



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:20 PM UTC

PDB ID : 6KZO / pdb_00006kzo
EMDB ID : EMD-0791
Title : membrane protein
Authors : Yan, N.
Deposited on : 2019-09-25
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

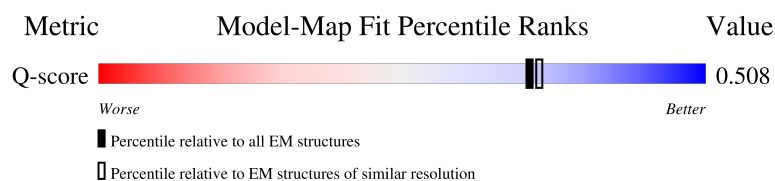
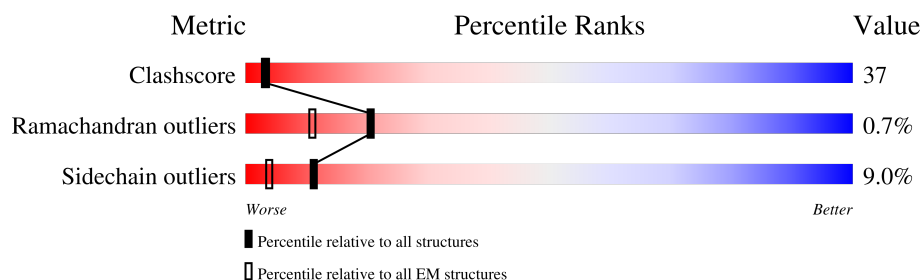
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	2261	26% 14% . 57%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8238 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.

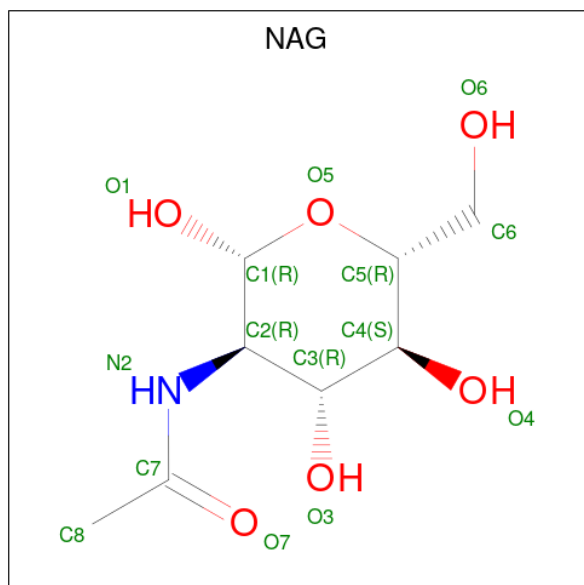
- Molecule 1 is a protein called Voltage-dependent T-type calcium channel subunit alpha-1G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	967	7739	5114	1248	1313	64	0	0

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

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Ca	0
			2	2	

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



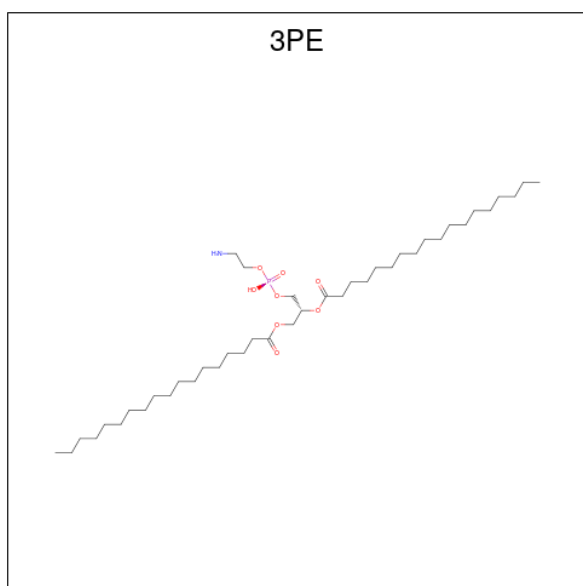
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



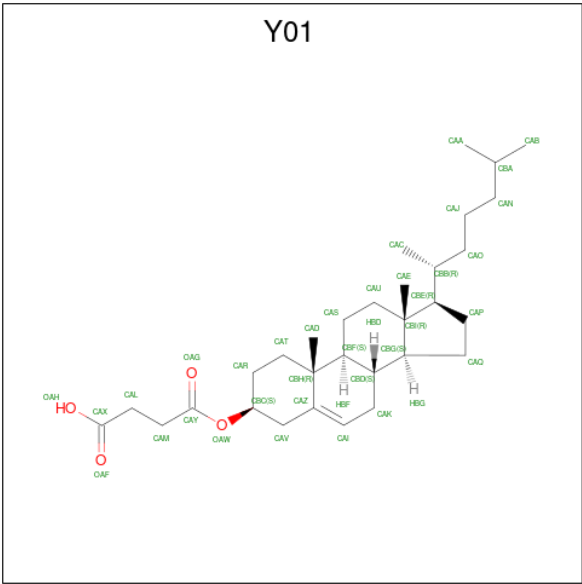
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
4	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
4	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
4	A	1	Total	C				0
			17	17				
4	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
4	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
4	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
4	A	1	Total	C	N	O	P	0
			39	29	1	8	1	

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Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	C	0
			17	17	
4	A	1	Total	C	0
			17	17	
4	A	1	Total	C	0
			14	14	
4	A	1	Total	C	0
			16	16	
4	A	1	Total	C	0
			17	17	

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			35	31	4	
5	A	1	Total	C	O	0
			35	31	4	



PRO	GLY	GLU	GLN	LYS	HIS	SER
SER	GLY	PRO	ALA	LEU	GLY	PRO
PRO	PRO	PRO	GLN	PRO	SER	LYS
LYS	GLY	SER	GLN	PRO	THR	PRO
ASP	ARG	ARG	SER	GLY	ALA	GLY
VAL	PRO	ASP	ARG	ARG	GLY	LEU
LEU	LYS	LEU	SER	SER	PRO	HIS
SER	LYS	LYS	HIS	PRO	LEU	ALA
LEU	LEU	LYS	SER	LEU	GLY	ALA
SER	LEU	CYS	LYS	ALA	HIS	ALA
GLY	SER	TYR	ILE	GLN	ARG	HIS
LEU	PRO	SER	SER	ARG	GLY	ALA
SER	PRO	VAL	LYS	PRO	THR	ARG
SER	PRO	GLU	HIS	LEU	SER	GLY
ASP	ILE	ALA	MET	ARG	LEU	ALA
PRO	THR	GLN	THR	ARG	PRO	SER
ALA	ILE	SER	PRO	GLN	LYS	HIS
ASP	ASP	CYS	PRO	ALA	ALA	PHE
LEU	PRO	GLN	ALA	ALA	GLN	SER
ASP	PRO	ARG	PRO	ILE	GLY	GLU
PRO	GLU	ARG	CYS	ARG	SER	HIS
	SER	PRO	PRO	THR	SER	PRO
	GLN	THR	GLY	ASP	VAL	PRO
	GLY	SER	PRO	SER	LEU	THR
	ARG	PRO	GLU	LEU	SER	MET
	THR	LEU	PRO	ASP	VAL	PRO
	PRO	GLU	TRP	GLN	SER	HIS
	PRO	GLN	GLY	GLY	GLN	PRO
	SER	ARG	LYS	LEU	PRO	THR
	GLY	HIS	PRO	SER	ASP	GLU
	ILE	SER	PRO	ARG	THR	PRO
	CYS	ILE	GLU	GLU	SER	GLY
	LEU	ALA	THR	ASP	TYR	PRO
	ARG	VAL	ARG	LEU	ILE	ASP
	ARG	SER	SER	LEU	LEU	LEU
	ALA	CYS	SER	ALA	GLN	LEU
	PRO	LEU	LEU	GLU	LEU	THR
	ALA	ASP	GLU	VAL	PRO	VAL
	SER	SER	LEU	SER	LYS	ARG
	SER	GLY	ASP	GLY	ASP	LYS
	ASP	SER	THR	PRO	ALA	SER
	SER	GLN	GLU	SER	GLY	GLY
	LYS	PRO	LEU	PRO	HIS	VAL
	ASP	HIS	SER	PRO	LEU	SER
	PRO	LEU	TRP	LEU	LEU	ARG
	LEU	GLY	ILE	ALA	GLN	THR
	THR	THR	SER	ARG	PRO	HIS
	ALA	THR	GLY	TYR	SER	LEU
	PRO	ASN	LEU	PHE	ALA	PRO
	ASP	LEU	PRO	THR	PRO	ASN
	SER	GLY	PRO	GLY	THR	ASP
	MET	GLN	GLY	SER	GLY	THR
	ALA	GLN	GLY	THR	THR	MET
	ALA	PRO	GLN	SER	ILE	CYS
	SER	ILE	THR	THR	DEU	ARG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105559	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	349.12, 349.12, 349.12	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.091, 1.091, 1.091	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: 3PE, Y01, CA, NAG

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	0.53	0/7904	0.86	14/10711 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ALA	N-CA-C	9.91	122.16	111.36
1	A	1674	VAL	N-CA-C	7.67	117.74	110.53
1	A	1447	ASP	N-CA-C	7.42	119.16	111.14
1	A	256	GLU	N-CA-C	7.31	119.25	111.28
1	A	327	GLU	N-CA-C	7.20	119.13	111.28
1	A	328	HIS	N-CA-C	6.91	121.10	109.76
1	A	199	ILE	N-CA-C	6.62	116.77	110.42
1	A	239	ASN	N-CA-C	6.55	119.25	110.35
1	A	1371	ARG	N-CA-C	6.23	118.15	111.36
1	A	379	ILE	N-CA-C	5.54	116.31	110.72
1	A	1673	GLU	N-CA-C	5.54	117.31	111.28
1	A	1412	LYS	N-CA-C	5.45	117.30	111.36
1	A	366	ALA	N-CA-C	5.12	116.95	111.36
1	A	1293	ILE	N-CA-C	5.09	115.32	110.53

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	7739	0	7919	592	0
2	A	2	0	0	0	0
3	A	70	0	65	7	0
4	A	357	0	508	52	0
5	A	70	0	98	17	0
All	All	8238	0	8590	620	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (620) 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:A:1420:GLY:HA3	1:A:1437:TYR:CD2	1.55	1.42
1:A:1672:ILE:HD12	1:A:1676:ALA:CB	1.64	1.26
1:A:1418:CYS:HB3	1:A:1439:TRP:CZ3	1.75	1.21
1:A:1672:ILE:CD1	1:A:1676:ALA:HB3	1.70	1.21
1:A:210:MET:HG2	1:A:397:GLN:NE2	1.57	1.19
4:A:2316:3PE:C31	5:A:2321:Y01:HBA	1.73	1.18
1:A:1417:VAL:HG11	1:A:1442:HIS:CE1	1.78	1.17
1:A:1272:MET:HE2	1:A:1287:LEU:HD21	1.23	1.15
1:A:184:VAL:O	1:A:187:PRO:HD2	1.45	1.14
1:A:200:LEU:CD1	1:A:871:LEU:HD23	1.77	1.14
1:A:1710:LEU:O	1:A:1713:VAL:HG12	1.48	1.14
1:A:217:LEU:HB2	1:A:1706:MET:HE3	1.15	1.12
1:A:820:TRP:CE3	1:A:833:LEU:HD11	1.86	1.11
1:A:217:LEU:CB	1:A:1706:MET:HE3	1.81	1.09
1:A:251:LEU:HD23	1:A:251:LEU:H	1.17	1.08
1:A:1626:ILE:O	1:A:1629:VAL:HG12	1.55	1.06
1:A:1419:GLN:HG3	1:A:1440:VAL:HG21	1.38	1.06
1:A:1672:ILE:CD1	1:A:1676:ALA:CB	2.32	1.05
1:A:197:MET:HE3	1:A:870:MET:HE2	1.37	1.04
1:A:210:MET:CB	1:A:397:GLN:HE22	1.69	1.03
1:A:1598:ILE:HD11	1:A:1698:LYS:CE	1.89	1.03
1:A:101:PHE:CE2	1:A:885:HIS:CD2	2.47	1.03
1:A:1420:GLY:HA3	1:A:1437:TYR:CE2	1.94	1.02
1:A:1419:GLN:CG	1:A:1440:VAL:HG21	1.90	1.02
1:A:1342:MET:HE3	1:A:1342:MET:HA	1.38	1.01
1:A:1420:GLY:CA	1:A:1437:TYR:HD2	1.73	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:GLY:CA	1:A:1437:TYR:CD2	2.43	1.00
1:A:101:PHE:CZ	1:A:885:HIS:CD2	2.48	1.00
1:A:197:MET:HE3	1:A:870:MET:CE	1.91	1.00
1:A:1417:VAL:HG11	1:A:1442:HIS:HE1	1.21	0.99
1:A:1712:THR:HG21	1:A:1830:HIS:CD2	1.96	0.99
1:A:1418:CYS:CB	1:A:1439:TRP:CE3	2.46	0.99
1:A:1417:VAL:CG1	1:A:1442:HIS:CE1	2.44	0.98
1:A:1418:CYS:HB3	1:A:1439:TRP:CE3	1.97	0.98
4:A:2313:3PE:C2A	4:A:2319:3PE:H3D1	1.93	0.98
1:A:1687:ILE:HG22	4:A:2312:3PE:H342	1.46	0.97
1:A:1598:ILE:HD11	1:A:1698:LYS:HE3	1.46	0.97
1:A:217:LEU:HB2	1:A:1706:MET:CE	1.94	0.97
1:A:1667:ILE:HG22	1:A:1671:GLU:OE2	1.65	0.95
1:A:194:VAL:HG11	1:A:870:MET:HE1	1.44	0.95
1:A:210:MET:CG	1:A:397:GLN:NE2	2.29	0.95
1:A:869:CYS:SG	4:A:2308:3PE:C29	2.55	0.95
1:A:1418:CYS:HB2	1:A:1439:TRP:HE3	1.32	0.94
1:A:200:LEU:CD1	1:A:871:LEU:CD2	2.46	0.94
1:A:200:LEU:HD13	1:A:871:LEU:CD2	1.98	0.93
1:A:1419:GLN:HG2	1:A:1440:VAL:CG2	1.99	0.93
1:A:1687:ILE:CG2	4:A:2312:3PE:H342	1.98	0.92
1:A:1333:ILE:O	1:A:1336:ILE:HG22	1.71	0.91
1:A:243:LEU:HD12	1:A:247:PHE:CE1	2.06	0.90
1:A:1687:ILE:HD12	1:A:1688:MET:N	1.87	0.90
1:A:125:PHE:HE1	1:A:163:GLY:HA3	1.36	0.90
1:A:128:PHE:CD2	1:A:189:ARG:NH1	2.40	0.89
1:A:279:MET:HE3	1:A:369:PHE:HB2	1.52	0.88
1:A:790:MET:O	1:A:794:LEU:HD23	1.73	0.88
1:A:945:ILE:HD13	4:A:2319:3PE:H3E2	1.56	0.88
1:A:125:PHE:CE1	1:A:163:GLY:HA3	2.07	0.87
1:A:1728:MET:HE1	1:A:1769:PHE:HZ	1.38	0.87
1:A:1419:GLN:HG2	1:A:1440:VAL:HG23	1.56	0.87
1:A:277:ASN:O	1:A:368:SER:HA	1.75	0.86
1:A:1419:GLN:CG	1:A:1440:VAL:CG2	2.53	0.86
1:A:1272:MET:HE2	1:A:1287:LEU:CD2	2.04	0.86
1:A:213:ASN:OD1	1:A:1705:GLY:C	2.20	0.84
4:A:2308:3PE:H122	4:A:2316:3PE:H3E2	1.58	0.84
5:A:2321:Y01:HAA2	5:A:2321:Y01:HAO2	1.57	0.84
1:A:858:LEU:HD11	1:A:1507:ASN:ND2	1.92	0.84
1:A:1426:ILE:HD11	1:A:1431:ASP:C	2.02	0.83
1:A:1418:CYS:HB2	1:A:1439:TRP:CE3	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:NH1	1:A:113:ARG:HB3	1.93	0.83
1:A:1418:CYS:HB3	1:A:1439:TRP:HZ3	1.39	0.82
1:A:1595:THR:HB	1:A:1702:MET:HE3	1.60	0.82
1:A:1616:LEU:HD23	1:A:1620:LEU:CD2	2.10	0.82
1:A:1420:GLY:HA3	1:A:1437:TYR:HD2	1.03	0.82
1:A:155:LEU:HD23	1:A:155:LEU:O	1.80	0.82
1:A:1375:LEU:HD23	1:A:1375:LEU:O	1.79	0.82
1:A:217:LEU:CB	1:A:1706:MET:CE	2.55	0.81
4:A:2313:3PE:C2A	4:A:2319:3PE:C3D	2.58	0.81
1:A:115:ARG:CZ	1:A:115:ARG:HA	2.11	0.81
4:A:2309:3PE:O14	4:A:2315:3PE:H232	1.80	0.81
1:A:128:PHE:CE2	1:A:189:ARG:NH1	2.49	0.81
1:A:210:MET:CG	1:A:397:GLN:HE22	1.91	0.81
1:A:210:MET:HB2	1:A:397:GLN:HE22	1.45	0.81
1:A:101:PHE:CZ	1:A:885:HIS:HD2	1.96	0.80
1:A:1426:ILE:HD12	1:A:1431:ASP:CG	2.07	0.80
1:A:1831:LEU:HD13	1:A:1831:LEU:O	1.82	0.80
1:A:1258:VAL:O	1:A:1261:VAL:HG12	1.82	0.80
1:A:1710:LEU:O	1:A:1713:VAL:CG1	2.28	0.79
1:A:1418:CYS:CB	1:A:1439:TRP:CZ3	2.61	0.79
1:A:1766:GLY:HA3	4:A:2314:3PE:O22	1.82	0.79
1:A:1333:ILE:O	1:A:1336:ILE:CG2	2.31	0.79
1:A:1716:ALA:HA	1:A:1829:LYS:HD2	1.64	0.79
1:A:1601:ASN:OD1	1:A:1695:ARG:HD3	1.83	0.79
1:A:1687:ILE:HG22	4:A:2312:3PE:H362	1.64	0.79
1:A:217:LEU:CA	1:A:1706:MET:HE3	2.12	0.79
1:A:1404:GLY:O	1:A:1408:VAL:HG23	1.83	0.78
1:A:858:LEU:CD1	1:A:1507:ASN:ND2	2.46	0.78
1:A:165:LEU:HD23	1:A:165:LEU:O	1.84	0.78
1:A:1672:ILE:O	1:A:1676:ALA:HB3	1.84	0.78
5:A:2322:Y01:HAC1	5:A:2322:Y01:HAU2	1.66	0.78
1:A:1416:PHE:HD2	1:A:1439:TRP:CD1	2.01	0.78
1:A:1716:ALA:CA	1:A:1829:LYS:HD2	2.13	0.78
1:A:113:ARG:HB3	1:A:113:ARG:HH11	1.49	0.78
1:A:210:MET:CB	1:A:397:GLN:NE2	2.47	0.78
1:A:243:LEU:HD12	1:A:247:PHE:CZ	2.18	0.77
1:A:1272:MET:CE	1:A:1287:LEU:HD21	2.10	0.77
1:A:1687:ILE:HG22	4:A:2312:3PE:C36	2.15	0.77
1:A:783:THR:CG2	1:A:818:SER:OG	2.32	0.76
1:A:197:MET:CE	1:A:870:MET:HE2	2.14	0.76
1:A:200:LEU:HD11	1:A:871:LEU:HD23	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PHE:O	1:A:160:VAL:CG1	2.34	0.76
1:A:256:GLU:O	1:A:257:ARG:CB	2.32	0.76
1:A:1669:LEU:O	1:A:1672:ILE:HG22	1.86	0.76
1:A:1421:GLU:H	1:A:1437:TYR:HE2	1.34	0.75
1:A:1299:LEU:HD13	1:A:1299:LEU:O	1.85	0.75
1:A:200:LEU:HD22	1:A:204:LEU:HD13	1.67	0.75
1:A:1667:ILE:CG2	1:A:1671:GLU:OE2	2.35	0.75
3:A:2306:NAG:O5	3:A:2306:NAG:H82	1.87	0.75
1:A:115:ARG:HA	1:A:115:ARG:NE	2.02	0.74
1:A:907:ASP:OD1	1:A:907:ASP:N	2.21	0.74
1:A:1728:MET:SD	4:A:2317:3PE:H3E2	2.28	0.74
1:A:878:ILE:O	1:A:881:ILE:HG22	1.87	0.74
4:A:2316:3PE:H331	5:A:2321:Y01:HAN1	1.69	0.74
1:A:1728:MET:HE1	1:A:1769:PHE:CZ	2.22	0.74
1:A:1324:ASN:H	1:A:1324:ASN:HD22	1.34	0.74
1:A:1709:LEU:C	1:A:1709:LEU:HD23	2.13	0.74
1:A:1421:GLU:N	1:A:1437:TYR:HE2	1.85	0.74
1:A:1712:THR:HG21	1:A:1830:HIS:CG	2.22	0.73
1:A:962:ILE:HD12	1:A:1506:LEU:HD21	1.70	0.73
1:A:1672:ILE:CD1	1:A:1676:ALA:HB1	2.17	0.73
1:A:1350:ILE:HD12	1:A:1350:ILE:N	2.03	0.73
1:A:217:LEU:C	1:A:217:LEU:HD23	2.13	0.73
1:A:945:ILE:CD1	4:A:2319:3PE:H3E2	2.18	0.73
1:A:1673:GLU:HG2	1:A:1679:PRO:HG3	1.70	0.73
1:A:1717:LEU:HD13	1:A:1717:LEU:C	2.14	0.73
1:A:1687:ILE:HG22	4:A:2312:3PE:C34	2.17	0.73
1:A:157:PHE:O	1:A:160:VAL:HG12	1.89	0.72
1:A:922:GLN:HE22	4:A:2320:3PE:C3H	2.02	0.72
1:A:1284:ARG:HE	1:A:1284:ARG:HA	1.52	0.72
1:A:1672:ILE:HD12	1:A:1672:ILE:O	1.89	0.72
1:A:1406:LEU:HD23	1:A:1406:LEU:O	1.88	0.72
1:A:279:MET:HE3	1:A:369:PHE:CD1	2.24	0.72
1:A:1326:LEU:HD13	1:A:1326:LEU:O	1.90	0.72
4:A:2310:3PE:O22	4:A:2311:3PE:H361	1.89	0.72
1:A:204:LEU:CD1	1:A:957:ASN:HD22	2.03	0.72
1:A:1506:LEU:HD12	1:A:1506:LEU:O	1.89	0.72
1:A:1672:ILE:HD12	1:A:1676:ALA:HB3	0.81	0.71
1:A:329:ASN:HB3	1:A:330:PRO:HD2	1.69	0.71
1:A:1272:MET:HE1	1:A:1287:LEU:HG	1.72	0.71
1:A:1836:LYS:NZ	1:A:1836:LYS:HB3	2.04	0.71
1:A:200:LEU:HD22	1:A:200:LEU:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:HB3	1:A:326:GLY:O	1.90	0.71
1:A:1389:ILE:HD12	1:A:1389:ILE:C	2.16	0.71
1:A:1323:TRP:NE1	1:A:1376:LYS:HE3	2.05	0.71
1:A:210:MET:HG2	1:A:397:GLN:HE21	1.52	0.70
1:A:1502:ALA:HB1	4:A:2308:3PE:H32	1.73	0.70
1:A:1693:ILE:O	1:A:1696:VAL:HG12	1.91	0.70
1:A:873:MET:HE3	1:A:873:MET:HA	1.73	0.70
1:A:1598:ILE:CD1	1:A:1698:LYS:HE3	2.21	0.70
1:A:881:ILE:O	1:A:881:ILE:HD13	1.91	0.70
1:A:204:LEU:HD11	1:A:957:ASN:HD22	1.56	0.70
1:A:783:THR:HG23	1:A:818:SER:OG	1.91	0.70
1:A:871:LEU:HD12	1:A:871:LEU:O	1.92	0.70
1:A:1342:MET:HE3	1:A:1342:MET:CA	2.20	0.70
1:A:1601:ASN:OD1	1:A:1695:ARG:CD	2.38	0.70
1:A:330:PRO:HD2	1:A:335:ILE:O	1.92	0.70
1:A:1824:ILE:O	1:A:1828:MET:CE	2.40	0.70
1:A:1728:MET:CE	1:A:1769:PHE:HZ	2.06	0.69
1:A:329:ASN:HB3	1:A:330:PRO:CD	2.22	0.69
1:A:213:ASN:OD1	1:A:1706:MET:N	2.25	0.69
1:A:184:VAL:O	1:A:187:PRO:CD	2.34	0.69
1:A:211:LEU:HD22	1:A:214:VAL:HG11	1.75	0.69
1:A:864:ASN:ND2	1:A:965:GLU:HG3	2.08	0.69
1:A:1445:ASN:C	1:A:1445:ASN:HD22	2.01	0.68
1:A:279:MET:CE	1:A:369:PHE:CD1	2.77	0.68
4:A:2316:3PE:C31	5:A:2321:Y01:CBA	2.63	0.68
1:A:186:ARG:HB2	1:A:187:PRO:HD3	1.74	0.68
1:A:1359:LEU:HD12	1:A:1740:GLU:HG2	1.75	0.68
1:A:118:GLN:C	1:A:118:GLN:HE21	2.00	0.68
1:A:389:LEU:HD21	1:A:1709:LEU:HD21	1.74	0.68
1:A:1388:PRO:HG3	1:A:1515:GLU:OE2	1.94	0.68
1:A:166:GLU:HA	1:A:179:VAL:HG21	1.76	0.67
1:A:1420:GLY:CA	1:A:1437:TYR:CE2	2.72	0.67
1:A:1697:LEU:O	1:A:1700:LEU:HB2	1.95	0.67
1:A:1716:ALA:HB2	1:A:1829:LYS:HB3	1.77	0.67
1:A:165:LEU:HD23	1:A:165:LEU:C	2.19	0.67
1:A:217:LEU:HA	1:A:1706:MET:CE	2.23	0.67
1:A:1333:ILE:C	1:A:1336:ILE:HG22	2.20	0.67
1:A:904:LYS:HD3	1:A:918:GLN:HE22	1.60	0.67
1:A:1299:LEU:HD13	1:A:1299:LEU:C	2.19	0.67
1:A:1616:LEU:CD2	1:A:1620:LEU:CD2	2.73	0.67
1:A:1399:PHE:CD2	1:A:1500:ILE:HD12	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1324:ASN:H	1:A:1324:ASN:ND2	1.93	0.66
5:A:2321:Y01:HAB3	5:A:2321:Y01:CAO	2.26	0.66
1:A:858:LEU:HD11	1:A:1507:ASN:CG	2.20	0.66
1:A:1616:LEU:HD23	1:A:1620:LEU:HD23	1.77	0.66
1:A:1828:MET:O	1:A:1832:GLU:HG2	1.94	0.66
1:A:1342:MET:HA	1:A:1342:MET:CE	2.22	0.66
1:A:1369:ILE:HG23	1:A:1375:LEU:HD22	1.77	0.66
1:A:1669:LEU:O	1:A:1672:ILE:CG2	2.44	0.66
1:A:1684:ILE:HD12	1:A:1684:ILE:N	2.11	0.66
1:A:200:LEU:HD22	1:A:200:LEU:C	2.21	0.66
1:A:223:PHE:CE1	1:A:227:ILE:HD11	2.31	0.65
1:A:279:MET:HE3	1:A:369:PHE:CB	2.24	0.65
1:A:1284:ARG:NH1	1:A:1287:LEU:CD1	2.60	0.65
1:A:279:MET:CE	1:A:369:PHE:HB2	2.25	0.65
5:A:2321:Y01:HAU2	5:A:2321:Y01:HAC1	1.78	0.65
1:A:1681:ASN:HB3	1:A:1684:ILE:HD13	1.78	0.65
1:A:1426:ILE:HD11	1:A:1432:CYS:N	2.11	0.64
1:A:1459:LEU:HD13	1:A:1465:TRP:HB2	1.79	0.64
1:A:1716:ALA:HB2	1:A:1829:LYS:CB	2.27	0.64
1:A:112:GLN:O	1:A:116:ILE:HG13	1.98	0.64
1:A:783:THR:HG21	1:A:818:SER:OG	1.96	0.64
1:A:1621:LYS:HZ3	1:A:1621:LYS:HB2	1.63	0.64
1:A:881:ILE:CD1	1:A:885:HIS:CE1	2.81	0.64
1:A:243:LEU:HD12	1:A:247:PHE:HE1	1.61	0.64
1:A:90:VAL:HG22	1:A:124:ILE:HG23	1.80	0.64
1:A:280:ARG:HH11	1:A:1758:ARG:NE	1.96	0.64
1:A:910:LEU:HB2	4:A:2309:3PE:H12	1.80	0.64
1:A:1323:TRP:CD1	1:A:1376:LYS:HE3	2.33	0.64
1:A:249:LEU:CD2	1:A:249:LEU:H	2.10	0.63
1:A:1692:ARG:O	1:A:1695:ARG:HG2	1.98	0.63
1:A:256:GLU:O	1:A:257:ARG:HB2	1.97	0.63
1:A:1416:PHE:CD2	1:A:1439:TRP:CD1	2.86	0.63
1:A:197:MET:HE3	1:A:870:MET:HE3	1.78	0.63
1:A:395:ALA:HB2	1:A:960:VAL:HG22	1.80	0.63
1:A:1272:MET:CE	1:A:1287:LEU:CD2	2.75	0.63
1:A:1712:THR:CG2	1:A:1830:HIS:CD2	2.80	0.63
1:A:223:PHE:CE1	1:A:1602:VAL:HG13	2.34	0.63
1:A:1836:LYS:HB3	1:A:1836:LYS:HZ1	1.63	0.63
1:A:753:ILE:O	1:A:757:THR:HG23	1.99	0.62
1:A:1673:GLU:OE1	1:A:1674:VAL:N	2.32	0.62
1:A:1272:MET:CE	1:A:1287:LEU:CG	2.76	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:HD21	1:A:159:ILE:HD11	1.81	0.62
1:A:1417:VAL:HG12	1:A:1442:HIS:CE1	2.34	0.62
1:A:199:ILE:N	1:A:199:ILE:HD13	2.15	0.62
1:A:1628:THR:HG21	1:A:1667:ILE:CD1	2.30	0.62
1:A:241:CYS:HB3	1:A:320:TYR:HB3	1.82	0.62
1:A:1284:ARG:HH11	1:A:1287:LEU:CD1	2.11	0.62
1:A:1598:ILE:CD1	1:A:1698:LYS:CE	2.74	0.62
1:A:1284:ARG:HA	1:A:1284:ARG:NE	2.15	0.61
1:A:396:THR:HG21	1:A:1830:HIS:CE1	2.36	0.61
1:A:155:LEU:HD23	1:A:155:LEU:C	2.25	0.61
1:A:157:PHE:C	1:A:160:VAL:HG12	2.25	0.61
1:A:864:ASN:HD22	1:A:965:GLU:HG3	1.65	0.61
1:A:1624:ASN:OD1	1:A:1692:ARG:NH2	2.33	0.61
1:A:1284:ARG:NH1	1:A:1287:LEU:HD12	2.15	0.61
1:A:1343:VAL:HG12	1:A:1343:VAL:O	2.00	0.61
1:A:211:LEU:HD13	4:A:2320:3PE:H381	1.83	0.61
1:A:1684:ILE:O	1:A:1687:ILE:HG13	2.00	0.61
1:A:1284:ARG:HH11	1:A:1287:LEU:HD12	1.65	0.60
1:A:251:LEU:H	1:A:251:LEU:CD2	1.94	0.60
1:A:1824:ILE:O	1:A:1828:MET:HE2	2.01	0.60
5:A:2321:Y01:HAB3	5:A:2321:Y01:HAO1	1.83	0.60
1:A:251:LEU:HD23	1:A:251:LEU:N	2.02	0.60
1:A:1375:LEU:HD23	1:A:1375:LEU:C	2.27	0.60
1:A:1624:ASN:HD22	1:A:1624:ASN:C	2.05	0.60
1:A:1684:ILE:HD12	1:A:1684:ILE:H	1.66	0.60
1:A:1734:PHE:HD1	1:A:1807:TYR:HE1	1.47	0.60
1:A:762:ILE:HG22	1:A:762:ILE:O	2.02	0.60
1:A:1364:ARG:HB2	1:A:1365:PRO:HD3	1.84	0.60
1:A:1517:PHE:CE1	1:A:1828:MET:SD	2.95	0.60
1:A:1697:LEU:HA	1:A:1700:LEU:HD13	1.84	0.60
1:A:1734:PHE:HD1	1:A:1807:TYR:CE1	2.19	0.60
1:A:1326:LEU:HD13	1:A:1326:LEU:C	2.26	0.59
1:A:1272:MET:CE	1:A:1287:LEU:HG	2.32	0.59
1:A:1681:ASN:OD1	1:A:1682:PRO:HD2	2.02	0.59
1:A:766:GLU:OE1	1:A:766:GLU:HA	2.03	0.59
1:A:910:LEU:HD12	4:A:2309:3PE:O22	2.03	0.59
1:A:1767:MET:CE	4:A:2314:3PE:O14	2.51	0.59
1:A:215:LEU:O	1:A:215:LEU:HD23	2.03	0.58
1:A:1373:GLN:HA	1:A:1373:GLN:OE1	2.03	0.58
1:A:217:LEU:CA	1:A:1706:MET:CE	2.78	0.58
3:A:2306:NAG:H82	3:A:2306:NAG:C5	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1725:LEU:HD13	1:A:1725:LEU:O	2.03	0.58
1:A:280:ARG:HH11	1:A:1758:ARG:CZ	2.17	0.58
1:A:125:PHE:HZ	1:A:164:MET:N	2.01	0.58
1:A:870:MET:HG3	4:A:2309:3PE:C3F	2.34	0.58
1:A:385:PHE:HE1	1:A:1713:VAL:HG21	1.68	0.58
5:A:2321:Y01:HAA2	5:A:2321:Y01:CAO	2.24	0.58
1:A:157:PHE:O	1:A:160:VAL:HG13	2.02	0.58
1:A:1256:ASP:OD1	1:A:1256:ASP:N	2.37	0.58
1:A:1687:ILE:HG23	4:A:2312:3PE:H342	1.83	0.58
1:A:208:LEU:HD12	4:A:2320:3PE:H352	1.86	0.57
1:A:287:THR:HG23	1:A:315:ASN:HD22	1.69	0.57
1:A:217:LEU:HA	1:A:1706:MET:HE1	1.85	0.57
1:A:253:VAL:HG11	1:A:316:TRP:CZ2	2.38	0.57
1:A:1383:MET:SD	1:A:1383:MET:N	2.77	0.57
1:A:1351:LEU:N	1:A:1351:LEU:HD22	2.20	0.57
1:A:873:MET:HA	1:A:873:MET:CE	2.32	0.57
1:A:1667:ILE:O	1:A:1671:GLU:HG3	2.05	0.57
3:A:2306:NAG:H83	3:A:2306:NAG:H3	1.86	0.57
1:A:186:ARG:N	1:A:187:PRO:HD2	2.19	0.57
1:A:1767:MET:HE2	4:A:2314:3PE:O14	2.05	0.57
1:A:1616:LEU:HD23	1:A:1620:LEU:HD22	1.87	0.57
3:A:2306:NAG:H3	3:A:2306:NAG:C8	2.35	0.57
1:A:132:MET:SD	1:A:160:VAL:HG11	2.44	0.56
1:A:1411:PHE:CD1	1:A:1446:PHE:HD2	2.23	0.56
3:A:2306:NAG:H82	3:A:2306:NAG:C4	2.35	0.56
1:A:820:TRP:CZ3	1:A:833:LEU:HD11	2.38	0.56
1:A:101:PHE:CZ	1:A:885:HIS:NE2	2.73	0.56
1:A:155:LEU:CD2	1:A:159:ILE:HD11	2.35	0.56
1:A:332:LYS:HG2	1:A:934:ALA:CB	2.36	0.56
1:A:1366:LEU:O	1:A:1369:ILE:HG13	2.06	0.56
1:A:1385:SER:O	1:A:1388:PRO:HD2	2.05	0.56
1:A:1766:GLY:CA	4:A:2314:3PE:O22	2.53	0.56
4:A:2308:3PE:C12	4:A:2316:3PE:H3E2	2.32	0.56
1:A:255:LEU:HD11	1:A:316:TRP:CD1	2.41	0.56
1:A:1833:GLU:HA	1:A:1833:GLU:OE1	2.05	0.56
1:A:236:LEU:CD1	1:A:367:HIS:HB2	2.36	0.56
1:A:279:MET:HE3	1:A:369:PHE:CG	2.41	0.56
1:A:1265:LEU:HD12	1:A:1294:PHE:HZ	1.71	0.56
1:A:1425:ASN:OD1	3:A:2305:NAG:O5	2.22	0.56
1:A:820:TRP:CE3	1:A:833:LEU:CD1	2.76	0.55
1:A:256:GLU:O	1:A:257:ARG:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1746:GLU:O	1:A:1790:ARG:NH1	2.40	0.55
1:A:204:LEU:HD21	1:A:954:VAL:HG12	1.87	0.55
1:A:1672:ILE:HD13	1:A:1676:ALA:CB	2.31	0.55
1:A:231:GLN:OE1	1:A:231:GLN:HA	2.06	0.55
1:A:1361:ARG:HG2	1:A:1364:ARG:HE	1.70	0.55
1:A:1831:LEU:HD13	1:A:1831:LEU:C	2.32	0.55
1:A:396:THR:HG21	1:A:1830:HIS:HE1	1.72	0.55
1:A:1406:LEU:HD23	1:A:1406:LEU:C	2.32	0.55
1:A:223:PHE:CE2	1:A:1693:ILE:HD11	2.42	0.55
1:A:1832:GLU:OE1	1:A:1832:GLU:HA	2.07	0.55
1:A:200:LEU:HD21	1:A:868:PHE:CE1	2.41	0.54
1:A:1450:GLY:O	5:A:2321:Y01:HAD2	2.06	0.54
1:A:887:PHE:HA	1:A:890:LYS:HD3	1.88	0.54
1:A:1284:ARG:HE	1:A:1284:ARG:CA	2.18	0.54
1:A:374:TYR:CD1	1:A:374:TYR:C	2.85	0.54
1:A:1272:MET:HE3	1:A:1287:LEU:HD11	1.90	0.54
1:A:280:ARG:NH1	1:A:1758:ARG:NE	2.55	0.54
1:A:820:TRP:HE3	1:A:833:LEU:HD11	1.60	0.54
1:A:1410:LEU:O	1:A:1414:LYS:NZ	2.39	0.54
1:A:1399:PHE:HD2	1:A:1500:ILE:HD12	1.71	0.54
1:A:1628:THR:OG1	1:A:1667:ILE:HD11	2.08	0.54
1:A:1739:VAL:HG23	1:A:1762:PHE:O	2.08	0.54
1:A:793:LYS:NZ	1:A:846:ARG:HH22	2.06	0.54
1:A:1364:ARG:N	1:A:1365:PRO:HD2	2.23	0.54
1:A:332:LYS:HG2	1:A:934:ALA:HB2	1.90	0.53
1:A:1284:ARG:HH11	1:A:1287:LEU:HB2	1.73	0.53
1:A:364:MET:HA	1:A:368:SER:O	2.08	0.53
1:A:1672:ILE:HD11	1:A:1677:SER:HB3	1.91	0.53
1:A:858:LEU:HD12	1:A:1507:ASN:ND2	2.22	0.53
1:A:884:MET:HE3	1:A:907:ASP:O	2.09	0.53
3:A:2306:NAG:C8	3:A:2306:NAG:C3	2.85	0.53
1:A:875:PHE:CD1	1:A:875:PHE:C	2.87	0.53
1:A:118:GLN:HE21	1:A:118:GLN:CA	2.22	0.53
1:A:125:PHE:CZ	1:A:163:GLY:C	2.87	0.53
1:A:1684:ILE:H	1:A:1684:ILE:CD1	2.22	0.53
1:A:1774:ARG:HH21	1:A:1780:ASN:HB3	1.74	0.53
5:A:2322:Y01:HAC1	5:A:2322:Y01:CAU	2.37	0.53
4:A:2309:3PE:O14	4:A:2315:3PE:C23	2.54	0.52
1:A:200:LEU:HD13	1:A:871:LEU:HD22	1.89	0.52
1:A:1269:THR:OG1	1:A:1287:LEU:HD23	2.09	0.52
1:A:224:ILE:HG21	4:A:2312:3PE:H2E2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:LEU:CD1	1:A:1507:ASN:CG	2.81	0.52
1:A:1399:PHE:CE2	1:A:1500:ILE:HD12	2.45	0.52
1:A:1657:LEU:C	1:A:1657:LEU:HD23	2.34	0.52
1:A:1359:LEU:CD1	1:A:1740:GLU:HG2	2.37	0.52
1:A:1279:PRO:O	1:A:1284:ARG:HG2	2.10	0.52
1:A:158:PHE:HA	1:A:161:ILE:HD11	1.90	0.52
1:A:1426:ILE:HD11	1:A:1432:CYS:CA	2.40	0.52
1:A:1672:ILE:HD13	1:A:1676:ALA:HB1	1.87	0.52
1:A:1727:PHE:CE1	1:A:1819:LEU:CD2	2.93	0.52
1:A:118:GLN:CA	1:A:118:GLN:NE2	2.73	0.52
1:A:350:VAL:HG11	1:A:378:LEU:HD23	1.91	0.52
1:A:1628:THR:HG21	1:A:1667:ILE:HD12	1.90	0.52
1:A:157:PHE:HA	1:A:160:VAL:CG1	2.40	0.51
1:A:188:LEU:HD21	1:A:878:ILE:CD1	2.40	0.51
1:A:204:LEU:CD1	1:A:957:ASN:ND2	2.71	0.51
1:A:1698:LYS:C	1:A:1700:LEU:H	2.17	0.51
1:A:1387:LYS:N	1:A:1388:PRO:HD2	2.26	0.51
1:A:1777:THR:HG22	4:A:2318:3PE:H3A2	1.92	0.51
1:A:194:VAL:HG11	1:A:870:MET:CE	2.30	0.51
1:A:249:LEU:H	1:A:249:LEU:HD22	1.75	0.51
1:A:1389:ILE:HD12	1:A:1389:ILE:O	2.10	0.51
1:A:118:GLN:NE2	1:A:118:GLN:O	2.28	0.51
1:A:1351:LEU:N	1:A:1351:LEU:CD2	2.74	0.51
1:A:186:ARG:N	1:A:187:PRO:CD	2.74	0.51
1:A:380:ILE:HG22	4:A:2318:3PE:H372	1.93	0.51
1:A:882:LEU:O	1:A:882:LEU:HD12	2.10	0.51
1:A:249:LEU:CD2	1:A:249:LEU:N	2.73	0.51
1:A:1411:PHE:HB3	1:A:1414:LYS:HB2	1.93	0.51
1:A:904:LYS:CD	1:A:918:GLN:HE22	2.23	0.51
1:A:1492:LEU:HD12	4:A:2315:3PE:H282	1.93	0.51
1:A:118:GLN:NE2	1:A:118:GLN:HA	2.25	0.51
1:A:197:MET:HE2	1:A:870:MET:HG2	1.92	0.51
1:A:872:LEU:HD12	1:A:872:LEU:O	2.10	0.51
1:A:1621:LYS:HZ3	1:A:1621:LYS:CB	2.20	0.50
1:A:115:ARG:NE	1:A:115:ARG:CA	2.73	0.50
1:A:1600:LEU:HD13	1:A:1600:LEU:O	2.11	0.50
1:A:1714:MET:SD	1:A:1714:MET:C	2.94	0.50
1:A:1364:ARG:N	1:A:1365:PRO:CD	2.74	0.50
1:A:1711:ASP:OD1	1:A:1712:THR:N	2.45	0.50
4:A:2313:3PE:C2A	4:A:2319:3PE:H3D2	2.40	0.50
1:A:179:VAL:O	1:A:182:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:CD2	1:A:204:LEU:HD13	2.40	0.50
1:A:1369:ILE:HG21	1:A:1379:VAL:HG21	1.92	0.50
1:A:1665:MET:O	1:A:1669:LEU:HG	2.12	0.50
1:A:125:PHE:CZ	1:A:164:MET:N	2.78	0.50
1:A:1426:ILE:HD11	1:A:1432:CYS:HA	1.94	0.50
1:A:215:LEU:HD12	4:A:2320:3PE:H351	1.93	0.50
1:A:1604:THR:HA	1:A:1607:MET:CG	2.42	0.50
1:A:1697:LEU:O	1:A:1700:LEU:HD13	2.12	0.50
1:A:204:LEU:HG	1:A:957:ASN:ND2	2.27	0.50
1:A:1598:ILE:HD11	1:A:1698:LYS:NZ	2.26	0.50
1:A:1629:VAL:HG13	1:A:1630:ILE:N	2.27	0.50
1:A:181:THR:O	1:A:184:VAL:HG13	2.12	0.50
1:A:764:TYR:CD1	1:A:764:TYR:C	2.90	0.50
1:A:1604:THR:HA	1:A:1607:MET:HG3	1.94	0.50
1:A:330:PRO:CD	1:A:335:ILE:O	2.60	0.49
1:A:1324:ASN:ND2	1:A:1324:ASN:N	2.60	0.49
1:A:277:ASN:O	1:A:368:SER:CA	2.56	0.49
1:A:1406:LEU:C	1:A:1406:LEU:CD2	2.85	0.49
1:A:1601:ASN:O	1:A:1601:ASN:ND2	2.44	0.49
1:A:91:ILE:HG21	1:A:190:ALA:HB2	1.94	0.49
1:A:186:ARG:CB	1:A:187:PRO:HD3	2.40	0.49
1:A:398:PHE:HD2	1:A:964:VAL:HG21	1.78	0.49
1:A:1284:ARG:NH1	1:A:1287:LEU:HD13	2.26	0.49
1:A:1366:LEU:HD11	1:A:1733:ILE:HD13	1.94	0.49
1:A:1448:ASN:ND2	5:A:2321:Y01:OAH	2.45	0.49
1:A:1727:PHE:CE1	1:A:1819:LEU:HD21	2.46	0.49
1:A:864:ASN:OD1	1:A:864:ASN:N	2.45	0.49
1:A:1326:LEU:C	1:A:1326:LEU:CD1	2.86	0.49
1:A:881:ILE:HD13	1:A:881:ILE:C	2.38	0.48
1:A:393:VAL:HG21	1:A:1709:LEU:HD11	1.95	0.48
1:A:1487:ASN:HD21	4:A:2310:3PE:H12	1.77	0.48
1:A:910:LEU:HD12	4:A:2309:3PE:H12	1.94	0.48
1:A:1487:ASN:ND2	4:A:2310:3PE:H12	2.27	0.48
1:A:1827:LEU:O	1:A:1831:LEU:HB2	2.13	0.48
1:A:134:VAL:O	1:A:137:VAL:HB	2.13	0.48
1:A:1369:ILE:HG23	1:A:1375:LEU:CD2	2.41	0.48
1:A:755:VAL:O	1:A:759:SER:HB2	2.14	0.48
1:A:157:PHE:HA	1:A:160:VAL:HG12	1.95	0.48
1:A:197:MET:HG3	1:A:870:MET:HE2	1.94	0.48
1:A:1351:LEU:CD2	1:A:1351:LEU:H	2.25	0.48
1:A:1416:PHE:HD2	1:A:1439:TRP:NE1	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1591:ASP:O	1:A:1595:THR:HG22	2.14	0.48
1:A:1453:LEU:HD23	5:A:2321:Y01:HAE3	1.96	0.48
1:A:123:PHE:CD1	1:A:123:PHE:C	2.91	0.47
1:A:904:LYS:HD3	1:A:918:GLN:NE2	2.29	0.47
1:A:200:LEU:C	1:A:200:LEU:CD2	2.85	0.47
1:A:1259:VAL:HG11	1:A:1371:ARG:HE	1.78	0.47
1:A:923:GLU:CD	1:A:1464:GLY:H	2.21	0.47
1:A:1506:LEU:HD12	1:A:1506:LEU:C	2.39	0.47
1:A:1714:MET:HG3	1:A:1715:GLN:N	2.28	0.47
1:A:1687:ILE:HG22	4:A:2312:3PE:C35	2.44	0.47
1:A:342:TYR:CE2	4:A:2319:3PE:H341	2.50	0.47
1:A:844:LEU:O	1:A:848:LEU:HD22	2.14	0.47
1:A:1684:ILE:N	1:A:1684:ILE:CD1	2.77	0.47
1:A:1701:LYS:HE3	1:A:1701:LYS:HB2	1.73	0.47
1:A:208:LEU:N	1:A:208:LEU:CD2	2.77	0.47
1:A:165:LEU:C	1:A:165:LEU:CD2	2.85	0.47
1:A:200:LEU:CD1	1:A:871:LEU:HD22	2.42	0.47
1:A:1621:LYS:HG2	1:A:1622:ILE:HD13	1.96	0.47
1:A:1698:LYS:C	1:A:1700:LEU:N	2.73	0.47
1:A:397:GLN:O	1:A:397:GLN:HG3	2.15	0.47
1:A:157:PHE:CA	1:A:160:VAL:HG12	2.45	0.47
1:A:223:PHE:CZ	1:A:1602:VAL:HG13	2.50	0.47
1:A:1389:ILE:C	1:A:1389:ILE:CD1	2.85	0.47
1:A:155:LEU:C	1:A:155:LEU:CD2	2.87	0.46
1:A:1717:LEU:HD22	1:A:1717:LEU:O	2.16	0.46
1:A:1601:ASN:OD1	1:A:1695:ARG:HD2	2.15	0.46
1:A:1624:ASN:C	1:A:1624:ASN:ND2	2.73	0.46
1:A:1628:THR:HG21	1:A:1667:ILE:HD11	1.96	0.46
1:A:1299:LEU:C	1:A:1299:LEU:CD1	2.85	0.46
1:A:101:PHE:HZ	1:A:885:HIS:HD2	1.56	0.46
1:A:249:LEU:N	1:A:249:LEU:HD23	2.30	0.46
1:A:764:TYR:O	1:A:765:HIS:C	2.59	0.46
1:A:873:MET:HE3	1:A:873:MET:CA	2.39	0.46
1:A:1333:ILE:CA	1:A:1336:ILE:HG22	2.46	0.46
1:A:369:PHE:CG	1:A:369:PHE:O	2.69	0.46
1:A:1303:THR:HA	1:A:1306:VAL:HG12	1.97	0.45
1:A:367:HIS:O	1:A:371:ASN:ND2	2.50	0.45
1:A:1687:ILE:HD12	1:A:1687:ILE:C	2.40	0.45
1:A:186:ARG:HB2	1:A:187:PRO:CD	2.44	0.45
1:A:1333:ILE:HA	1:A:1336:ILE:HG22	1.98	0.45
1:A:241:CYS:O	1:A:258:TYR:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLU:HG3	1:A:260:GLN:CD	2.42	0.45
1:A:962:ILE:CD1	1:A:1506:LEU:HD21	2.43	0.45
1:A:1495:ILE:HG21	4:A:2315:3PE:H2C2	1.98	0.45
1:A:371:ASN:N	1:A:371:ASN:HD22	2.15	0.45
1:A:881:ILE:CD1	1:A:885:HIS:HE1	2.28	0.45
1:A:1265:LEU:HD22	1:A:1268:ILE:HD12	1.99	0.45
1:A:1284:ARG:NE	1:A:1284:ARG:CA	2.79	0.45
1:A:1450:GLY:O	5:A:2321:Y01:CAD	2.65	0.45
1:A:97:THR:HA	1:A:117:LEU:CD1	2.46	0.45
1:A:287:THR:CG2	1:A:315:ASN:HD22	2.29	0.45
1:A:369:PHE:CD1	1:A:369:PHE:O	2.70	0.45
1:A:1601:ASN:ND2	1:A:1601:ASN:C	2.73	0.45
1:A:1388:PRO:HG3	1:A:1515:GLU:HG2	1.99	0.45
1:A:200:LEU:HD12	1:A:871:LEU:HD23	1.87	0.45
1:A:211:LEU:CD2	1:A:214:VAL:HG11	2.45	0.45
1:A:780:ILE:HD13	1:A:780:ILE:HA	1.77	0.45
1:A:871:LEU:HD12	1:A:871:LEU:C	2.42	0.45
1:A:1601:ASN:C	1:A:1601:ASN:HD22	2.19	0.45
1:A:1824:ILE:O	1:A:1828:MET:HE3	2.17	0.45
1:A:917:PHE:HE1	4:A:2308:3PE:H241	1.82	0.45
1:A:1333:ILE:O	1:A:1336:ILE:HG23	2.15	0.45
1:A:1380:GLU:N	1:A:1380:GLU:OE1	2.50	0.45
1:A:1728:MET:SD	4:A:2317:3PE:H3C2	2.57	0.45
1:A:188:LEU:CD2	1:A:878:ILE:HD11	2.47	0.44
1:A:394:ILE:HG23	1:A:960:VAL:HG21	1.99	0.44
1:A:764:TYR:CD1	1:A:765:HIS:O	2.69	0.44
1:A:881:ILE:HD11	1:A:885:HIS:CE1	2.52	0.44
1:A:1414:LYS:HB3	1:A:1475:ALA:HB1	1.98	0.44
1:A:90:VAL:HG11	1:A:127:PHE:CE1	2.51	0.44
1:A:200:LEU:HD12	1:A:871:LEU:CD2	2.43	0.44
1:A:255:LEU:CD1	1:A:316:TRP:CG	2.99	0.44
1:A:1266:ASN:O	1:A:1266:ASN:ND2	2.51	0.44
1:A:1272:MET:CE	1:A:1287:LEU:HD11	2.47	0.44
1:A:1389:ILE:HG21	1:A:1508:MET:O	2.17	0.44
1:A:1416:PHE:CD2	1:A:1439:TRP:NE1	2.86	0.44
1:A:158:PHE:O	1:A:158:PHE:CD1	2.70	0.44
1:A:1486:HIS:CE1	4:A:2310:3PE:H111	2.53	0.44
1:A:1621:LYS:HB2	1:A:1621:LYS:NZ	2.28	0.44
4:A:2316:3PE:H3F2	4:A:2318:3PE:C3F	2.48	0.44
1:A:1451:GLN:HE21	5:A:2321:Y01:CAX	2.31	0.44
1:A:1612:GLN:NE2	1:A:1617:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PHE:O	1:A:247:PHE:CD1	2.70	0.44
1:A:764:TYR:CD1	1:A:764:TYR:O	2.70	0.44
1:A:1517:PHE:HZ	1:A:1831:LEU:HG	1.82	0.44
1:A:200:LEU:HD13	1:A:871:LEU:HD23	1.59	0.44
1:A:279:MET:CE	1:A:369:PHE:CG	3.00	0.44
1:A:1411:PHE:HA	1:A:1414:LYS:HD3	2.00	0.43
1:A:1687:ILE:CG2	4:A:2312:3PE:H362	2.43	0.43
1:A:80:ASN:HB2	1:A:83:PHE:H	1.82	0.43
1:A:1672:ILE:HD12	1:A:1672:ILE:C	2.42	0.43
1:A:256:GLU:HG3	1:A:260:GLN:NE2	2.33	0.43
1:A:1598:ILE:HD11	1:A:1698:LYS:HE2	1.93	0.43
1:A:836:PHE:C	1:A:838:LEU:N	2.76	0.43
1:A:1375:LEU:C	1:A:1375:LEU:CD2	2.91	0.43
1:A:1411:PHE:HD1	1:A:1446:PHE:HD2	1.63	0.43
5:A:2321:Y01:HAO2	5:A:2321:Y01:HAB3	1.98	0.43
1:A:1621:LYS:HG2	1:A:1622:ILE:CD1	2.48	0.43
1:A:764:TYR:O	1:A:764:TYR:CG	2.70	0.43
1:A:1342:MET:HE2	1:A:1342:MET:O	2.18	0.43
1:A:1673:GLU:CD	1:A:1673:GLU:C	2.86	0.43
1:A:125:PHE:CE1	1:A:163:GLY:CA	2.91	0.43
1:A:155:LEU:O	1:A:159:ILE:HG13	2.19	0.43
1:A:847:PHE:C	1:A:848:LEU:HD13	2.43	0.43
1:A:881:ILE:CD1	1:A:881:ILE:C	2.92	0.43
1:A:907:ASP:HB2	1:A:908:SER:H	1.63	0.43
1:A:1669:LEU:C	1:A:1672:ILE:HG22	2.43	0.43
1:A:817:ILE:HG23	1:A:833:LEU:HD22	2.00	0.42
1:A:1323:TRP:CD1	1:A:1376:LYS:CE	3.01	0.42
1:A:158:PHE:CD1	1:A:158:PHE:C	2.97	0.42
1:A:1828:MET:HE2	1:A:1828:MET:N	2.35	0.42
1:A:1799:TYR:HD1	1:A:1799:TYR:HA	1.70	0.42
1:A:113:ARG:H	1:A:113:ARG:HG2	1.56	0.42
1:A:120:PHE:O	1:A:124:ILE:HG13	2.18	0.42
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.80	0.42
1:A:1445:ASN:C	1:A:1445:ASN:ND2	2.73	0.42
1:A:1709:LEU:C	1:A:1709:LEU:CD2	2.86	0.42
1:A:1719:GLN:HA	1:A:1719:GLN:OE1	2.18	0.42
1:A:357:VAL:HG13	1:A:361:TYR:CZ	2.54	0.42
1:A:881:ILE:HD12	1:A:885:HIS:CE1	2.55	0.42
1:A:791:LEU:C	1:A:791:LEU:HD13	2.44	0.42
1:A:1681:ASN:HB3	1:A:1684:ILE:CD1	2.46	0.42
1:A:186:ARG:CB	1:A:187:PRO:CD	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ILE:N	1:A:199:ILE:CD1	2.83	0.42
1:A:208:LEU:CD1	4:A:2320:3PE:H352	2.49	0.42
1:A:223:PHE:CE1	1:A:227:ILE:CD1	3.02	0.42
1:A:1600:LEU:CD1	1:A:1600:LEU:C	2.92	0.42
1:A:1677:SER:OG	1:A:1678:LEU:N	2.53	0.42
1:A:1710:LEU:HA	1:A:1710:LEU:HD23	1.81	0.42
1:A:1389:ILE:O	1:A:1393:VAL:HG23	2.19	0.42
1:A:1716:ALA:CB	1:A:1829:LYS:HD2	2.50	0.42
1:A:208:LEU:N	1:A:208:LEU:HD22	2.34	0.42
1:A:236:LEU:HD23	1:A:236:LEU:HA	1.73	0.42
1:A:1517:PHE:CZ	1:A:1831:LEU:HG	2.55	0.42
1:A:842:LEU:HA	1:A:842:LEU:HD12	1.81	0.42
1:A:909:LEU:O	1:A:912:ALA:N	2.41	0.42
1:A:1723:LEU:HD13	1:A:1723:LEU:HA	1.88	0.42
1:A:217:LEU:HD23	1:A:217:LEU:O	2.19	0.41
1:A:1607:MET:HE3	1:A:1607:MET:HB3	1.95	0.41
1:A:97:THR:HA	1:A:117:LEU:HD11	2.01	0.41
1:A:105:GLU:N	1:A:105:GLU:OE1	2.53	0.41
1:A:204:LEU:HG	1:A:957:ASN:HD21	1.85	0.41
1:A:269:PHE:CE2	1:A:280:ARG:NH2	2.85	0.41
1:A:367:HIS:O	1:A:367:HIS:CG	2.70	0.41
1:A:1323:TRP:NE1	1:A:1376:LYS:CE	2.81	0.41
1:A:1662:LEU:O	1:A:1688:MET:HE3	2.20	0.41
1:A:1831:LEU:C	1:A:1831:LEU:CD1	2.93	0.41
1:A:791:LEU:HD13	1:A:791:LEU:O	2.21	0.41
1:A:1418:CYS:O	1:A:1418:CYS:SG	2.78	0.41
1:A:1695:ARG:HE	1:A:1695:ARG:HB3	1.68	0.41
1:A:1717:LEU:HD13	1:A:1717:LEU:O	2.20	0.41
1:A:901:PRO:HB2	1:A:905:ASN:HD22	1.85	0.41
1:A:1621:LYS:NZ	1:A:1670:GLU:CD	2.78	0.41
1:A:1717:LEU:C	1:A:1717:LEU:CD1	2.85	0.41
1:A:244:PRO:HD2	1:A:247:PHE:HE1	1.85	0.41
1:A:805:ASN:HA	1:A:806:PRO:HD3	1.85	0.41
1:A:1342:MET:CA	1:A:1342:MET:CE	2.92	0.41
1:A:1426:ILE:HD12	1:A:1431:ASP:CB	2.50	0.41
1:A:158:PHE:HA	1:A:161:ILE:CD1	2.51	0.41
1:A:188:LEU:CD2	1:A:878:ILE:CD1	2.99	0.41
1:A:1500:ILE:O	1:A:1504:PHE:CD2	2.73	0.41
1:A:1709:LEU:HD23	1:A:1709:LEU:O	2.19	0.41
4:A:2314:3PE:C32	4:A:2314:3PE:O21	2.69	0.41
1:A:855:LEU:HD23	1:A:855:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:LEU:CD1	4:A:2309:3PE:H12	2.51	0.41
1:A:948:MET:HE3	1:A:948:MET:HB3	1.92	0.41
1:A:1624:ASN:ND2	1:A:1624:ASN:O	2.40	0.41
1:A:1629:VAL:CG1	1:A:1630:ILE:N	2.84	0.41
1:A:185:LEU:HD22	1:A:188:LEU:HD12	2.03	0.41
1:A:965:GLU:HA	1:A:965:GLU:OE1	2.21	0.41
1:A:1284:ARG:O	1:A:1288:THR:HG23	2.20	0.41
1:A:1422:ASP:HB2	1:A:1437:TYR:OH	2.21	0.41
1:A:1595:THR:CB	1:A:1702:MET:HE3	2.43	0.41
1:A:227:ILE:O	1:A:231:GLN:HG2	2.21	0.40
1:A:1462:LYS:HE3	1:A:1498:LEU:HD22	2.02	0.40
1:A:155:LEU:HD23	1:A:159:ILE:HG13	2.02	0.40
1:A:329:ASN:OD1	1:A:336:ASN:ND2	2.54	0.40
1:A:1377:LEU:HA	1:A:1377:LEU:HD13	1.68	0.40
1:A:1517:PHE:HE1	1:A:1828:MET:SD	2.42	0.40
1:A:387:ILE:HG21	4:A:2320:3PE:H3G2	2.04	0.40
1:A:1426:ILE:CD1	1:A:1431:ASP:CG	2.87	0.40
5:A:2321:Y01:HAO2	5:A:2321:Y01:HAP2	1.95	0.40
1:A:1774:ARG:NH2	1:A:1780:ASN:HB3	2.36	0.40
1:A:1717:LEU:HB3	1:A:1718:PRO:HD3	2.04	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	941/2261 (42%)	903 (96%)	31 (3%)	7 (1%)	18 49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ARG

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Mol	Chain	Res	Type
1	A	907	ASP
1	A	765	HIS
1	A	837	ARG
1	A	107	ILE
1	A	763	GLU
1	A	764	TYR

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	855/1946 (44%)	778 (91%)	77 (9%)	9 31

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	113	ARG
1	A	115	ARG
1	A	133	VAL
1	A	164	MET
1	A	184	VAL
1	A	199	ILE
1	A	200	LEU
1	A	202	THR
1	A	203	LEU
1	A	206	ASP
1	A	218	CYS
1	A	237	LEU
1	A	240	ARG
1	A	249	LEU
1	A	251	LEU
1	A	271	CYS
1	A	283	ARG
1	A	285	VAL
1	A	288	LEU

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Mol	Chain	Res	Type
1	A	318	GLN
1	A	332	LYS
1	A	368	SER
1	A	374	TYR
1	A	377	LEU
1	A	397	GLN
1	A	759	SER
1	A	764	TYR
1	A	775	LEU
1	A	777	ILE
1	A	780	ILE
1	A	848	LEU
1	A	861	THR
1	A	864	ASN
1	A	872	LEU
1	A	881	ILE
1	A	907	ASP
1	A	908	SER
1	A	1259	VAL
1	A	1265	LEU
1	A	1324	ASN
1	A	1326	LEU
1	A	1342	MET
1	A	1350	ILE
1	A	1351	LEU
1	A	1377	LEU
1	A	1380	GLU
1	A	1383	MET
1	A	1411	PHE
1	A	1418	CYS
1	A	1445	ASN
1	A	1462	LYS
1	A	1463	ASP
1	A	1506	LEU
1	A	1507	ASN
1	A	1515	GLU
1	A	1595	THR
1	A	1600	LEU
1	A	1604	THR
1	A	1620	LEU
1	A	1621	LYS
1	A	1622	ILE

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Mol	Chain	Res	Type
1	A	1623	CYS
1	A	1672	ILE
1	A	1674	VAL
1	A	1684	ILE
1	A	1685	ILE
1	A	1701	LYS
1	A	1712	THR
1	A	1714	MET
1	A	1717	LEU
1	A	1723	LEU
1	A	1725	LEU
1	A	1739	VAL
1	A	1799	TYR
1	A	1828	MET
1	A	1831	LEU

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

Mol	Chain	Res	Type
1	A	112	GLN
1	A	118	GLN
1	A	349	GLN
1	A	371	ASN
1	A	388	ASN
1	A	397	GLN
1	A	773	ASN
1	A	852	GLN
1	A	885	HIS
1	A	922	GLN
1	A	957	ASN
1	A	1266	ASN
1	A	1291	ASN
1	A	1324	ASN
1	A	1409	GLN
1	A	1419	GLN
1	A	1442	HIS
1	A	1448	ASN
1	A	1486	HIS
1	A	1507	ASN
1	A	1516	ASN
1	A	1722	ASN
1	A	1780	ASN

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Mol	Chain	Res	Type
1	A	1830	HIS

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 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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$
4	3PE	A	2310	-	34,34,50	1.19	2 (5%)	37,39,55	1.22	4 (10%)
3	NAG	A	2304	1	14,14,15	0.23	0	17,19,21	0.53	0
3	NAG	A	2306	1	14,14,15	0.43	0	17,19,21	1.59	4 (23%)
4	3PE	A	2312	-	43,43,50	1.05	2 (4%)	46,48,55	1.03	4 (8%)
4	3PE	A	2313	-	34,34,50	1.14	2 (5%)	37,39,55	1.11	2 (5%)
4	3PE	A	2318	-	13,13,50	0.23	0	12,12,55	0.61	0
4	3PE	A	2308	-	30,30,50	1.24	2 (6%)	33,35,55	1.09	3 (9%)
5	Y01	A	2321	-	38,38,38	4.24	12 (31%)	57,57,57	2.37	20 (35%)
4	3PE	A	2309	-	37,37,50	1.10	2 (5%)	40,42,55	1.07	3 (7%)
3	NAG	A	2305	1	14,14,15	0.29	0	17,19,21	0.57	0
4	3PE	A	2320	-	16,16,50	0.24	0	15,15,55	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	Y01	A	2322	-	38,38,38	4.17	12 (31%)	57,57,57	1.96	14 (24%)
4	3PE	A	2311	-	16,16,50	0.28	0	15,15,55	0.50	0
3	NAG	A	2303	1	14,14,15	0.40	0	17,19,21	0.44	0
3	NAG	A	2307	1	14,14,15	0.37	0	17,19,21	0.48	0
4	3PE	A	2315	-	38,38,50	1.11	2 (5%)	41,43,55	0.94	3 (7%)
4	3PE	A	2314	-	36,36,50	1.11	2 (5%)	39,41,55	1.25	3 (7%)
4	3PE	A	2316	-	16,16,50	0.24	0	15,15,55	0.57	0
4	3PE	A	2319	-	15,15,50	0.26	0	14,14,55	0.51	0
4	3PE	A	2317	-	16,16,50	0.35	0	15,15,55	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3PE	A	2310	-	-	15/38/38/54	-
3	NAG	A	2304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2306	1	-	6/6/23/26	0/1/1/1
4	3PE	A	2312	-	-	11/47/47/54	-
4	3PE	A	2313	-	-	5/38/38/54	-
4	3PE	A	2318	-	-	0/11/11/54	-
4	3PE	A	2308	-	-	5/34/34/54	-
5	Y01	A	2321	-	-	8/19/77/77	0/4/4/4
4	3PE	A	2309	-	-	13/41/41/54	-
3	NAG	A	2305	1	-	0/6/23/26	0/1/1/1
4	3PE	A	2320	-	-	0/14/14/54	-
5	Y01	A	2322	-	-	4/19/77/77	0/4/4/4
4	3PE	A	2311	-	-	0/14/14/54	-
3	NAG	A	2303	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2307	1	-	2/6/23/26	0/1/1/1
4	3PE	A	2315	-	-	5/42/42/54	-
4	3PE	A	2314	-	-	10/40/40/54	-
4	3PE	A	2316	-	-	0/14/14/54	-
4	3PE	A	2319	-	-	0/13/13/54	-
4	3PE	A	2317	-	-	0/14/14/54	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2321	Y01	CAI-CAZ	17.68	1.69	1.33
5	A	2322	Y01	CAI-CAZ	17.59	1.69	1.33
5	A	2322	Y01	CBH-CBF	7.40	1.67	1.56
5	A	2321	Y01	CBH-CBF	7.16	1.67	1.56
5	A	2321	Y01	CAU-CBI	-7.14	1.41	1.54
5	A	2321	Y01	CAQ-CAP	6.95	1.73	1.54
5	A	2322	Y01	CAQ-CAP	6.87	1.72	1.54
5	A	2321	Y01	CBB-CBE	-6.63	1.43	1.54
5	A	2322	Y01	CAK-CBD	6.57	1.63	1.53
5	A	2322	Y01	CAU-CAS	6.42	1.66	1.53
5	A	2321	Y01	CAK-CBD	6.37	1.63	1.53
5	A	2321	Y01	CAU-CAS	6.21	1.65	1.53
5	A	2322	Y01	CBI-CBE	5.70	1.65	1.55
5	A	2321	Y01	CBI-CBE	5.47	1.65	1.55
5	A	2322	Y01	CAU-CBI	-5.28	1.44	1.54
5	A	2321	Y01	CAQ-CBG	5.17	1.64	1.54
5	A	2322	Y01	CAQ-CBG	5.05	1.64	1.54
5	A	2322	Y01	CBB-CBE	-5.05	1.45	1.54
4	A	2308	3PE	O31-C31	4.54	1.46	1.33
4	A	2312	3PE	O21-C21	4.50	1.47	1.34
4	A	2309	3PE	O31-C31	4.45	1.46	1.33
4	A	2312	3PE	O31-C31	4.44	1.46	1.33
4	A	2314	3PE	O31-C31	4.43	1.46	1.33
4	A	2310	3PE	O21-C21	4.42	1.46	1.34
4	A	2313	3PE	O31-C31	4.42	1.46	1.33
4	A	2315	3PE	O21-C21	4.40	1.46	1.34
4	A	2315	3PE	O31-C31	4.37	1.46	1.33
4	A	2310	3PE	O31-C31	4.34	1.46	1.33
4	A	2308	3PE	O21-C21	4.32	1.46	1.34
4	A	2309	3PE	O21-C21	4.17	1.46	1.34
4	A	2313	3PE	O21-C21	4.10	1.45	1.34
4	A	2314	3PE	O21-C21	3.79	1.45	1.34
5	A	2322	Y01	OAW-CAY	3.04	1.42	1.34
5	A	2321	Y01	OAW-CAY	2.69	1.41	1.34
5	A	2322	Y01	CAO-CBB	2.54	1.60	1.54
5	A	2321	Y01	CBH-CAZ	-2.48	1.48	1.52
5	A	2321	Y01	CAO-CBB	2.13	1.59	1.54
5	A	2322	Y01	CAE-CBI	2.02	1.57	1.54

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2321	Y01	CBI-CBE-CBB	-5.81	110.53	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2321	Y01	CBG-CBI-CBE	5.47	106.38	100.10
5	A	2322	Y01	CAD-CBH-CBF	-5.18	105.85	111.66
5	A	2322	Y01	CAK-CAI-CAZ	-4.82	116.89	125.02
5	A	2321	Y01	CAV-CAZ-CBH	-4.80	110.28	116.42
4	A	2314	3PE	O21-C21-C22	4.76	121.77	111.48
4	A	2310	3PE	O21-C21-C22	4.59	121.42	111.48
3	A	2306	NAG	C4-C3-C2	4.38	117.43	111.02
5	A	2321	Y01	CAK-CAI-CAZ	-4.32	117.72	125.02
5	A	2321	Y01	CAU-CBI-CBE	4.13	122.69	116.60
4	A	2312	3PE	O21-C21-C22	4.09	120.33	111.48
5	A	2321	Y01	OAW-CAY-CAM	4.02	120.19	111.48
5	A	2322	Y01	CBI-CBE-CBB	-4.00	113.32	119.50
5	A	2321	Y01	CBH-CAZ-CAI	-3.96	117.15	122.93
4	A	2309	3PE	O21-C21-C22	3.94	120.00	111.48
5	A	2321	Y01	CAE-CBI-CAU	-3.92	104.83	110.61
4	A	2313	3PE	O21-C21-C22	3.89	119.89	111.48
5	A	2322	Y01	CAV-CAZ-CBH	-3.88	111.45	116.42
5	A	2321	Y01	CAD-CBH-CBF	-3.85	107.34	111.66
5	A	2321	Y01	CAE-CBI-CBG	-3.85	104.69	111.68
5	A	2322	Y01	CAE-CBI-CBG	-3.81	104.77	111.68
5	A	2322	Y01	OAW-CAY-CAM	3.75	119.60	111.48
5	A	2322	Y01	CAE-CBI-CBE	-3.45	105.41	111.68
5	A	2321	Y01	CAE-CBI-CBE	-3.43	105.45	111.68
3	A	2306	NAG	C3-C4-C5	3.19	116.02	110.23
5	A	2322	Y01	CBH-CAZ-CAI	-3.15	118.33	122.93
5	A	2322	Y01	CAU-CBI-CBG	3.11	111.89	107.25
4	A	2313	3PE	O31-C31-C32	3.09	121.25	111.83
4	A	2315	3PE	O31-C31-C32	3.07	121.19	111.83
4	A	2314	3PE	O31-C31-C32	2.90	120.69	111.83
4	A	2308	3PE	O21-C21-C22	2.86	117.68	111.48
4	A	2310	3PE	O31-C31-C32	2.82	120.42	111.83
5	A	2321	Y01	CBF-CBD-CBG	2.78	112.72	109.09
4	A	2308	3PE	O31-C31-C32	2.78	120.32	111.83
4	A	2315	3PE	O21-C21-C22	2.75	117.42	111.48
5	A	2322	Y01	CAU-CBI-CBE	2.73	120.61	116.60
5	A	2321	Y01	CAU-CBI-CBG	2.70	111.29	107.25
5	A	2322	Y01	CBF-CBD-CBG	2.68	112.58	109.09
4	A	2312	3PE	O31-C31-C32	2.64	119.88	111.83
4	A	2310	3PE	O21-C21-O22	-2.62	117.58	123.70
4	A	2308	3PE	O21-C21-O22	-2.52	117.82	123.70
4	A	2314	3PE	O21-C21-O22	-2.45	117.98	123.70
5	A	2321	Y01	CBI-CBG-CBD	-2.44	110.95	114.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2321	Y01	CAR-CBC-CAV	2.44	114.36	110.97
3	A	2306	NAG	O5-C1-C2	-2.41	107.56	111.29
4	A	2309	3PE	O31-C31-C32	2.41	119.17	111.83
5	A	2322	Y01	CAK-CBD-CBF	2.35	112.44	109.72
5	A	2321	Y01	CBC-CAV-CAZ	2.32	114.88	111.45
4	A	2312	3PE	O21-C21-O22	-2.22	118.51	123.70
5	A	2322	Y01	OAH-CAX-CAL	2.20	120.94	114.00
5	A	2321	Y01	CBF-CBH-CAZ	2.17	112.84	109.65
4	A	2310	3PE	C2-O21-C21	-2.13	112.69	117.80
5	A	2322	Y01	CAS-CBF-CBH	-2.10	110.50	113.08
5	A	2321	Y01	CAS-CBF-CBH	-2.06	110.54	113.08
5	A	2321	Y01	CBH-CBF-CBD	-2.05	109.71	112.71
4	A	2312	3PE	O31-C31-O32	-2.05	118.51	123.63
4	A	2309	3PE	C3-O31-C31	2.03	124.55	117.12
4	A	2315	3PE	O21-C21-O22	-2.03	118.97	123.70
5	A	2321	Y01	CAC-CBB-CBE	-2.02	109.86	112.88
3	A	2306	NAG	C1-O5-C5	-2.01	109.49	112.19

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2306	NAG	C8-C7-N2-C2
3	A	2306	NAG	O7-C7-N2-C2
4	A	2308	3PE	C1-O11-P-O13
4	A	2308	3PE	C1-O11-P-O14
4	A	2309	3PE	C11-O13-P-O11
4	A	2309	3PE	C11-O13-P-O12
4	A	2309	3PE	C11-O13-P-O14
4	A	2309	3PE	C22-C21-O21-C2
4	A	2310	3PE	C1-O11-P-O12
4	A	2310	3PE	C1-O11-P-O13
4	A	2310	3PE	C1-O11-P-O14
4	A	2310	3PE	C11-O13-P-O11
4	A	2310	3PE	C11-O13-P-O12
4	A	2310	3PE	C12-C11-O13-P
4	A	2310	3PE	O22-C21-O21-C2
4	A	2312	3PE	C1-O11-P-O12
4	A	2312	3PE	C1-O11-P-O13
4	A	2312	3PE	C11-O13-P-O11
4	A	2313	3PE	C11-O13-P-O11
4	A	2313	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
4	A	2313	3PE	C11-O13-P-O14
4	A	2314	3PE	C1-O11-P-O14
4	A	2315	3PE	C1-O11-P-O14
5	A	2322	Y01	CAM-CAY-OAW-CBC
5	A	2322	Y01	CAR-CBC-OAW-CAY
4	A	2310	3PE	O32-C31-O31-C3
4	A	2314	3PE	O32-C31-O31-C3
4	A	2309	3PE	O22-C21-O21-C2
5	A	2322	Y01	OAG-CAY-OAW-CBC
4	A	2314	3PE	C32-C31-O31-C3
4	A	2310	3PE	C22-C21-O21-C2
3	A	2307	NAG	O5-C5-C6-O6
4	A	2310	3PE	C32-C31-O31-C3
5	A	2321	Y01	CAJ-CAO-CBB-CAC
4	A	2308	3PE	O32-C31-O31-C3
4	A	2308	3PE	C32-C31-O31-C3
3	A	2307	NAG	C4-C5-C6-O6
3	A	2306	NAG	O5-C5-C6-O6
5	A	2321	Y01	CAJ-CAO-CBB-CBE
4	A	2314	3PE	C21-C22-C23-C24
4	A	2314	3PE	C27-C28-C29-C2A
5	A	2322	Y01	CAV-CBC-OAW-CAY
4	A	2312	3PE	C22-C21-O21-C2
3	A	2306	NAG	C4-C5-C6-O6
4	A	2312	3PE	O22-C21-O21-C2
4	A	2314	3PE	C22-C21-O21-C2
4	A	2314	3PE	O22-C21-O21-C2
4	A	2315	3PE	C22-C21-O21-C2
5	A	2321	Y01	CAM-CAY-OAW-CBC
3	A	2304	NAG	C4-C5-C6-O6
4	A	2310	3PE	C25-C26-C27-C28
4	A	2309	3PE	C32-C31-O31-C3
5	A	2321	Y01	OAG-CAY-OAW-CBC
3	A	2304	NAG	O5-C5-C6-O6
4	A	2309	3PE	O32-C31-O31-C3
4	A	2312	3PE	C32-C31-O31-C3
4	A	2310	3PE	C23-C24-C25-C26
4	A	2315	3PE	O22-C21-O21-C2
4	A	2312	3PE	C2-C1-O11-P
3	A	2306	NAG	C1-C2-N2-C7
4	A	2312	3PE	O32-C31-O31-C3
4	A	2314	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
5	A	2321	Y01	CAJ-CAN-CBA-CAA
4	A	2309	3PE	O31-C31-C32-C33
4	A	2313	3PE	C22-C21-O21-C2
4	A	2313	3PE	O22-C21-O21-C2
4	A	2308	3PE	C1-O11-P-O12
4	A	2309	3PE	C1-O11-P-O12
4	A	2309	3PE	C1-O11-P-O13
4	A	2309	3PE	C1-O11-P-O14
4	A	2312	3PE	C1-O11-P-O14
4	A	2312	3PE	C11-O13-P-O14
4	A	2315	3PE	C1-O11-P-O13
4	A	2312	3PE	O31-C31-C32-C33
5	A	2321	Y01	CAC-CBB-CBE-CBI
4	A	2314	3PE	C1-C2-O21-C21
5	A	2321	Y01	CAJ-CAN-CBA-CAB
5	A	2321	Y01	CAX-CAL-CAM-CAY
4	A	2310	3PE	C1-C2-O21-C21
4	A	2310	3PE	C3-C2-O21-C21
4	A	2314	3PE	O11-C1-C2-C3
3	A	2306	NAG	C3-C2-N2-C7
4	A	2315	3PE	O21-C21-C22-C23
4	A	2310	3PE	C2-C3-O31-C31
4	A	2309	3PE	C1-C2-O21-C21
4	A	2309	3PE	O32-C31-C32-C33

There are no ring outliers.

17 monomers are involved in 73 short contacts:

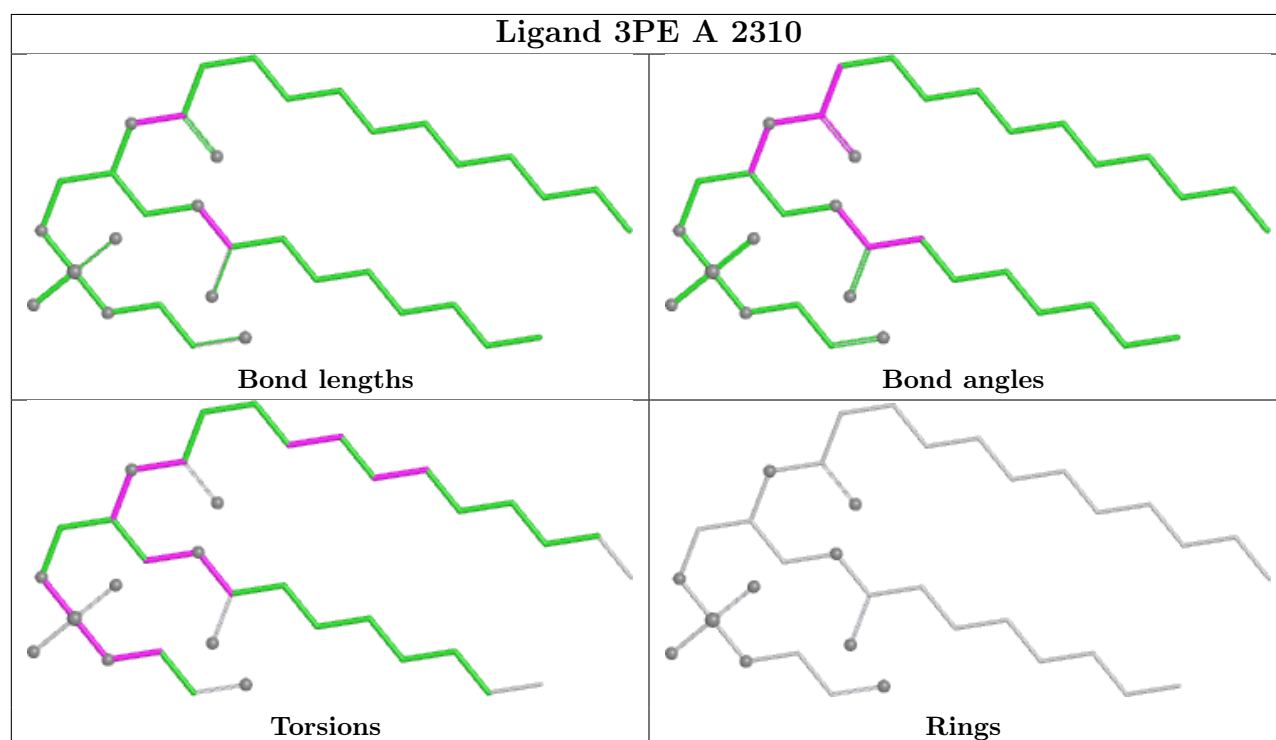
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2310	3PE	4	0
3	A	2306	NAG	6	0
4	A	2312	3PE	9	0
4	A	2313	3PE	3	0
4	A	2318	3PE	3	0
4	A	2308	3PE	5	0
5	A	2321	Y01	15	0
4	A	2309	3PE	7	0
3	A	2305	NAG	1	0
4	A	2320	3PE	6	0
5	A	2322	Y01	2	0
4	A	2311	3PE	1	0
4	A	2315	3PE	4	0

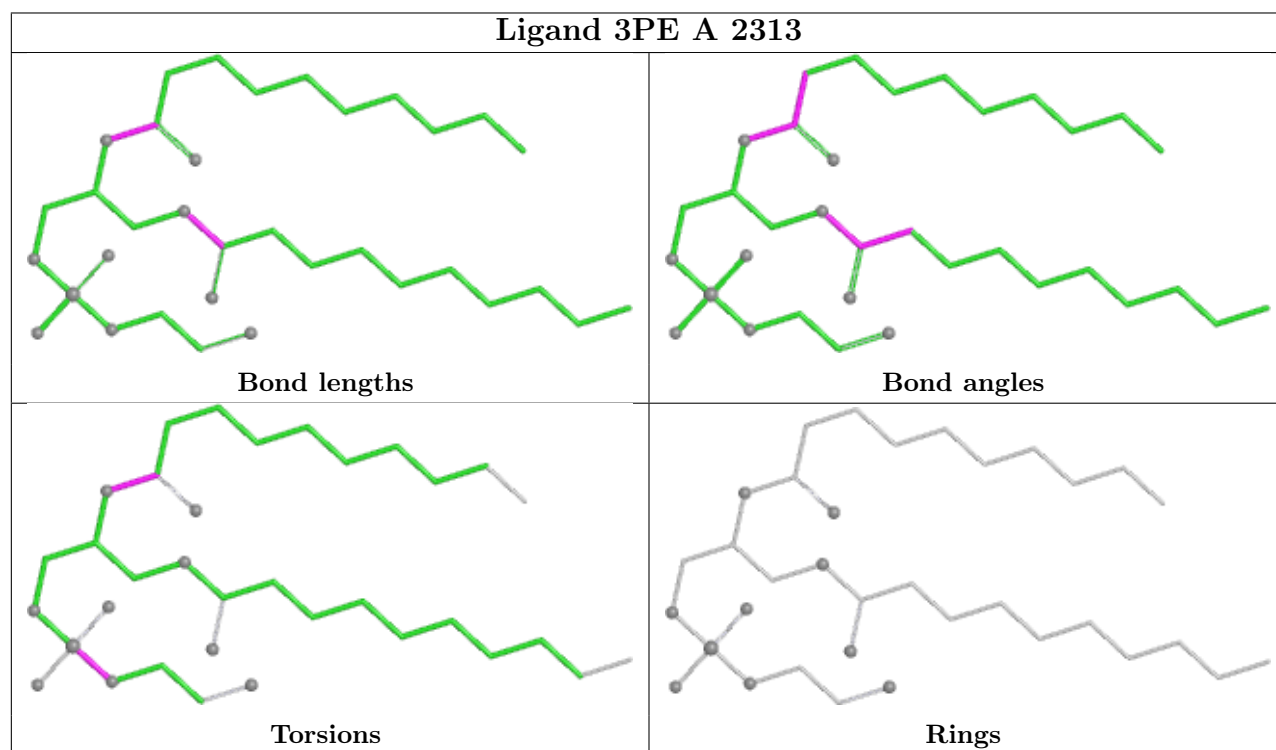
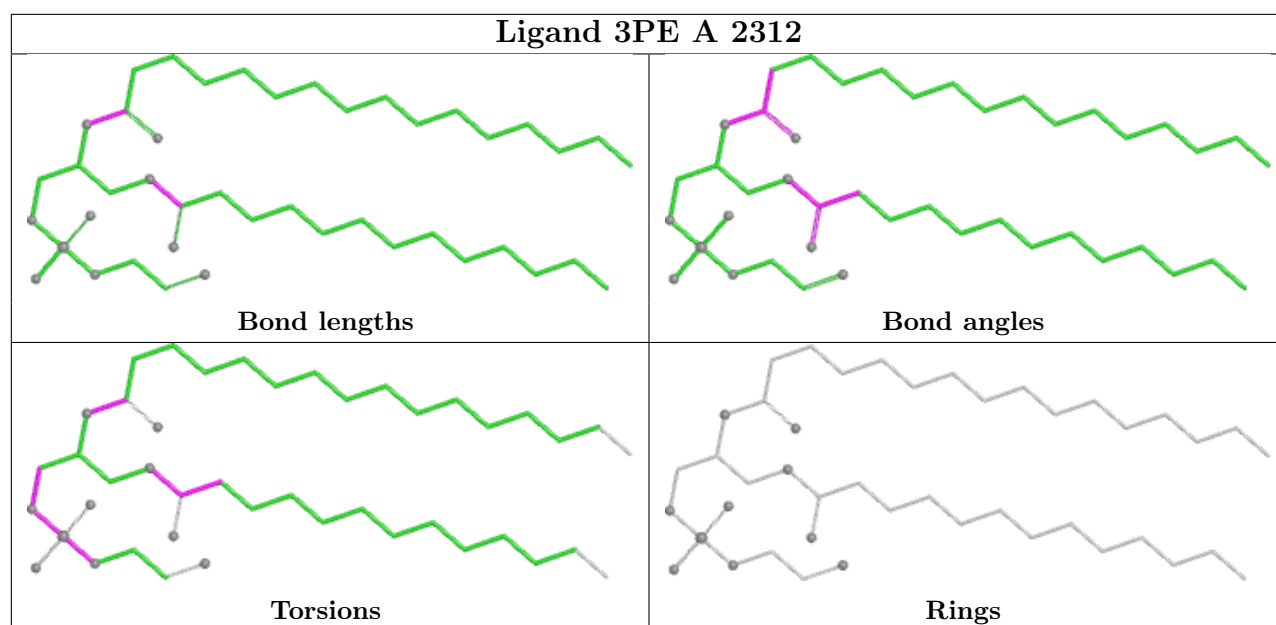
Continued on next page...

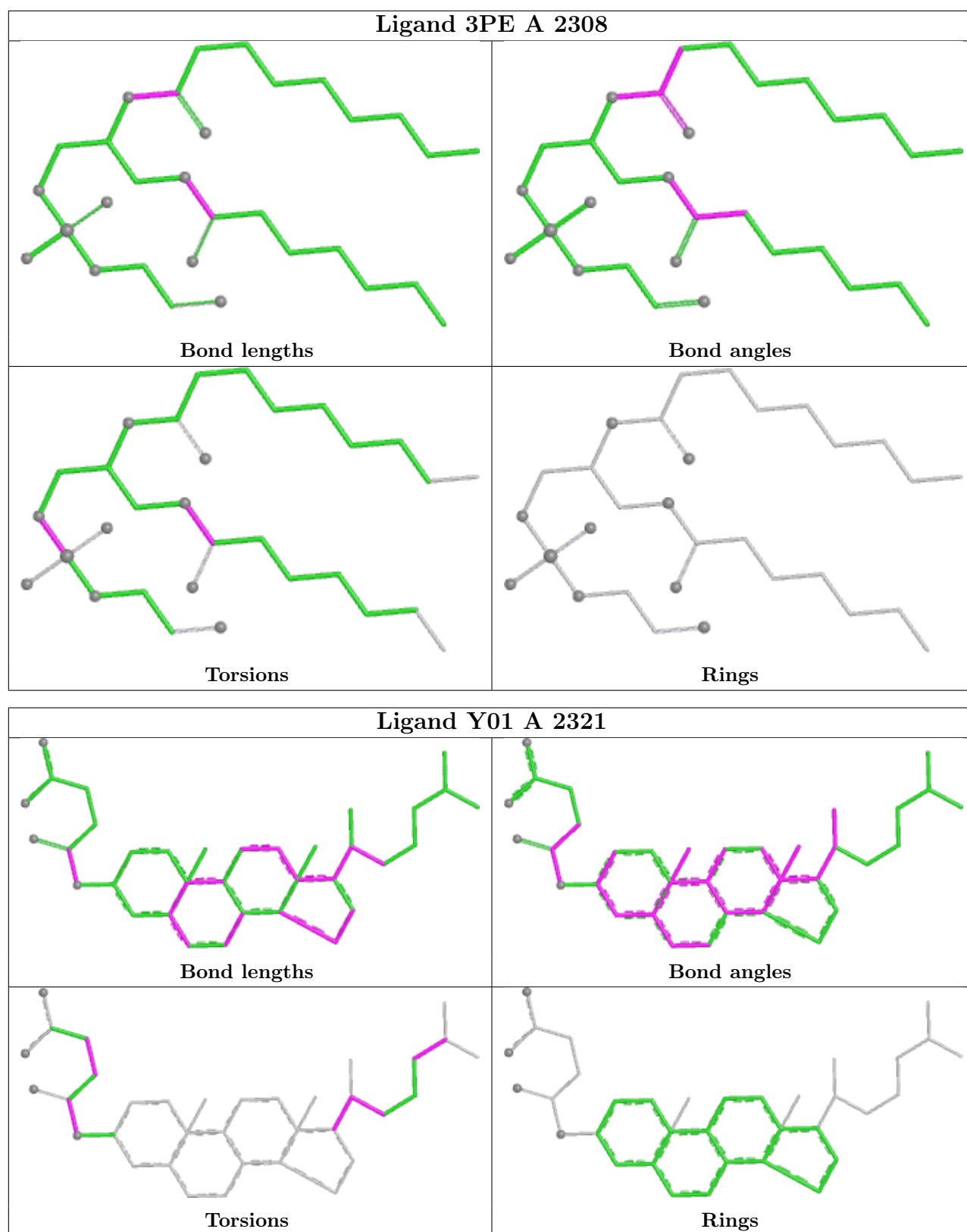
Continued from previous page...

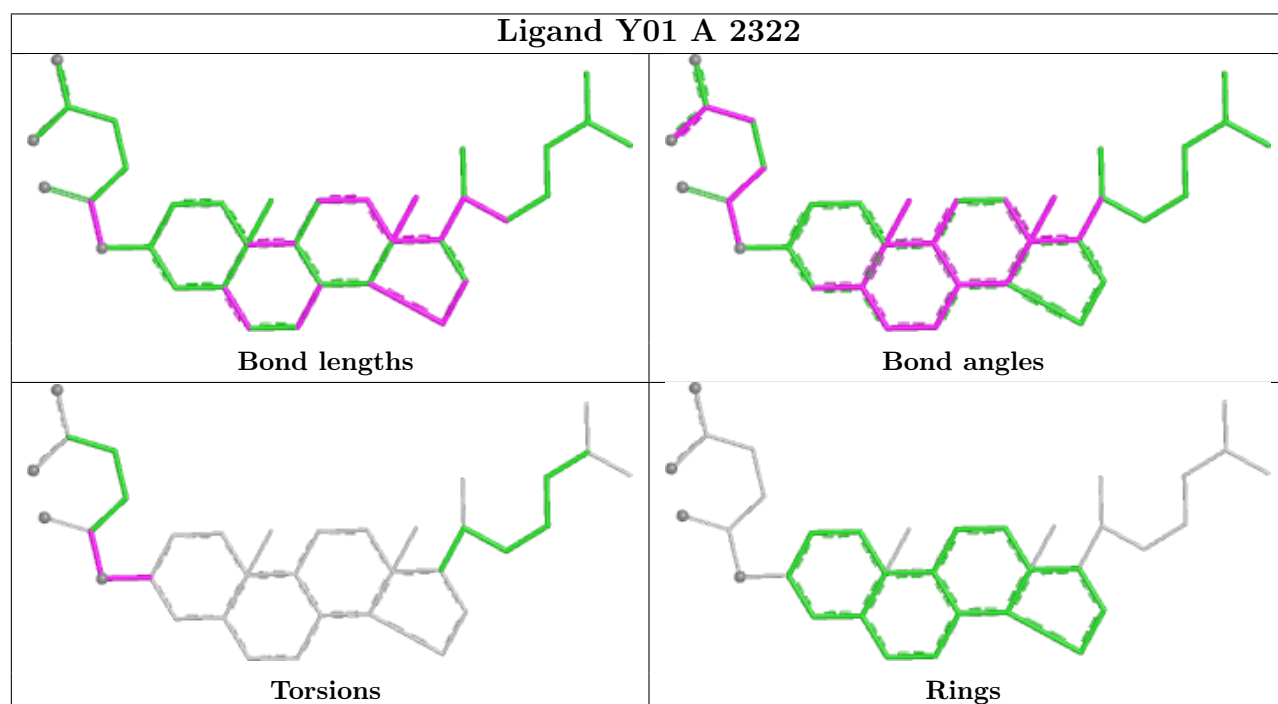
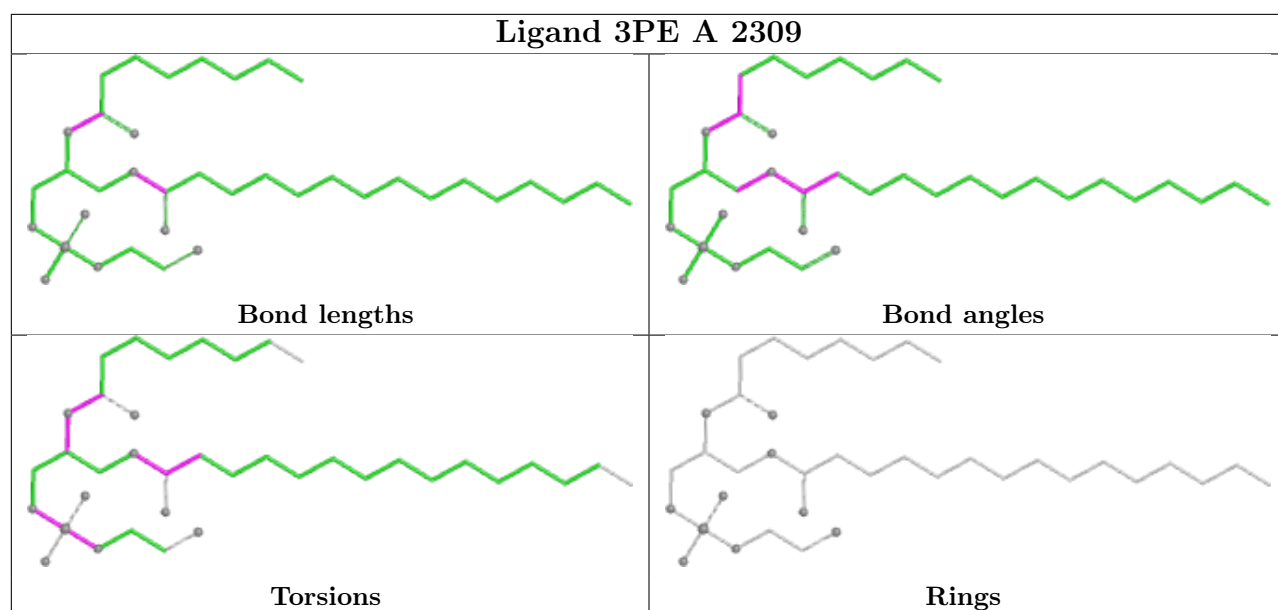
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2314	3PE	5	0
4	A	2316	3PE	6	0
4	A	2319	3PE	6	0
4	A	2317	3PE	2	0

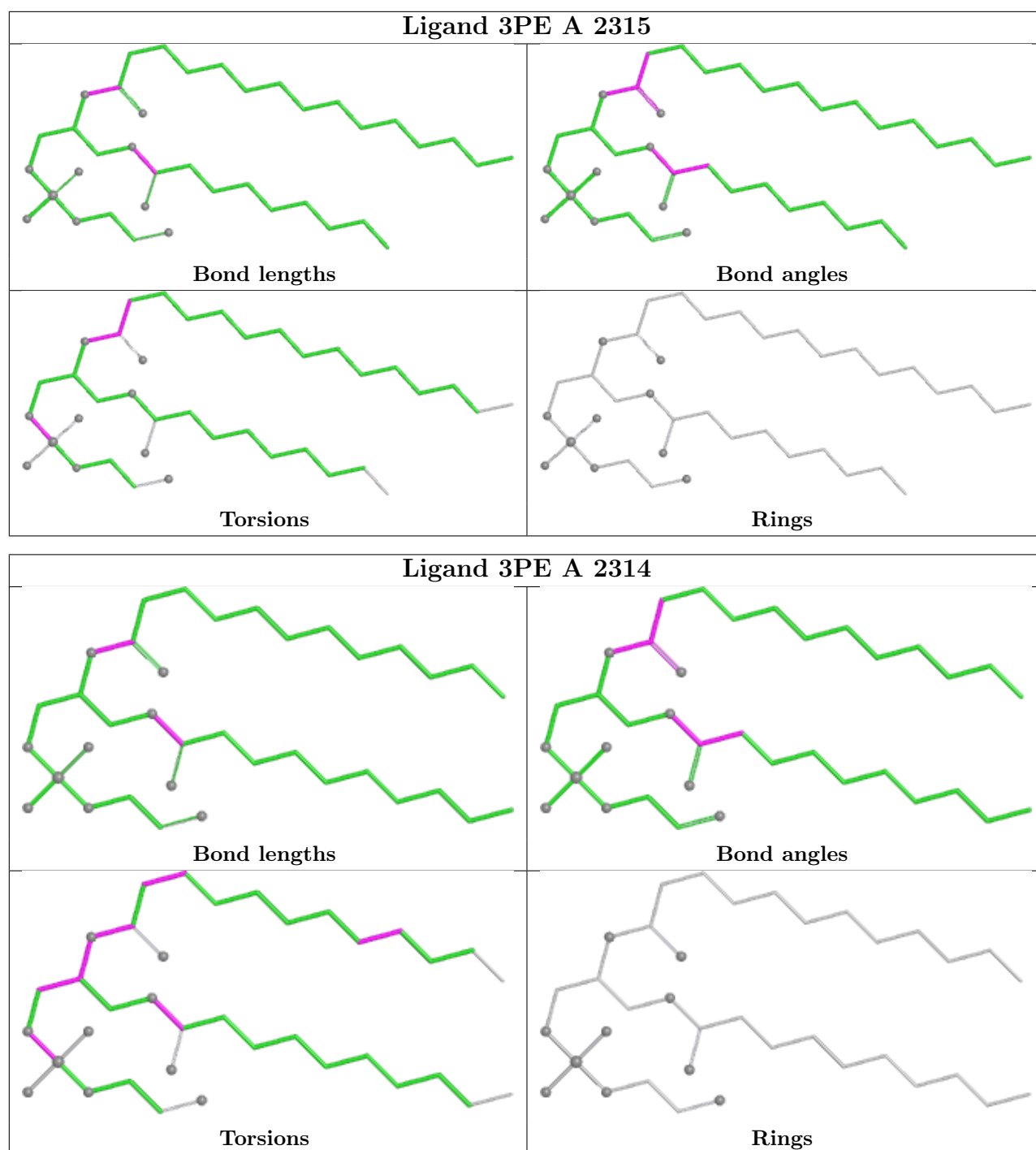
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

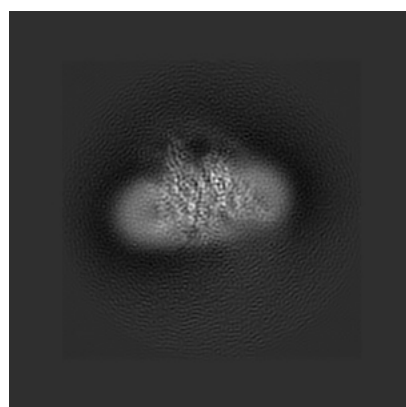
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0791. These allow visual inspection of the internal detail of the map and identification of artifacts.

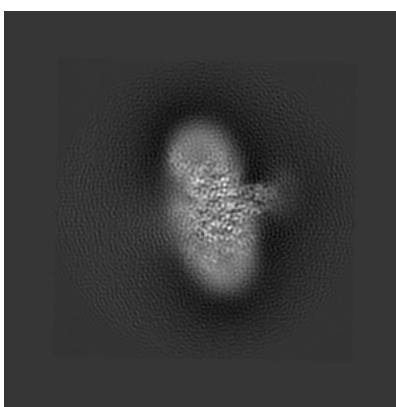
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

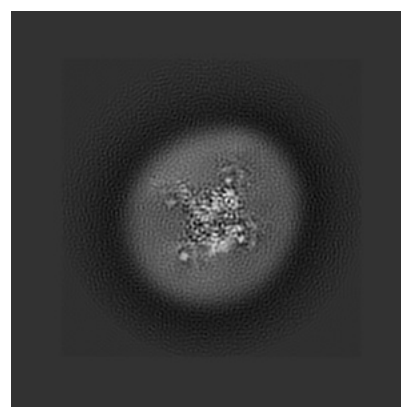
6.1.1 Primary map



X



Y

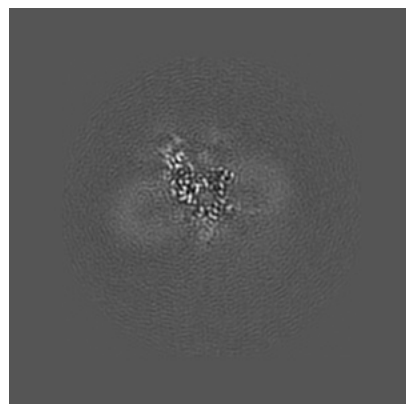


Z

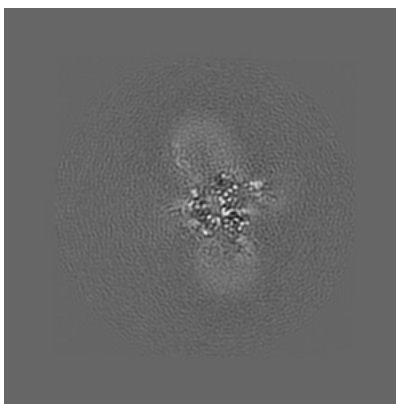
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

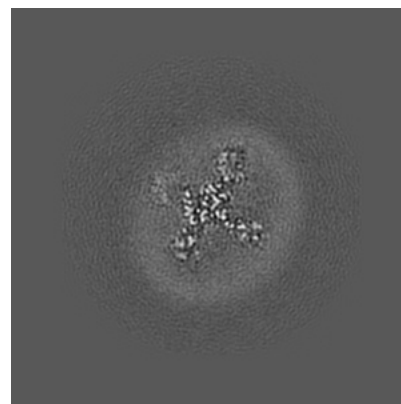
6.2.1 Primary map



X Index: 160



Y Index: 160

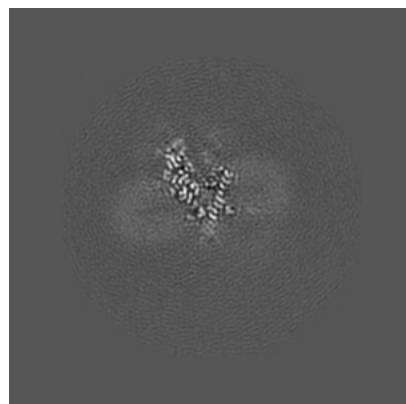


Z Index: 160

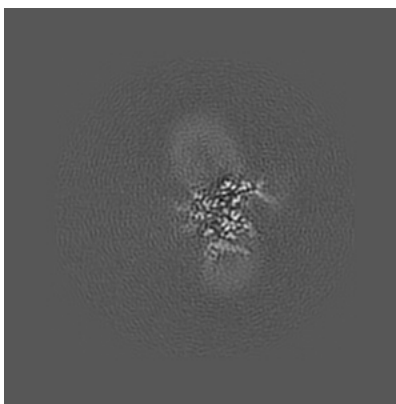
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

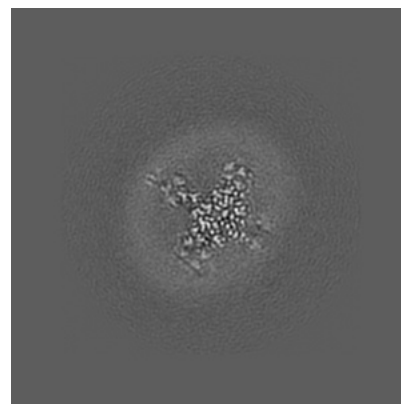
6.3.1 Primary map



X Index: 161



Y Index: 166

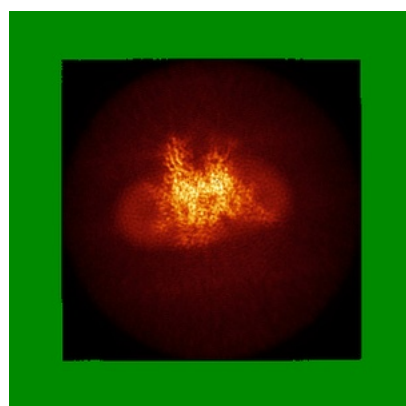


Z Index: 175

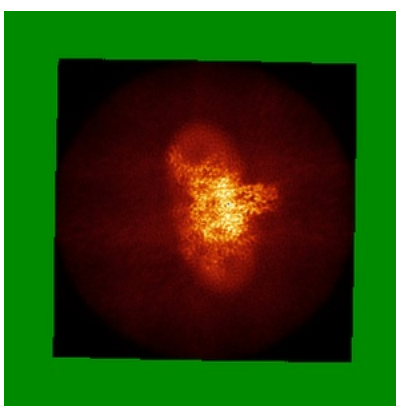
The images above show the largest variance slices of the map in three orthogonal directions.

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

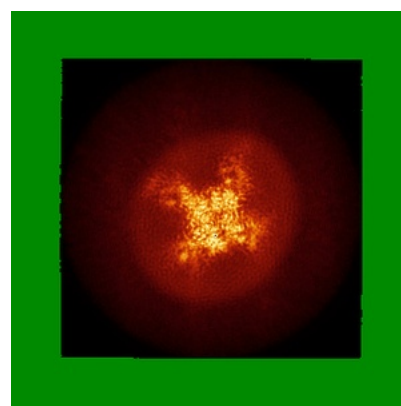
6.4.1 Primary map



X



Y

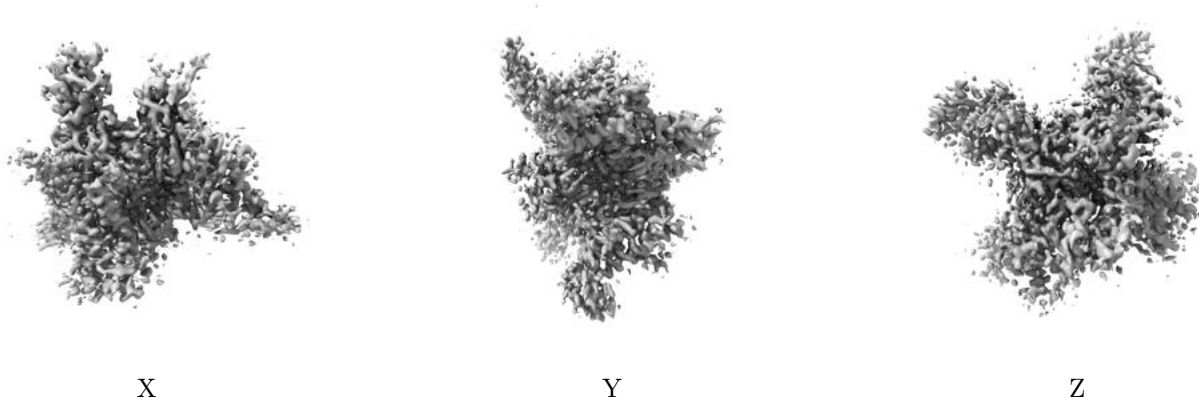


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

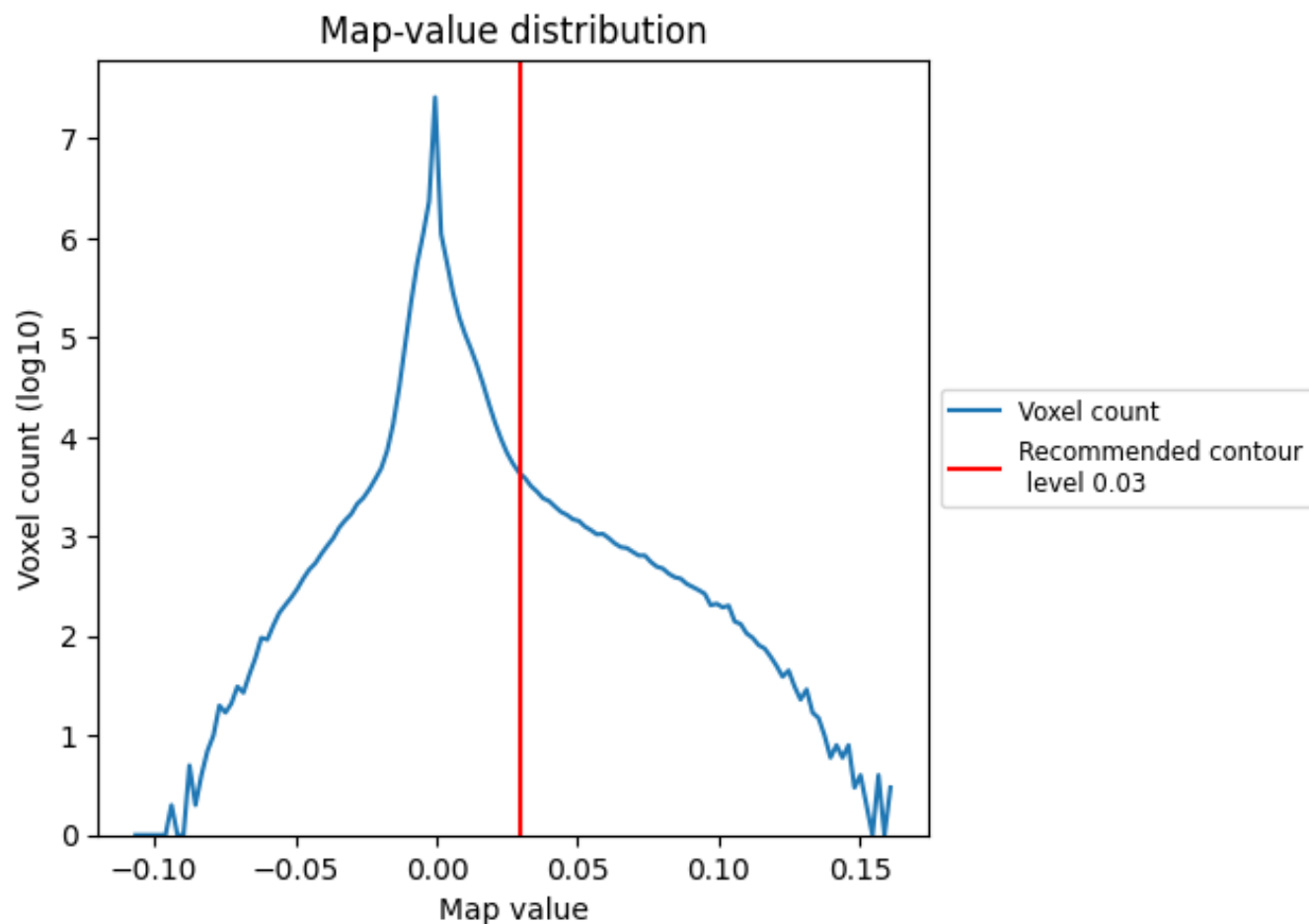
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

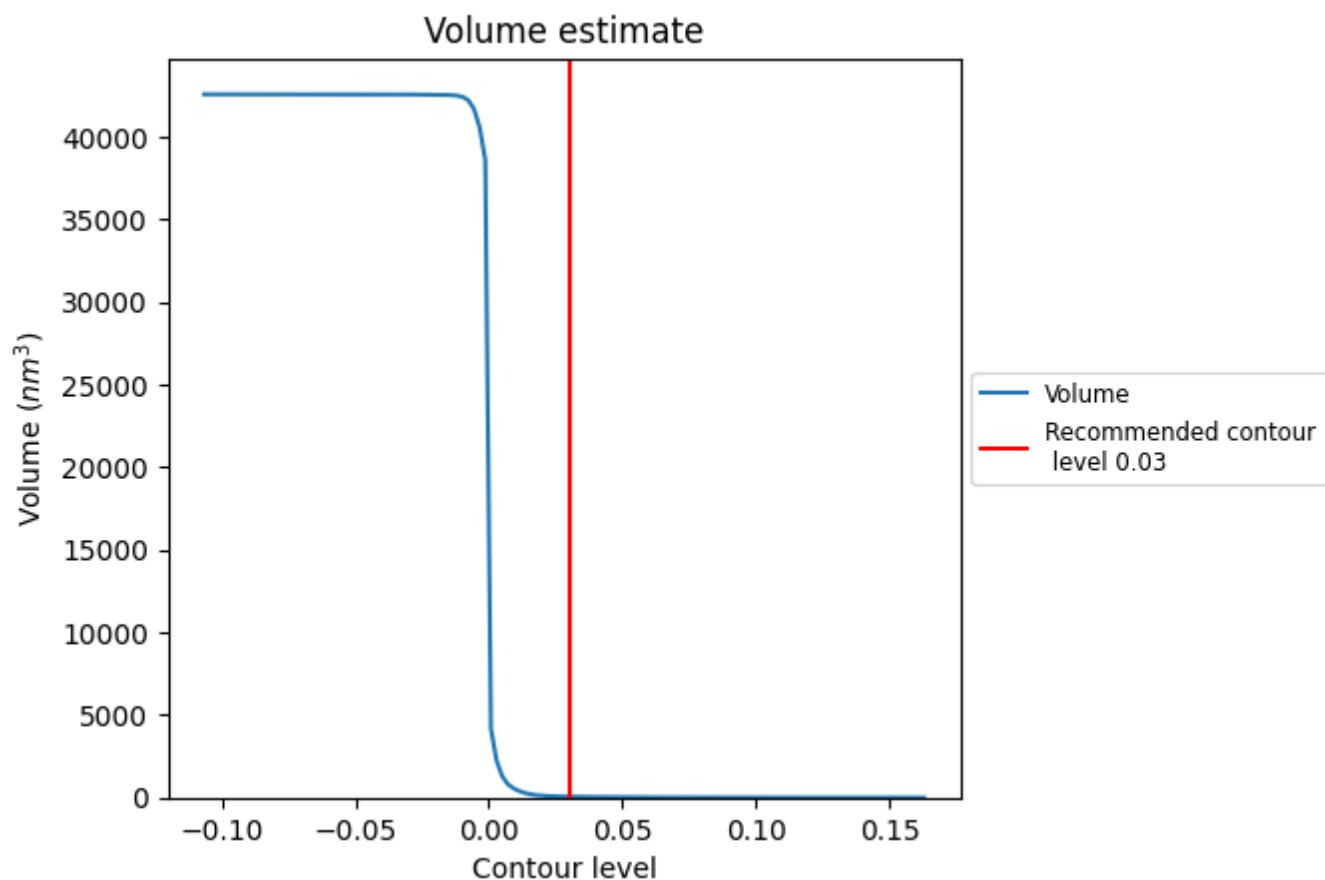
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

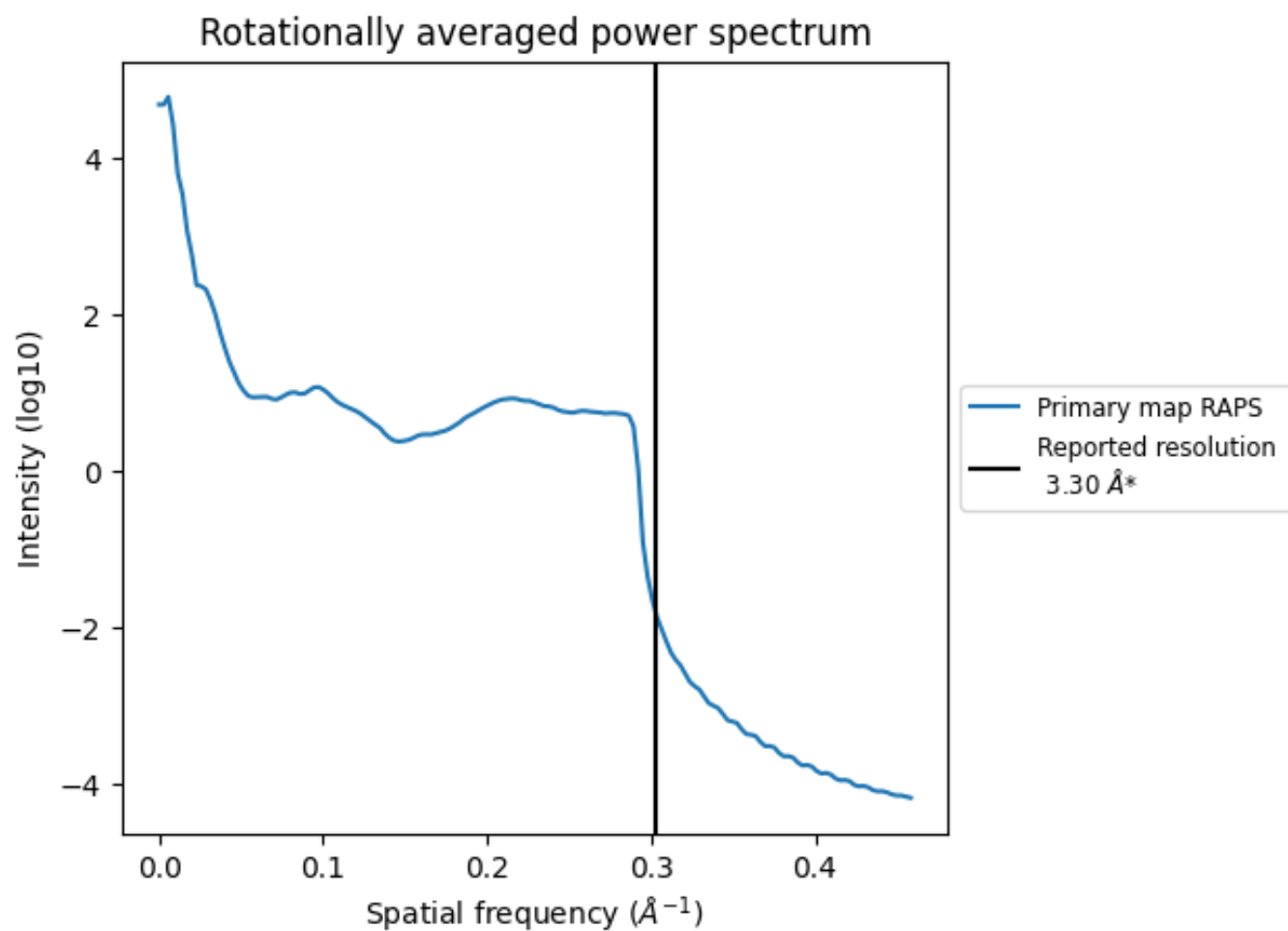
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 54 nm³; this corresponds to an approximate mass of 48 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 0.303 Å⁻¹

8 Fourier-Shell correlation

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

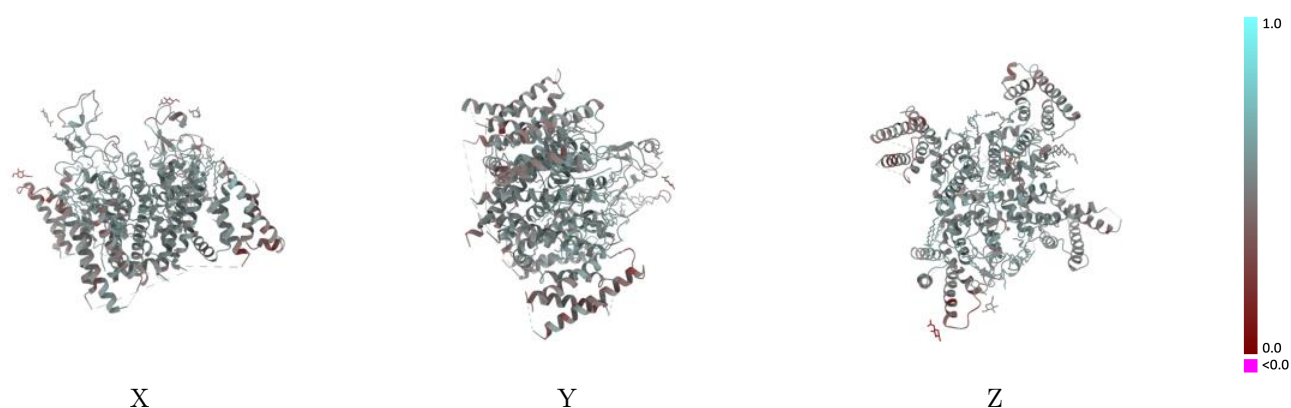
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0791 and PDB model 6KZO. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

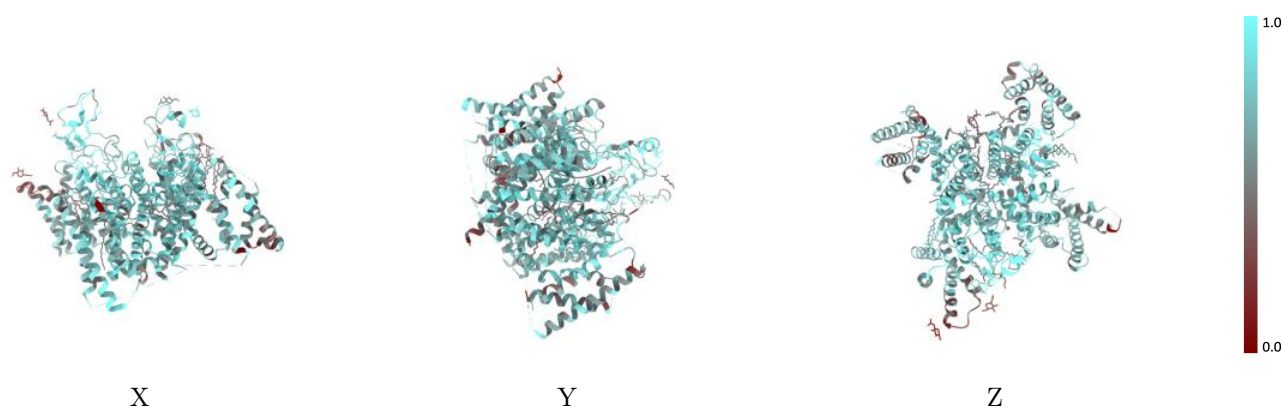
This section was not generated.

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



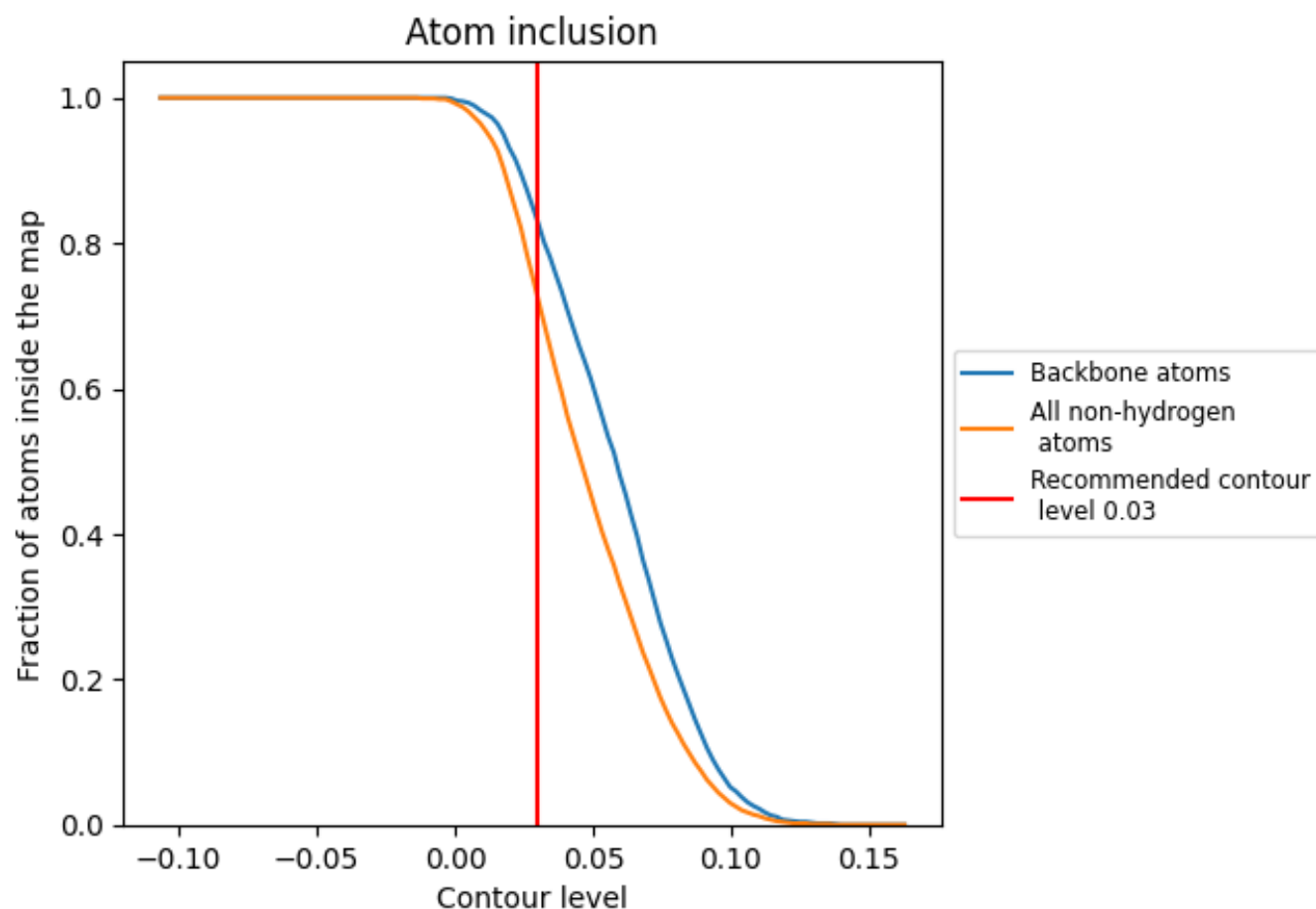
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 72% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.5080
A	0.7250	0.5080

