
2	6OU	C	1106	-	-	6/11/11/52	-
2	6OU	B	1403	-	-	1/11/11/52	-
2	6OU	A	1503	-	-	1/11/11/52	-
2	6OU	A	1505	-	-	15/30/30/52	-
2	6OU	D	1102	-	-	5/11/11/52	-
2	6OU	D	1104	-	-	5/11/11/52	-
3	EQK	D	1101	-	-	9/26/31/31	0/3/3/3
2	6OU	B	1402	-	-	2/11/11/52	-
2	6OU	A	1502	-	-	5/11/11/52	-
2	6OU	C	1105	-	-	3/11/11/52	-
3	EQK	A	1506	-	-	7/26/31/31	0/3/3/3
2	6OU	A	1507	-	-	4/9/9/52	-
2	6OU	C	1102	-	-	9/30/30/52	-
3	EQK	C	1101	-	-	11/26/31/31	0/3/3/3

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1101	EQK	C31-N12	8.43	1.49	1.33
3	D	1101	EQK	C31-N13	8.40	1.49	1.33
3	C	1101	EQK	C31-N12	7.95	1.48	1.33
3	B	1406	EQK	C31-N12	7.94	1.48	1.33
3	C	1101	EQK	C31-N13	7.74	1.48	1.33
3	B	1406	EQK	C31-N13	7.70	1.48	1.33
3	D	1101	EQK	C17-C15	7.59	1.53	1.39
3	B	1406	EQK	C17-C15	7.37	1.52	1.39
3	C	1101	EQK	C17-C15	7.35	1.52	1.39
3	D	1101	EQK	C21-C24	7.17	1.53	1.38
3	A	1506	EQK	C17-C15	7.16	1.52	1.39
3	D	1101	EQK	C30-N13	7.07	1.45	1.32
3	D	1101	EQK	C29-N12	7.01	1.45	1.32
3	D	1101	EQK	C15-N08	6.88	1.49	1.34
3	D	1101	EQK	C24-N08	6.87	1.49	1.34
3	A	1506	EQK	O07-C27	-6.86	1.09	1.23
3	C	1101	EQK	C21-C24	6.72	1.52	1.38
3	B	1406	EQK	C21-C24	6.68	1.52	1.38
3	C	1101	EQK	C15-N08	6.51	1.48	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1406	EQK	C15-N08	6.47	1.48	1.34
3	C	1101	EQK	C24-N08	6.37	1.48	1.34
3	B	1406	EQK	C24-N08	6.36	1.48	1.34
3	B	1406	EQK	C29-N12	5.96	1.43	1.32
3	C	1101	EQK	C29-N12	5.95	1.43	1.32
3	B	1406	EQK	C30-N13	5.90	1.43	1.32
3	C	1101	EQK	C30-N13	5.90	1.43	1.32
3	D	1101	EQK	C28-C30	5.85	1.49	1.41
3	D	1101	EQK	C28-C29	5.83	1.49	1.41
3	D	1101	EQK	C17-C16	5.67	1.49	1.39
3	A	1506	EQK	C15-N08	5.47	1.46	1.34
3	B	1406	EQK	C28-C30	5.46	1.48	1.41
3	C	1101	EQK	C28-C30	5.40	1.48	1.41
3	B	1406	EQK	C17-C16	5.32	1.49	1.39
3	C	1101	EQK	C17-C16	5.32	1.49	1.39
3	D	1101	EQK	C25-N10	5.15	1.45	1.36
3	A	1506	EQK	C21-C24	5.10	1.48	1.38
3	D	1101	EQK	C16-C20	5.05	1.53	1.48
3	A	1506	EQK	C31-N12	4.95	1.43	1.33
3	D	1101	EQK	C21-C16	4.85	1.49	1.39
3	A	1506	EQK	C31-N13	4.85	1.42	1.33
3	B	1406	EQK	C28-C29	4.78	1.47	1.41
3	C	1101	EQK	C28-C29	4.73	1.47	1.41
3	A	1506	EQK	C28-C27	-4.39	1.44	1.51
3	B	1406	EQK	C21-C16	4.35	1.48	1.39
3	C	1101	EQK	C21-C16	4.34	1.48	1.39
3	A	1506	EQK	C17-C16	4.19	1.47	1.39
3	D	1101	EQK	C22-N09	4.18	1.57	1.36
3	A	1506	EQK	C24-N08	4.17	1.43	1.34
3	C	1101	EQK	C16-C20	3.90	1.52	1.48
3	B	1406	EQK	C25-N10	3.82	1.43	1.36
3	C	1101	EQK	C25-N10	3.77	1.43	1.36
3	B	1406	EQK	C16-C20	3.74	1.51	1.48
2	A	1502	6OU	C06-C05	-3.72	1.30	1.51
3	D	1101	EQK	C27-N10	3.66	1.45	1.35
3	C	1101	EQK	C22-N09	3.64	1.54	1.36
2	B	1402	6OU	C06-C05	-3.63	1.31	1.51
3	B	1406	EQK	C22-N09	3.61	1.54	1.36
3	A	1506	EQK	C28-C30	3.46	1.45	1.41
3	D	1101	EQK	O05-C29	3.28	1.40	1.35
3	D	1101	EQK	O06-C30	3.24	1.40	1.35
3	A	1506	EQK	O06-C33	-3.12	1.33	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1406	EQK	O07-C27	-3.10	1.17	1.23
3	C	1101	EQK	O06-C30	3.09	1.39	1.35
3	C	1101	EQK	O07-C27	-3.07	1.17	1.23
3	B	1406	EQK	O06-C30	3.03	1.39	1.35
3	A	1506	EQK	C21-C16	2.89	1.45	1.39
3	B	1406	EQK	C27-N10	2.70	1.42	1.35
3	C	1101	EQK	C27-N10	2.70	1.42	1.35
3	A	1506	EQK	C22-N09	2.50	1.49	1.36
3	A	1506	EQK	C28-C29	2.46	1.44	1.41
3	B	1406	EQK	O05-C29	2.44	1.38	1.35
3	C	1101	EQK	O05-C29	2.41	1.38	1.35
3	A	1506	EQK	O05-C32	-2.39	1.35	1.42
3	A	1506	EQK	C29-N12	2.30	1.36	1.32
2	A	1505	6OU	O30-C31	2.29	1.40	1.33
2	D	1105	6OU	O30-C31	2.27	1.40	1.33
3	D	1101	EQK	O07-C27	-2.16	1.18	1.23
2	C	1102	6OU	O30-C31	2.12	1.39	1.33
2	B	1405	6OU	O30-C31	2.01	1.39	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1506	EQK	C26-C22-C20	6.09	135.07	129.29
3	D	1101	EQK	N13-C31-N12	-5.69	119.69	128.60
3	C	1101	EQK	N13-C31-N12	-5.35	120.23	128.60
3	B	1406	EQK	N13-C31-N12	-5.30	120.31	128.60
3	D	1101	EQK	C26-C22-N09	5.25	125.96	119.69
3	A	1506	EQK	C19-C14-C23	4.95	115.16	107.25
3	A	1506	EQK	C21-C24-N08	-4.86	117.92	123.96
3	A	1506	EQK	F03-C26-F02	-4.32	89.88	105.72
3	A	1506	EQK	F02-C26-C22	4.08	118.72	112.32
3	A	1506	EQK	C24-C21-C16	3.97	125.48	119.57
3	A	1506	EQK	N13-C31-N12	-3.94	122.43	128.60
3	A	1506	EQK	C31-N13-C30	3.77	122.19	115.88
3	B	1406	EQK	C21-C24-N08	-3.60	119.49	123.96
3	D	1101	EQK	C26-C22-C20	-3.56	125.91	129.29
3	C	1101	EQK	C21-C24-N08	-3.56	119.54	123.96
3	A	1506	EQK	C19-C14-C15	-3.50	104.98	111.79
3	B	1406	EQK	C32-O05-C29	-3.39	113.85	117.21
3	C	1101	EQK	C32-O05-C29	-3.37	113.87	117.21
3	D	1101	EQK	C33-O06-C30	-3.37	113.87	117.21
3	D	1101	EQK	C32-O05-C29	-3.26	113.99	117.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1101	EQK	C21-C24-N08	-3.21	119.97	123.96
3	C	1101	EQK	C26-C22-N09	3.20	123.51	119.69
3	B	1406	EQK	C26-C22-N09	3.19	123.50	119.69
3	A	1506	EQK	F04-C26-F03	2.96	116.58	105.72
3	D	1101	EQK	C14-C15-N08	2.93	120.09	115.22
2	A	1505	6OU	O30-C31-C33	2.87	120.92	111.91
3	D	1101	EQK	C28-C27-N10	2.69	119.97	114.91
2	C	1102	6OU	O30-C31-C33	2.68	120.31	111.91
3	D	1101	EQK	C25-N10-C27	-2.65	120.08	126.64
3	A	1506	EQK	C25-N10-C27	-2.59	120.23	126.64
3	A	1506	EQK	C16-C17-C15	-2.57	116.68	119.73
3	C	1101	EQK	C31-N13-C30	2.54	120.14	115.88
3	D	1101	EQK	C31-N12-C29	2.54	120.13	115.88
3	D	1101	EQK	C31-N13-C30	2.54	120.13	115.88
3	B	1406	EQK	C31-N13-C30	2.53	120.11	115.88
2	D	1105	6OU	O30-C31-C33	2.51	119.80	111.91
3	C	1101	EQK	C31-N12-C29	2.51	120.09	115.88
3	B	1406	EQK	C31-N12-C29	2.47	120.02	115.88
3	C	1101	EQK	F02-C26-C22	-2.42	108.53	112.32
3	B	1406	EQK	F02-C26-C22	-2.39	108.58	112.32
3	C	1101	EQK	C19-C14-C23	2.37	111.05	107.25
3	B	1406	EQK	C19-C14-C23	2.36	111.02	107.25
3	A	1506	EQK	C33-O06-C30	2.32	119.51	117.21
3	B	1406	EQK	C14-C15-N08	2.32	119.08	115.22
2	B	1405	6OU	O30-C31-C33	2.32	119.18	111.91
3	A	1506	EQK	C18-C14-C23	2.29	110.92	107.25
3	C	1101	EQK	C25-N10-C27	-2.29	120.98	126.64
3	C	1101	EQK	C14-C15-N08	2.28	119.02	115.22
3	B	1406	EQK	C25-N10-C27	-2.28	121.00	126.64
3	D	1101	EQK	C17-C15-N08	-2.06	119.97	123.31
3	B	1406	EQK	C24-N08-C15	2.05	120.30	117.49
3	D	1101	EQK	C24-N08-C15	2.03	120.26	117.49

There are no chirality outliers.

All (155) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1102	6OU	O26-C27-C28-N29
2	A	1505	6OU	C21-O22-P23-O24
2	A	1505	6OU	C21-O22-P23-O25
2	A	1505	6OU	C21-O22-P23-O26
2	A	1505	6OU	C27-O26-P23-O22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1505	6OU	C27-O26-P23-O24
2	A	1505	6OU	C27-O26-P23-O25
2	A	1505	6OU	O26-C27-C28-N29
2	A	1507	6OU	C38-C39-C40-C41
2	D	1105	6OU	C27-O26-P23-O24
2	D	1105	6OU	C27-O26-P23-O25
3	B	1406	EQK	C23-C14-C15-N08
3	C	1101	EQK	C23-C14-C15-N08
3	A	1506	EQK	C23-C14-C15-N08
3	D	1101	EQK	C23-C14-C15-N08
3	D	1101	EQK	N10-C27-C28-C30
3	D	1101	EQK	O07-C27-C28-C30
3	B	1406	EQK	C17-C16-C20-C22
3	B	1406	EQK	C21-C16-C20-C22
3	C	1101	EQK	C17-C16-C20-C22
3	C	1101	EQK	C21-C16-C20-C22
3	A	1506	EQK	C17-C16-C20-C22
3	A	1506	EQK	C21-C16-C20-C22
2	D	1105	6OU	C31-C33-C34-C35
3	D	1101	EQK	C21-C16-C20-C22
2	A	1505	6OU	C31-C33-C34-C35
2	D	1105	6OU	C27-O26-P23-O22
2	C	1103	6OU	C44-C45-C46-C47
2	A	1502	6OU	C09-C10-C11-C12
2	A	1502	6OU	C10-C11-C12-C13
2	B	1401	6OU	C42-C43-C44-C45
2	B	1401	6OU	C43-C44-C45-C46
2	B	1404	6OU	C43-C44-C45-C46
2	A	1504	6OU	C43-C44-C45-C46
2	D	1103	6OU	C43-C44-C45-C46
3	D	1101	EQK	C17-C16-C20-C22
2	C	1102	6OU	C44-C45-C46-C47
2	C	1106	6OU	C37-C38-C39-C40
3	B	1406	EQK	N09-C22-C26-F04
3	C	1101	EQK	N09-C22-C26-F04
3	D	1101	EQK	N09-C22-C26-F04
2	B	1404	6OU	C42-C43-C44-C45
2	A	1504	6OU	C42-C43-C44-C45
2	C	1106	6OU	C42-C43-C44-C45
2	D	1103	6OU	C42-C43-C44-C45
2	A	1505	6OU	C34-C35-C36-C37
2	D	1102	6OU	C43-C44-C45-C46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1103	6OU	C43-C44-C45-C46
2	A	1501	6OU	C44-C45-C46-C47
2	A	1502	6OU	C08-C09-C10-C11
2	C	1105	6OU	C37-C38-C39-C40
2	D	1102	6OU	C41-C42-C43-C44
2	D	1105	6OU	C44-C45-C46-C47
2	D	1104	6OU	C42-C43-C44-C45
2	C	1106	6OU	C44-C45-C46-C47
2	A	1504	6OU	C46-C47-C48-C49
2	B	1401	6OU	C41-C42-C43-C44
2	B	1405	6OU	C37-C38-C39-C40
2	A	1501	6OU	C37-C38-C39-C40
2	D	1104	6OU	C41-C42-C43-C44
2	A	1507	6OU	C44-C45-C46-C47
2	A	1503	6OU	C42-C43-C44-C45
2	B	1401	6OU	C37-C38-C39-C40
2	B	1404	6OU	C41-C42-C43-C44
2	A	1504	6OU	C41-C42-C43-C44
2	D	1103	6OU	C41-C42-C43-C44
2	D	1105	6OU	C41-C42-C43-C44
2	B	1403	6OU	C43-C44-C45-C46
2	A	1507	6OU	C43-C44-C45-C46
2	D	1104	6OU	C46-C47-C48-C49
2	D	1104	6OU	C38-C39-C40-C41
2	B	1404	6OU	C36-C37-C38-C39
2	A	1504	6OU	C36-C37-C38-C39
2	D	1103	6OU	C36-C37-C38-C39
2	D	1102	6OU	C36-C37-C38-C39
2	A	1505	6OU	C33-C31-O30-C20
3	B	1406	EQK	N09-C22-C26-F02
3	B	1406	EQK	N09-C22-C26-F03
3	C	1101	EQK	N09-C22-C26-F02
3	C	1101	EQK	N09-C22-C26-F03
3	D	1101	EQK	N09-C22-C26-F02
3	D	1101	EQK	N09-C22-C26-F03
2	C	1103	6OU	C37-C38-C39-C40
2	D	1102	6OU	C40-C41-C42-C43
2	B	1402	6OU	C09-C10-C11-C12
2	D	1105	6OU	C36-C37-C38-C39
2	A	1505	6OU	O32-C31-O30-C20
2	C	1105	6OU	C41-C42-C43-C44
2	C	1106	6OU	C41-C42-C43-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1406	EQK	O07-C27-C28-C30
3	C	1101	EQK	O07-C27-C28-C30
3	A	1506	EQK	O07-C27-C28-C30
2	C	1102	6OU	C45-C46-C47-C48
2	C	1106	6OU	C45-C46-C47-C48
2	A	1505	6OU	C41-C42-C43-C44
3	B	1406	EQK	N10-C27-C28-C29
3	B	1406	EQK	N10-C27-C28-C30
3	C	1101	EQK	N10-C27-C28-C29
3	C	1101	EQK	N10-C27-C28-C30
3	A	1506	EQK	N10-C27-C28-C30
2	D	1105	6OU	C33-C34-C35-C36
2	B	1402	6OU	C11-C12-C13-C14
2	C	1103	6OU	C45-C46-C47-C48
2	C	1104	6OU	C44-C45-C46-C47
2	D	1105	6OU	C37-C38-C39-C40
2	D	1105	6OU	C43-C44-C45-C46
2	C	1106	6OU	C36-C37-C38-C39
2	C	1102	6OU	C43-C44-C45-C46
2	B	1405	6OU	C27-O26-P23-O22
2	C	1102	6OU	C27-O26-P23-O22
2	D	1105	6OU	C21-O22-P23-O26
2	B	1405	6OU	C38-C39-C40-C41
2	C	1105	6OU	C40-C41-C42-C43
3	C	1101	EQK	O07-C27-C28-C29
3	A	1506	EQK	O07-C27-C28-C29
2	A	1501	6OU	C40-C41-C42-C43
2	D	1104	6OU	C37-C38-C39-C40
2	C	1104	6OU	C46-C47-C48-C49
2	A	1501	6OU	C45-C46-C47-C48
2	B	1405	6OU	C36-C37-C38-C39
2	B	1405	6OU	C40-C41-C42-C43
2	C	1103	6OU	C40-C41-C42-C43
2	A	1505	6OU	C38-C39-C40-C41
2	B	1401	6OU	C38-C39-C40-C41
3	B	1406	EQK	C23-C14-C15-C17
3	C	1101	EQK	C23-C14-C15-C17
3	B	1406	EQK	O07-C27-C28-C29
2	C	1102	6OU	C40-C41-C42-C43
2	C	1103	6OU	C38-C39-C40-C41
2	C	1104	6OU	C38-C39-C40-C41
2	A	1501	6OU	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1404	6OU	C40-C41-C42-C43
2	A	1504	6OU	C40-C41-C42-C43
2	A	1505	6OU	C40-C41-C42-C43
2	D	1103	6OU	C40-C41-C42-C43
2	D	1105	6OU	C40-C41-C42-C43
2	A	1501	6OU	C41-C42-C43-C44
2	A	1505	6OU	C44-C45-C46-C47
2	A	1502	6OU	C11-C12-C13-C14
2	A	1504	6OU	C45-C46-C47-C48
3	A	1506	EQK	N10-C27-C28-C29
2	C	1102	6OU	C38-C39-C40-C41
2	D	1105	6OU	C38-C39-C40-C41
2	B	1401	6OU	C46-C47-C48-C49
2	C	1104	6OU	C40-C41-C42-C43
2	D	1102	6OU	C38-C39-C40-C41
2	A	1502	6OU	C07-C08-C09-C10
2	B	1404	6OU	C38-C39-C40-C41
2	A	1504	6OU	C38-C39-C40-C41
2	B	1405	6OU	C27-O26-P23-O24
3	D	1101	EQK	C19-C14-C15-N08
2	D	1103	6OU	C38-C39-C40-C41
2	C	1102	6OU	O30-C31-C33-C34
2	C	1102	6OU	O32-C31-C33-C34
2	A	1507	6OU	C42-C43-C44-C45

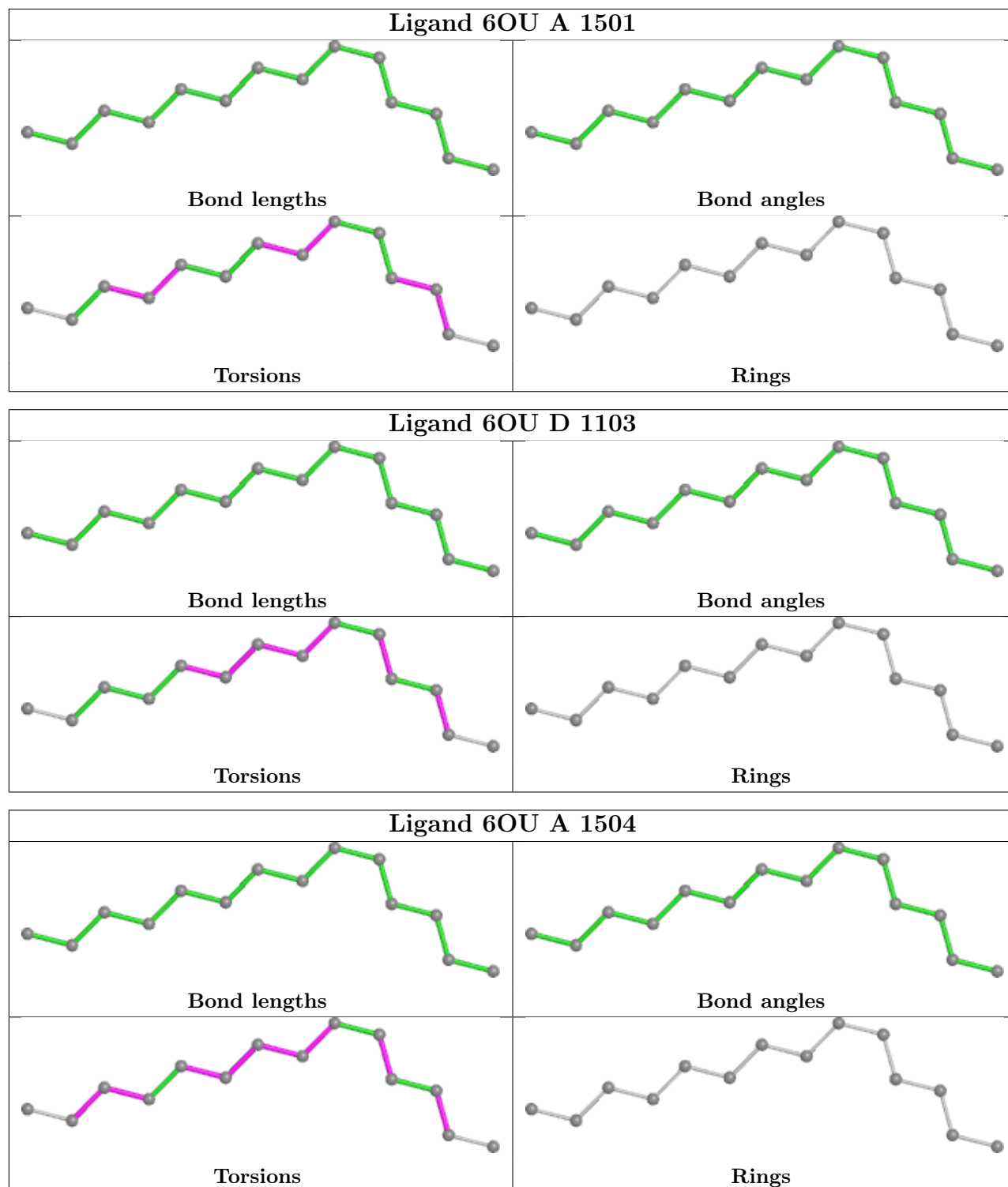
There are no ring outliers.

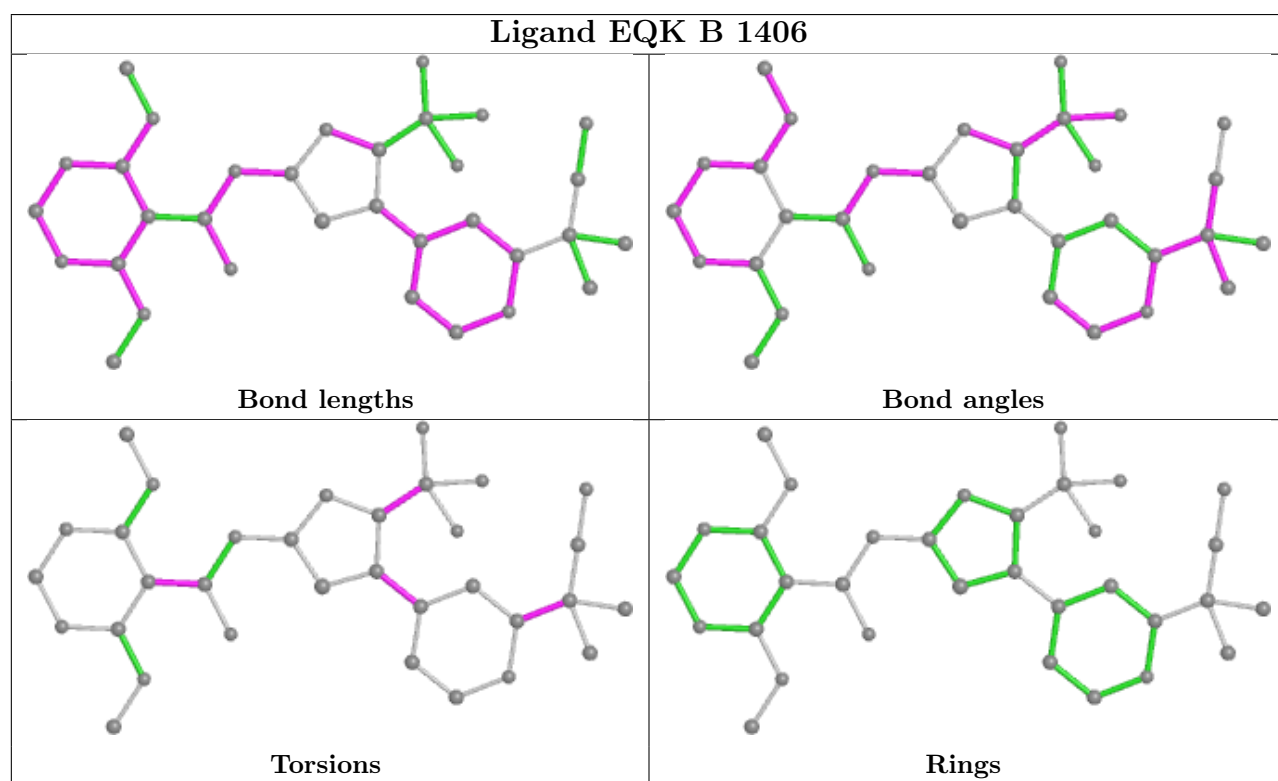
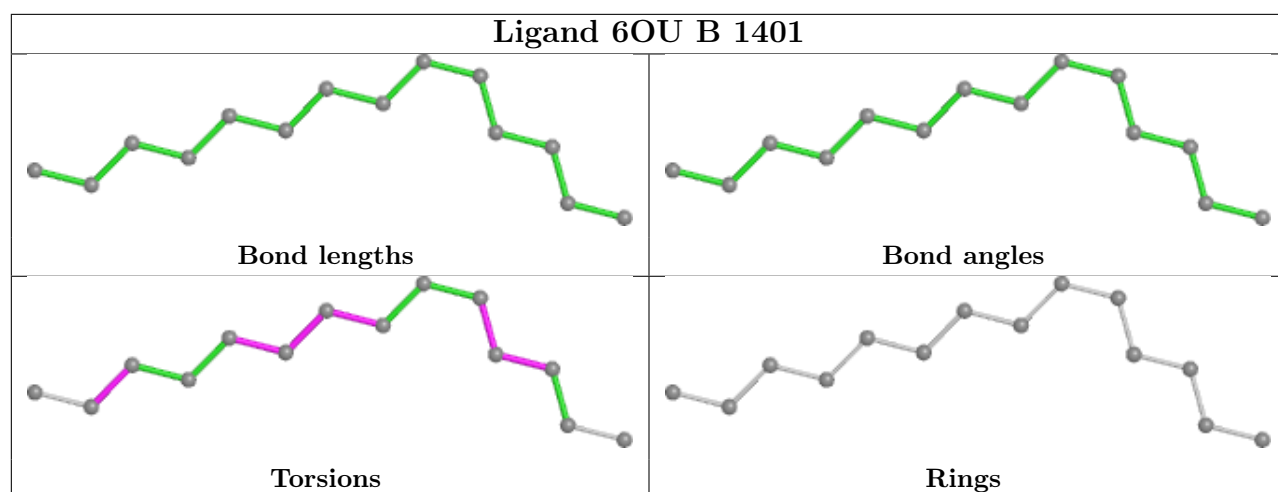
7 monomers are involved in 22 short contacts:

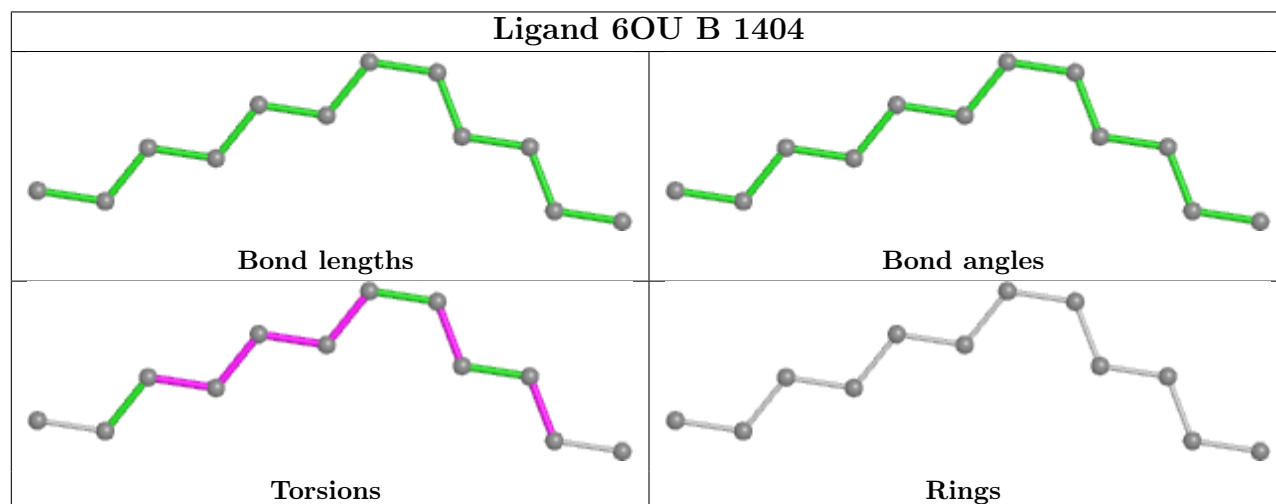
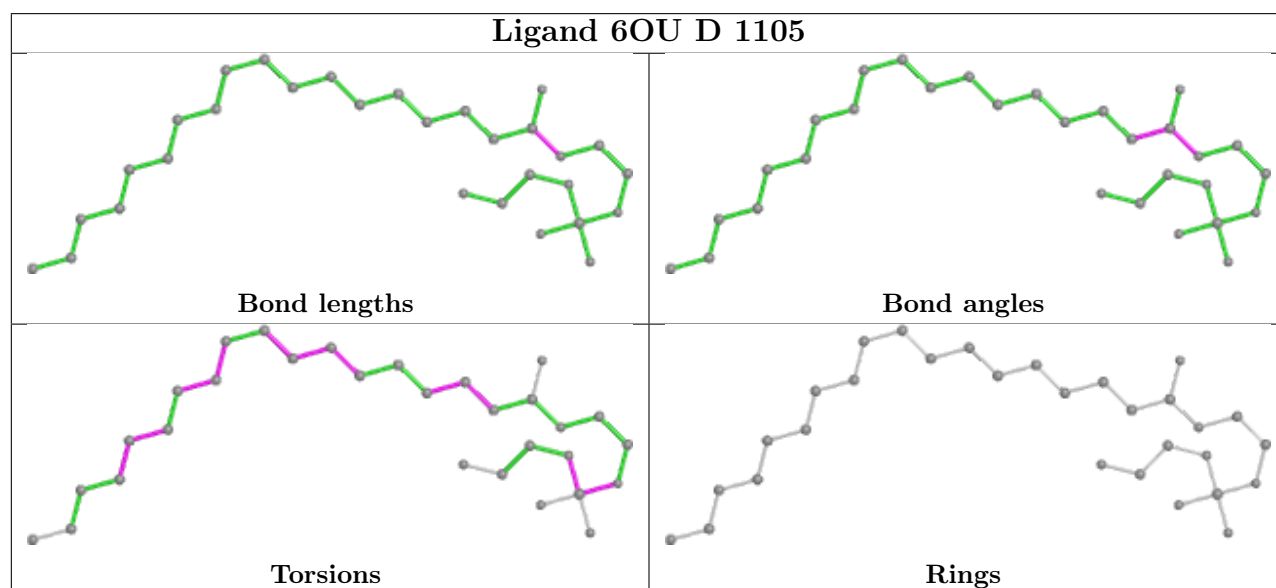
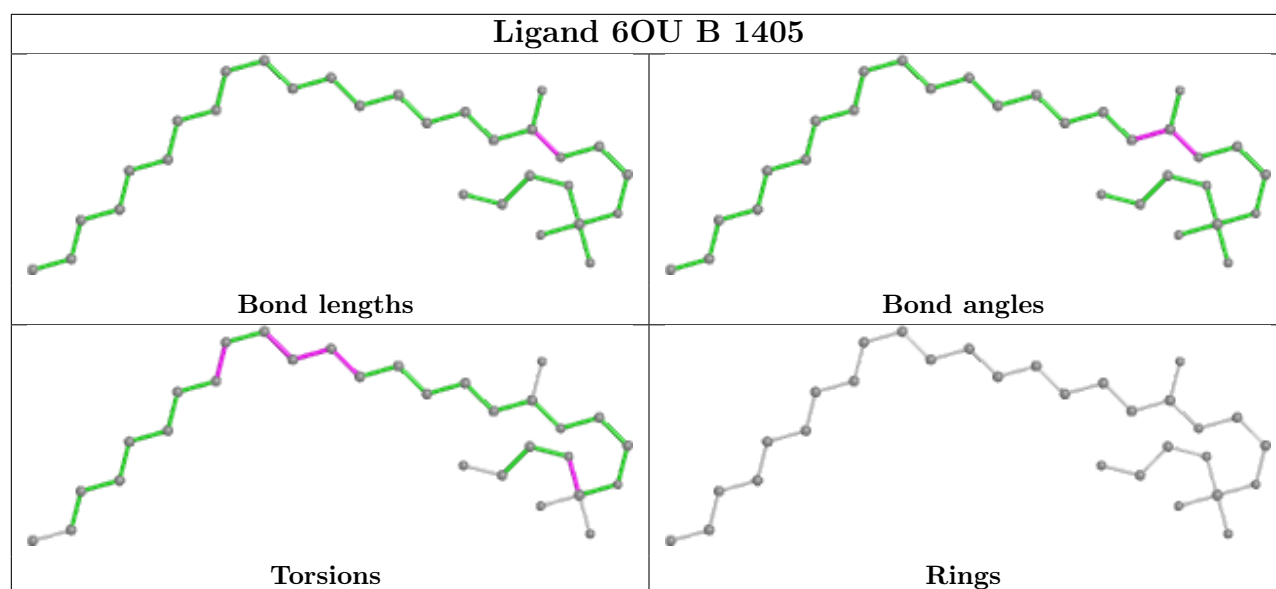
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1406	EQK	5	0
2	C	1104	6OU	1	0
2	A	1505	6OU	2	0
3	D	1101	EQK	5	0
2	C	1105	6OU	1	0
3	A	1506	EQK	3	0
3	C	1101	EQK	5	0

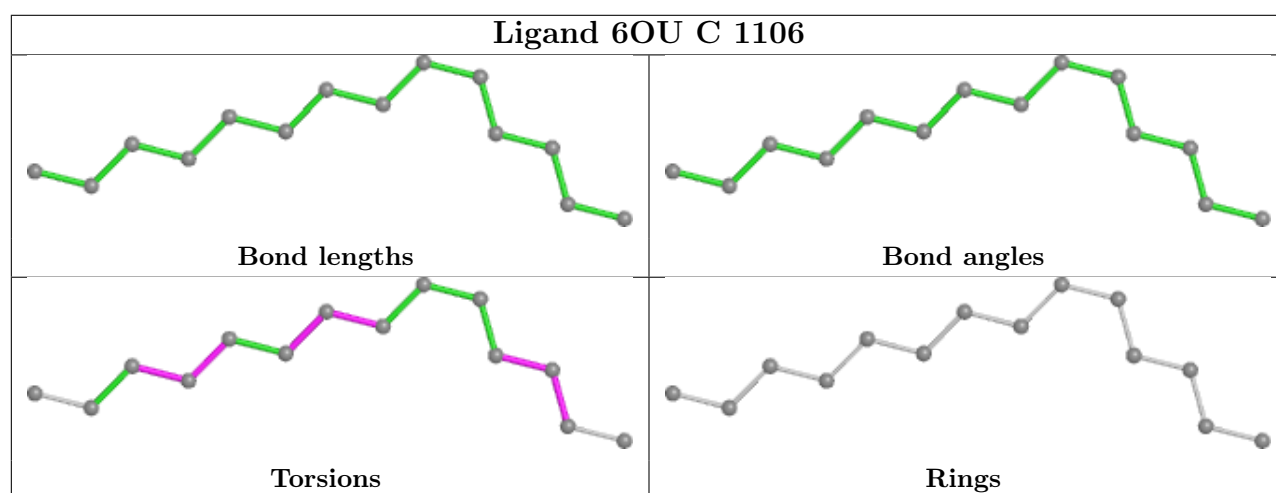
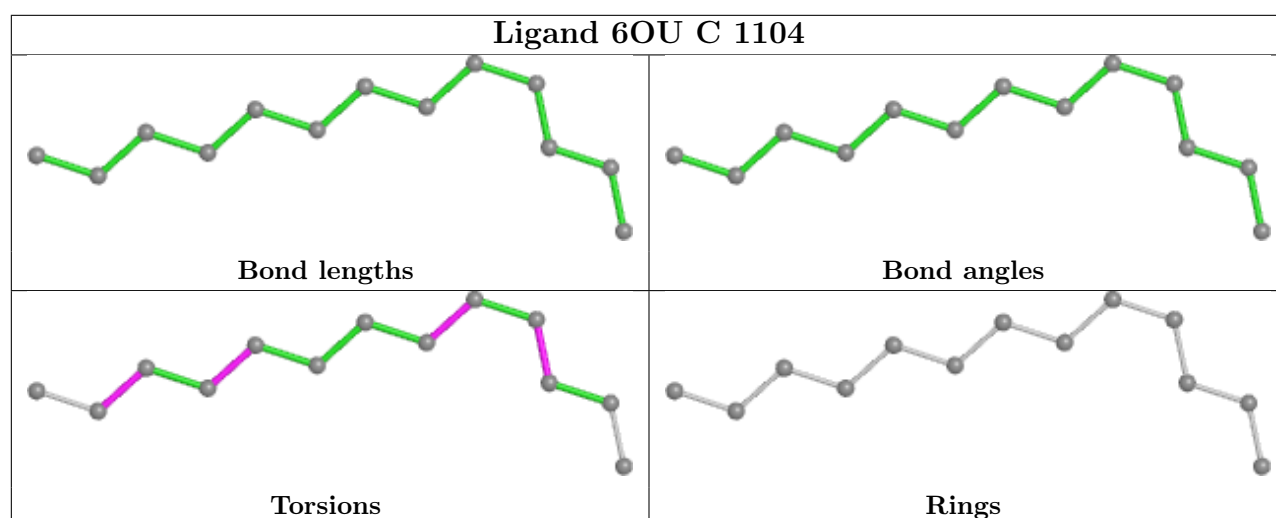
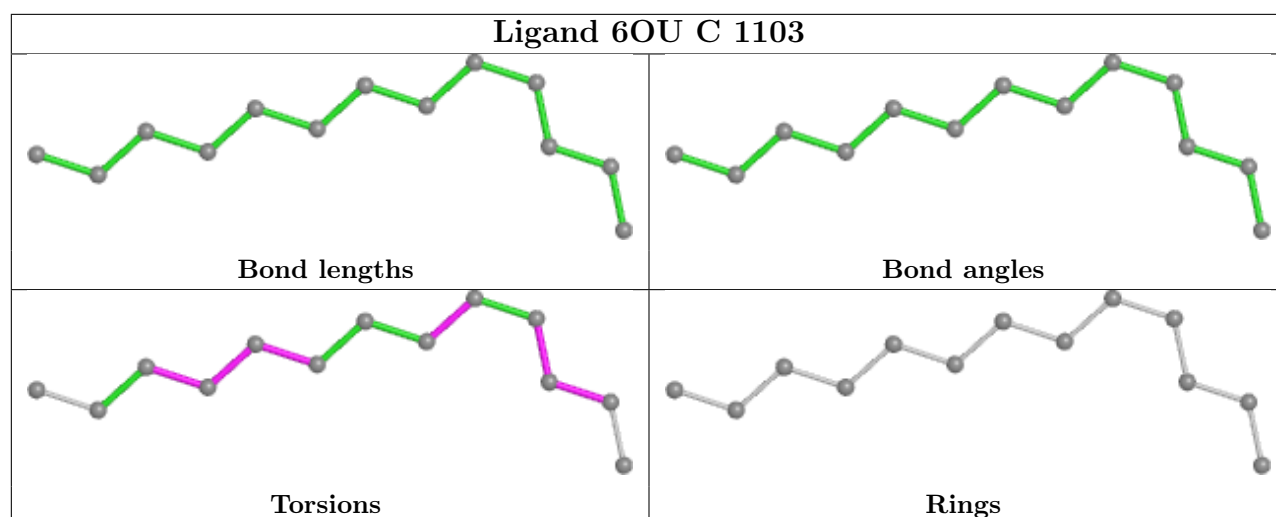
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

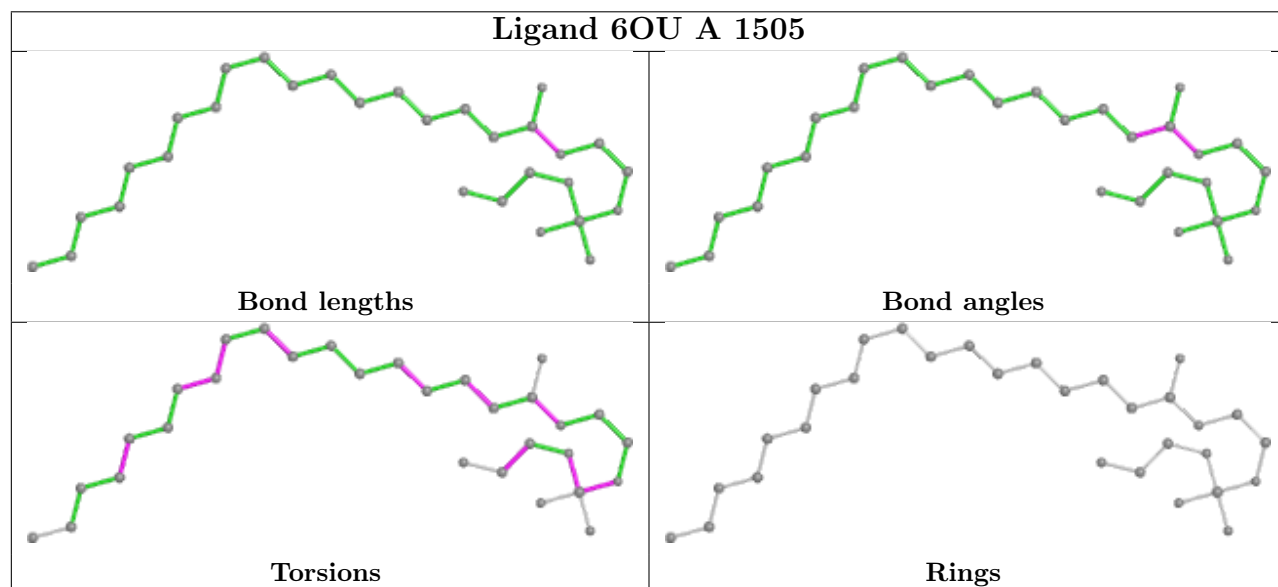
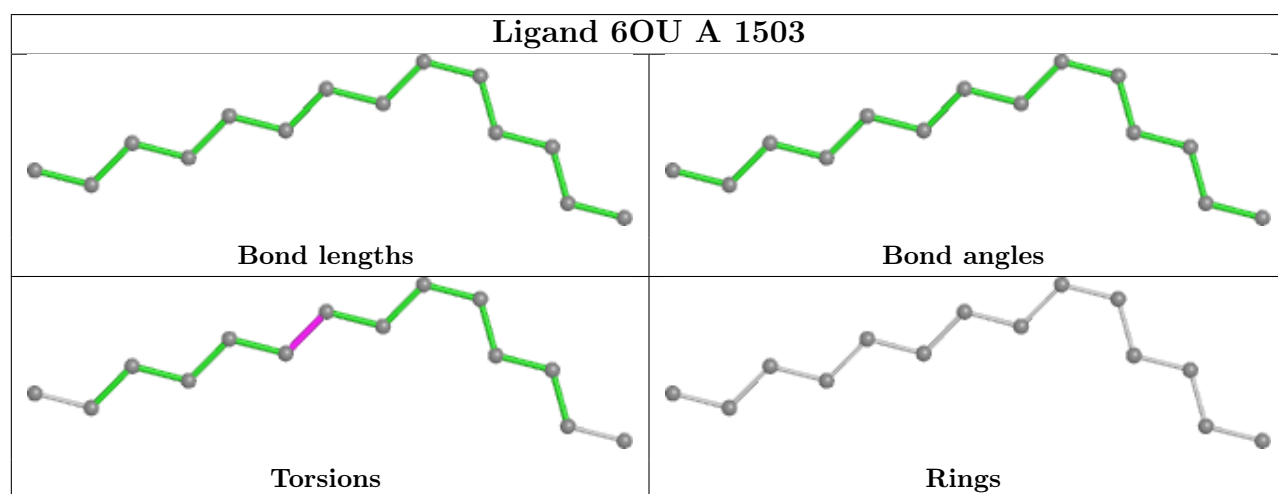
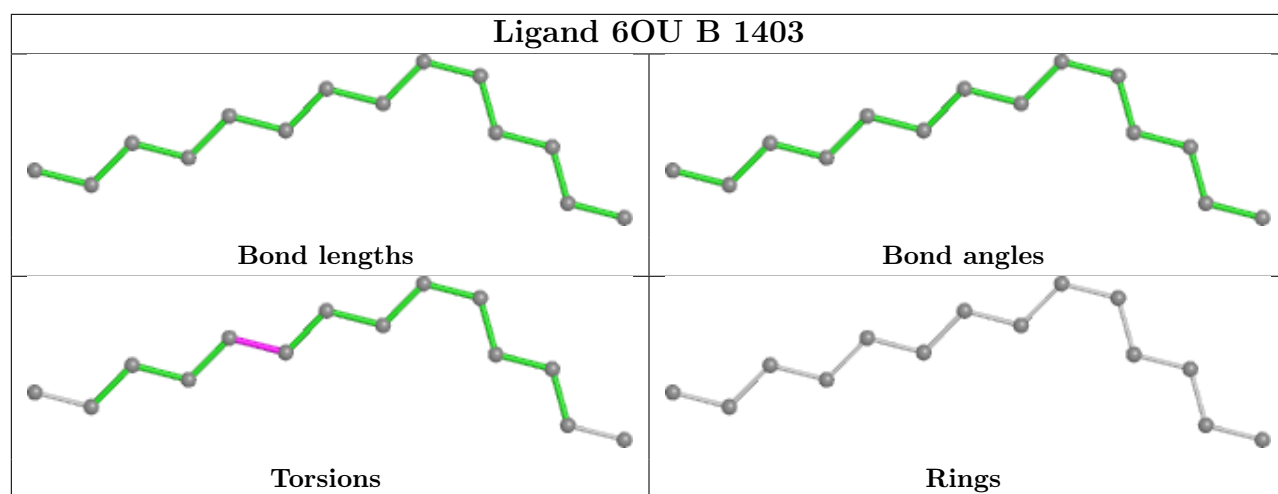
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

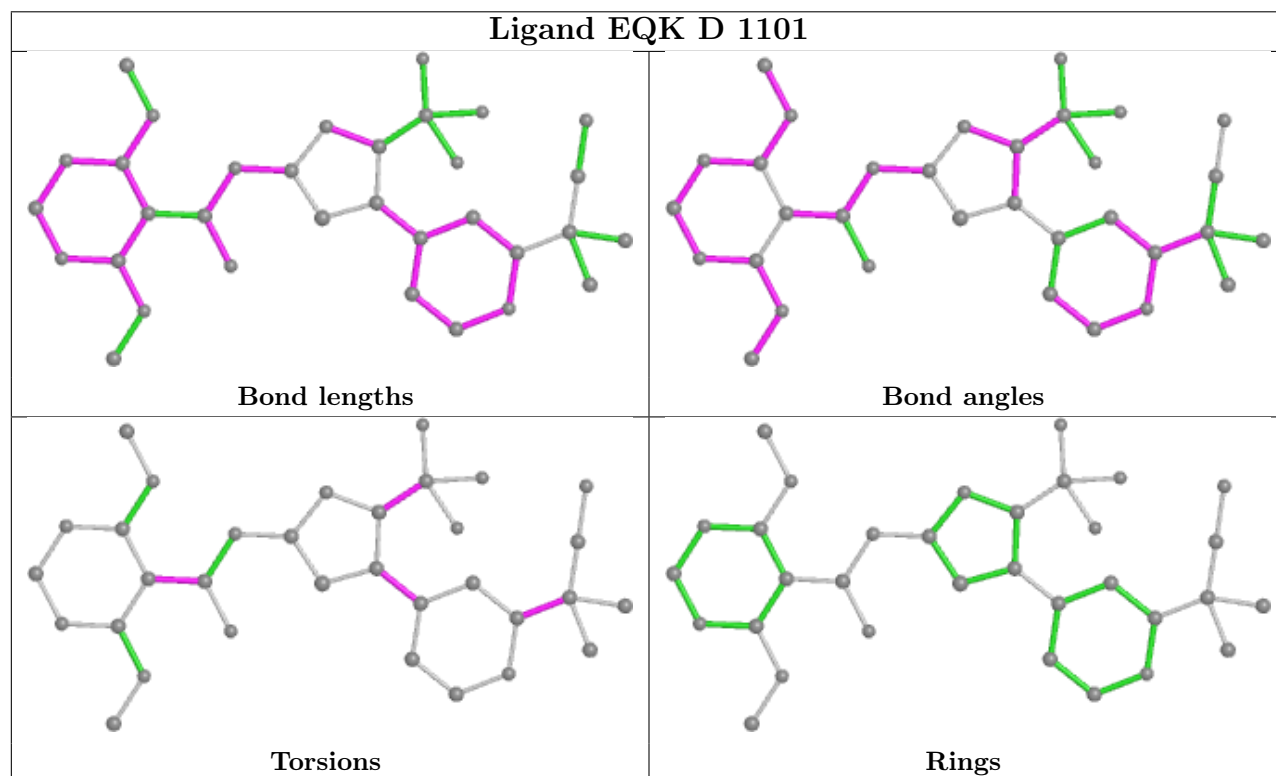
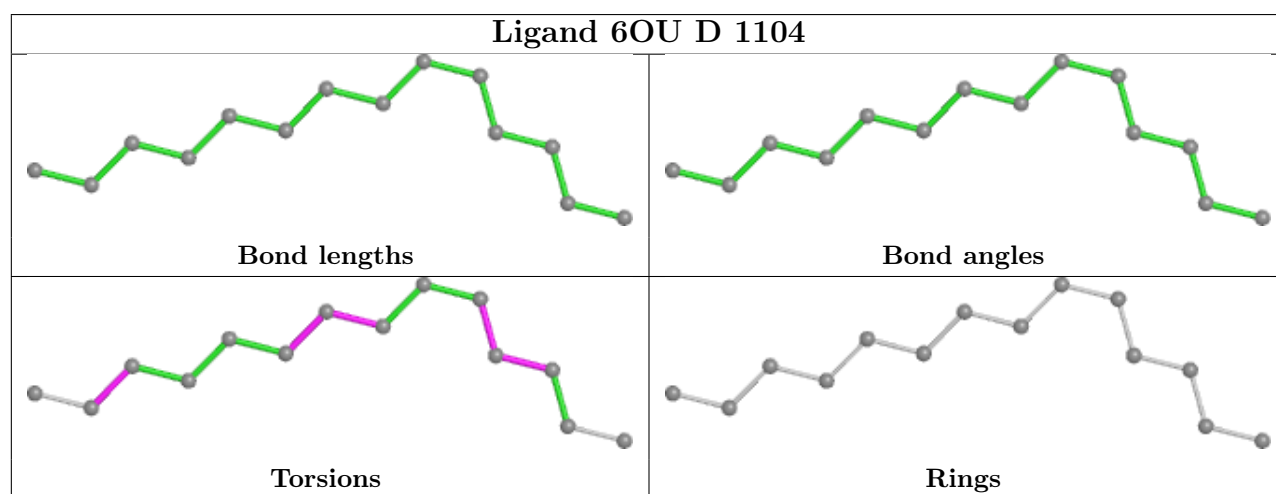
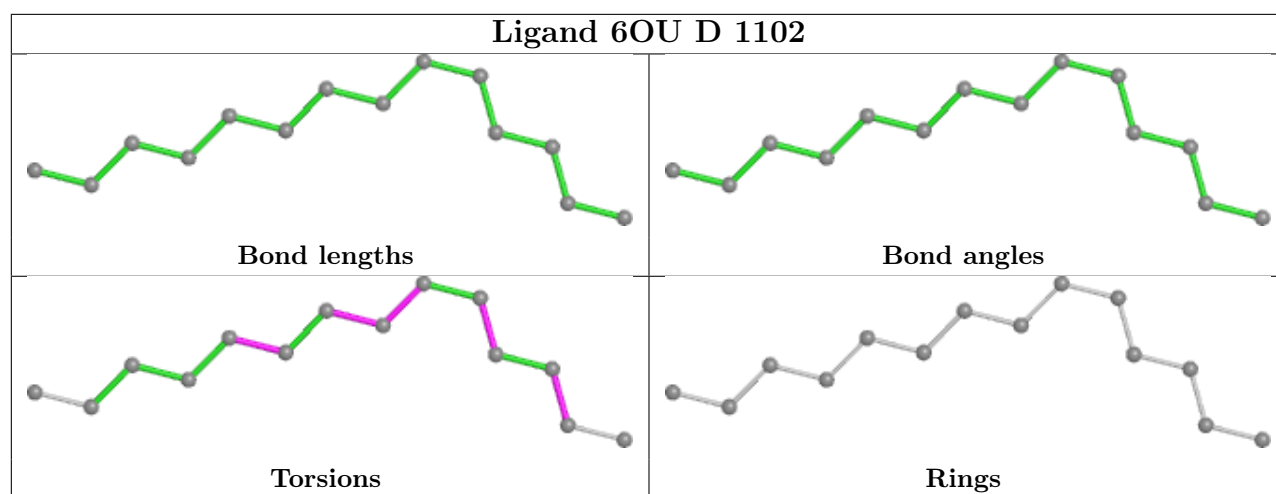


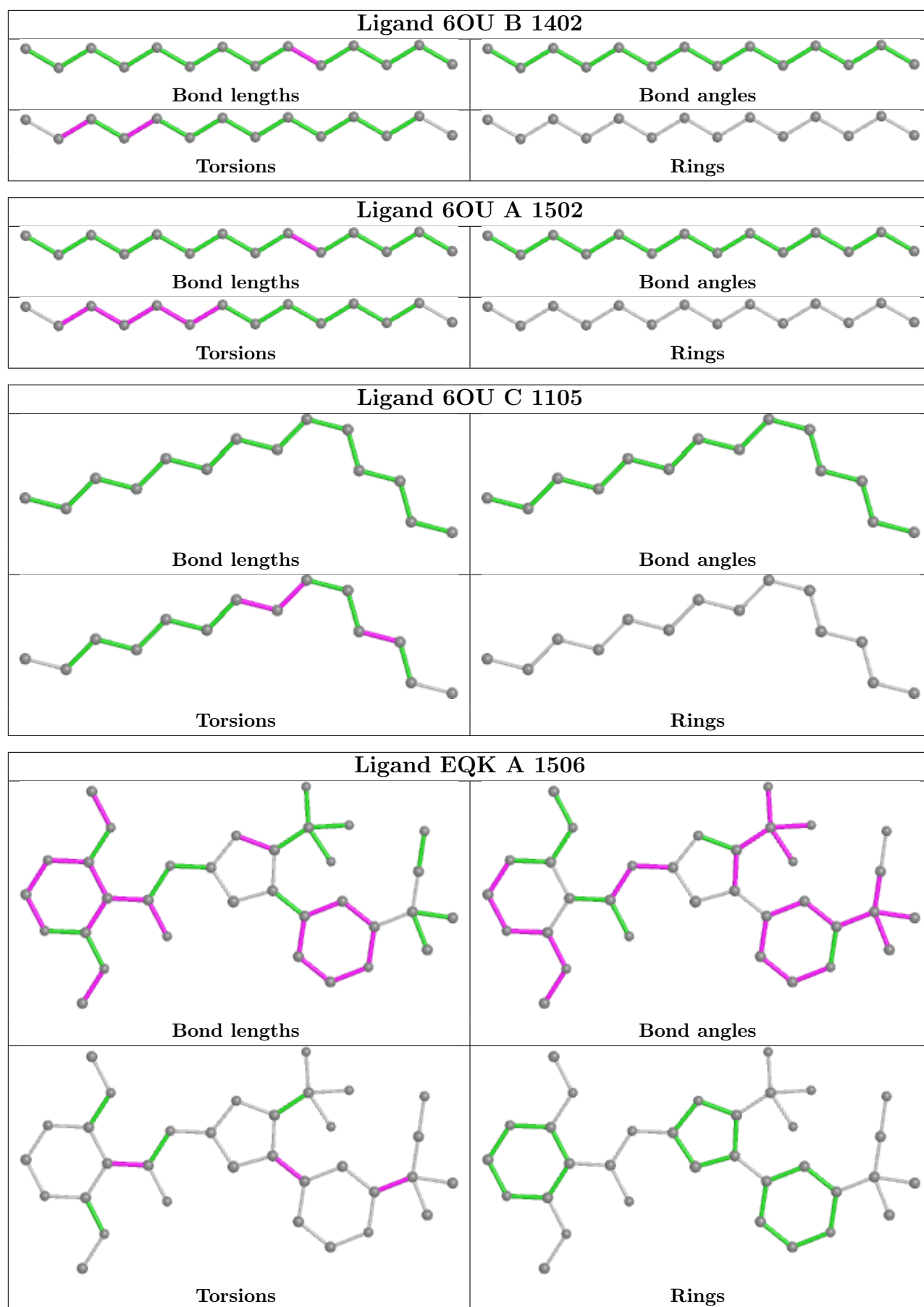


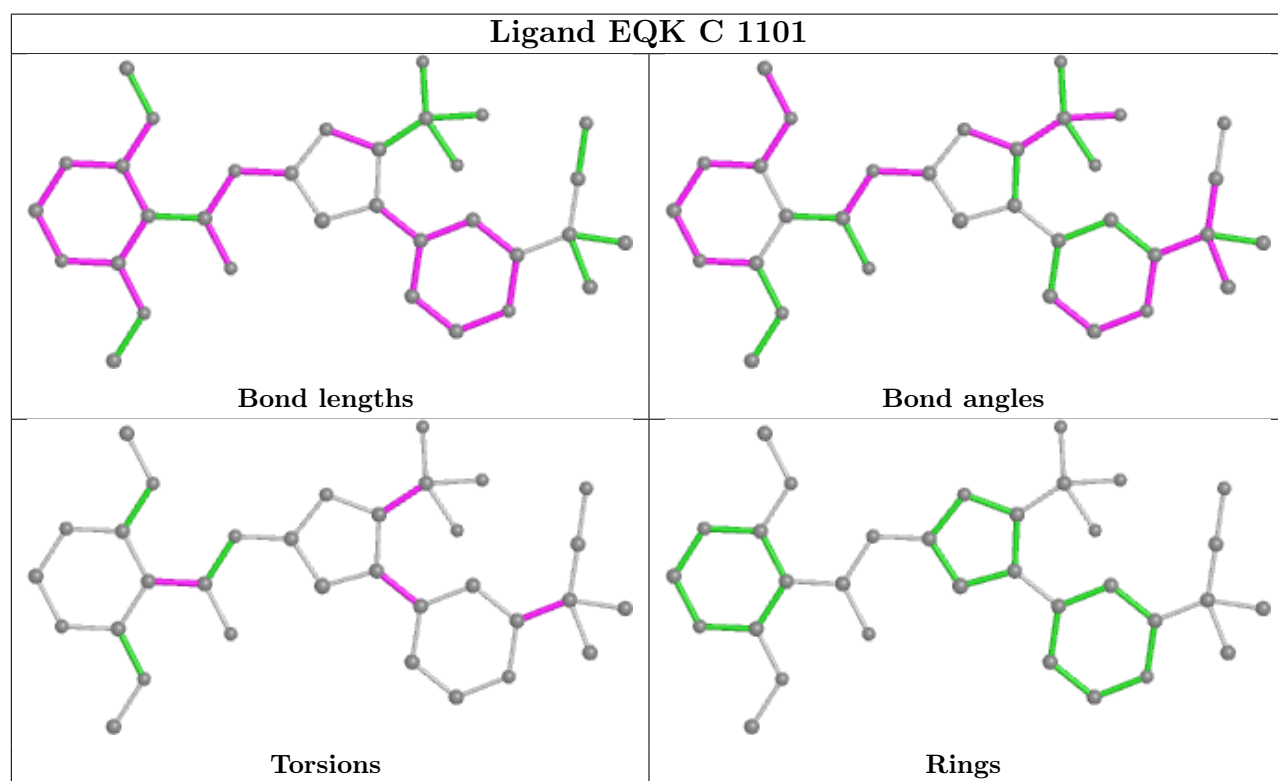
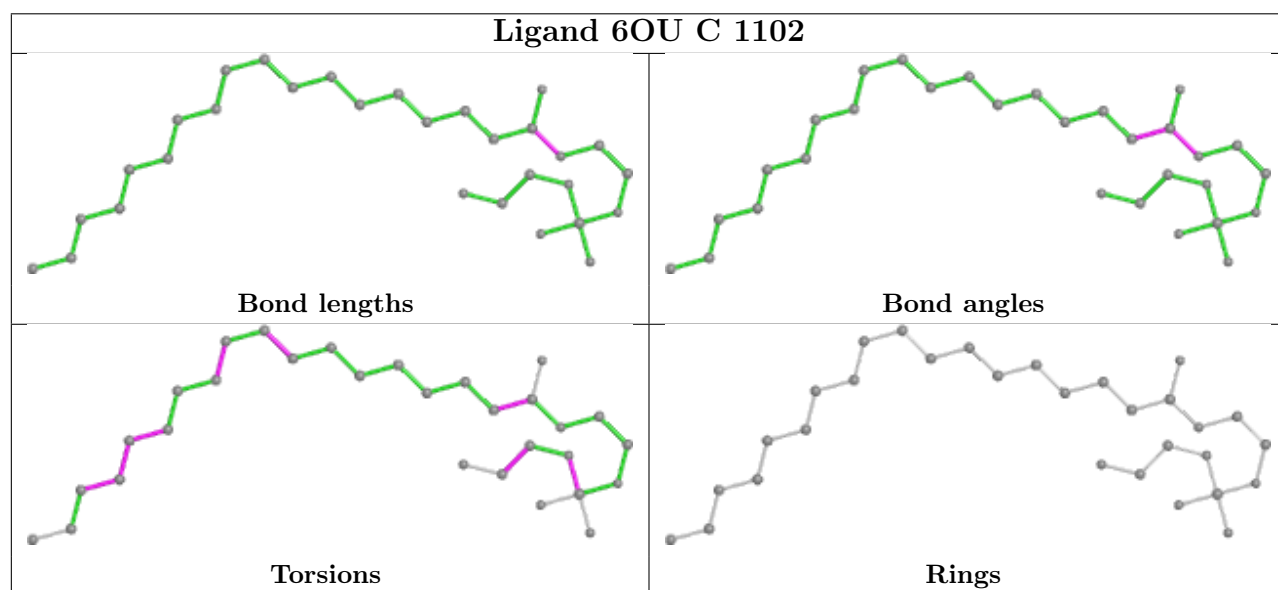
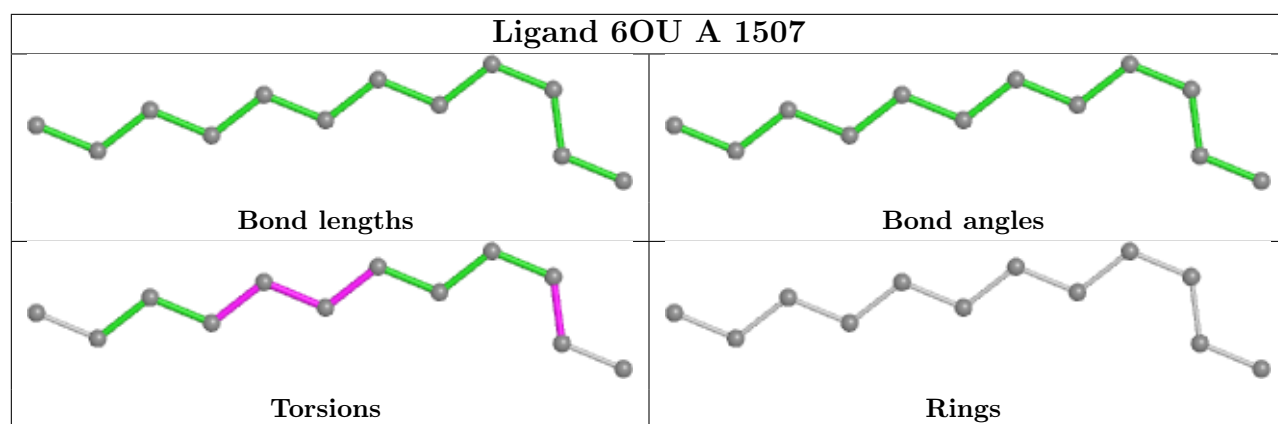












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

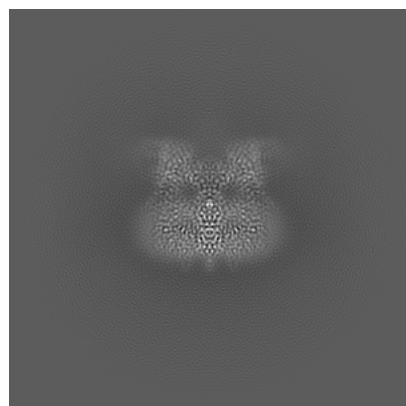
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33214. These allow visual inspection of the internal detail of the map and identification of artifacts.

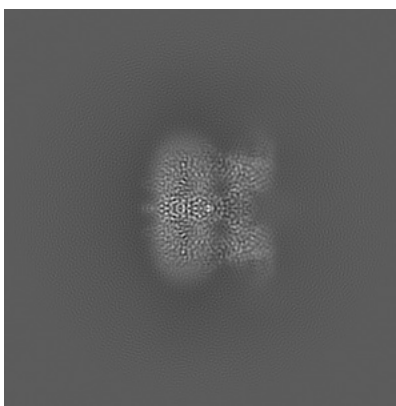
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

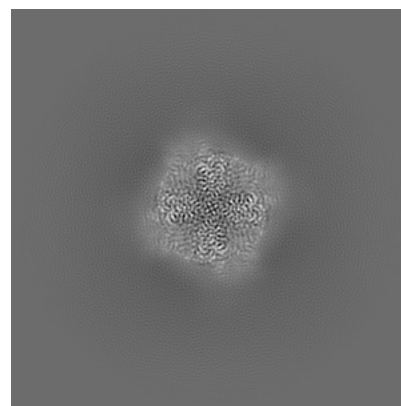
6.1.1 Primary map



X

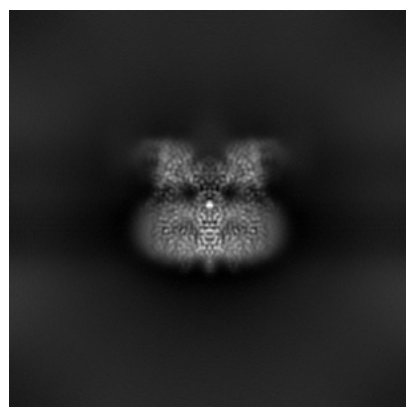


Y

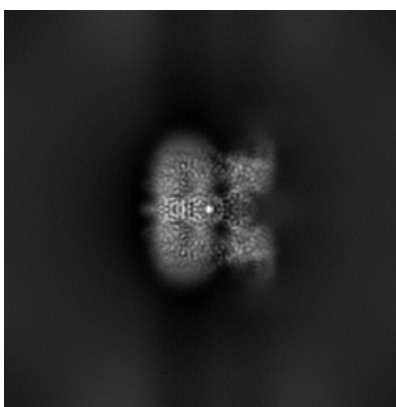


Z

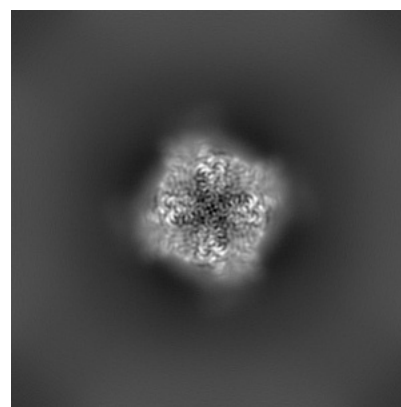
6.1.2 Raw map



X



Y

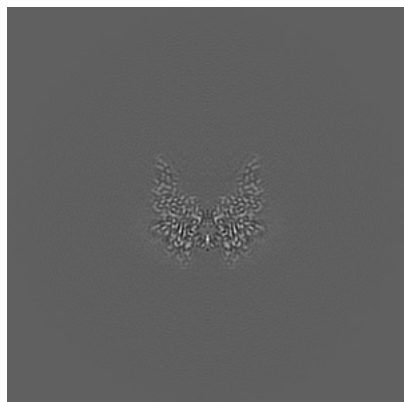


Z

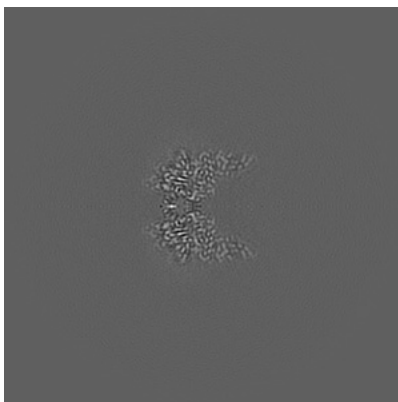
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

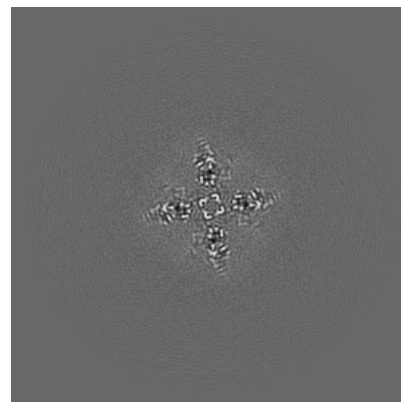
6.2.1 Primary map



X Index: 160

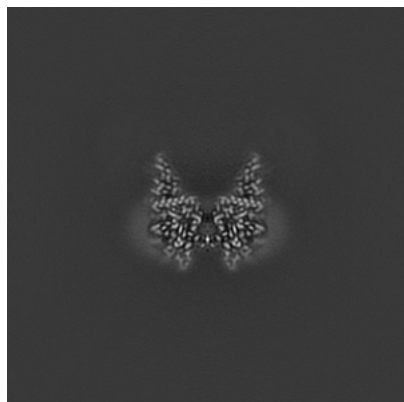


Y Index: 160

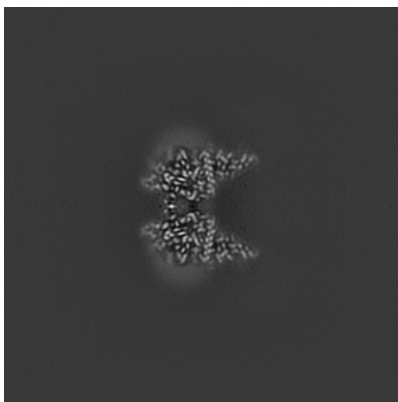


Z Index: 160

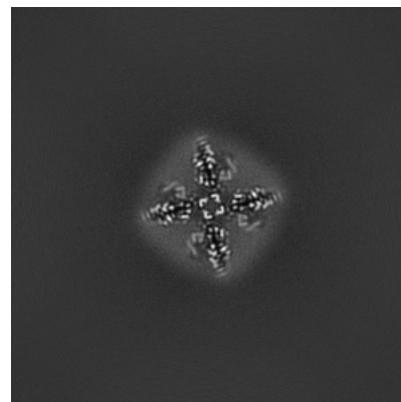
6.2.2 Raw map



X Index: 160



Y Index: 160

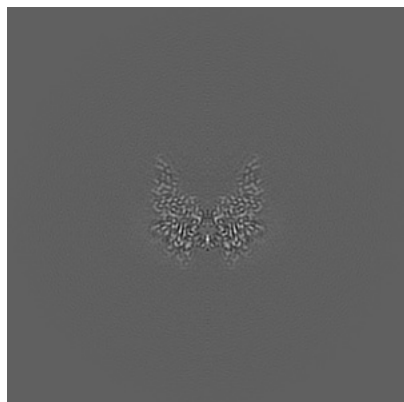


Z Index: 160

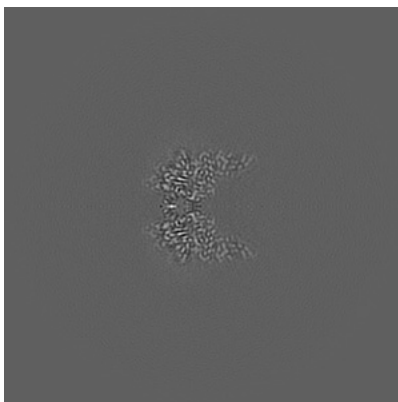
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

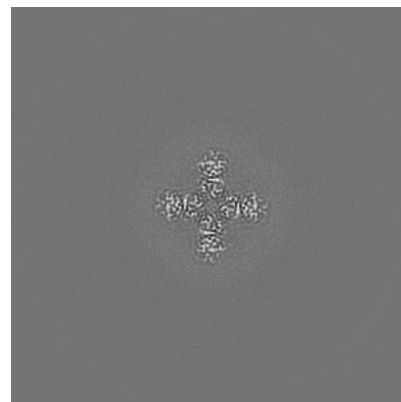
6.3.1 Primary map



X Index: 160

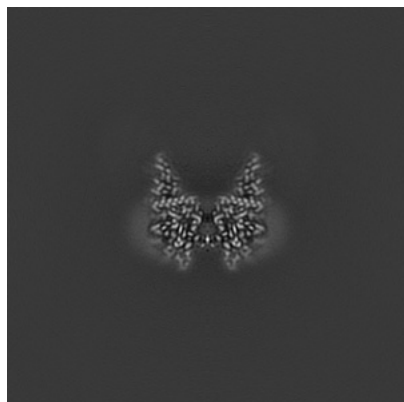


Y Index: 160

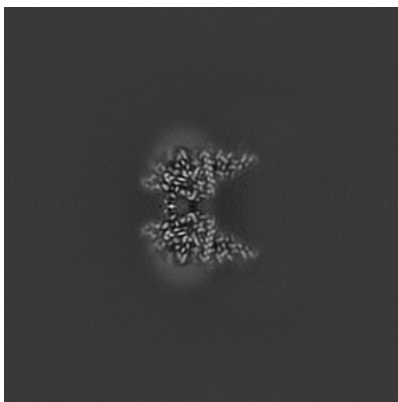


Z Index: 143

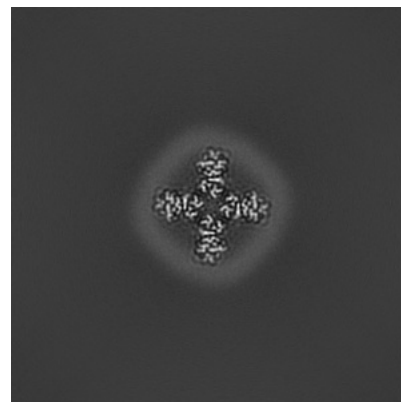
6.3.2 Raw map



X Index: 160



Y Index: 160

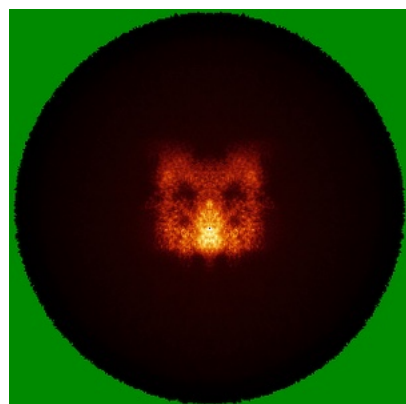


Z Index: 143

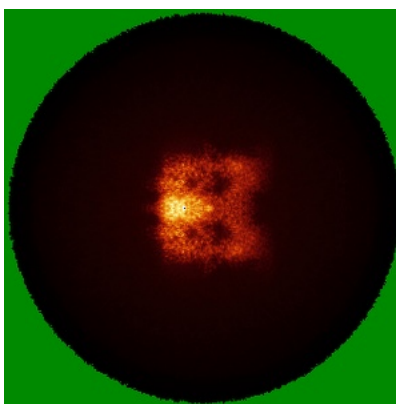
The images above show the largest variance slices of the map in three orthogonal directions.

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

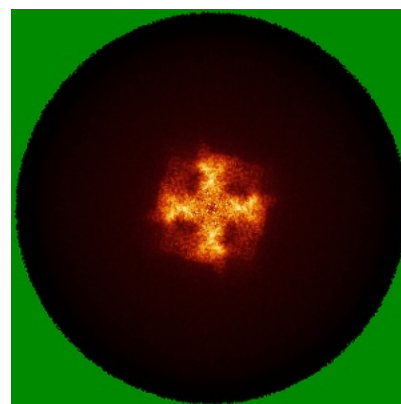
6.4.1 Primary map



X

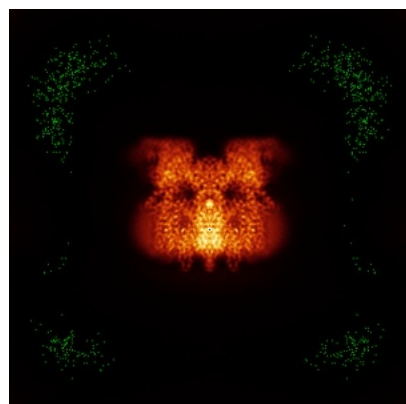


Y

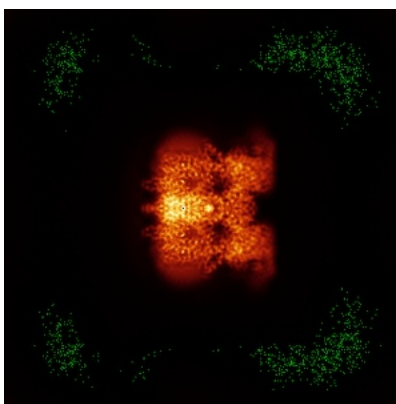


Z

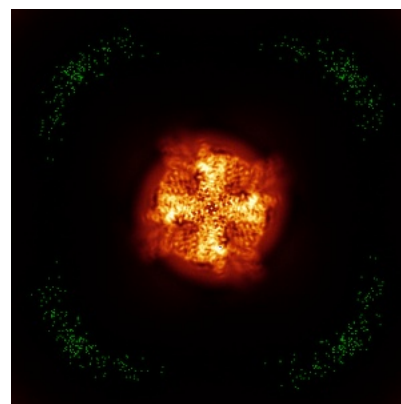
6.4.2 Raw map



X



Y

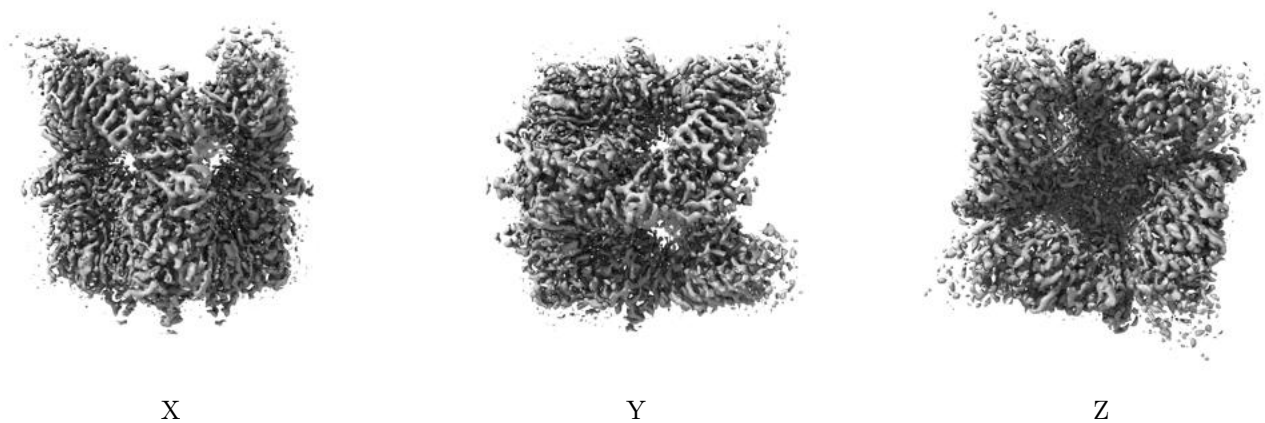


Z

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.

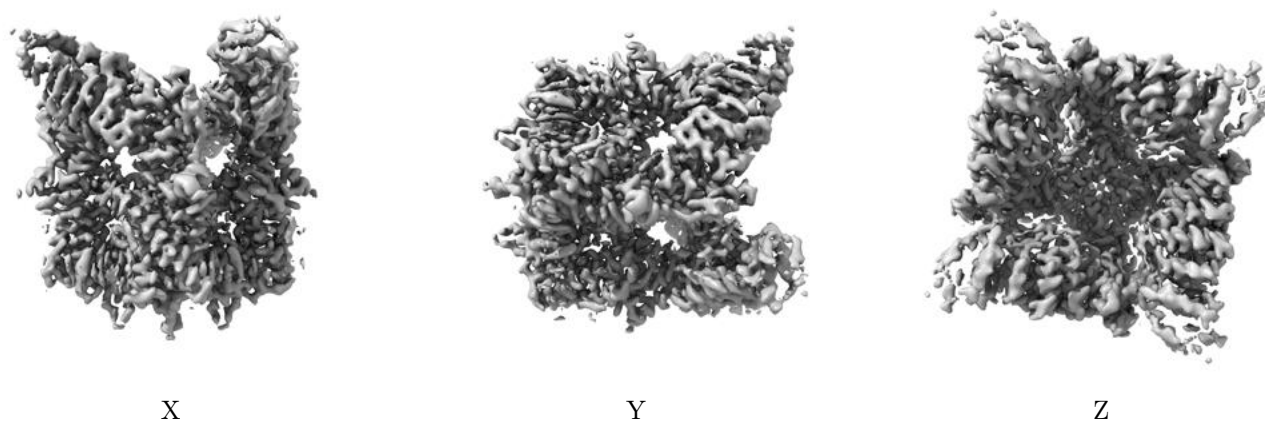
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

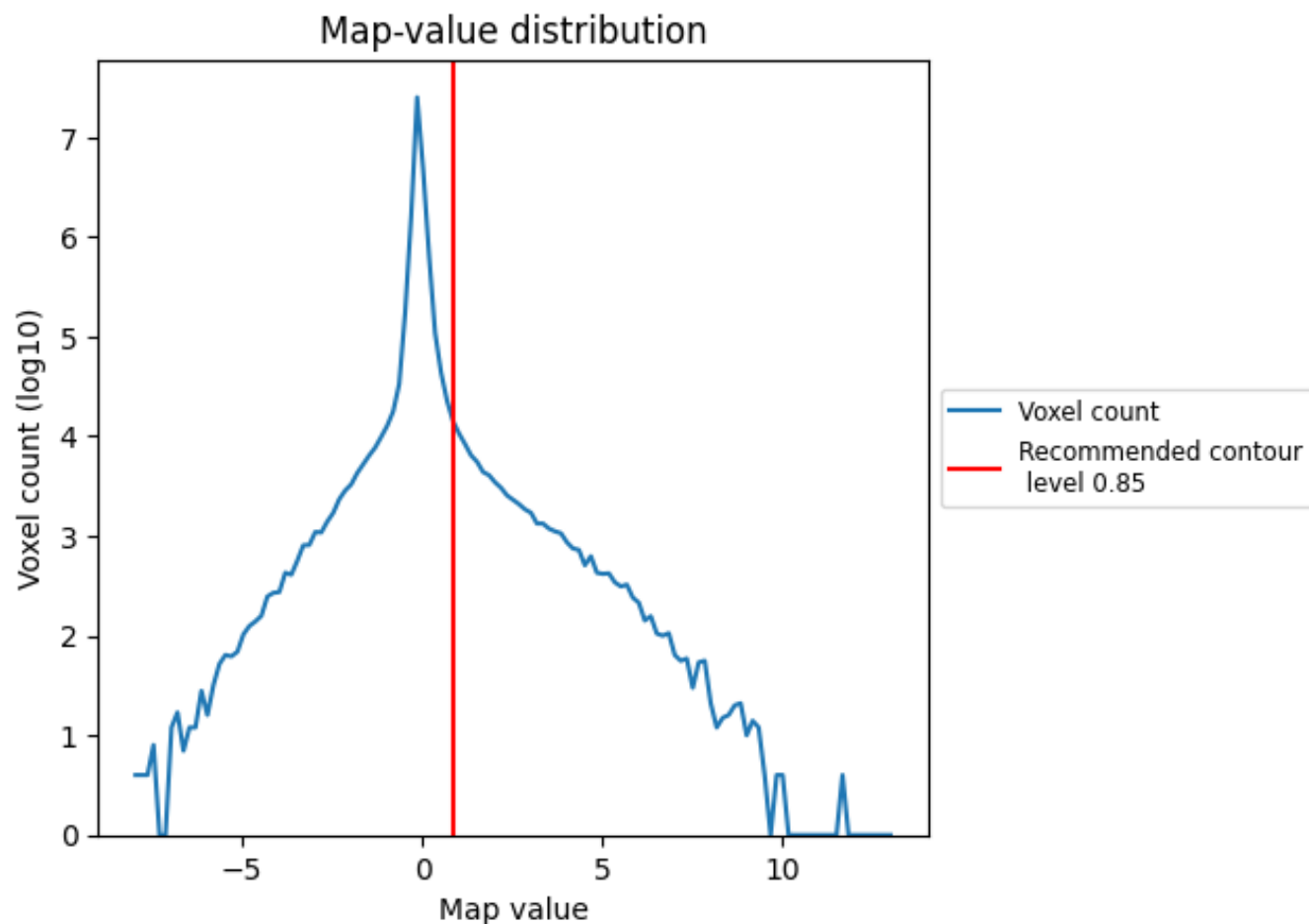
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

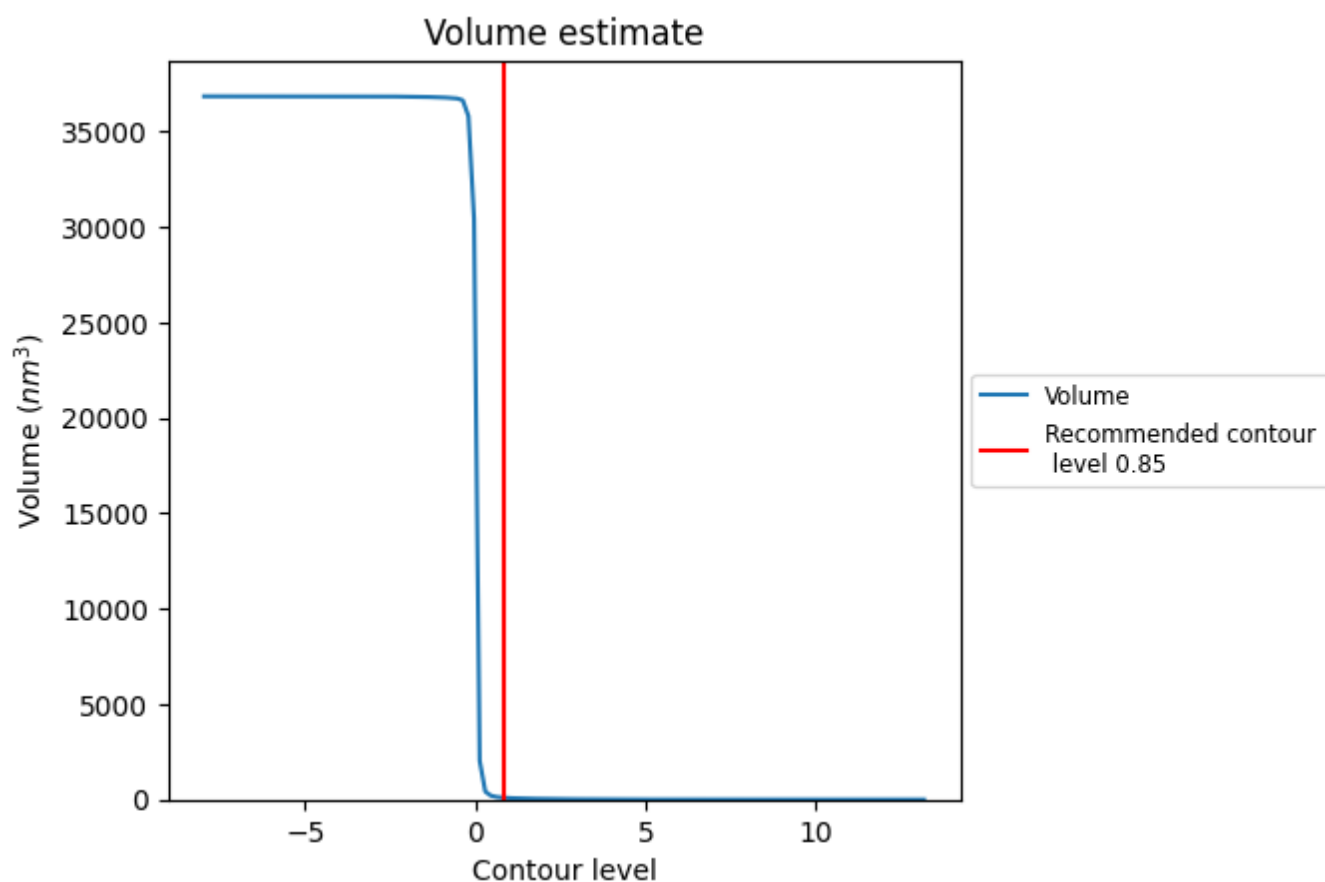
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

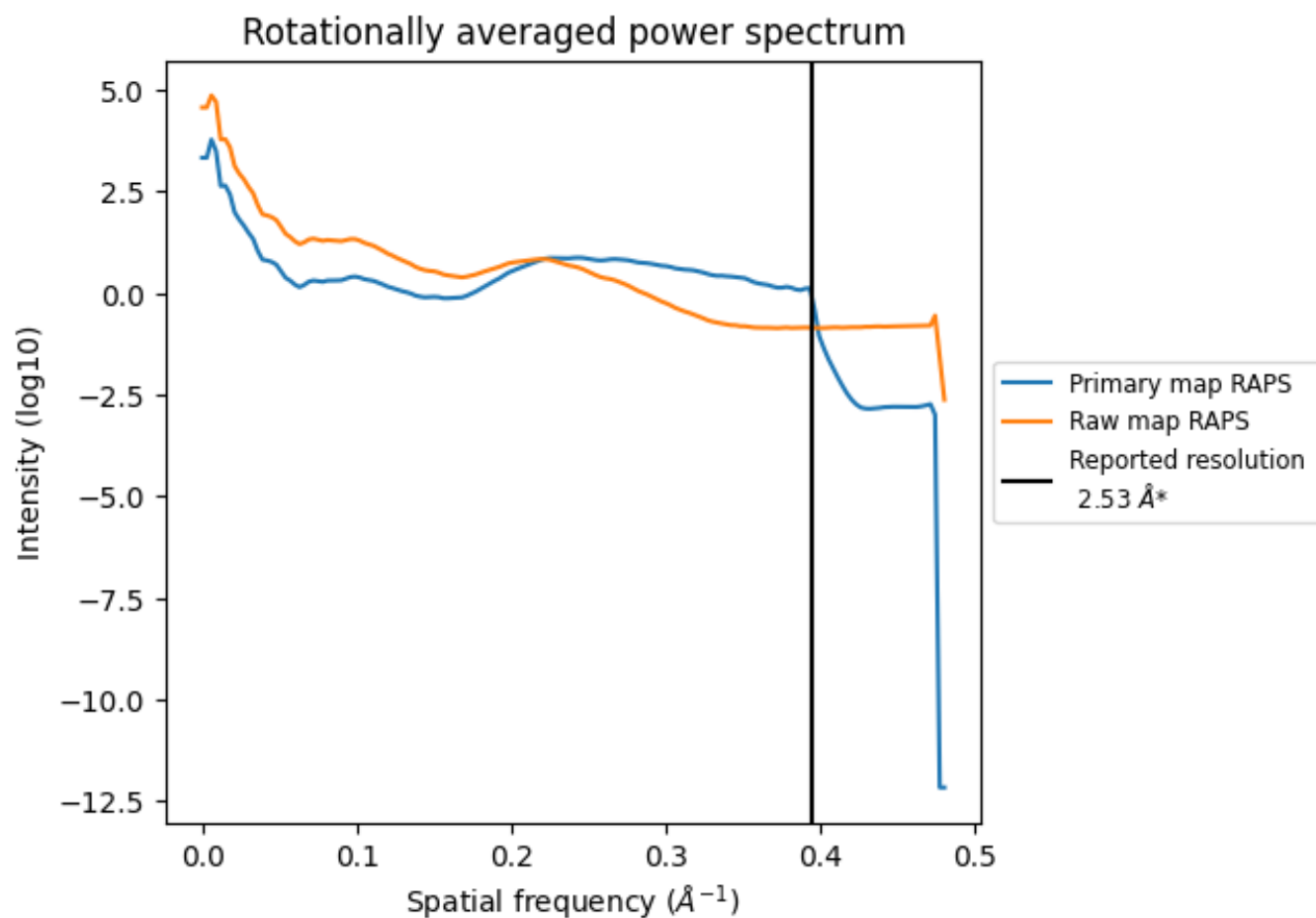
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm^3 ; this corresponds to an approximate mass of 87 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 ⓘ

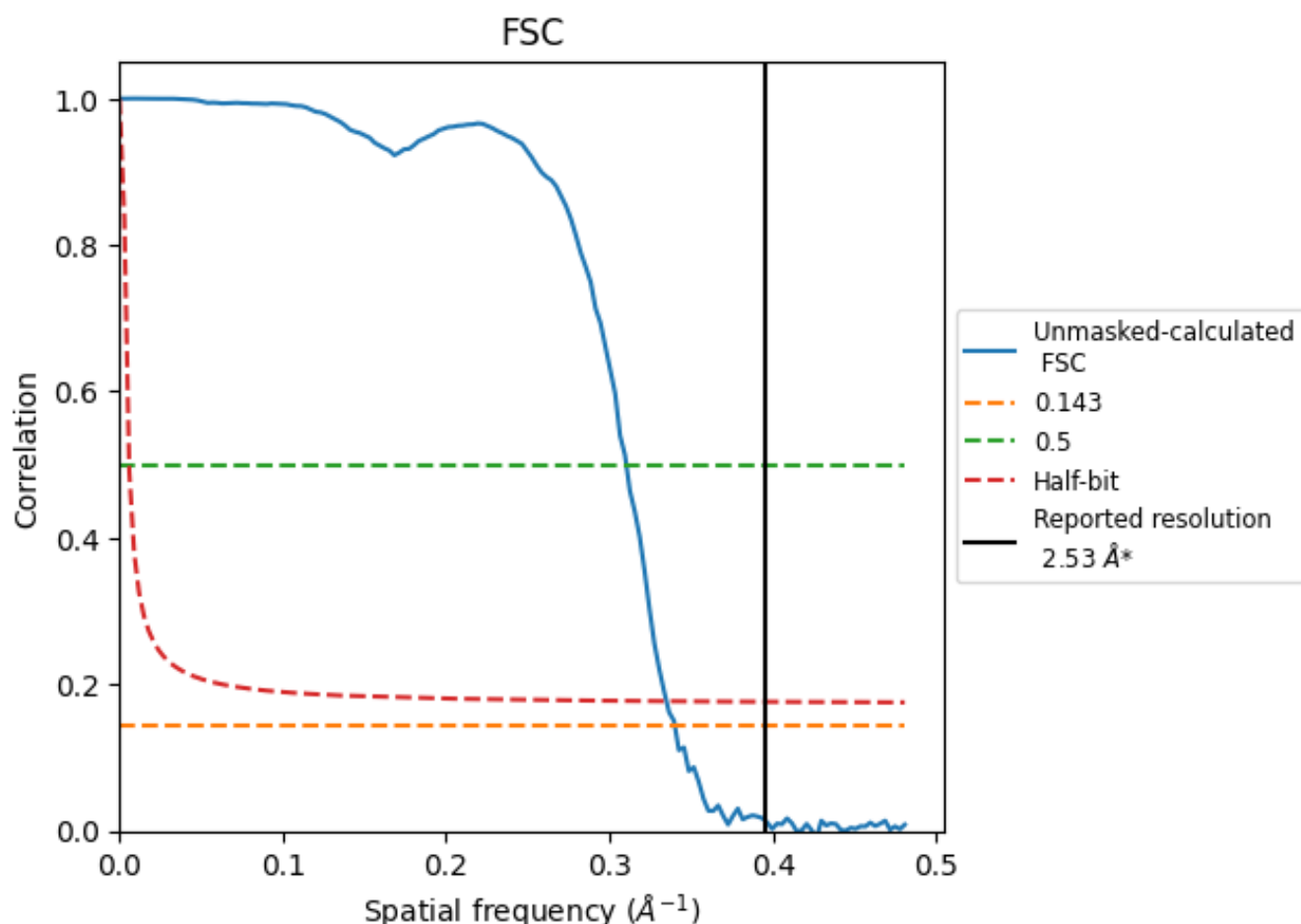


*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

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 0.395 \AA^{-1}

8.2 Resolution estimates [i](#)

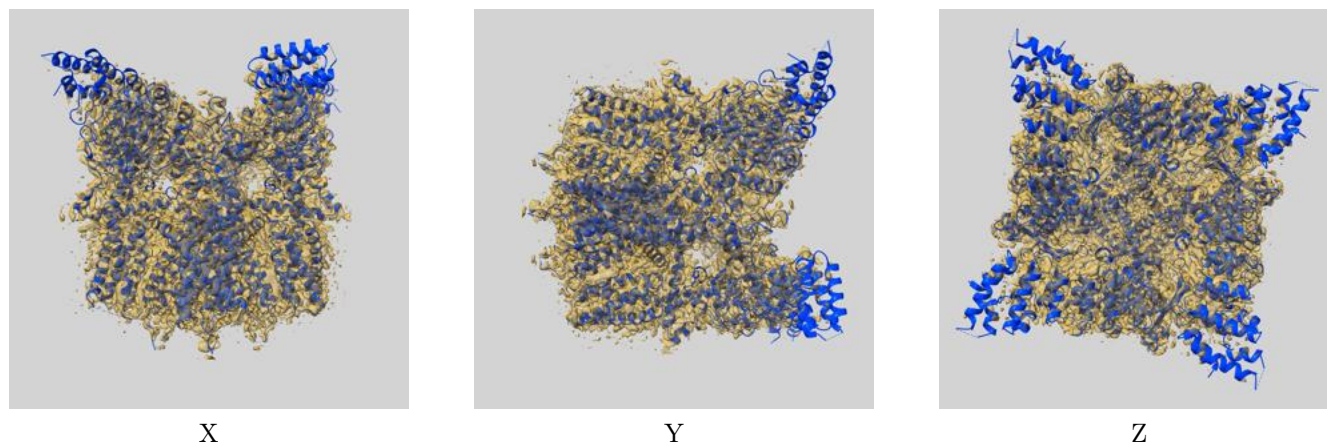
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.94	3.22	2.99

*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 2.94 differs from the reported value 2.53 by more than 10 %

9 Map-model fit [i](#)

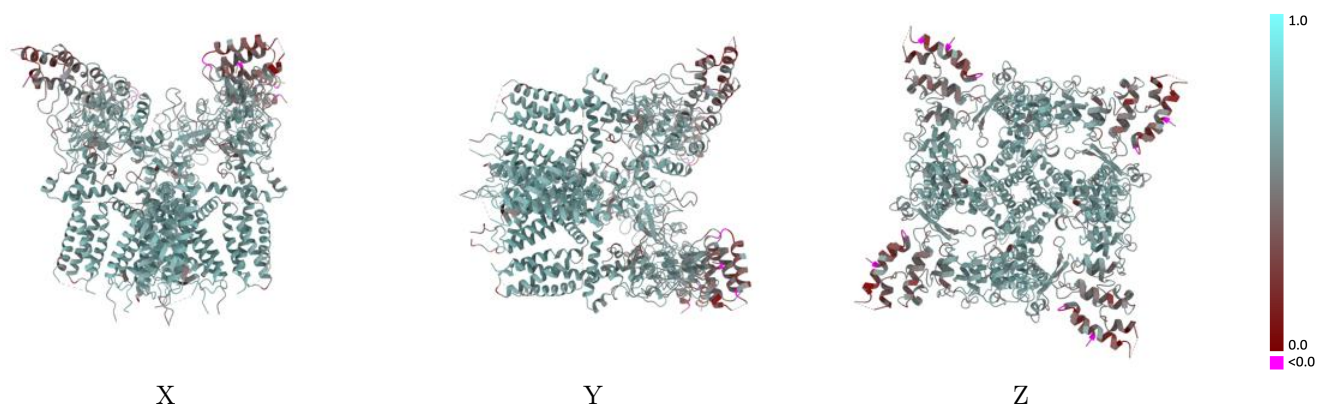
This section contains information regarding the fit between EMDB map EMD-33214 and PDB model 7XJ0. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



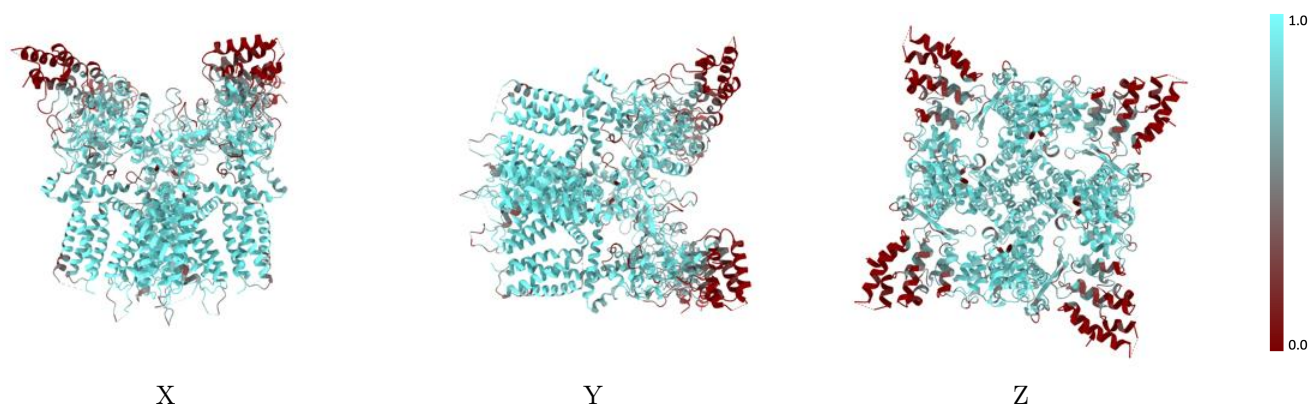
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



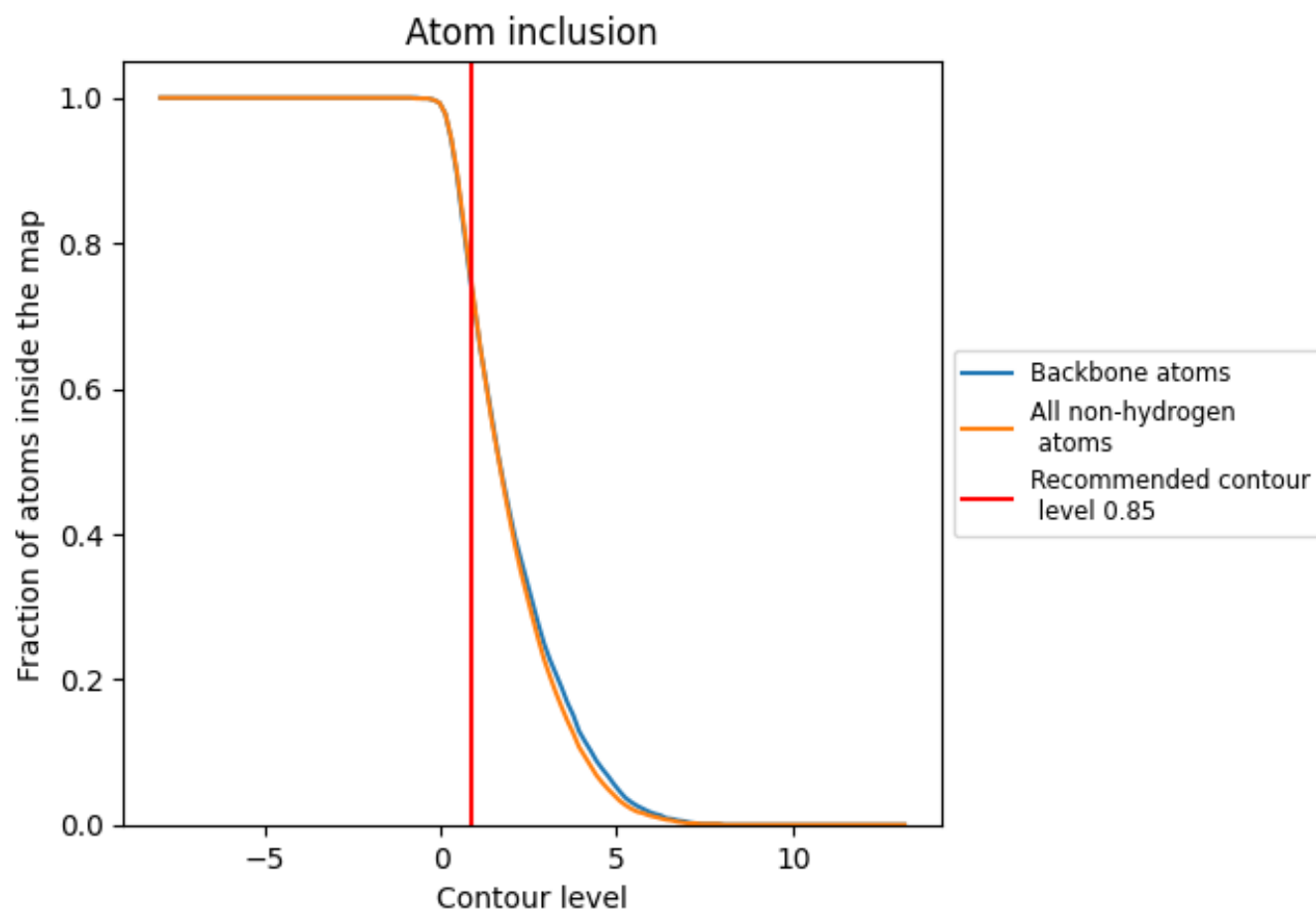
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.85).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7530	<div></div> 0.5760
A	<div></div> 0.7500	<div></div> 0.5780
B	<div></div> 0.7520	<div></div> 0.5750
C	<div></div> 0.7550	<div></div> 0.5780
D	<div></div> 0.7540	<div></div> 0.5750

