



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:25 AM UTC

PDB ID : 9CR0 / pdb_00009cr0
EMDB ID : EMD-45829
Title : Azotobacter vinelandii Reduced MoFeP (C2 symmetry) obtained using the SPT Labtech chameleon of 20 mM sodium dithionite under Al's oil
Authors : Cook, B.D.; Narehood, S.M.; McGuire, K.L.; Li, Y.; Tezcan, F.A.; Herzik, M.A.
Deposited on : 2024-07-19
Resolution : 2.08 Å (reported)
Based on initial model : 6NBC

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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

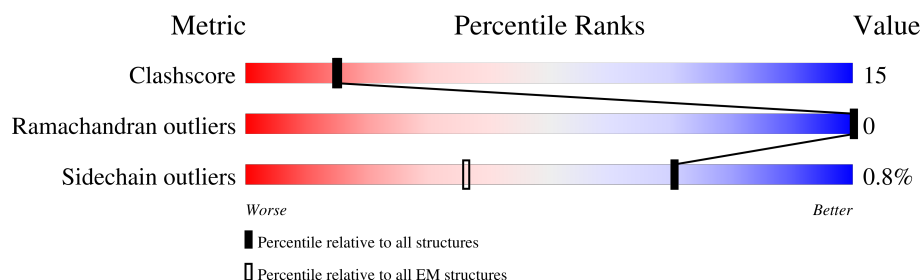
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.08 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	492	71% 25% .
1	C	492	72% 24% ..
2	B	523	78% 21%
2	D	523	78% 22%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ICS	A	502	-	-	X	-
4	ICS	C	502	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17763 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.

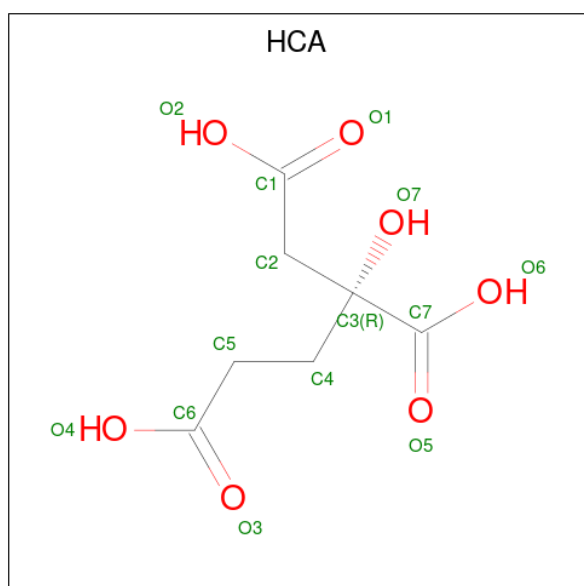
- Molecule 1 is a protein called Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	477	Total	C	N	O	S	1	0
			3793	2412	646	709	26		
1	C	477	Total	C	N	O	S	1	0
			3790	2410	646	709	25		

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

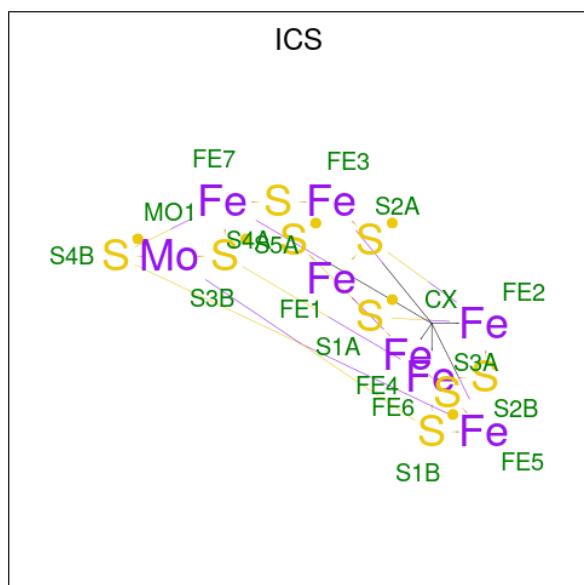
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	522	Total	C	N	O	S	0	0
			4174	2666	705	775	28		
2	D	522	Total	C	N	O	S	0	0
			4174	2666	705	775	28		

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			14	7	7	
3	C	1	Total	C	O	0
			14	7	7	

- Molecule 4 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICS) (formula: CFe_7MoS_9) (labeled as "Ligand of Interest" by depositor).

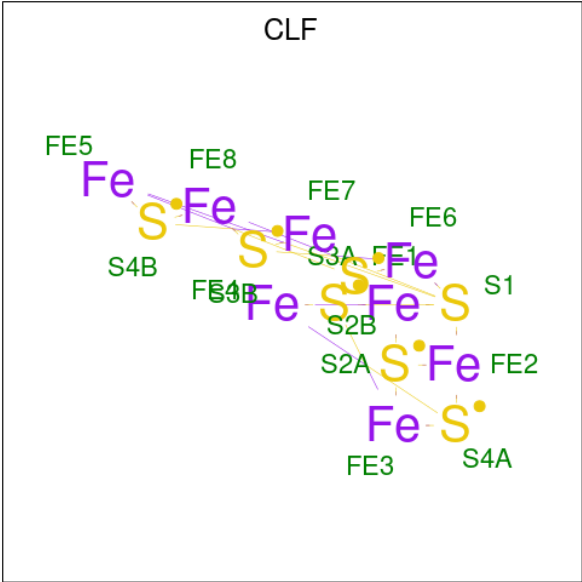


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
4	C	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	B	2	Total	Fe	0
			2	2	

- Molecule 6 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe_8S_7) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	Fe	S	0
			15	8	7	
6	D	1	Total	Fe	S	0
			15	8	7	

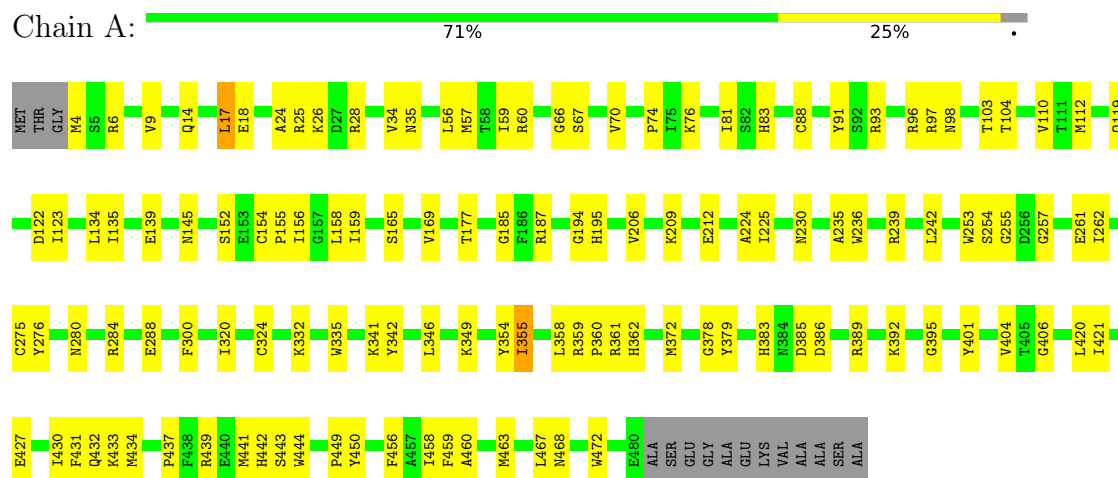
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	360	Total	O	0
			360	360	
7	B	507	Total	O	0
			507	507	
7	C	365	Total	O	0
			365	365	
7	D	504	Total	O	0
			504	504	

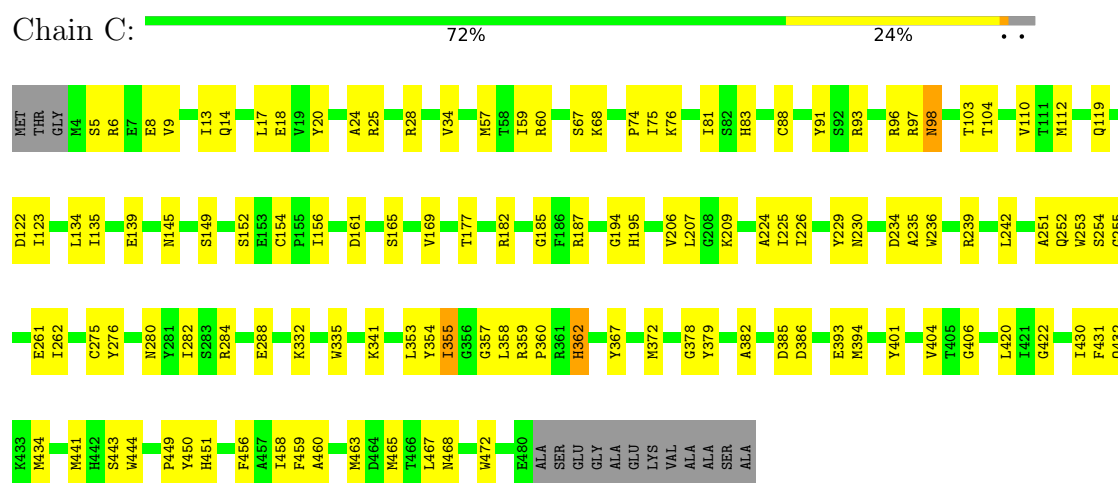
3 Residue-property plots

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. 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. 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.

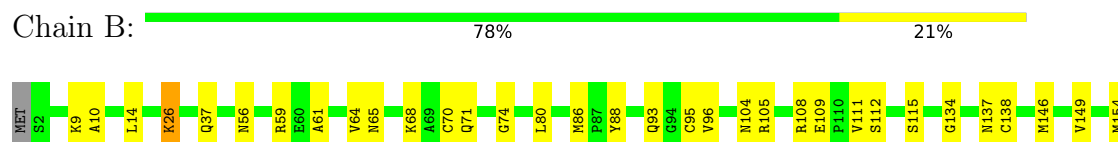
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

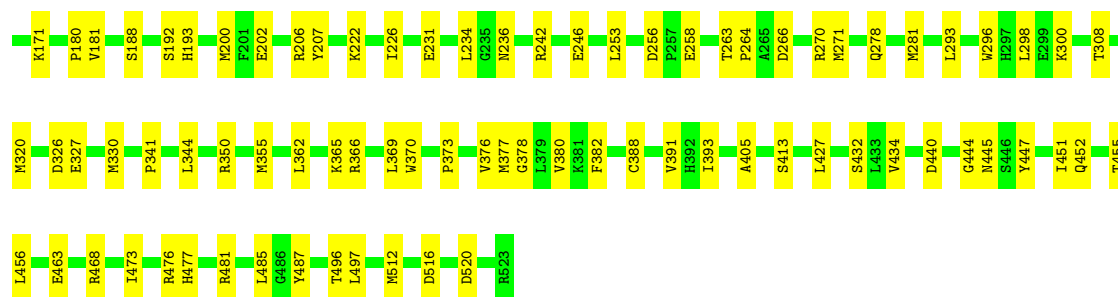


- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



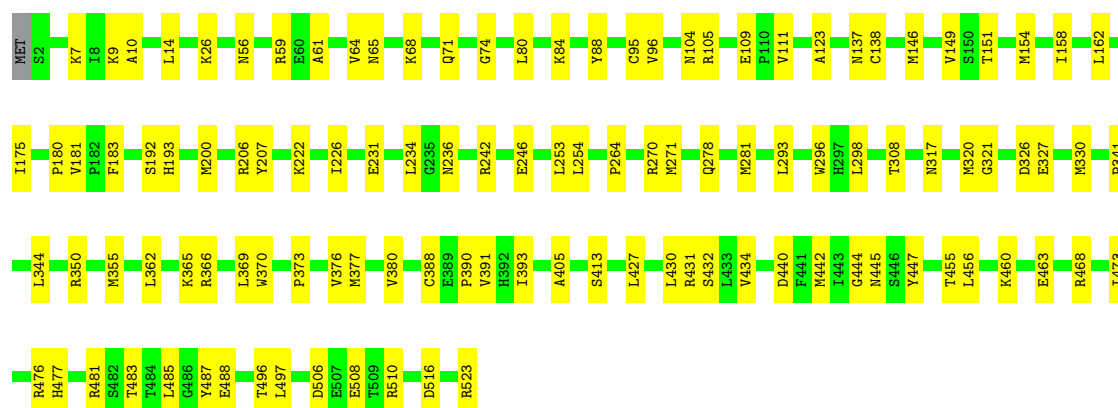
- Molecule 2: Nitrogenase molybdenum-iron protein beta chain





- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain D: 78% 22%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	95009	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	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: ICS, CLF, FE, HCA

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	0.13	0/3884	0.34	0/5237
1	C	0.14	0/3881	0.34	0/5234
2	B	0.13	0/4280	0.31	0/5786
2	D	0.13	0/4280	0.31	0/5786
All	All	0.13	0/16325	0.33	0/22043

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	3793	0	3734	120	0
1	C	3790	0	3727	124	0
2	B	4174	0	4088	108	0
2	D	4174	0	4088	110	0
3	A	14	0	7	2	0
3	C	14	0	7	2	0
4	A	18	0	0	4	0
4	C	18	0	0	6	0
5	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	15	0	0	0	0
6	D	15	0	0	0	0
7	A	360	0	0	85	0
7	B	507	0	0	77	0
7	C	365	0	0	94	0
7	D	504	0	0	76	0
All	All	17763	0	15651	471	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (471) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:502:ICS:S4A	7:C:904:HOH:O	2.32	0.87
2:D:242:ARG:NH1	7:D:706:HOH:O	2.12	0.83
2:B:271:MET:SD	7:B:1199:HOH:O	2.37	0.82
2:B:242:ARG:NH1	7:B:708:HOH:O	2.13	0.80
4:A:502:ICS:S4A	7:A:753:HOH:O	2.40	0.79
1:A:17:LEU:O	7:A:602:HOH:O	2.01	0.79
1:A:383:HIS:O	7:A:601:HOH:O	2.00	0.78
1:C:420:LEU:O	7:C:601:HOH:O	2.02	0.77
1:C:25:ARG:NH1	7:C:602:HOH:O	2.16	0.77
2:B:362:LEU:O	7:B:702:HOH:O	2.02	0.77
2:D:362:LEU:O	7:D:702:HOH:O	2.02	0.76
2:D:137:ASN:ND2	7:D:710:HOH:O	2.18	0.75
2:D:271:MET:SD	7:D:1195:HOH:O	2.43	0.75
1:A:360:PRO:O	7:A:603:HOH:O	2.05	0.75
1:C:17:LEU:O	7:C:602:HOH:O	2.05	0.75
2:B:520:ASP:O	7:B:703:HOH:O	2.04	0.74
2:B:146:MET:HB2	2:B:180:PRO:HG2	1.69	0.74
1:C:97:ARG:NH1	7:C:623:HOH:O	2.19	0.74
2:D:281:MET:SD	7:D:1125:HOH:O	2.46	0.74
1:C:83:HIS:O	7:C:603:HOH:O	2.06	0.74
1:C:93:ARG:NH1	7:C:625:HOH:O	2.21	0.73
1:A:421:ILE:O	7:A:605:HOH:O	2.07	0.73
2:D:9:LYS:HB2	2:D:14:LEU:HB2	1.70	0.73
4:C:502:ICS:S1A	7:C:658:HOH:O	2.46	0.73
1:A:83:HIS:O	7:A:606:HOH:O	2.07	0.73
1:A:93:ARG:NH1	7:A:626:HOH:O	2.21	0.73
1:C:154:CYS:SG	7:C:644:HOH:O	2.48	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:ASN:ND2	7:C:630:HOH:O	2.22	0.72
2:B:281:MET:SD	7:B:1111:HOH:O	2.47	0.72
2:B:134:GLY:O	7:B:704:HOH:O	2.06	0.72
1:C:119:GLN:O	7:C:605:HOH:O	2.07	0.72
2:B:355:MET:SD	7:B:1112:HOH:O	2.47	0.72
1:A:88:CYS:O	7:A:608:HOH:O	2.08	0.71
1:C:431:PHE:O	7:C:606:HOH:O	2.08	0.71
2:D:236:ASN:OD1	7:D:704:HOH:O	2.09	0.71
1:A:119:GLN:O	7:A:607:HOH:O	2.08	0.71
2:D:355:MET:SD	7:D:1120:HOH:O	2.49	0.71
1:A:139:GLU:OE1	7:A:609:HOH:O	2.09	0.70
2:B:445:ASN:OD1	7:B:705:HOH:O	2.09	0.70
2:B:236:ASN:OD1	7:B:706:HOH:O	2.09	0.70
2:D:445:ASN:OD1	7:D:703:HOH:O	2.08	0.70
4:C:502:ICS:S4A	7:C:678:HOH:O	2.50	0.70
1:A:431:PHE:O	7:A:610:HOH:O	2.10	0.69
1:A:154:CYS:SG	7:A:643:HOH:O	2.49	0.69
2:B:68:LYS:O	7:B:707:HOH:O	2.10	0.69
4:A:502:ICS:S4A	7:A:671:HOH:O	2.49	0.69
1:C:88:CYS:O	7:C:607:HOH:O	2.09	0.69
1:A:26:LYS:NZ	7:A:629:HOH:O	2.22	0.69
1:A:57:MET:O	7:A:611:HOH:O	2.11	0.69
1:A:450:TYR:O	7:A:613:HOH:O	2.12	0.68
2:D:68:LYS:O	7:D:705:HOH:O	2.10	0.68
1:C:57:MET:O	7:C:608:HOH:O	2.11	0.68
1:A:456:PHE:O	7:A:612:HOH:O	2.11	0.68
1:A:97:ARG:NH1	7:A:620:HOH:O	2.19	0.68
4:C:502:ICS:S1A	7:C:878:HOH:O	2.52	0.67
1:C:456:PHE:O	7:C:609:HOH:O	2.12	0.67
1:A:156:ILE:HG13	7:A:606:HOH:O	1.95	0.67
1:C:443:SER:OG	7:C:604:HOH:O	2.06	0.67
1:C:362:HIS:ND1	7:C:637:HOH:O	2.27	0.67
1:C:450:TYR:O	7:C:610:HOH:O	2.13	0.66
1:C:161:ASP:O	1:C:182:ARG:NH2	2.28	0.66
2:B:320:MET:O	7:B:710:HOH:O	2.14	0.66
1:A:35:ASN:ND2	1:A:395:GLY:O	2.27	0.66
4:A:502:ICS:S1A	7:A:874:HOH:O	2.53	0.66
1:C:6:ARG:HG3	1:C:34:VAL:HG11	1.76	0.65
1:A:152:SER:HA	7:A:606:HOH:O	1.96	0.65
2:B:154:MET:SD	7:B:1137:HOH:O	2.54	0.65
1:C:185:GLY:N	7:C:644:HOH:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:455:THR:OG1	7:D:701:HOH:O	2.01	0.65
2:D:154:MET:SD	7:D:1152:HOH:O	2.55	0.65
2:B:476:ARG:O	7:B:711:HOH:O	2.15	0.64
2:D:476:ARG:O	7:D:707:HOH:O	2.14	0.64
1:A:185:GLY:N	7:A:643:HOH:O	2.28	0.64
2:D:146:MET:HB2	2:D:180:PRO:HG2	1.79	0.64
2:B:9:LYS:HB2	2:B:14:LEU:HB2	1.80	0.64
3:A:501:HCA:O1	3:A:501:HCA:O7	2.15	0.64
1:A:25:ARG:NH1	7:A:602:HOH:O	2.19	0.64
1:A:284:ARG:O	1:A:288:GLU:HG3	1.98	0.63
2:D:104:ASN:ND2	2:D:109:GLU:O	2.30	0.63
1:C:432:GLN:O	7:C:613:HOH:O	2.16	0.63
1:C:422:GLY:O	7:C:611:HOH:O	2.15	0.63
3:C:501:HCA:O7	3:C:501:HCA:O1	2.17	0.62
1:C:284:ARG:O	1:C:288:GLU:HG3	1.98	0.62
2:B:138:CYS:SG	7:B:1140:HOH:O	2.51	0.62
1:A:385:ASP:OD2	1:A:385:ASP:N	2.33	0.62
1:C:152:SER:HA	7:C:603:HOH:O	1.98	0.62
1:A:187:ARG:HG3	7:A:664:HOH:O	2.00	0.61
2:B:104:ASN:ND2	2:B:109:GLU:O	2.33	0.61
1:C:359:ARG:HG3	7:C:904:HOH:O	1.99	0.61
1:C:60:ARG:O	7:C:614:HOH:O	2.16	0.61
1:A:432:GLN:O	7:A:614:HOH:O	2.16	0.61
1:A:255:GLY:HA2	7:A:641:HOH:O	2.00	0.61
2:D:477:HIS:ND1	7:D:752:HOH:O	2.31	0.61
1:A:443:SER:OG	7:A:604:HOH:O	2.06	0.60
1:C:187:ARG:HG3	7:C:667:HOH:O	2.01	0.60
1:A:253:TRP:O	7:A:616:HOH:O	2.16	0.60
2:B:231:GLU:CD	2:B:236:ASN:HD22	2.10	0.60
1:C:139:GLU:OE1	7:C:612:HOH:O	2.15	0.60
1:A:359:ARG:HG3	7:A:753:HOH:O	2.01	0.60
2:B:61:ALA:O	7:B:713:HOH:O	2.17	0.59
1:C:230:ASN:HA	1:C:235:ALA:H	1.66	0.59
1:A:468:ASN:OD1	7:A:615:HOH:O	2.16	0.59
2:B:455:THR:OG1	7:B:701:HOH:O	2.00	0.59
2:D:231:GLU:CD	2:D:236:ASN:HD22	2.11	0.59
1:A:123:ILE:HG12	7:A:607:HOH:O	2.02	0.59
1:A:104:THR:O	7:A:617:HOH:O	2.17	0.58
2:D:508:GLU:OE1	7:D:708:HOH:O	2.17	0.58
1:C:123:ILE:HG12	7:C:605:HOH:O	2.02	0.58
1:C:357:GLY:N	7:C:658:HOH:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:MET:HE3	7:B:754:HOH:O	2.04	0.58
2:B:242:ARG:O	2:B:246:GLU:HG3	2.04	0.58
1:A:6:ARG:HG3	1:A:34:VAL:HG11	1.85	0.58
2:D:431:ARG:NH2	7:D:723:HOH:O	2.24	0.58
1:C:463:MET:SD	7:C:942:HOH:O	2.57	0.58
2:D:270:ARG:NH1	7:D:712:HOH:O	2.34	0.58
1:C:360:PRO:O	7:C:618:HOH:O	2.17	0.58
1:C:251:ALA:O	7:C:616:HOH:O	2.17	0.57
2:B:56:ASN:OD1	7:B:715:HOH:O	2.18	0.57
1:A:434:MET:HB2	7:A:610:HOH:O	2.05	0.57
2:D:242:ARG:O	2:D:246:GLU:HG3	2.04	0.57
2:B:226:ILE:HB	2:B:253:LEU:HD12	1.87	0.57
1:C:449:PRO:HB2	7:C:738:HOH:O	2.04	0.57
2:D:434:VAL:HG23	7:D:969:HOH:O	2.03	0.57
1:C:385:ASP:OD2	1:C:385:ASP:N	2.37	0.57
2:B:300:LYS:NZ	7:B:779:HOH:O	2.37	0.56
1:C:74:PRO:O	7:C:617:HOH:O	2.17	0.56
1:C:104:THR:O	7:C:619:HOH:O	2.18	0.56
1:C:187:ARG:N	7:C:667:HOH:O	2.38	0.56
1:A:442:HIS:NE2	7:A:619:HOH:O	2.22	0.56
2:B:516:ASP:OD2	7:B:716:HOH:O	2.18	0.56
2:B:326:ASP:OD1	2:B:487:TYR:OH	2.19	0.56
2:D:317:ASN:ND2	7:D:757:HOH:O	2.33	0.56
1:A:230:ASN:HA	1:A:235:ALA:H	1.70	0.56
2:D:138:CYS:SG	7:D:1145:HOH:O	2.52	0.56
1:A:145:ASN:HB2	7:A:713:HOH:O	2.06	0.55
2:B:378:GLY:O	7:B:714:HOH:O	2.17	0.55
1:C:261:GLU:OE2	7:C:620:HOH:O	2.18	0.55
1:C:367:TYR:OH	7:C:615:HOH:O	2.17	0.55
1:A:324:CYS:HB2	7:A:635:HOH:O	2.05	0.55
1:C:96:ARG:NH2	4:C:502:ICS:S5A	2.74	0.55
2:D:326:ASP:OD1	2:D:487:TYR:OH	2.20	0.55
1:C:194:GLY:HA2	7:C:929:HOH:O	2.07	0.54
2:B:138:CYS:N	7:B:704:HOH:O	2.40	0.54
2:B:341:PRO:HD2	2:B:344:LEU:HD12	1.88	0.54
1:A:187:ARG:N	7:A:664:HOH:O	2.38	0.54
1:A:354:TYR:O	7:A:619:HOH:O	2.19	0.54
1:A:433:LYS:NZ	2:B:263:THR:O	2.38	0.54
1:A:194:GLY:HA2	7:A:921:HOH:O	2.07	0.54
1:A:386:ASP:HB2	7:A:601:HOH:O	2.06	0.54
1:C:434:MET:HB2	7:C:606:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLU:H	1:A:212:GLU:CD	2.15	0.54
2:B:434:VAL:HG23	7:B:991:HOH:O	2.07	0.54
2:D:105:ARG:NH2	7:D:781:HOH:O	2.39	0.54
2:D:181:VAL:HG12	7:D:777:HOH:O	2.08	0.54
1:A:460:ALA:HB2	7:A:612:HOH:O	2.07	0.54
1:C:177:THR:OG1	1:C:209:LYS:NZ	2.41	0.54
2:D:264:PRO:O	7:D:712:HOH:O	2.19	0.54
2:B:468:ARG:NH1	7:B:738:HOH:O	2.27	0.53
2:D:341:PRO:HD2	2:D:344:LEU:HD12	1.89	0.53
2:B:95:CYS:HB2	7:B:1032:HOH:O	2.08	0.53
1:A:4:MET:HE3	1:A:4:MET:O	2.09	0.53
1:C:28:ARG:NH2	7:C:649:HOH:O	2.31	0.53
1:C:145:ASN:HB2	7:C:728:HOH:O	2.08	0.53
2:D:200:MET:HE3	7:D:762:HOH:O	2.08	0.53
2:B:181:VAL:HG12	7:B:786:HOH:O	2.08	0.52
1:C:156:ILE:HG23	1:C:161:ASP:HB2	1.91	0.52
1:A:359:ARG:NE	7:A:671:HOH:O	2.42	0.52
2:B:96:VAL:HG23	7:B:1032:HOH:O	2.10	0.52
1:C:460:ALA:HB2	7:C:609:HOH:O	2.09	0.52
1:A:60:ARG:O	7:A:618:HOH:O	2.19	0.52
1:A:74:PRO:O	7:A:621:HOH:O	2.19	0.52
2:D:390:PRO:HD3	7:D:770:HOH:O	2.09	0.52
1:A:261:GLU:OE2	7:A:622:HOH:O	2.19	0.52
2:D:14:LEU:HD23	7:D:1171:HOH:O	2.09	0.52
2:D:293:LEU:HB3	7:D:1139:HOH:O	2.10	0.52
2:B:59:ARG:NE	7:B:715:HOH:O	2.39	0.52
2:D:369:LEU:HD11	2:D:393:ILE:HG12	1.90	0.52
2:B:14:LEU:HD23	7:B:1168:HOH:O	2.10	0.52
2:B:266:ASP:OD1	7:B:717:HOH:O	2.19	0.52
2:D:65:ASN:ND2	7:D:788:HOH:O	2.43	0.52
2:D:485:LEU:HD22	7:D:861:HOH:O	2.10	0.52
1:A:449:PRO:HB2	7:A:680:HOH:O	2.09	0.51
2:B:65:ASN:ND2	7:B:794:HOH:O	2.42	0.51
2:D:56:ASN:OD1	7:D:711:HOH:O	2.18	0.51
2:D:393:ILE:HD12	7:D:978:HOH:O	2.10	0.51
1:A:358:LEU:HB3	7:A:753:HOH:O	2.11	0.51
2:B:104:ASN:ND2	2:B:111:VAL:HG23	2.25	0.51
2:D:95:CYS:HB2	7:D:952:HOH:O	2.11	0.51
2:B:105:ARG:NH2	7:B:792:HOH:O	2.42	0.51
1:C:75:ILE:HD11	1:C:254:SER:HB2	1.93	0.51
1:C:225:ILE:HD11	1:C:242:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:477:HIS:ND1	7:B:765:HOH:O	2.34	0.51
2:B:270:ARG:NH1	7:B:717:HOH:O	2.24	0.51
1:A:158:LEU:HD11	2:B:154:MET:HG2	1.93	0.51
2:D:440:ASP:HB2	7:D:793:HOH:O	2.11	0.51
1:A:81:ILE:HD12	1:A:134:LEU:HD21	1.94	0.50
2:B:440:ASP:HB2	7:B:799:HOH:O	2.11	0.50
1:C:359:ARG:NE	7:C:678:HOH:O	2.43	0.50
3:C:501:HCA:O1	7:C:624:HOH:O	2.20	0.50
2:D:96:VAL:HG23	7:D:952:HOH:O	2.10	0.50
1:C:229:TYR:O	7:C:622:HOH:O	2.19	0.50
1:C:372:MET:SD	7:C:965:HOH:O	2.60	0.50
1:A:83:HIS:HB3	7:A:606:HOH:O	2.10	0.50
2:D:253:LEU:HG	7:D:891:HOH:O	2.12	0.50
1:A:320:ILE:HG22	7:A:635:HOH:O	2.12	0.50
2:B:37:GLN:OE1	7:B:718:HOH:O	2.20	0.50
2:B:393:ILE:HD12	7:B:976:HOH:O	2.11	0.50
2:D:473:ILE:HG12	7:D:909:HOH:O	2.12	0.50
2:B:473:ILE:HG12	7:B:967:HOH:O	2.12	0.49
1:C:9:VAL:HG11	7:C:812:HOH:O	2.12	0.49
2:D:445:ASN:HA	7:D:909:HOH:O	2.12	0.49
1:C:252:GLN:NE2	1:C:255:GLY:O	2.45	0.49
2:D:298:LEU:HD12	7:D:728:HOH:O	2.12	0.49
1:A:206:VAL:HG12	7:A:709:HOH:O	2.12	0.49
2:B:350:ARG:NH2	7:B:722:HOH:O	2.21	0.49
1:A:165:SER:O	1:A:169:VAL:HG23	2.12	0.49
1:C:13:ILE:O	1:C:17:LEU:HG	2.12	0.49
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.94	0.49
1:A:177:THR:OG1	1:A:209:LYS:NZ	2.46	0.48
1:C:332:LYS:HA	1:C:335:TRP:NE1	2.28	0.48
1:C:355:ILE:HD12	1:C:359:ARG:HB3	1.95	0.48
2:B:293:LEU:HB3	7:B:1148:HOH:O	2.13	0.48
2:B:455:THR:HB	2:B:463:GLU:HA	1.94	0.48
1:C:14:GLN:O	1:C:18:GLU:HG3	2.13	0.48
1:A:156:ILE:HG12	7:A:859:HOH:O	2.13	0.48
1:C:149:SER:HB2	7:C:936:HOH:O	2.14	0.48
1:C:206:VAL:HG12	7:C:709:HOH:O	2.12	0.48
2:D:226:ILE:HB	2:D:253:LEU:HD12	1.96	0.48
1:A:96:ARG:NH2	4:A:502:ICS:S5A	2.79	0.48
1:A:439:ARG:O	7:A:605:HOH:O	2.20	0.48
2:B:298:LEU:HD12	7:B:731:HOH:O	2.13	0.48
2:B:388:CYS:HA	7:B:702:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:SER:O	1:C:169:VAL:HG23	2.14	0.48
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.49	0.48
2:D:468:ARG:NH1	7:D:735:HOH:O	2.27	0.48
2:B:93:GLN:NE2	7:B:805:HOH:O	2.47	0.48
1:C:28:ARG:HB2	7:C:842:HOH:O	2.14	0.48
1:C:472:TRP:NE1	7:C:665:HOH:O	2.37	0.48
2:B:264:PRO:O	7:B:717:HOH:O	2.20	0.47
1:C:81:ILE:HD12	1:C:134:LEU:HD21	1.96	0.47
1:C:5:SER:HB3	1:C:8:GLU:HG3	1.96	0.47
1:C:156:ILE:HG13	7:C:603:HOH:O	2.15	0.47
3:A:501:HCA:O1	7:A:623:HOH:O	2.19	0.47
2:B:365:LYS:N	7:B:702:HOH:O	2.22	0.47
1:C:234:ASP:HB3	1:C:451:HIS:CD2	2.50	0.47
1:C:280:ASN:HB2	7:C:775:HOH:O	2.14	0.47
1:C:459:PHE:O	1:C:463:MET:HG2	2.15	0.47
1:A:103:THR:HB	7:A:653:HOH:O	2.14	0.47
1:A:459:PHE:O	1:A:463:MET:HG2	2.14	0.47
1:C:156:ILE:HG12	7:C:849:HOH:O	2.13	0.47
1:C:25:ARG:HA	7:C:842:HOH:O	2.14	0.47
1:A:9:VAL:HG11	7:A:810:HOH:O	2.14	0.47
1:C:59:ILE:HD13	1:C:354:TYR:HE2	1.79	0.47
2:D:236:ASN:CG	2:D:485:LEU:HG	2.39	0.47
2:D:485:LEU:HD13	7:D:1146:HOH:O	2.14	0.47
2:B:320:MET:HG3	7:B:941:HOH:O	2.14	0.47
1:C:355:ILE:HD12	1:C:359:ARG:CB	2.44	0.47
2:D:326:ASP:O	2:D:330:MET:HG3	2.15	0.47
2:B:447:TYR:O	7:B:720:HOH:O	2.21	0.47
2:D:388:CYS:HA	7:D:702:HOH:O	2.13	0.47
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.50	0.47
2:B:452:GLN:O	2:B:455:THR:OG1	2.33	0.47
2:B:481:ARG:NH1	7:B:809:HOH:O	2.48	0.47
1:A:300:PHE:HA	7:A:613:HOH:O	2.15	0.46
1:A:280:ASN:HB2	7:A:801:HOH:O	2.15	0.46
2:D:104:ASN:ND2	2:D:111:VAL:HG23	2.31	0.46
1:A:74:PRO:HB3	7:A:641:HOH:O	2.16	0.46
1:C:406:GLY:N	7:C:608:HOH:O	2.48	0.46
1:C:444:TRP:HD1	7:C:693:HOH:O	1.97	0.46
1:A:155:PRO:HD2	7:A:859:HOH:O	2.14	0.46
1:A:253:TRP:HA	1:A:254:SER:HA	1.64	0.46
1:A:420:LEU:HD13	7:A:917:HOH:O	2.14	0.46
2:D:26:LYS:HE2	2:D:26:LYS:HB2	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLN:O	1:A:18:GLU:HG3	2.15	0.46
1:C:59:ILE:HD13	1:C:354:TYR:CE2	2.51	0.46
1:C:98:ASN:HB3	7:C:666:HOH:O	2.14	0.46
1:A:332:LYS:HA	1:A:335:TRP:NE1	2.29	0.46
2:B:369:LEU:HD11	2:B:393:ILE:HG12	1.98	0.46
1:C:103:THR:HB	7:C:655:HOH:O	2.15	0.46
1:C:449:PRO:HA	7:C:693:HOH:O	2.16	0.46
1:A:24:ALA:HB1	7:A:879:HOH:O	2.15	0.46
1:A:59:ILE:HD13	1:A:354:TYR:CE2	2.51	0.46
1:A:59:ILE:HD13	1:A:354:TYR:HE2	1.79	0.46
1:A:406:GLY:N	7:A:611:HOH:O	2.49	0.46
2:B:373:PRO:HD2	7:B:977:HOH:O	2.16	0.46
1:C:252:GLN:HB3	7:C:692:HOH:O	2.16	0.46
2:D:506:ASP:OD1	7:D:715:HOH:O	2.21	0.46
1:C:195:HIS:HA	7:C:627:HOH:O	2.16	0.46
2:D:206:ARG:HB2	7:D:804:HOH:O	2.16	0.46
2:D:350:ARG:NH2	7:D:717:HOH:O	2.21	0.46
2:D:447:TYR:HB2	7:D:703:HOH:O	2.16	0.46
1:A:195:HIS:HA	7:A:628:HOH:O	2.15	0.46
1:C:253:TRP:CZ2	1:C:262:ILE:HG23	2.50	0.46
1:A:67:SER:HA	7:A:628:HOH:O	2.16	0.45
1:C:122:ASP:HB2	7:C:605:HOH:O	2.16	0.45
1:A:122:ASP:HB2	7:A:607:HOH:O	2.16	0.45
1:A:472:TRP:NE1	7:A:661:HOH:O	2.38	0.45
2:B:202:GLU:O	7:B:719:HOH:O	2.20	0.45
2:B:264:PRO:O	7:B:721:HOH:O	2.21	0.45
2:D:61:ALA:O	7:D:714:HOH:O	2.21	0.45
2:D:497:LEU:HB3	7:D:1188:HOH:O	2.16	0.45
1:C:276:TYR:O	1:C:280:ASN:HB3	2.16	0.45
2:B:380:VAL:HG21	7:B:1191:HOH:O	2.15	0.45
2:D:455:THR:HB	2:D:463:GLU:HA	1.98	0.45
1:A:225:ILE:HD11	1:A:242:LEU:HD12	1.99	0.45
1:A:355:ILE:HB	1:A:360:PRO:HD3	1.97	0.45
2:D:123:ALA:HA	2:D:158:ILE:HD11	1.98	0.45
2:D:111:VAL:HG12	7:D:1078:HOH:O	2.16	0.45
1:A:253:TRP:CZ2	1:A:262:ILE:HG23	2.52	0.45
2:B:86:MET:HE1	2:B:112:SER:HB3	1.99	0.45
2:B:202:GLU:HG3	2:B:300:LYS:HG2	1.98	0.45
1:A:91:TYR:HB2	7:A:608:HOH:O	2.17	0.45
2:B:447:TYR:HB2	7:B:705:HOH:O	2.17	0.45
2:D:481:ARG:NH1	7:D:801:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ALA:HA	7:A:638:HOH:O	2.17	0.44
2:B:497:LEU:HB3	7:B:1189:HOH:O	2.16	0.44
1:C:224:ALA:HA	7:C:616:HOH:O	2.17	0.44
2:D:254:LEU:HD22	7:D:984:HOH:O	2.16	0.44
2:D:456:LEU:HD13	7:D:795:HOH:O	2.17	0.44
2:B:376:VAL:HG12	7:B:1086:HOH:O	2.17	0.44
1:C:463:MET:HA	7:C:942:HOH:O	2.16	0.44
2:D:373:PRO:HD2	7:D:1014:HOH:O	2.16	0.44
2:D:380:VAL:HG21	7:D:1191:HOH:O	2.16	0.44
2:B:393:ILE:HG21	7:B:1191:HOH:O	2.17	0.44
1:C:275:CYS:HA	1:C:358:LEU:HD22	2.00	0.44
2:D:516:ASP:OD2	7:D:716:HOH:O	2.21	0.44
1:A:346:LEU:HB3	1:A:372:MET:SD	2.57	0.44
1:C:24:ALA:HB1	7:C:874:HOH:O	2.16	0.44
2:D:376:VAL:HG12	7:D:1090:HOH:O	2.17	0.44
2:B:388:CYS:SG	7:B:993:HOH:O	2.61	0.44
1:C:76:LYS:HA	1:C:110:VAL:HG23	1.99	0.44
1:C:378:GLY:HA3	1:C:401:TYR:CD1	2.53	0.44
1:A:430:ILE:HG13	7:A:813:HOH:O	2.17	0.44
1:A:361:ARG:NH2	7:A:654:HOH:O	2.51	0.44
2:B:445:ASN:HA	7:B:876:HOH:O	2.17	0.44
2:B:456:LEU:HD13	7:B:755:HOH:O	2.16	0.44
1:C:255:GLY:HA2	7:C:622:HOH:O	2.17	0.44
2:B:256:ASP:HB2	7:B:852:HOH:O	2.16	0.43
1:C:149:SER:HB3	7:C:767:HOH:O	2.17	0.43
1:C:358:LEU:HB3	7:C:904:HOH:O	2.16	0.43
1:C:441:MET:HE3	7:C:919:HOH:O	2.17	0.43
1:C:91:TYR:HB2	7:C:607:HOH:O	2.17	0.43
2:B:327:GLU:HA	2:B:330:MET:HE3	1.99	0.43
1:C:206:VAL:HA	1:C:209:LYS:HD3	1.99	0.43
1:A:135:ILE:HG12	7:A:957:HOH:O	2.18	0.43
1:C:67:SER:HA	7:C:627:HOH:O	2.16	0.43
1:C:225:ILE:HD13	7:C:852:HOH:O	2.18	0.43
1:C:335:TRP:NE1	7:C:698:HOH:O	2.51	0.43
1:A:76:LYS:HA	1:A:110:VAL:HG23	2.01	0.43
2:B:496:THR:HG22	7:B:811:HOH:O	2.18	0.43
2:D:355:MET:SD	7:D:1183:HOH:O	2.62	0.43
1:C:355:ILE:HB	1:C:360:PRO:HD3	2.00	0.43
4:C:502:ICS:S4A	7:C:793:HOH:O	2.62	0.43
2:D:391:VAL:HB	7:D:981:HOH:O	2.19	0.43
1:A:355:ILE:HD12	1:A:359:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:ARG:NH2	7:B:758:HOH:O	2.51	0.43
2:B:88:TYR:O	2:B:149:VAL:HA	2.19	0.43
1:A:225:ILE:HD13	7:A:842:HOH:O	2.18	0.43
1:A:341:LYS:O	7:A:627:HOH:O	2.22	0.43
7:A:839:HOH:O	2:B:64:VAL:HG13	2.19	0.43
2:B:391:VAL:HB	7:B:990:HOH:O	2.18	0.43
2:B:413:SER:HB3	7:B:785:HOH:O	2.18	0.43
1:C:68:LYS:HE2	7:C:954:HOH:O	2.19	0.43
2:D:523:ARG:NH2	7:D:715:HOH:O	2.51	0.43
1:A:236:TRP:HD1	7:A:930:HOH:O	2.02	0.42
1:A:458:ILE:HA	7:A:711:HOH:O	2.18	0.42
2:B:80:LEU:HD12	7:B:1138:HOH:O	2.19	0.42
2:D:88:TYR:O	2:D:149:VAL:HA	2.19	0.42
1:A:389:ARG:HA	1:A:392:LYS:HE3	2.01	0.42
2:B:180:PRO:HA	2:B:207:TYR:OH	2.19	0.42
7:B:802:HOH:O	2:D:510:ARG:HD3	2.18	0.42
1:C:253:TRP:HA	1:C:254:SER:HA	1.64	0.42
2:D:296:TRP:NE1	2:D:377:MET:HE1	2.35	0.42
2:D:321:GLY:HA3	7:D:803:HOH:O	2.19	0.42
1:A:276:TYR:O	1:A:280:ASN:HB3	2.19	0.42
1:A:441:MET:HE3	7:A:894:HOH:O	2.19	0.42
2:B:512:MET:HG2	1:C:103:THR:HG23	2.01	0.42
1:C:20:TYR:N	7:C:602:HOH:O	2.51	0.42
1:C:382:ALA:HB1	1:C:386:ASP:HB2	2.00	0.42
2:D:10:ALA:O	2:D:14:LEU:HB3	2.19	0.42
2:D:278:GLN:HA	7:D:1166:HOH:O	2.18	0.42
2:D:496:THR:HG22	7:D:797:HOH:O	2.19	0.42
1:A:206:VAL:HA	1:A:209:LYS:HD3	2.00	0.42
1:A:257:GLY:HA2	7:A:668:HOH:O	2.20	0.42
2:B:296:TRP:HE1	2:B:377:MET:HE1	1.84	0.42
2:D:71:GLN:HG2	2:D:192:SER:O	2.20	0.42
2:B:485:LEU:HD22	7:B:941:HOH:O	2.19	0.42
7:C:625:HOH:O	2:D:427:LEU:HD12	2.20	0.42
2:D:80:LEU:HD12	7:D:1144:HOH:O	2.19	0.42
2:D:180:PRO:HA	2:D:207:TYR:OH	2.19	0.42
2:D:320:MET:HG3	7:D:861:HOH:O	2.19	0.42
2:D:388:CYS:SG	7:D:993:HOH:O	2.60	0.42
2:D:393:ILE:HG21	7:D:1191:HOH:O	2.20	0.42
2:D:413:SER:HB3	7:D:780:HOH:O	2.19	0.42
1:A:378:GLY:HA3	1:A:401:TYR:CD1	2.53	0.42
1:C:353:LEU:HD13	7:C:843:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:321:GLY:O	7:D:713:HOH:O	2.21	0.42
1:A:155:PRO:O	1:A:159:ILE:HG12	2.19	0.42
1:C:226:ILE:HA	1:C:253:TRP:HB2	2.02	0.42
7:C:846:HOH:O	2:D:64:VAL:HG13	2.19	0.42
2:D:366:ARG:NH2	7:D:758:HOH:O	2.51	0.42
2:B:137:ASN:HB2	7:B:704:HOH:O	2.19	0.42
1:A:112:MET:HB3	7:A:839:HOH:O	2.20	0.42
1:A:349:LYS:HG3	1:A:467:LEU:HD21	2.01	0.42
1:C:458:ILE:HA	7:C:720:HOH:O	2.18	0.42
2:D:370:TRP:HZ3	2:D:442:MET:HB3	1.84	0.42
2:B:296:TRP:NE1	2:B:377:MET:HE1	2.35	0.42
1:C:341:LYS:O	7:C:629:HOH:O	2.22	0.42
1:C:360:PRO:HB2	1:C:379:TYR:CZ	2.55	0.42
2:D:296:TRP:HE1	2:D:377:MET:HE1	1.85	0.42
2:B:71:GLN:HG2	2:B:192:SER:O	2.20	0.41
1:C:207:LEU:HD22	1:C:282:ILE:HD11	2.02	0.41
2:D:7:LYS:HD2	2:D:7:LYS:HA	1.84	0.41
7:A:626:HOH:O	2:B:427:LEU:HD12	2.19	0.41
2:B:293:LEU:N	7:B:731:HOH:O	2.53	0.41
2:B:382:PHE:HB2	7:B:714:HOH:O	2.20	0.41
2:B:451:ILE:HG13	7:B:720:HOH:O	2.20	0.41
1:C:83:HIS:HB3	7:C:603:HOH:O	2.21	0.41
1:A:437:PRO:HA	1:A:472:TRP:CZ2	2.55	0.41
1:C:430:ILE:HG13	7:C:796:HOH:O	2.21	0.41
2:B:70:CYS:HB2	2:B:188:SER:HB2	2.01	0.41
2:B:222:LYS:HB2	2:B:222:LYS:HE3	1.84	0.41
2:D:84:LYS:HB3	2:D:84:LYS:HE3	1.80	0.41
2:D:405:ALA:HB3	7:D:800:HOH:O	2.20	0.41
1:A:360:PRO:HB2	1:A:379:TYR:CZ	2.56	0.41
2:B:96:VAL:HG21	2:B:115:SER:HB3	2.03	0.41
2:B:108:ARG:HD3	7:B:765:HOH:O	2.20	0.41
2:D:146:MET:HE1	7:D:1204:HOH:O	2.20	0.41
2:D:460:LYS:HA	7:D:795:HOH:O	2.20	0.41
1:C:394:MET:HG2	7:C:641:HOH:O	2.21	0.41
2:D:293:LEU:N	7:D:728:HOH:O	2.53	0.41
2:D:74:GLY:HA3	2:D:193:HIS:O	2.21	0.41
2:D:308:THR:HB	7:D:729:HOH:O	2.20	0.41
2:B:26:LYS:HB2	2:B:26:LYS:HE2	1.71	0.41
2:B:74:GLY:HA3	2:B:193:HIS:O	2.21	0.41
2:B:234:LEU:HD12	7:B:809:HOH:O	2.20	0.41
2:B:405:ALA:HB3	7:B:801:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:LEU:HB3	7:C:630:HOH:O	2.20	0.41
2:D:183:PHE:HB3	7:D:777:HOH:O	2.20	0.41
2:D:430:LEU:O	2:D:434:VAL:HG22	2.21	0.41
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.91	0.41
1:A:341:LYS:HD3	1:A:342:TYR:CE2	2.55	0.41
1:A:355:ILE:HD12	1:A:359:ARG:CB	2.51	0.41
2:B:206:ARG:HB2	7:B:719:HOH:O	2.21	0.41
2:B:278:GLN:HA	7:B:1166:HOH:O	2.21	0.41
2:B:308:THR:HB	7:B:735:HOH:O	2.19	0.41
1:C:112:MET:HB3	7:C:846:HOH:O	2.20	0.41
2:D:222:LYS:HE3	2:D:222:LYS:HB2	1.90	0.41
1:A:28:ARG:HB2	7:A:882:HOH:O	2.20	0.40
1:A:81:ILE:HG13	7:A:956:HOH:O	2.21	0.40
1:A:444:TRP:CD1	7:A:710:HOH:O	2.73	0.40
1:C:135:ILE:HG12	7:C:963:HOH:O	2.20	0.40
1:A:66:GLY:O	1:A:70:VAL:HB	2.20	0.40
1:A:427:GLU:N	1:A:427:GLU:CD	2.79	0.40
1:C:393:GLU:HB2	7:C:641:HOH:O	2.20	0.40
2:D:234:LEU:HD12	7:D:801:HOH:O	2.20	0.40
2:D:370:TRP:CE2	2:D:444:GLY:HA3	2.56	0.40
1:A:66:GLY:O	7:A:628:HOH:O	2.22	0.40
2:B:370:TRP:CE2	2:B:444:GLY:HA3	2.56	0.40
1:C:74:PRO:HB3	7:C:622:HOH:O	2.21	0.40
1:C:450:TYR:HB2	7:C:714:HOH:O	2.21	0.40
2:D:151:THR:HG23	2:D:162:LEU:HD11	2.03	0.40
2:D:365:LYS:N	7:D:702:HOH:O	2.22	0.40
2:D:483:THR:HG21	2:D:488:GLU:HG2	2.03	0.40
1:A:28:ARG:NH2	7:A:649:HOH:O	2.32	0.40
2:B:10:ALA:O	2:B:14:LEU:HB3	2.21	0.40
1:C:236:TRP:HD1	7:C:944:HOH:O	2.03	0.40
2:D:59:ARG:NE	7:D:711:HOH:O	2.39	0.40
2:D:327:GLU:HA	2:D:330:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/492 (97%)	460 (97%)	16 (3%)	0	100	100
1	C	476/492 (97%)	457 (96%)	19 (4%)	0	100	100
2	B	520/523 (99%)	510 (98%)	10 (2%)	0	100	100
2	D	520/523 (99%)	510 (98%)	10 (2%)	0	100	100
All	All	1992/2030 (98%)	1937 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	408/415 (98%)	404 (99%)	4 (1%)	68	75
1	C	407/415 (98%)	403 (99%)	4 (1%)	68	75
2	B	454/455 (100%)	450 (99%)	4 (1%)	70	77
2	D	454/455 (100%)	452 (100%)	2 (0%)	84	89
All	All	1723/1740 (99%)	1709 (99%)	14 (1%)	70	80

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	98	ASN
1	A	355	ILE
1	A	362	HIS
2	B	26	LYS
2	B	171	LYS
2	B	258	GLU
2	B	432	SER

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Mol	Chain	Res	Type
1	C	98	ASN
1	C	355	ILE
1	C	362	HIS
1	C	465	MET
2	D	175	ILE
2	D	432	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	98	ASN
1	A	321	GLN
2	B	53	GLN
2	B	93	GLN
2	B	163	ASN
1	C	321	GLN
1	C	468	ASN
2	D	18	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HCA	C	501	-	13,13,13	1.09	1 (7%)	15,18,18	1.28	1 (6%)
4	ICS	A	502	7,1	6,30,30	1.61	1 (16%)	-		
4	ICS	C	502	7,1	6,30,30	1.60	1 (16%)	-		
3	HCA	A	501	-	13,13,13	1.08	0	15,18,18	1.26	1 (6%)
6	CLF	D	601	2,1	0,24,24	-	-	-		
6	CLF	B	602	2,1	0,24,24	-	-	-		

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
6	CLF	D	601	2,1	-	-	0/12/10/10
3	HCA	C	501	-	-	5/17/17/17	-
6	CLF	B	602	2,1	-	-	0/12/10/10
3	HCA	A	501	-	-	5/17/17/17	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	ICS	S2B-FE6	-3.04	2.17	2.24
4	C	502	ICS	S2B-FE6	-3.03	2.17	2.24
3	C	501	HCA	C3-C7	-2.00	1.51	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	HCA	O6-C7-C3	2.78	118.47	113.14
3	A	501	HCA	O6-C7-C3	2.74	118.39	113.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

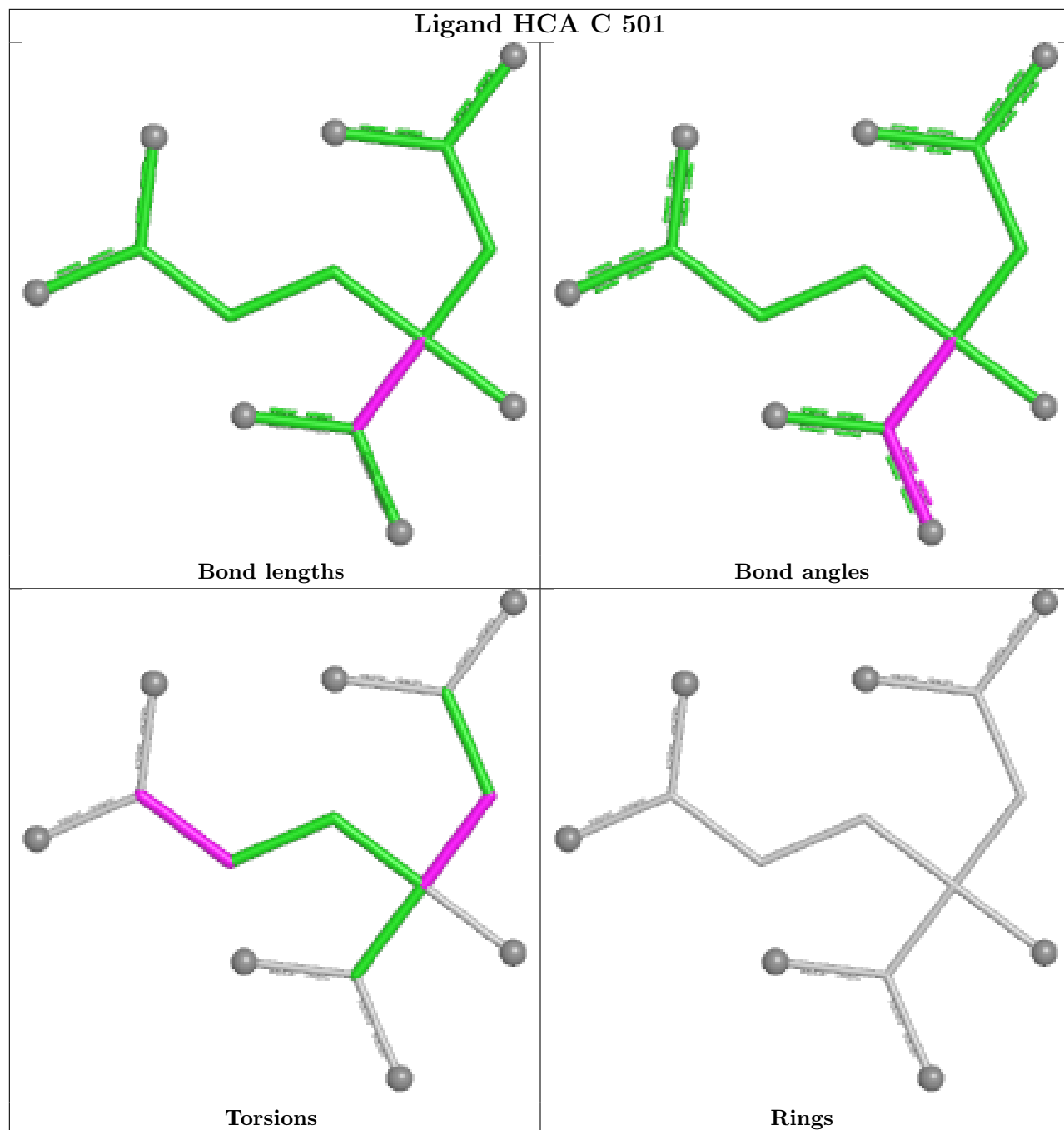
Mol	Chain	Res	Type	Atoms
3	A	501	HCA	C1-C2-C3-C7
3	A	501	HCA	C1-C2-C3-C4
3	C	501	HCA	C1-C2-C3-C7
3	A	501	HCA	C1-C2-C3-O7
3	C	501	HCA	C1-C2-C3-C4
3	C	501	HCA	C1-C2-C3-O7
3	A	501	HCA	C4-C5-C6-O3
3	C	501	HCA	C4-C5-C6-O3
3	A	501	HCA	C4-C5-C6-O4
3	C	501	HCA	C4-C5-C6-O4

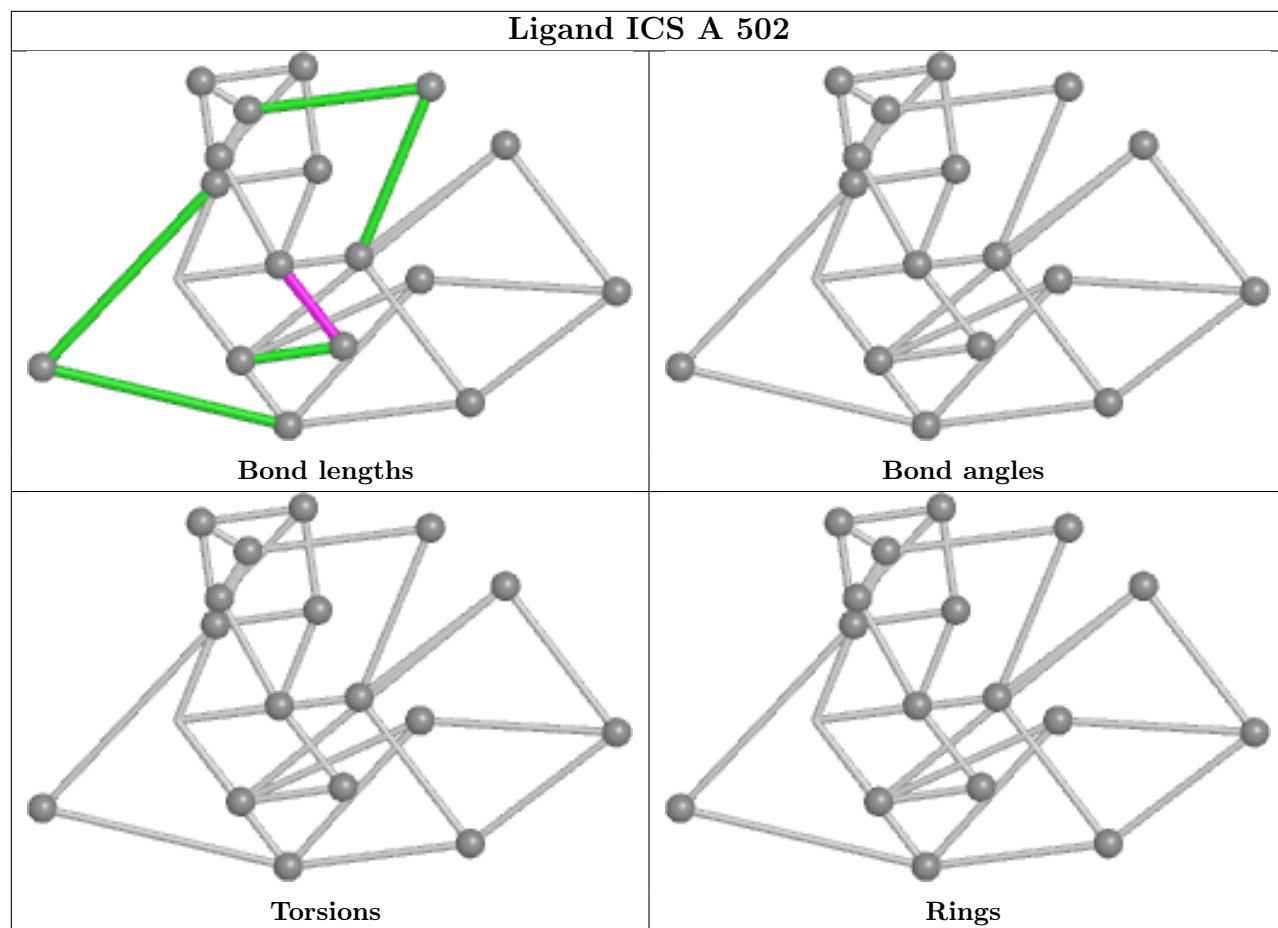
There are no ring outliers.

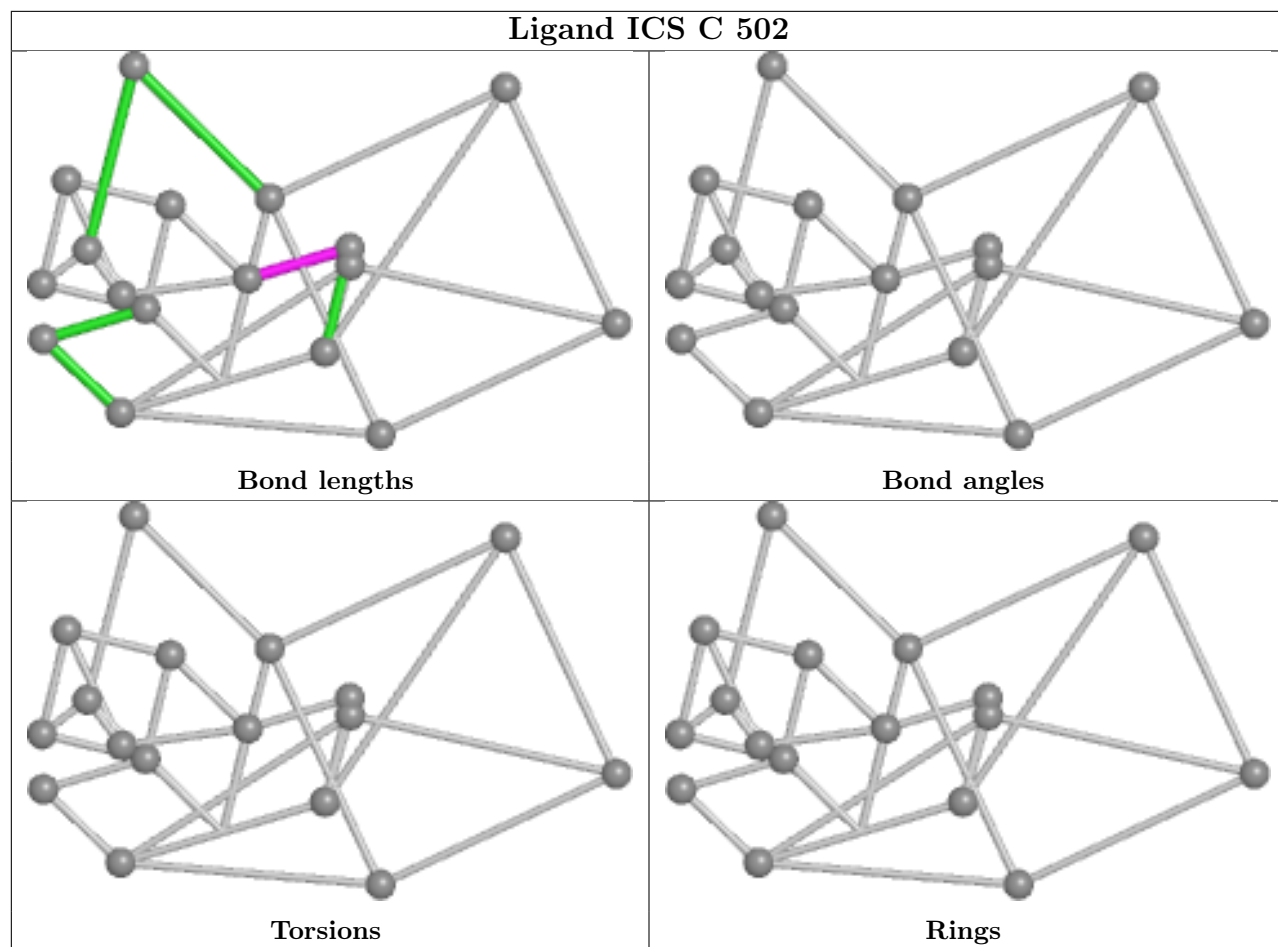
4 monomers are involved in 14 short contacts:

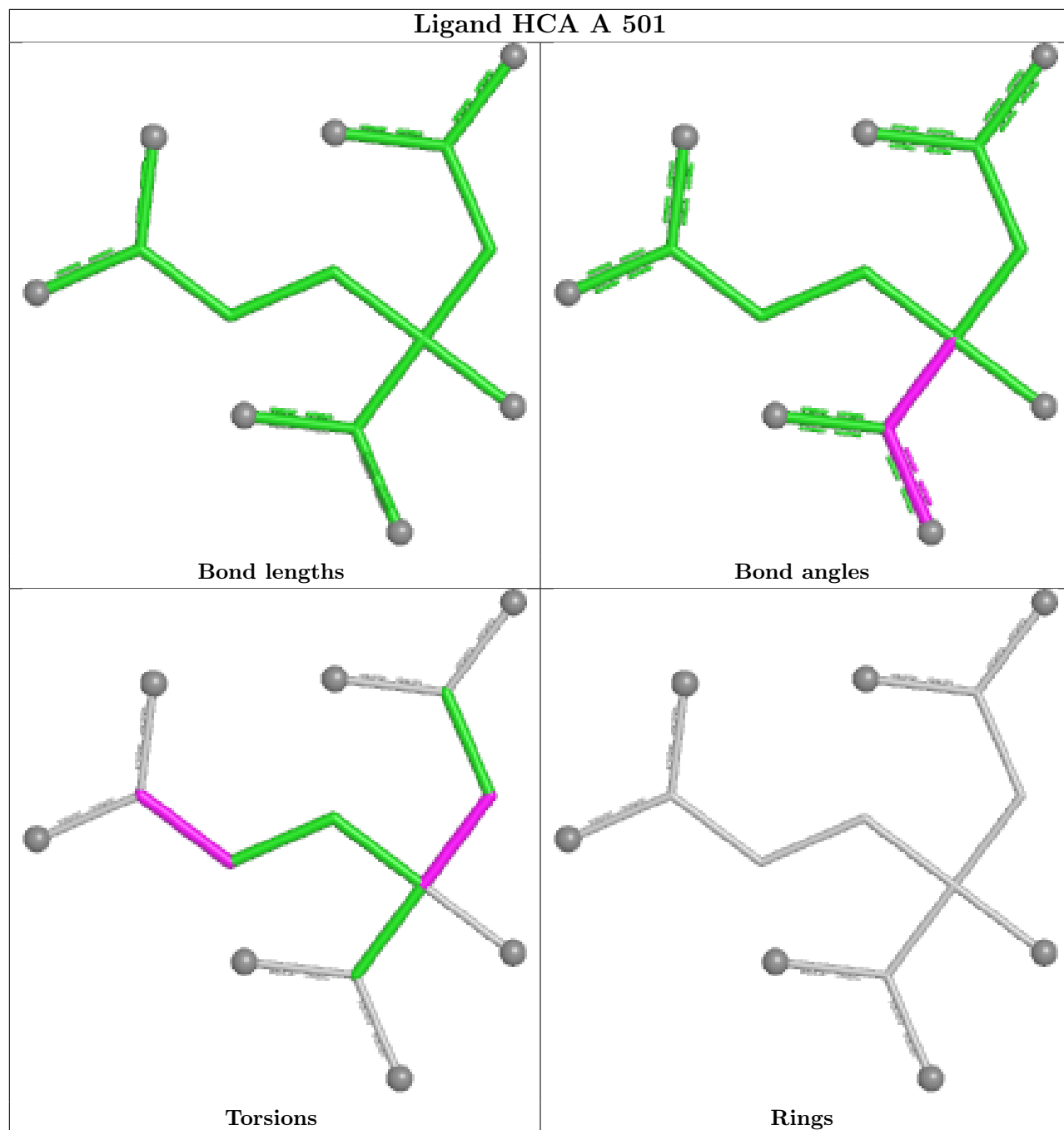
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	HCA	2	0
4	A	502	ICS	4	0
4	C	502	ICS	6	0
3	A	501	HCA	2	0

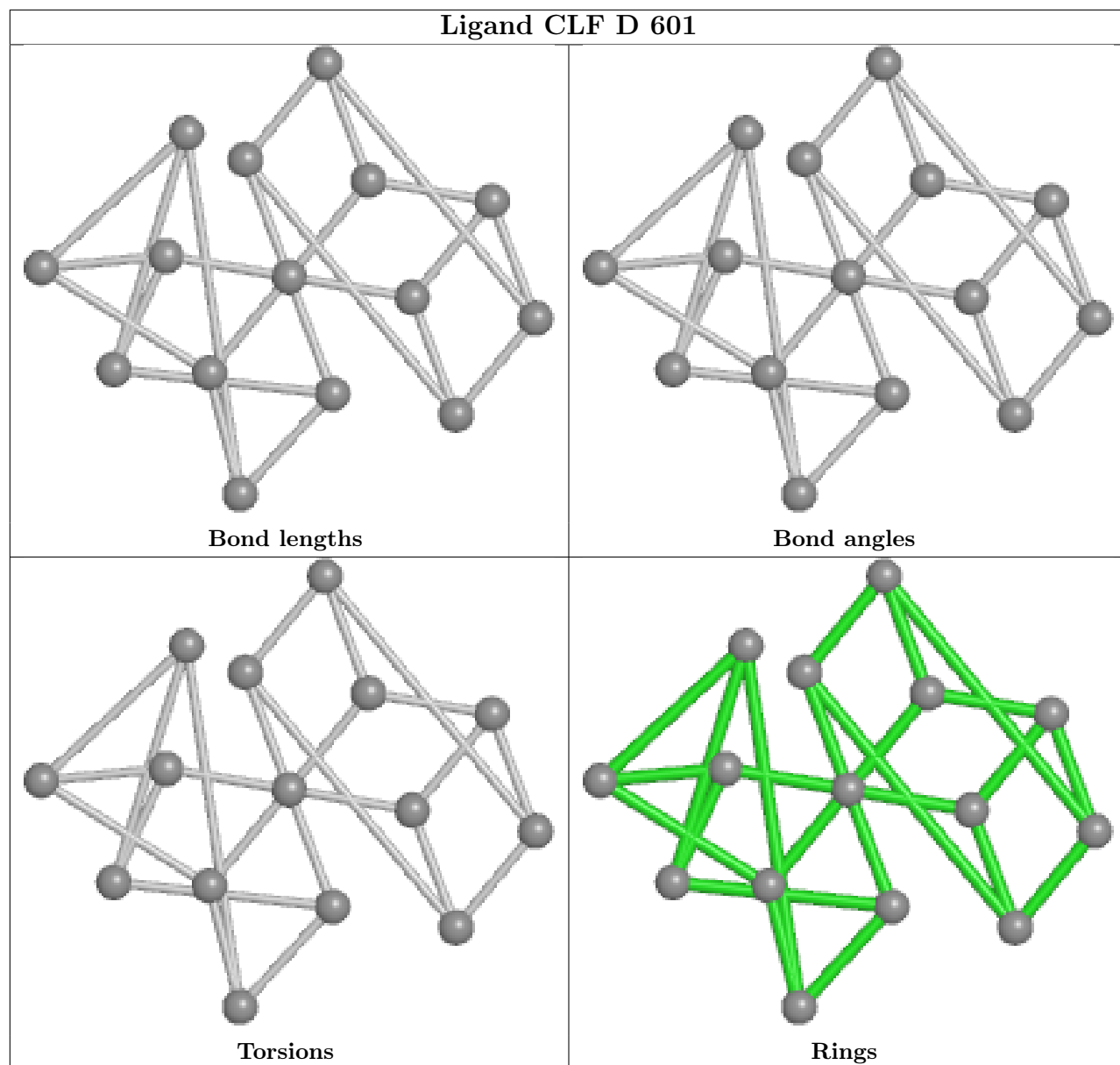
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

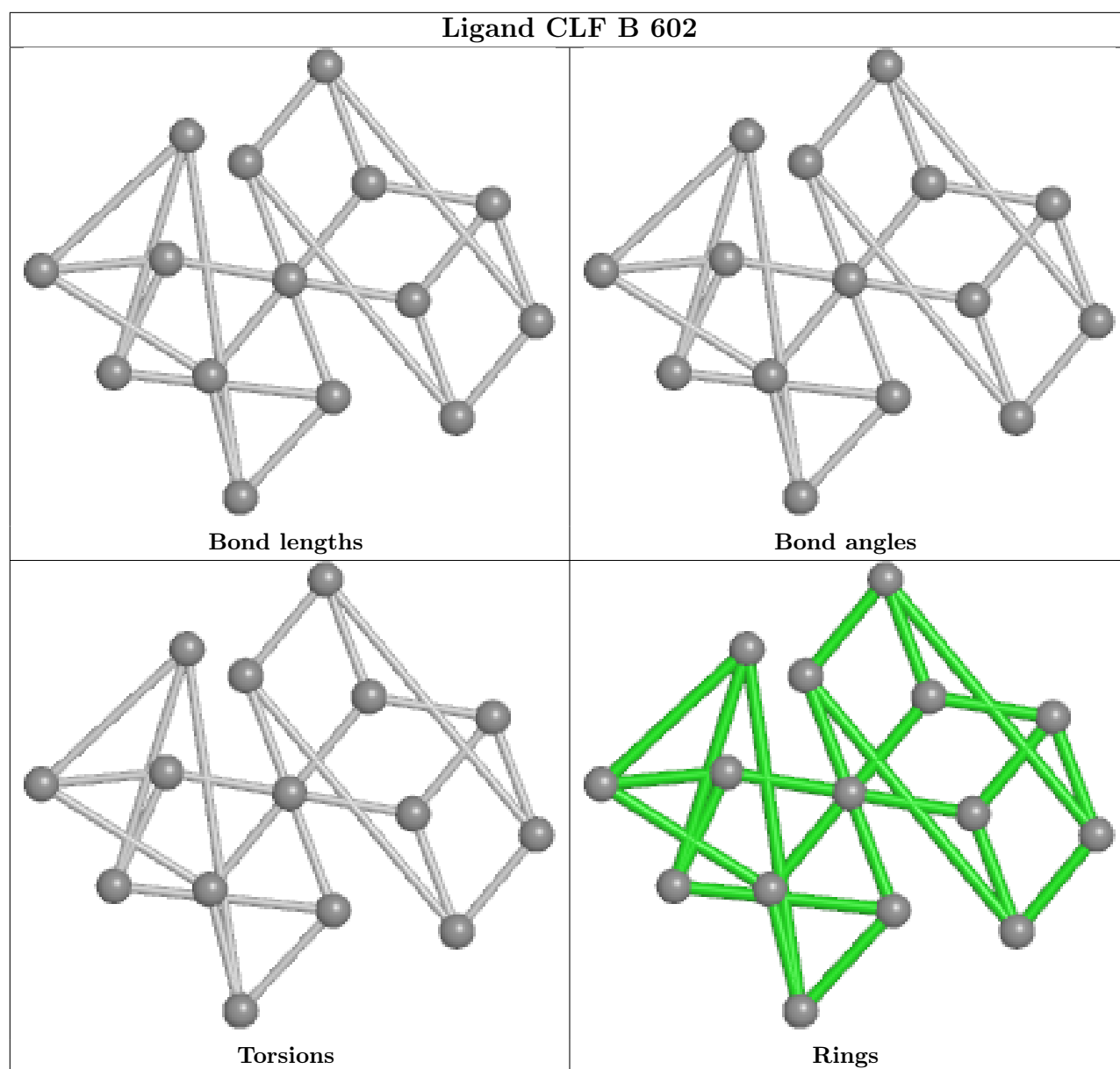












5.7 Other polymers [i](#)

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

This section contains visualisations of the EMDB entry EMD-45829. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.