



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:13 PM UTC

PDB ID : 6JZO / pdb_00006jzo
EMDB ID : EMD-9898
Title : Structure of the mouse TRPC4 ion channel
Authors : Duan, J.; Li, Z.; Li, J.; Zhang, J.
Deposited on : 2019-05-03
Resolution : 3.28 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:

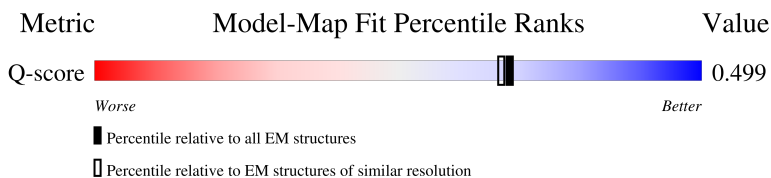
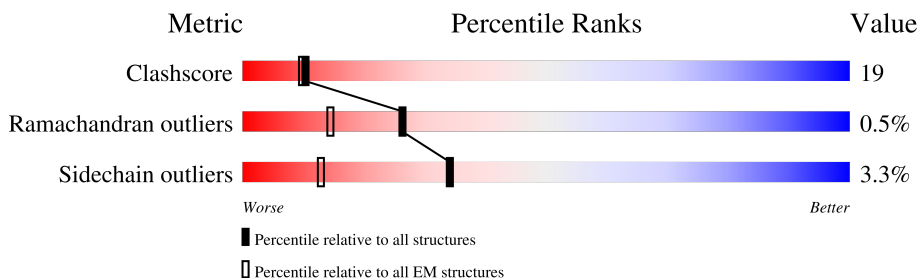
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.28 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	14492 (2.78 - 3.78)

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	755	
1	B	755	
1	C	755	
1	D	755	

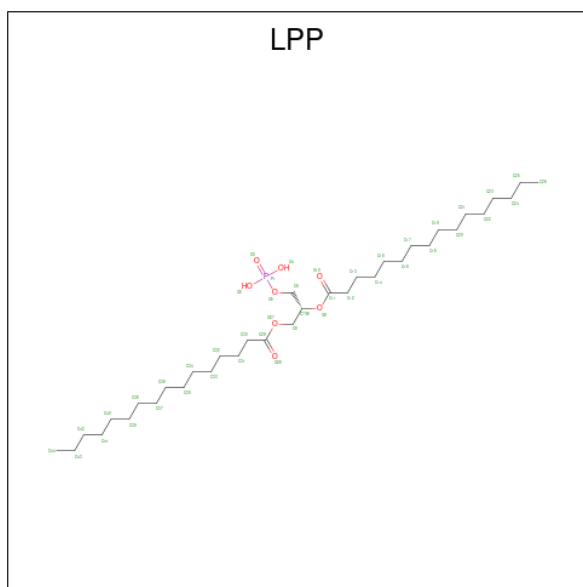
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	Y01	B	801	-	-	X	-
2	Y01	C	801	-	-	X	-
2	Y01	D	801	-	-	X	-
3	LPP	A	802	-	-	X	-
3	LPP	A	803	-	-	X	-
3	LPP	C	802	-	-	X	-
3	LPP	D	802	-	-	X	-

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Mol	Chain	Residues	Atoms			AltConf
2	C	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	

- Molecule 3 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			44	35	8	1	
3	A	1	Total	C	O	P	0
			44	35	8	1	
3	C	1	Total	C	O	P	0
			44	35	8	1	
3	D	1	Total	C	O	P	0
			44	35	8	1	

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Na	0
			1	1	
4	B	1	Total	Na	0
			1	1	

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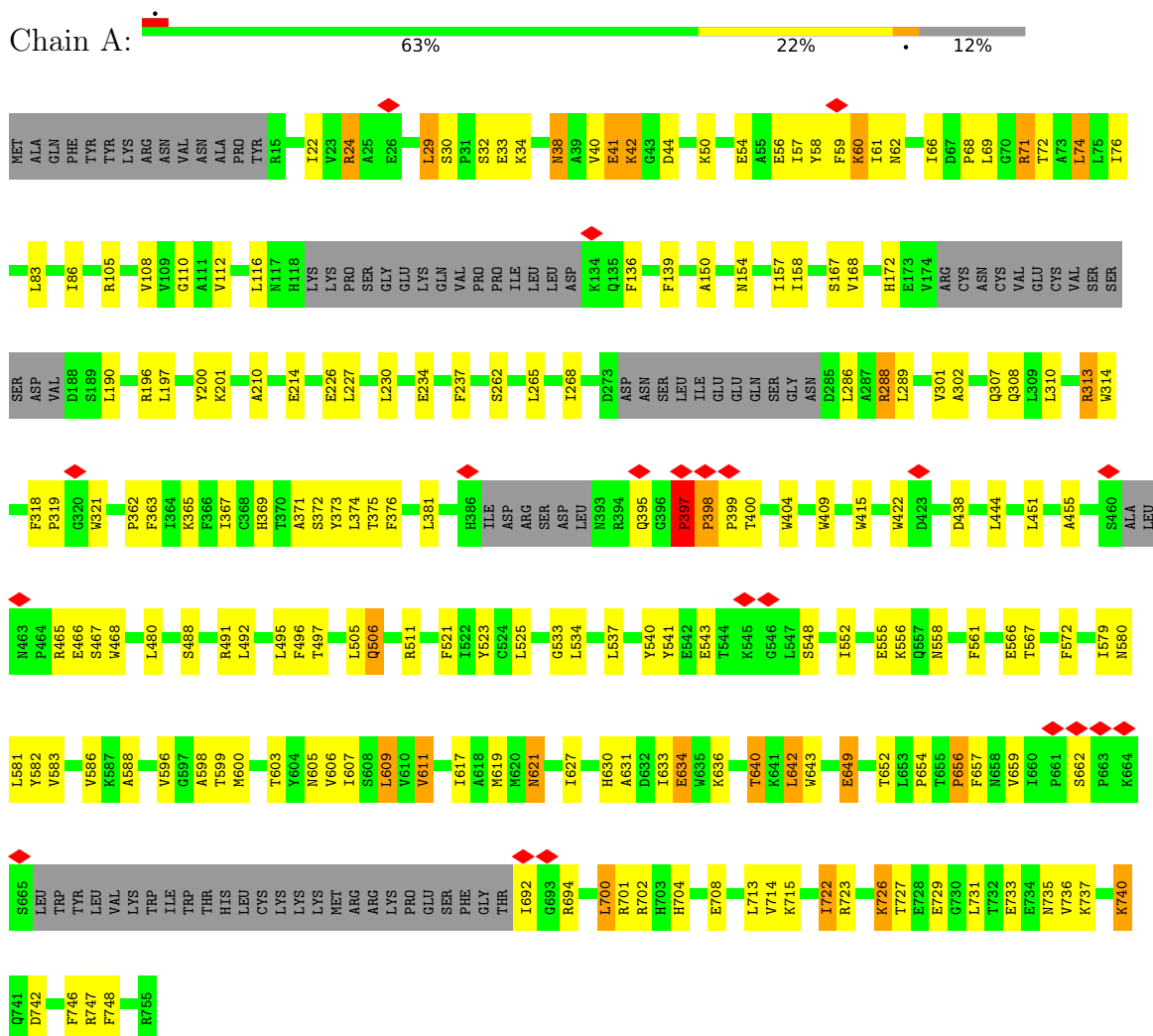
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Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total 1	Na 1	0
4	D	1	Total 1	Na 1	0

3 Residue-property plots

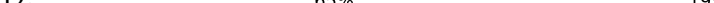
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

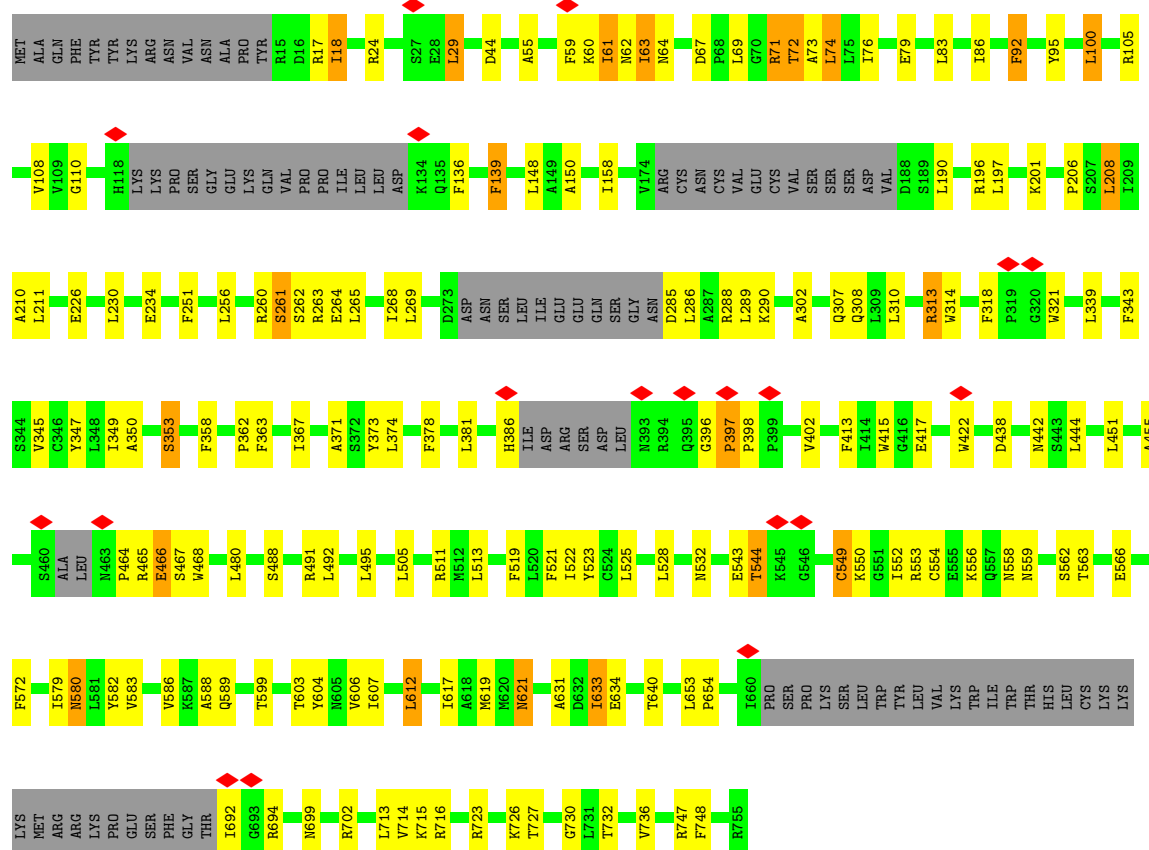
- Molecule 1: Short transient receptor potential channel 4



- Molecule 1: Short transient receptor potential channel 4



- Chain D:  65% 19% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	232858	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	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	0.236	Depositor
Minimum map value	-0.162	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	314.88, 314.88, 314.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	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: NA, Y01, LPP

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	0.42	1/5419 (0.0%)	0.80	22/7357 (0.3%)
1	B	0.38	0/5389	0.74	18/7313 (0.2%)
1	C	0.36	0/5389	0.69	10/7315 (0.1%)
1	D	0.37	0/5378	0.71	15/7301 (0.2%)
All	All	0.39	1/21575 (0.0%)	0.74	65/29286 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	397	PRO	C-N	5.29	1.39	1.33

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	PRO	N-CA-C	-10.69	97.66	110.70
1	C	60	LYS	N-CA-C	10.58	127.16	112.45
1	A	57	ILE	N-CA-C	-10.19	95.38	108.84
1	C	558	ASN	N-CA-C	9.94	121.88	111.14
1	A	656	PRO	CA-N-CD	-9.54	98.64	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	558	ASN	N-CA-C	8.86	120.55	111.07
1	B	71	ARG	N-CA-C	8.85	122.08	111.02
1	C	550	LYS	N-CA-C	8.69	123.19	112.59
1	B	74	LEU	N-CA-C	-8.54	101.71	112.90
1	B	465	ARG	N-CA-C	8.15	119.79	111.07
1	A	42	LYS	N-CA-C	-8.02	103.70	113.97
1	D	465	ARG	N-CA-C	7.65	119.26	111.07
1	A	172	HIS	N-CA-C	7.53	120.60	110.35
1	D	208	LEU	N-CA-C	-7.50	103.59	112.89
1	C	465	ARG	N-CA-C	7.45	119.04	111.07
1	C	172	HIS	N-CA-C	7.44	120.46	110.35
1	B	172	HIS	N-CA-C	7.39	120.40	110.35
1	A	611	VAL	N-CA-C	7.26	118.05	110.72
1	D	71	ARG	N-CA-C	7.23	121.64	111.52
1	A	59	PHE	N-CA-C	7.22	119.15	111.28
1	B	58	TYR	N-CA-C	7.11	119.03	111.28
1	A	397	PRO	CA-C-N	-7.10	113.07	120.38
1	A	397	PRO	C-N-CA	-7.10	113.07	120.38
1	B	609	LEU	N-CA-C	7.01	119.00	111.36
1	B	558	ASN	N-CA-C	7.00	118.56	111.07
1	A	722	ILE	N-CA-C	-6.91	103.75	110.72
1	A	58	TYR	N-CA-C	6.88	118.78	111.28
1	D	550	LYS	N-CA-C	6.78	121.23	112.41
1	B	611	VAL	N-CA-C	6.65	117.43	110.72
1	A	71	ARG	N-CA-C	6.62	120.38	111.24
1	B	59	PHE	N-CA-C	6.55	118.42	111.28
1	D	562	SER	N-CA-C	6.49	118.36	111.28
1	A	38	ASN	N-CA-C	-6.43	104.48	112.90
1	B	236	GLU	N-CA-C	-6.41	101.90	110.55
1	A	631	ALA	N-CA-C	6.33	118.25	111.36
1	B	60	LYS	N-CA-C	6.29	117.80	111.07
1	D	59	PHE	N-CA-C	6.13	118.04	111.36
1	B	541	TYR	N-CA-C	6.11	118.02	111.36
1	D	60	LYS	N-CA-C	6.10	120.79	112.68
1	A	60	LYS	N-CA-C	6.07	117.57	111.07
1	B	631	ALA	N-CA-C	6.07	117.90	111.28
1	C	632	ASP	N-CA-C	5.98	117.88	111.36
1	D	631	ALA	N-CA-C	5.91	117.80	111.36
1	C	612	LEU	N-CA-C	5.91	117.80	111.36
1	B	540	TYR	N-CA-C	5.82	117.42	111.14
1	B	632	ASP	N-CA-C	5.74	117.61	111.36
1	A	56	GLU	N-CA-C	-5.71	105.05	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	631	ALA	N-CA-C	5.68	117.47	111.28
1	D	612	LEU	N-CA-C	5.65	117.52	111.36
1	A	541	TYR	N-CA-C	5.64	117.43	111.28
1	B	18	ILE	CA-C-N	-5.54	114.27	120.14
1	B	18	ILE	C-N-CA	-5.54	114.27	120.14
1	C	136	PHE	N-CA-C	5.53	119.20	111.74
1	A	521	PHE	N-CA-C	-5.47	105.23	111.14
1	D	29	LEU	CA-CB-CG	5.47	135.45	116.30
1	A	609	LEU	N-CA-C	5.42	117.27	111.36
1	C	72	THR	N-CA-C	-5.38	103.43	110.53
1	A	649	GLU	N-CA-C	-5.31	101.51	109.79
1	D	549	CYS	N-CA-C	-5.25	100.84	109.40
1	A	465	ARG	N-CA-C	5.24	116.84	111.03
1	D	139	PHE	N-CA-C	5.22	118.00	109.59
1	D	61	ILE	N-CA-C	5.08	116.32	108.44
1	B	519	PHE	N-CA-C	5.08	117.71	111.82
1	A	558	ASN	N-CA-C	5.04	116.46	111.07
1	D	72	THR	N-CA-C	-5.02	103.52	110.35

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	397	PRO	Peptide
1	B	398	PRO	Peptide
1	C	397	PRO	Peptide
1	C	398	PRO	Peptide
1	D	397	PRO	Peptide
1	D	398	PRO	Peptide

5.2 Too-close contacts ⓘ

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	5296	0	5238	251	0
1	B	5268	0	5215	210	0
1	C	5266	0	5217	157	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5255	0	5212	230	0
2	A	35	0	47	19	0
2	B	35	0	49	26	0
2	C	35	0	49	21	0
2	D	35	0	49	22	0
3	A	88	0	134	51	0
3	C	44	0	67	21	0
3	D	44	0	67	25	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	21405	0	21344	811	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 19.

All (811) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:PHE:CE1	2:B:801:Y01:HAB1	1.45	1.52
1:B:378:PHE:CZ	2:B:801:Y01:HAB1	1.47	1.48
1:D:378:PHE:CZ	2:D:801:Y01:HAB1	1.51	1.44
1:B:378:PHE:CE1	2:B:801:Y01:CAB	2.01	1.43
1:D:386:HIS:HE1	1:D:402:VAL:CG2	1.31	1.41
1:C:539:PHE:CZ	1:C:540:TYR:CE2	2.14	1.35
1:B:378:PHE:CD1	2:B:801:Y01:HAB2	1.61	1.33
1:D:196:ARG:NH1	1:D:234:GLU:OE2	1.57	1.33
1:D:378:PHE:CE1	2:D:801:Y01:CAB	2.11	1.32
1:A:467:SER:O	1:A:468:TRP:CD1	1.84	1.30
1:A:467:SER:O	1:A:468:TRP:HD1	1.15	1.30
1:D:64:ASN:ND2	1:D:95:TYR:H	1.30	1.27
1:D:378:PHE:CE1	2:D:801:Y01:HAB1	1.67	1.27
1:D:549:CYS:CB	1:D:554:CYS:SG	2.23	1.26
1:D:386:HIS:CE1	1:D:402:VAL:CG2	2.17	1.26
1:D:386:HIS:CE1	1:D:402:VAL:HG23	1.73	1.22
1:A:511:ARG:CZ	1:A:634:GLU:OE1	1.88	1.22
1:C:539:PHE:CZ	1:C:540:TYR:CZ	2.31	1.18
1:D:378:PHE:CD1	2:D:801:Y01:HAB2	1.77	1.18
1:C:539:PHE:CE1	1:C:540:TYR:CE2	2.31	1.17
3:A:803:LPP:H443	3:A:803:LPP:H401	1.20	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:PHE:CZ	2:D:801:Y01:CAB	2.24	1.16
1:C:539:PHE:HZ	1:C:540:TYR:CZ	1.64	1.16
3:C:802:LPP:H401	3:C:802:LPP:H443	1.20	1.15
1:C:539:PHE:CE1	1:C:540:TYR:CD2	2.34	1.15
1:D:549:CYS:SG	1:D:554:CYS:SG	1.30	1.15
3:A:802:LPP:H401	3:A:802:LPP:H443	1.20	1.12
1:D:64:ASN:HD21	1:D:95:TYR:N	1.45	1.12
1:B:139:PHE:CE2	1:B:148:LEU:HD11	1.84	1.11
1:B:139:PHE:HE2	1:B:148:LEU:HD11	1.13	1.10
1:B:44:ASP:O	1:B:48:VAL:HG23	1.53	1.09
1:B:378:PHE:CZ	2:B:801:Y01:CAB	2.21	1.09
3:D:802:LPP:H401	3:D:802:LPP:H443	1.20	1.09
1:C:72:THR:OG1	1:C:75:LEU:HG	1.53	1.08
1:A:237:PHE:HE2	1:B:308:GLN:NE2	1.52	1.06
1:D:549:CYS:SG	1:D:554:CYS:CB	2.42	1.06
1:D:378:PHE:CE1	2:D:801:Y01:HAB2	1.81	1.06
1:D:386:HIS:CE1	1:D:402:VAL:HG21	1.87	1.06
1:A:533:GLY:C	1:A:600:MET:HE1	1.81	1.05
1:B:544:THR:OG1	1:B:559:ASN:ND2	1.90	1.04
1:D:64:ASN:HD22	1:D:95:TYR:HB3	1.19	1.03
1:D:386:HIS:HE1	1:D:402:VAL:HG23	0.91	1.03
1:C:617:ILE:O	1:C:621:ASN:ND2	1.92	1.02
1:A:511:ARG:NE	1:A:634:GLU:OE1	1.93	1.02
1:A:398:PRO:HB3	1:A:404:TRP:NE1	1.74	1.01
1:D:64:ASN:HD22	1:D:95:TYR:CB	1.75	1.00
1:B:237:PHE:HE2	1:C:308:GLN:NE2	1.58	1.00
1:A:66:ILE:HG12	1:A:72:THR:HG22	1.42	1.00
1:A:533:GLY:C	1:A:600:MET:CE	2.35	1.00
3:A:803:LPP:HC61	1:B:572:PHE:CD2	1.96	1.00
1:D:572:PHE:CD2	3:D:802:LPP:HC61	1.97	0.99
1:B:548:SER:O	1:B:549:CYS:SG	2.21	0.99
1:B:606:VAL:HG11	3:C:802:LPP:H331	1.45	0.98
1:B:378:PHE:CD1	2:B:801:Y01:CAB	2.32	0.97
1:A:398:PRO:CB	1:A:404:TRP:HE1	1.78	0.97
1:B:139:PHE:CE2	1:B:148:LEU:CD1	2.47	0.96
1:C:50:LYS:O	1:C:54:GLU:HG2	1.63	0.96
1:A:533:GLY:O	1:A:600:MET:HE1	1.65	0.96
1:D:519:PHE:CD2	1:D:619:MET:HE1	2.01	0.96
1:B:464:PRO:O	1:B:468:TRP:NE1	1.97	0.96
1:A:617:ILE:O	1:A:621:ASN:ND2	1.98	0.95
1:A:395:GLN:O	1:A:397:PRO:HD3	1.63	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:LEU:CD2	1:A:600:MET:HE2	1.96	0.95
1:D:64:ASN:ND2	1:D:95:TYR:CB	2.30	0.94
1:A:397:PRO:HB2	1:A:398:PRO:CD	1.97	0.94
1:C:572:PHE:CD2	3:C:802:LPP:HC61	2.03	0.94
1:D:139:PHE:CE2	1:D:148:LEU:HD11	2.02	0.94
1:A:372:SER:O	1:A:409:TRP:HZ3	1.51	0.94
1:A:66:ILE:HG12	1:A:72:THR:CG2	1.96	0.94
1:A:599:THR:HA	3:A:803:LPP:HC81	1.50	0.93
1:B:519:PHE:CD2	1:B:619:MET:HE1	2.02	0.93
1:B:532:ASN:OD1	1:C:381:LEU:HD23	1.68	0.92
1:A:534:LEU:HD23	1:A:600:MET:HE2	1.49	0.92
1:A:656:PRO:HD2	1:A:657:PHE:H	1.33	0.91
1:D:464:PRO:O	1:D:468:TRP:NE1	2.04	0.91
1:B:225:TRP:HZ3	1:B:296:ARG:HE	1.18	0.90
3:D:802:LPP:H401	3:D:802:LPP:C44	2.01	0.90
1:B:519:PHE:CE2	1:B:619:MET:HE1	2.07	0.90
1:A:381:LEU:HD23	1:D:532:ASN:OD1	1.70	0.89
1:D:64:ASN:ND2	1:D:95:TYR:N	2.08	0.89
1:D:519:PHE:CE2	1:D:619:MET:HE1	2.06	0.89
1:A:237:PHE:CE2	1:B:308:GLN:NE2	2.41	0.89
1:B:374:LEU:HD21	2:B:801:Y01:HAE2	1.53	0.89
1:C:237:PHE:HE2	1:D:308:GLN:NE2	1.69	0.89
1:D:139:PHE:HE2	1:D:148:LEU:HD11	1.37	0.89
1:B:50:LYS:O	1:B:54:GLU:HG2	1.73	0.89
1:A:376:PHE:HB2	1:A:409:TRP:CE3	2.08	0.88
1:A:534:LEU:N	1:A:600:MET:CE	2.37	0.88
1:A:636:LYS:O	1:A:640:THR:HG23	1.74	0.87
1:C:547:LEU:CB	1:C:558:ASN:HD22	1.87	0.87
1:A:534:LEU:CG	1:A:600:MET:HE2	2.05	0.87
3:A:802:LPP:H331	1:D:606:VAL:HG11	1.57	0.86
1:A:372:SER:O	1:A:409:TRP:CZ3	2.27	0.86
1:A:50:LYS:O	1:A:54:GLU:HG2	1.76	0.86
1:B:378:PHE:CG	2:B:801:Y01:HAB2	2.11	0.85
1:A:29:LEU:HD23	1:A:34:LYS:HG3	1.57	0.85
1:C:464:PRO:O	1:C:468:TRP:NE1	2.08	0.85
1:A:731:LEU:CD2	1:A:735:ASN:ND2	2.39	0.85
1:B:547:LEU:CB	1:B:558:ASN:HD22	1.89	0.85
1:B:79:GLU:OE2	1:C:726:LYS:NZ	2.10	0.84
1:C:188:ASP:N	1:D:262:SER:HG	1.76	0.84
3:A:803:LPP:H401	3:A:803:LPP:C44	2.01	0.83
3:C:802:LPP:H401	3:C:802:LPP:C44	2.01	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:PRO:HB3	1:A:404:TRP:HE1	1.36	0.83
1:D:208:LEU:O	1:D:211:LEU:O	1.95	0.83
1:B:547:LEU:CB	1:B:558:ASN:ND2	2.42	0.83
1:D:350:ALA:O	1:D:353:SER:OG	1.97	0.82
1:C:539:PHE:HZ	1:C:540:TYR:CE2	1.73	0.82
1:B:525:LEU:HD21	2:C:801:Y01:CAN	2.09	0.82
1:C:606:VAL:HG11	3:D:802:LPP:H331	1.62	0.82
1:A:376:PHE:HB2	1:A:409:TRP:CZ3	2.15	0.81
1:A:603:THR:HG22	3:A:803:LPP:H311	1.63	0.81
1:A:599:THR:HG23	3:A:803:LPP:HC82	1.61	0.81
1:B:237:PHE:CE2	1:C:308:GLN:NE2	2.47	0.81
1:B:495:LEU:HD23	2:B:801:Y01:HAD3	1.63	0.80
1:B:378:PHE:CE2	2:B:801:Y01:CAB	2.64	0.80
1:A:731:LEU:HD22	1:A:735:ASN:ND2	1.96	0.80
1:B:525:LEU:CD2	2:C:801:Y01:HAN1	2.11	0.80
1:D:617:ILE:O	1:D:621:ASN:ND2	2.15	0.80
1:A:495:LEU:HD23	2:A:801:Y01:HAD3	1.63	0.80
1:A:731:LEU:HD22	1:A:735:ASN:HD22	1.48	0.79
1:C:532:ASN:OD1	1:D:381:LEU:HD23	1.81	0.79
1:A:552:ILE:HD12	1:A:566:GLU:OE2	1.83	0.79
1:D:343:PHE:CE1	1:D:358:PHE:CE2	2.70	0.79
1:A:41:GLU:HB3	1:A:76:ILE:HG21	1.65	0.78
1:D:44:ASP:OD1	1:D:748:PHE:CG	2.36	0.78
1:A:374:LEU:HD21	2:A:801:Y01:HAE2	1.64	0.78
1:B:33:GLU:HG2	1:B:61:ILE:HG23	1.64	0.78
1:A:523:TYR:CD1	3:A:802:LPP:H263	2.19	0.78
1:B:363:PHE:HE1	2:B:801:Y01:HAL2	1.47	0.78
1:A:603:THR:HG22	3:A:803:LPP:H302	1.65	0.78
1:B:525:LEU:HD21	2:C:801:Y01:HAN2	1.63	0.78
1:D:378:PHE:CD1	2:D:801:Y01:CAB	2.53	0.77
3:D:802:LPP:HC7	3:D:802:LPP:O2	1.84	0.77
3:A:803:LPP:HC7	3:A:803:LPP:O2	1.84	0.76
1:A:29:LEU:HD23	1:A:34:LYS:CG	2.16	0.76
3:A:802:LPP:HC7	3:A:802:LPP:O2	1.84	0.76
1:A:656:PRO:HD2	1:A:657:PHE:N	1.99	0.76
3:C:802:LPP:HC7	3:C:802:LPP:O2	1.84	0.76
1:A:397:PRO:HB2	1:A:398:PRO:HD3	1.66	0.75
1:C:539:PHE:CZ	1:C:540:TYR:CD2	2.67	0.75
1:D:105:ARG:HD2	1:D:139:PHE:HZ	1.51	0.75
3:A:803:LPP:C6	1:B:572:PHE:CE2	2.69	0.75
1:D:572:PHE:CE2	3:D:802:LPP:C6	2.70	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:GLY:C	1:A:600:MET:HE3	2.11	0.74
1:A:700:LEU:HD13	1:A:704:HIS:CD2	2.22	0.74
1:A:642:LEU:HD23	1:A:643:TRP:N	2.01	0.74
1:B:37:LEU:HD21	1:B:73:ALA:HB2	1.69	0.74
1:D:64:ASN:HD21	1:D:95:TYR:H	0.75	0.74
1:D:139:PHE:CE2	1:D:148:LEU:CD1	2.70	0.74
1:A:534:LEU:HG	1:A:600:MET:HE2	1.68	0.74
1:C:363:PHE:HE1	2:C:801:Y01:HAL1	1.52	0.73
1:D:343:PHE:CE1	1:D:358:PHE:CD2	2.76	0.73
3:A:803:LPP:C6	1:B:572:PHE:CD2	2.72	0.73
1:D:343:PHE:CD1	1:D:358:PHE:HD2	2.07	0.73
1:D:563:THR:OG1	1:D:566:GLU:HB2	1.89	0.73
1:C:467:SER:O	1:C:468:TRP:HD1	1.72	0.73
2:A:801:Y01:HAE2	2:A:801:Y01:HAO1	1.69	0.73
1:C:547:LEU:CB	1:C:558:ASN:ND2	2.52	0.72
1:A:398:PRO:HB2	1:A:404:TRP:HE1	1.53	0.72
1:A:636:LYS:O	1:A:640:THR:CG2	2.37	0.72
1:B:633:ILE:HD12	1:B:633:ILE:C	2.15	0.72
3:A:802:LPP:H401	3:A:802:LPP:C44	2.01	0.72
1:D:572:PHE:CD2	3:D:802:LPP:C6	2.72	0.72
1:A:534:LEU:CA	1:A:600:MET:CE	2.67	0.72
1:A:642:LEU:HD23	1:A:642:LEU:C	2.15	0.72
1:B:374:LEU:HD21	2:B:801:Y01:CAE	2.20	0.72
1:B:378:PHE:CG	2:B:801:Y01:CAB	2.72	0.72
1:D:633:ILE:HD12	1:D:633:ILE:C	2.15	0.72
1:A:534:LEU:N	1:A:600:MET:HE3	2.04	0.71
1:A:715:LYS:HG3	1:D:136:PHE:CE1	2.25	0.71
1:A:497:THR:HG23	1:A:506:GLN:HE22	1.54	0.71
3:A:803:LPP:HC61	1:B:572:PHE:CE2	2.24	0.71
1:D:378:PHE:CE2	2:D:801:Y01:CAB	2.73	0.71
1:C:237:PHE:CE2	1:D:308:GLN:NE2	2.58	0.71
1:C:633:ILE:C	1:C:633:ILE:HD12	2.15	0.71
1:D:63:ILE:N	1:D:63:ILE:HD12	2.05	0.71
1:B:363:PHE:CE1	2:B:801:Y01:HAL2	2.26	0.71
1:C:539:PHE:HE1	1:C:540:TYR:CE2	2.07	0.71
1:D:467:SER:O	1:D:468:TRP:HD1	1.73	0.71
1:A:731:LEU:CD2	1:A:735:ASN:HD22	2.00	0.71
1:B:525:LEU:CD2	2:C:801:Y01:CAN	2.67	0.71
1:D:519:PHE:CD2	1:D:619:MET:CE	2.73	0.71
1:A:740:LYS:HE3	1:B:742:ASP:OD2	1.91	0.71
1:D:363:PHE:HE1	2:D:801:Y01:HAL1	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:THR:HG1	1:A:409:TRP:HH2	1.35	0.70
1:B:495:LEU:HD23	2:B:801:Y01:CAD	2.21	0.70
1:D:572:PHE:CE2	3:D:802:LPP:HC62	2.26	0.70
1:D:572:PHE:CE2	3:D:802:LPP:HC61	2.26	0.70
1:D:64:ASN:ND2	1:D:95:TYR:HB3	1.97	0.70
1:A:398:PRO:HB3	1:A:404:TRP:CE2	2.26	0.70
1:A:603:THR:CG2	3:A:803:LPP:H302	2.22	0.70
1:B:44:ASP:O	1:B:48:VAL:CG2	2.35	0.70
1:A:572:PHE:CD2	3:A:802:LPP:HC61	2.27	0.70
1:B:467:SER:O	1:B:468:TRP:HD1	1.74	0.70
1:D:374:LEU:HD21	2:D:801:Y01:HAE2	1.74	0.70
1:B:519:PHE:CD2	1:B:619:MET:CE	2.73	0.70
1:A:534:LEU:HA	1:A:600:MET:CE	2.22	0.70
1:A:606:VAL:HG11	3:A:803:LPP:H331	1.74	0.69
1:B:519:PHE:HD2	1:B:619:MET:HE1	1.55	0.69
1:A:722:ILE:CD1	1:D:69:LEU:HD21	2.21	0.69
1:B:525:LEU:HD23	2:C:801:Y01:HAN1	1.73	0.69
1:B:44:ASP:OD1	1:B:748:PHE:CG	2.46	0.69
1:C:580:ASN:H	1:C:580:ASN:ND2	1.90	0.69
2:C:801:Y01:HAC1	2:C:801:Y01:HAU2	1.73	0.69
1:C:72:THR:HG1	1:C:75:LEU:HG	1.54	0.69
3:A:803:LPP:HC62	1:B:572:PHE:CE2	2.27	0.68
1:B:50:LYS:O	1:B:54:GLU:CG	2.40	0.68
1:D:64:ASN:ND2	1:D:95:TYR:HB2	2.09	0.68
2:A:801:Y01:CAP	1:D:525:LEU:HD21	2.22	0.68
1:B:60:LYS:O	1:B:61:ILE:CG1	2.41	0.68
1:C:572:PHE:CE2	3:C:802:LPP:C6	2.76	0.68
1:A:363:PHE:HE1	2:A:801:Y01:HAL1	1.58	0.68
2:D:801:Y01:HAC1	2:D:801:Y01:HAU2	1.75	0.68
1:B:560:ALA:CB	1:B:583:VAL:HG13	2.23	0.68
1:A:726:LYS:O	1:D:732:THR:OG1	2.08	0.68
2:A:801:Y01:HAP1	1:D:525:LEU:HD21	1.75	0.68
1:D:63:ILE:HD12	1:D:63:ILE:H	1.59	0.68
1:A:525:LEU:HD21	2:B:801:Y01:HAP2	1.76	0.68
1:A:726:LYS:NZ	1:D:79:GLU:OE2	2.19	0.68
1:D:519:PHE:HD2	1:D:619:MET:HE1	1.54	0.67
1:A:603:THR:HG22	3:A:803:LPP:C31	2.25	0.67
1:B:732:THR:OG1	1:C:726:LYS:O	2.10	0.67
1:C:363:PHE:CE1	2:C:801:Y01:HAL1	2.29	0.67
1:C:495:LEU:HD23	2:C:801:Y01:HAD3	1.75	0.67
1:A:715:LYS:HG3	1:D:136:PHE:CZ	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:LEU:HD23	1:A:735:ASN:ND2	2.09	0.67
1:B:30:SER:OG	1:B:31:PRO:HD2	1.94	0.67
1:D:261:SER:OG	1:D:264:GLU:HG3	1.95	0.67
1:D:580:ASN:H	1:D:580:ASN:ND2	1.92	0.67
1:C:79:GLU:OE2	1:D:726:LYS:NZ	2.21	0.66
1:A:467:SER:C	1:A:468:TRP:CD1	2.72	0.66
1:A:525:LEU:HD21	2:B:801:Y01:CAP	2.26	0.66
1:B:378:PHE:CE2	2:B:801:Y01:HAB3	2.30	0.66
1:A:599:THR:HG23	3:A:803:LPP:C8	2.23	0.66
1:B:552:ILE:HG21	1:B:579:ILE:HD11	1.78	0.66
1:C:523:TYR:HH	1:C:604:TYR:HH	1.40	0.66
1:A:41:GLU:HB3	1:A:76:ILE:CG2	2.25	0.66
1:C:523:TYR:CD1	3:C:802:LPP:H263	2.31	0.66
1:A:621:ASN:N	1:A:621:ASN:HD22	1.94	0.66
1:C:374:LEU:HD21	2:C:801:Y01:HAE2	1.78	0.65
1:D:549:CYS:HB2	1:D:554:CYS:SG	2.31	0.65
1:B:580:ASN:ND2	1:B:580:ASN:H	1.94	0.65
1:B:105:ARG:NH2	1:C:723:ARG:HG3	2.12	0.65
1:C:572:PHE:CE2	3:C:802:LPP:HC62	2.32	0.65
1:A:534:LEU:HA	1:A:600:MET:HE1	1.79	0.65
1:B:105:ARG:CD	1:B:139:PHE:HZ	2.10	0.65
1:C:582:TYR:HA	1:D:553:ARG:O	1.96	0.65
1:C:603:THR:HG22	3:D:802:LPP:H302	1.78	0.65
1:C:71:ARG:HA	1:C:71:ARG:NE	2.12	0.65
1:D:589:GLN:O	1:D:589:GLN:HG2	1.96	0.65
1:C:572:PHE:CD2	3:C:802:LPP:C6	2.77	0.65
1:D:285:ASP:HB2	1:D:290:LYS:NZ	2.12	0.65
1:A:603:THR:HG22	3:A:803:LPP:C30	2.26	0.64
1:B:560:ALA:HB3	1:B:583:VAL:HG13	1.78	0.64
1:D:519:PHE:CE2	1:D:619:MET:CE	2.80	0.64
1:D:495:LEU:HD23	2:D:801:Y01:HAD3	1.78	0.64
1:A:375:THR:OG1	1:A:409:TRP:HH2	1.78	0.64
1:A:511:ARG:NH2	1:A:634:GLU:OE1	2.29	0.64
1:A:729:GLU:HG2	1:D:730:GLY:HA3	1.78	0.64
1:A:611:VAL:HG11	3:A:803:LPP:H391	1.78	0.64
1:A:534:LEU:HG	1:A:600:MET:CE	2.28	0.64
1:D:363:PHE:CE1	2:D:801:Y01:HAL1	2.32	0.64
1:B:617:ILE:O	1:B:621:ASN:ND2	2.32	0.63
1:C:543:GLU:HA	1:C:543:GLU:OE1	1.97	0.63
1:A:607:ILE:HG12	3:A:803:LPP:H392	1.81	0.63
1:A:656:PRO:CD	1:A:657:PHE:H	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HD22	1:B:100:LEU:O	1.99	0.63
1:C:572:PHE:CE2	3:C:802:LPP:HC61	2.32	0.63
1:D:523:TYR:HH	1:D:604:TYR:HH	1.38	0.63
1:D:543:GLU:OE1	1:D:543:GLU:HA	1.97	0.63
1:B:611:VAL:HG11	3:C:802:LPP:H391	1.80	0.63
1:A:32:SER:CB	1:A:61:ILE:HD11	2.28	0.63
1:C:196:ARG:NH1	1:C:234:GLU:OE2	2.32	0.63
1:D:196:ARG:NH1	1:D:234:GLU:CD	2.52	0.63
1:B:138:GLU:O	1:B:138:GLU:HG2	1.99	0.63
1:D:580:ASN:H	1:D:580:ASN:HD22	1.47	0.63
1:B:519:PHE:CE2	1:B:619:MET:CE	2.80	0.62
1:A:38:ASN:O	1:A:42:LYS:HG3	1.98	0.62
1:A:649:GLU:HA	1:A:649:GLU:OE2	1.99	0.62
1:B:196:ARG:NH1	1:B:234:GLU:OE2	2.32	0.62
1:C:599:THR:HA	3:D:802:LPP:HC81	1.81	0.62
1:D:343:PHE:CE1	1:D:358:PHE:HE2	2.17	0.62
1:A:642:LEU:CD2	1:A:643:TRP:HD1	2.13	0.62
1:D:417:GLU:HG3	1:D:442:ASN:HD22	1.65	0.62
1:A:301:VAL:CG1	1:A:640:THR:HG21	2.30	0.62
1:A:722:ILE:HD12	1:D:69:LEU:HD11	1.81	0.62
1:B:50:LYS:HZ3	1:B:50:LYS:HB3	1.64	0.62
1:B:606:VAL:CG1	3:C:802:LPP:H331	2.26	0.62
1:A:196:ARG:NH1	1:A:234:GLU:OE2	2.32	0.62
1:B:32:SER:HB2	1:B:61:ILE:HD11	1.80	0.62
2:B:801:Y01:HAU2	2:B:801:Y01:HAC1	1.81	0.62
1:A:511:ARG:CD	1:A:634:GLU:OE1	2.48	0.62
1:B:415:TRP:HH2	1:B:422:TRP:CH2	2.18	0.62
1:B:60:LYS:O	1:B:61:ILE:HG13	2.00	0.62
1:A:237:PHE:HE2	1:B:308:GLN:HE21	1.44	0.61
1:A:700:LEU:HD13	1:A:704:HIS:HD2	1.63	0.61
1:B:32:SER:CB	1:B:61:ILE:HD11	2.29	0.61
1:A:552:ILE:CD1	1:A:566:GLU:OE2	2.48	0.61
1:B:48:VAL:O	1:B:52:LEU:HG	2.01	0.61
1:B:511:ARG:NH2	1:B:634:GLU:OE1	2.33	0.61
1:B:525:LEU:HD21	2:C:801:Y01:HAP2	1.81	0.61
1:D:343:PHE:CD1	1:D:358:PHE:CD2	2.88	0.61
1:B:139:PHE:HE2	1:B:148:LEU:CD1	1.95	0.61
1:B:521:PHE:CE1	2:C:801:Y01:HAB1	2.36	0.61
1:C:525:LEU:HD21	2:D:801:Y01:HAP2	1.82	0.61
1:A:74:LEU:HD23	1:A:74:LEU:O	2.01	0.61
1:A:136:PHE:CZ	1:B:715:LYS:HG3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:ASN:H	1:C:580:ASN:HD22	1.49	0.60
1:A:154:ASN:HD22	1:A:157:ILE:CD1	2.14	0.60
1:C:136:PHE:CZ	1:D:715:LYS:HG3	2.36	0.60
2:A:801:Y01:HAO1	2:A:801:Y01:CAE	2.31	0.60
1:D:543:GLU:O	1:D:544:THR:HG22	2.01	0.60
1:B:532:ASN:OD1	1:C:381:LEU:CD2	2.46	0.60
1:B:580:ASN:H	1:B:580:ASN:HD22	1.47	0.60
1:A:543:GLU:OE1	1:A:543:GLU:HA	2.02	0.60
1:C:343:PHE:CD1	1:C:358:PHE:HD2	2.19	0.60
1:B:313:ARG:CG	1:B:313:ARG:HH21	2.15	0.60
1:D:523:TYR:CD1	3:D:802:LPP:H263	2.37	0.60
1:A:154:ASN:HD22	1:A:157:ILE:HD12	1.67	0.59
1:A:168:VAL:O	1:D:18:ILE:HG22	2.02	0.59
3:A:802:LPP:H302	1:D:603:THR:HG22	1.84	0.59
1:C:343:PHE:CE1	1:C:358:PHE:CD2	2.91	0.59
1:B:69:LEU:O	1:B:71:ARG:HG2	2.03	0.59
1:A:365:LYS:O	1:A:369:HIS:HD2	1.85	0.59
1:A:398:PRO:CB	1:A:404:TRP:NE1	2.45	0.59
1:C:188:ASP:N	1:D:262:SER:OG	2.35	0.59
1:D:285:ASP:HB2	1:D:290:LYS:HZ2	1.67	0.59
1:A:40:VAL:O	1:A:41:GLU:HG2	2.03	0.59
1:A:656:PRO:CD	1:A:657:PHE:N	2.66	0.59
1:C:69:LEU:HG	1:C:69:LEU:O	2.01	0.59
3:A:802:LPP:H443	3:A:802:LPP:C40	2.13	0.58
1:B:430:ILE:O	1:B:430:ILE:HG22	2.02	0.58
1:A:374:LEU:HD21	2:A:801:Y01:CAE	2.33	0.58
1:A:715:LYS:CG	1:D:136:PHE:CE1	2.85	0.58
1:B:519:PHE:HD2	1:B:619:MET:CE	2.14	0.58
1:D:260:ARG:HG2	1:D:716:ARG:NH1	2.18	0.58
1:D:339:LEU:HB2	1:D:343:PHE:HE2	1.68	0.58
1:D:543:GLU:O	1:D:559:ASN:ND2	2.36	0.58
1:A:29:LEU:CD2	1:A:34:LYS:CG	2.80	0.58
1:C:74:LEU:HD23	1:C:74:LEU:O	2.04	0.58
1:D:67:ASP:HB2	1:D:71:ARG:HB2	1.85	0.58
1:B:377:LEU:HB3	2:B:801:Y01:HAA2	1.85	0.58
1:D:64:ASN:ND2	1:D:95:TYR:CA	2.66	0.58
1:D:519:PHE:HD2	1:D:619:MET:CE	2.14	0.58
1:B:378:PHE:CD2	2:B:801:Y01:CAB	2.87	0.58
1:B:105:ARG:HD2	1:B:139:PHE:CZ	2.39	0.58
1:D:544:THR:HG23	1:D:544:THR:O	2.04	0.58
1:A:552:ILE:HD12	1:A:552:ILE:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:ARG:CZ	1:B:634:GLU:OE1	2.52	0.57
1:B:582:TYR:HA	1:C:553:ARG:O	2.04	0.57
2:C:801:Y01:HAN2	2:C:801:Y01:HAP2	1.85	0.57
1:C:599:THR:HG23	3:D:802:LPP:HC82	1.85	0.57
1:A:313:ARG:HH21	1:A:313:ARG:HG3	1.70	0.57
1:A:381:LEU:CD2	1:D:532:ASN:OD1	2.51	0.57
1:D:226:GLU:O	1:D:230:LEU:HB2	2.05	0.57
1:D:378:PHE:CG	2:D:801:Y01:HAB2	2.36	0.57
1:C:539:PHE:HE1	1:C:540:TYR:CD2	2.14	0.57
1:C:466:GLU:OE2	1:C:467:SER:N	2.38	0.56
1:A:495:LEU:HD23	2:A:801:Y01:CAD	2.33	0.56
1:B:519:PHE:HD2	1:B:619:MET:SD	2.28	0.56
1:C:67:ASP:OD2	1:C:71:ARG:HB2	2.05	0.56
1:C:226:GLU:O	1:C:230:LEU:HB2	2.05	0.56
1:C:313:ARG:HH21	1:C:313:ARG:HG3	1.70	0.56
1:B:607:ILE:HG23	3:C:802:LPP:H422	1.88	0.56
1:C:71:ARG:HA	1:C:71:ARG:HE	1.68	0.56
1:C:511:ARG:NH2	1:C:634:GLU:OE1	2.38	0.56
1:A:226:GLU:O	1:A:230:LEU:HB2	2.05	0.56
1:D:313:ARG:HH21	1:D:313:ARG:HG3	1.68	0.56
1:A:363:PHE:CE1	2:A:801:Y01:HAL1	2.40	0.56
1:A:415:TRP:CD1	1:A:659:VAL:HG22	2.40	0.56
1:B:226:GLU:O	1:B:230:LEU:HB2	2.05	0.56
1:D:519:PHE:HE2	1:D:619:MET:HE1	1.66	0.56
1:A:154:ASN:HD22	1:A:157:ILE:CG1	2.17	0.56
1:C:67:ASP:HB2	1:C:71:ARG:HB2	1.87	0.56
1:D:289:LEU:HD13	1:D:310:LEU:HD21	1.88	0.56
1:A:534:LEU:CA	1:A:600:MET:HE1	2.34	0.56
1:D:589:GLN:O	1:D:589:GLN:CG	2.54	0.56
1:A:66:ILE:HG12	1:A:72:THR:CB	2.36	0.56
1:C:136:PHE:CE1	1:D:715:LYS:HG3	2.41	0.55
1:B:552:ILE:HD12	1:B:552:ILE:H	1.71	0.55
1:C:72:THR:OG1	1:C:75:LEU:CG	2.41	0.55
1:A:32:SER:C	1:A:61:ILE:HD11	2.30	0.55
1:D:63:ILE:H	1:D:63:ILE:CD1	2.18	0.55
1:A:496:PHE:HB2	1:A:506:GLN:HE21	1.72	0.55
1:A:605:ASN:O	1:A:609:LEU:HB2	2.07	0.55
1:C:67:ASP:OD2	1:C:71:ARG:CB	2.55	0.55
1:C:415:TRP:HH2	1:C:422:TRP:CH2	2.24	0.55
1:A:552:ILE:HD11	1:A:566:GLU:HG3	1.88	0.55
1:B:555:GLU:CD	1:B:555:GLU:H	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:803:LPP:H443	3:A:803:LPP:C40	2.13	0.55
3:A:803:LPP:H263	1:B:523:TYR:CD1	2.42	0.55
1:B:621:ASN:N	1:B:621:ASN:HD22	2.05	0.55
1:A:29:LEU:CD2	1:A:34:LYS:HG2	2.37	0.54
1:A:66:ILE:CG1	1:A:72:THR:HG22	2.27	0.54
1:A:534:LEU:N	1:A:600:MET:HE1	2.11	0.54
1:B:269:LEU:HD22	1:B:289:LEU:HG	1.89	0.54
1:B:611:VAL:HG11	3:C:802:LPP:H412	1.89	0.54
3:A:802:LPP:HC81	1:D:599:THR:HA	1.88	0.54
1:B:313:ARG:HH21	1:B:313:ARG:HG3	1.71	0.54
1:B:525:LEU:HD21	2:C:801:Y01:CAP	2.37	0.54
1:D:108:VAL:HG12	1:D:110:GLY:H	1.73	0.54
1:D:61:ILE:HG22	1:D:62:ASN:N	2.22	0.54
1:A:108:VAL:HG12	1:A:110:GLY:H	1.73	0.54
1:A:598:ALA:C	3:A:803:LPP:O3	2.50	0.54
1:B:549:CYS:SG	1:B:549:CYS:O	2.66	0.54
1:A:582:TYR:HB3	1:B:553:ARG:O	2.07	0.54
3:C:802:LPP:H443	3:C:802:LPP:C40	2.13	0.54
1:D:206:PRO:HB3	1:D:251:PHE:CD1	2.43	0.54
1:D:511:ARG:NH2	1:D:634:GLU:OE1	2.41	0.54
1:C:466:GLU:OE2	1:C:467:SER:CA	2.56	0.54
1:C:467:SER:O	1:C:468:TRP:CD1	2.59	0.54
1:D:345:VAL:HG12	1:D:349:ILE:CD1	2.38	0.54
1:A:496:PHE:HE2	1:D:522:ILE:HG12	1.73	0.54
1:B:68:PRO:O	1:C:715:LYS:NZ	2.39	0.54
1:B:340:PHE:CD1	1:B:340:PHE:C	2.86	0.54
1:B:605:ASN:O	1:B:609:LEU:HB2	2.08	0.54
1:D:415:TRP:HH2	1:D:422:TRP:CH2	2.25	0.54
1:C:269:LEU:HD22	1:C:289:LEU:HG	1.89	0.54
1:A:154:ASN:ND2	1:A:157:ILE:HG13	2.23	0.54
1:C:599:THR:HG23	3:D:802:LPP:C8	2.38	0.53
3:A:803:LPP:HC62	1:B:572:PHE:HE2	1.72	0.53
1:D:519:PHE:HD2	1:D:619:MET:SD	2.30	0.53
1:A:66:ILE:HG23	1:A:72:THR:HG22	1.91	0.53
1:A:154:ASN:HD22	1:A:157:ILE:HG13	1.73	0.53
1:B:108:VAL:HG12	1:B:110:GLY:H	1.73	0.53
1:D:417:GLU:HG3	1:D:442:ASN:ND2	2.23	0.53
1:B:60:LYS:O	1:B:61:ILE:HG12	2.07	0.53
1:A:38:ASN:O	1:A:42:LYS:CG	2.57	0.53
1:A:60:LYS:O	1:A:61:ILE:HG13	2.09	0.53
3:D:802:LPP:H443	3:D:802:LPP:C40	2.13	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:TYR:C	1:A:540:TYR:CD1	2.85	0.53
2:A:801:Y01:CAE	2:A:801:Y01:CAO	2.86	0.53
1:B:60:LYS:C	1:B:61:ILE:HG13	2.34	0.53
1:C:68:PRO:O	1:D:715:LYS:NZ	2.41	0.53
1:D:74:LEU:O	1:D:74:LEU:HD23	2.09	0.53
1:D:467:SER:O	1:D:468:TRP:CD1	2.60	0.53
1:B:75:LEU:O	1:B:78:ILE:N	2.38	0.53
1:B:374:LEU:CD2	2:B:801:Y01:HAE2	2.33	0.53
1:C:108:VAL:HG12	1:C:110:GLY:H	1.73	0.53
1:C:539:PHE:CZ	1:C:540:TYR:CE1	2.96	0.53
1:D:313:ARG:HH21	1:D:313:ARG:CG	2.22	0.53
1:A:105:ARG:HD2	1:A:139:PHE:HZ	1.74	0.53
1:B:492:LEU:O	1:B:495:LEU:HB2	2.08	0.53
1:D:345:VAL:CG1	1:D:349:ILE:HD11	2.38	0.52
1:A:167:SER:OG	1:D:17:ARG:NH2	2.34	0.52
1:A:167:SER:HG	1:D:17:ARG:HH21	1.54	0.52
1:B:525:LEU:CD2	2:C:801:Y01:HAN2	2.35	0.52
1:A:466:GLU:OE2	1:A:467:SER:N	2.42	0.52
1:B:105:ARG:HH22	1:C:723:ARG:HG3	1.74	0.52
1:C:105:ARG:HD2	1:C:139:PHE:HZ	1.74	0.52
1:B:50:LYS:NZ	1:B:50:LYS:CB	2.73	0.52
1:D:339:LEU:O	1:D:343:PHE:CD2	2.63	0.52
1:D:723:ARG:HH12	1:D:727:THR:CG2	2.23	0.52
1:A:365:LYS:O	1:A:369:HIS:CD2	2.63	0.52
1:C:525:LEU:HD21	2:D:801:Y01:CAP	2.40	0.51
1:D:378:PHE:CE2	2:D:801:Y01:HAB3	2.46	0.51
2:A:801:Y01:HAP2	1:D:525:LEU:HD21	1.91	0.51
1:C:532:ASN:OD1	1:D:381:LEU:CD2	2.57	0.51
1:C:607:ILE:HG12	3:D:802:LPP:H392	1.93	0.51
1:A:32:SER:OG	1:A:61:ILE:HD11	2.10	0.51
1:B:44:ASP:OD1	1:B:748:PHE:CD1	2.64	0.51
1:B:467:SER:O	1:B:468:TRP:CD1	2.60	0.51
1:B:139:PHE:CD2	1:B:148:LEU:CD1	2.94	0.51
1:D:572:PHE:HE2	3:D:802:LPP:HC62	1.72	0.51
1:B:377:LEU:HD22	1:B:492:LEU:HD21	1.92	0.51
1:C:136:PHE:CE1	1:D:715:LYS:CG	2.94	0.50
1:B:52:LEU:HB3	1:B:92:PHE:CE2	2.46	0.50
1:B:723:ARG:HH12	1:B:727:THR:CG2	2.24	0.50
1:D:92:PHE:N	1:D:92:PHE:CD1	2.78	0.50
1:A:29:LEU:HD13	1:A:29:LEU:N	2.26	0.50
1:A:318:PHE:HB3	1:A:321:TRP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:GLU:OE2	1:D:467:SER:N	2.45	0.50
1:A:511:ARG:NH2	1:A:627:ILE:HG23	2.27	0.50
1:A:723:ARG:HH12	1:A:727:THR:CG2	2.25	0.50
1:A:747:ARG:NH2	1:B:749:GLU:OE1	2.41	0.50
3:A:802:LPP:HC82	1:D:599:THR:HG23	1.92	0.50
1:D:63:ILE:N	1:D:63:ILE:CD1	2.73	0.50
1:B:519:PHE:HE2	1:B:619:MET:HE1	1.67	0.50
1:C:606:VAL:CG1	3:D:802:LPP:H331	2.39	0.50
1:A:313:ARG:HH21	1:A:313:ARG:CG	2.24	0.50
1:D:286:LEU:HD13	1:D:289:LEU:HD12	1.94	0.50
1:A:572:PHE:CE2	3:A:802:LPP:C6	2.95	0.50
1:C:723:ARG:HH12	1:C:727:THR:CG2	2.25	0.50
1:A:415:TRP:HA	1:A:415:TRP:CE3	2.47	0.50
3:A:802:LPP:O9	3:A:802:LPP:H141	2.12	0.50
1:B:607:ILE:HG12	3:C:802:LPP:H392	1.94	0.50
1:C:603:THR:HG22	3:D:802:LPP:H311	1.94	0.50
3:D:802:LPP:H141	3:D:802:LPP:O9	2.12	0.50
1:A:41:GLU:CB	1:A:76:ILE:CG2	2.90	0.49
3:A:802:LPP:H422	1:D:607:ILE:HG23	1.94	0.49
1:B:525:LEU:HD21	2:C:801:Y01:HAN1	1.80	0.49
1:C:699:ASN:OD1	1:C:702:ARG:NH2	2.45	0.49
1:D:347:TYR:HD2	1:D:653:LEU:HD21	1.77	0.49
1:A:497:THR:CG2	1:A:506:GLN:HE22	2.25	0.49
1:C:197:LEU:O	1:C:201:LYS:HB2	2.12	0.49
1:C:269:LEU:HA	1:C:288:ARG:HB3	1.92	0.49
1:D:269:LEU:HA	1:D:288:ARG:HB3	1.92	0.49
1:A:399:PRO:C	1:A:400:THR:HG23	2.37	0.49
1:B:699:ASN:OD1	1:B:702:ARG:NH2	2.45	0.49
1:D:699:ASN:OD1	1:D:702:ARG:NH2	2.45	0.49
1:A:654:PRO:O	1:A:656:PRO:HD2	2.12	0.49
1:A:722:ILE:HD12	1:D:69:LEU:HD21	1.94	0.49
3:A:803:LPP:H141	3:A:803:LPP:O9	2.12	0.49
1:C:268:ILE:HD11	1:C:713:LEU:HD11	1.95	0.49
1:C:580:ASN:ND2	1:C:580:ASN:N	2.60	0.49
1:A:523:TYR:CG	3:A:802:LPP:H263	2.47	0.49
1:B:50:LYS:HB3	1:B:50:LYS:NZ	2.26	0.49
1:B:136:PHE:CE1	1:C:715:LYS:HG3	2.47	0.49
1:D:345:VAL:HG12	1:D:349:ILE:HD11	1.93	0.49
1:B:430:ILE:O	1:B:430:ILE:CG2	2.61	0.49
1:C:313:ARG:HH21	1:C:313:ARG:CG	2.25	0.49
1:B:197:LEU:O	1:B:201:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:LYS:O	1:B:556:LYS:HD3	2.12	0.49
1:A:268:ILE:HD11	1:A:713:LEU:HD11	1.95	0.49
1:B:313:ARG:CG	1:B:313:ARG:NH2	2.73	0.49
1:B:603:THR:HG22	3:C:802:LPP:H302	1.95	0.49
1:C:572:PHE:HE2	3:C:802:LPP:HC62	1.78	0.49
1:A:496:PHE:CE2	1:D:522:ILE:HG12	2.48	0.49
1:D:197:LEU:O	1:D:201:LYS:HB2	2.12	0.49
1:B:105:ARG:HD2	1:B:139:PHE:HZ	1.73	0.48
1:A:534:LEU:CG	1:A:600:MET:CE	2.86	0.48
1:A:642:LEU:CD2	1:A:643:TRP:CD1	2.96	0.48
1:B:378:PHE:CD2	2:B:801:Y01:HAB3	2.47	0.48
1:C:60:LYS:O	1:C:61:ILE:HG13	2.13	0.48
1:D:466:GLU:OE2	1:D:467:SER:CA	2.61	0.48
1:A:308:GLN:OE1	1:D:190:LEU:HD23	2.13	0.48
1:A:415:TRP:HA	1:A:415:TRP:HE3	1.78	0.48
1:B:580:ASN:ND2	1:B:580:ASN:N	2.60	0.48
1:D:511:ARG:CZ	1:D:634:GLU:OE1	2.60	0.48
1:A:572:PHE:CE2	3:A:802:LPP:HC61	2.48	0.48
3:A:802:LPP:H392	1:D:607:ILE:HG12	1.96	0.48
1:B:92:PHE:N	1:B:92:PHE:CD1	2.81	0.48
1:D:268:ILE:HD11	1:D:713:LEU:HD11	1.94	0.48
1:B:268:ILE:HD11	1:B:713:LEU:HD11	1.94	0.48
1:D:339:LEU:HB2	1:D:343:PHE:CE2	2.46	0.48
1:D:621:ASN:N	1:D:621:ASN:HD22	2.11	0.48
1:A:397:PRO:O	1:A:399:PRO:HD3	2.14	0.48
1:A:607:ILE:HA	1:A:611:VAL:HB	1.96	0.48
1:A:197:LEU:O	1:A:201:LYS:HB2	2.12	0.48
1:A:190:LEU:HD11	1:B:265:LEU:HD22	1.96	0.48
1:B:522:ILE:HG12	1:C:496:PHE:HE2	1.78	0.48
1:D:580:ASN:ND2	1:D:580:ASN:N	2.60	0.48
1:C:603:THR:CG2	3:D:802:LPP:H302	2.44	0.48
1:D:378:PHE:CG	2:D:801:Y01:CAB	2.97	0.48
1:A:61:ILE:CG2	1:A:62:ASN:N	2.76	0.47
3:C:802:LPP:O9	3:C:802:LPP:H141	2.12	0.47
1:D:72:THR:O	1:D:73:ALA:C	2.55	0.47
1:A:44:ASP:OD1	1:A:748:PHE:CD2	2.68	0.47
1:B:237:PHE:HE2	1:C:308:GLN:HE21	1.54	0.47
1:B:318:PHE:HB3	1:B:321:TRP:HB2	1.96	0.47
1:B:72:THR:O	1:B:73:ALA:HB3	2.15	0.47
1:C:136:PHE:O	1:C:136:PHE:CG	2.68	0.47
1:D:619:MET:HB2	1:D:619:MET:HE3	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:SER:O	1:A:33:GLU:N	2.48	0.47
1:A:492:LEU:O	1:A:495:LEU:HB2	2.15	0.47
1:A:29:LEU:HD11	1:A:68:PRO:HD3	1.96	0.47
3:A:802:LPP:C8	1:D:599:THR:HG23	2.44	0.47
1:B:136:PHE:CG	1:B:136:PHE:O	2.68	0.47
1:B:544:THR:OG1	1:B:559:ASN:CG	2.56	0.47
1:D:339:LEU:O	1:D:343:PHE:HD2	1.98	0.47
1:B:136:PHE:CZ	1:C:715:LYS:HG3	2.49	0.47
1:D:260:ARG:HG2	1:D:716:ARG:HH12	1.78	0.47
1:D:343:PHE:HE1	1:D:358:PHE:CE2	2.25	0.47
1:A:289:LEU:HD13	1:A:310:LEU:HD21	1.96	0.47
1:D:92:PHE:N	1:D:92:PHE:HD1	2.12	0.47
1:D:586:VAL:HG12	1:D:588:ALA:H	1.80	0.47
1:A:286:LEU:HD13	1:A:289:LEU:HD12	1.97	0.47
1:A:654:PRO:O	1:A:656:PRO:CD	2.63	0.47
1:B:723:ARG:NH1	1:B:727:THR:CG2	2.78	0.47
1:C:343:PHE:CD1	1:C:358:PHE:CD2	3.02	0.47
1:A:606:VAL:CG1	3:A:803:LPP:H331	2.43	0.46
1:B:18:ILE:HG13	1:C:170:ARG:CG	2.45	0.46
1:B:586:VAL:HG12	1:B:588:ALA:H	1.80	0.46
1:B:607:ILE:CG2	3:C:802:LPP:H422	2.45	0.46
1:C:100:LEU:O	1:C:100:LEU:HD23	2.14	0.46
1:D:61:ILE:CG2	1:D:62:ASN:N	2.78	0.46
1:D:492:LEU:O	1:D:495:LEU:HB2	2.15	0.46
1:A:598:ALA:O	3:A:803:LPP:O3	2.33	0.46
1:B:552:ILE:HD12	1:B:566:GLU:OE2	2.15	0.46
1:C:492:LEU:O	1:C:495:LEU:HB2	2.15	0.46
1:D:67:ASP:OD2	1:D:71:ARG:HB2	2.15	0.46
1:A:265:LEU:HD22	1:D:190:LEU:HD11	1.96	0.46
1:A:723:ARG:HH12	1:A:727:THR:HG21	1.80	0.46
2:A:801:Y01:HAQ2	1:D:521:PHE:HE2	1.79	0.46
1:D:71:ARG:HA	1:D:71:ARG:NE	2.31	0.46
1:A:598:ALA:CB	1:B:553:ARG:NH1	2.78	0.46
1:B:105:ARG:CD	1:B:139:PHE:CZ	2.94	0.46
1:B:225:TRP:CZ3	1:B:296:ARG:NE	2.76	0.46
1:C:92:PHE:CD1	1:C:92:PHE:N	2.81	0.46
1:D:396:GLY:HA2	1:D:397:PRO:HD3	1.67	0.46
1:C:71:ARG:NE	1:C:71:ARG:CA	2.77	0.46
1:C:367:ILE:O	1:C:371:ALA:CB	2.64	0.46
1:A:534:LEU:CA	1:A:600:MET:HE2	2.44	0.46
1:A:736:VAL:O	1:A:740:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ARG:HA	1:D:71:ARG:HE	1.81	0.46
1:A:302:ALA:H	1:A:307:GLN:HE21	1.64	0.46
1:A:657:PHE:HE1	1:A:662:SER:H	1.61	0.46
2:A:801:Y01:HAQ2	1:D:521:PHE:CE2	2.50	0.46
1:C:586:VAL:HG12	1:C:588:ALA:H	1.80	0.46
1:D:313:ARG:CG	1:D:313:ARG:NH2	2.78	0.46
1:A:586:VAL:HG12	1:A:588:ALA:H	1.80	0.46
1:A:607:ILE:CG2	3:A:803:LPP:H422	2.46	0.46
1:C:396:GLY:HA2	1:C:397:PRO:HD3	1.66	0.46
1:D:55:ALA:HB1	1:D:63:ILE:HD11	1.98	0.46
1:D:302:ALA:H	1:D:307:GLN:HE21	1.64	0.46
1:A:534:LEU:HA	1:A:600:MET:HE2	1.96	0.46
1:B:60:LYS:C	1:B:61:ILE:CG1	2.89	0.46
1:C:607:ILE:HG23	3:D:802:LPP:H422	1.97	0.46
1:A:367:ILE:O	1:A:371:ALA:CB	2.64	0.46
1:A:555:GLU:CD	1:A:555:GLU:H	2.24	0.46
1:D:139:PHE:CD2	1:D:148:LEU:CD1	2.99	0.46
1:D:607:ILE:O	1:D:612:LEU:HB2	2.16	0.46
1:A:731:LEU:HD11	1:D:736:VAL:HG23	1.98	0.45
1:B:190:LEU:HB2	1:C:262:SER:HB3	1.99	0.45
2:A:801:Y01:HAP1	2:A:801:Y01:HAO2	1.55	0.45
1:A:69:LEU:O	1:A:71:ARG:HG2	2.16	0.45
1:A:723:ARG:NH1	1:A:727:THR:CG2	2.79	0.45
3:A:802:LPP:H331	1:D:606:VAL:CG1	2.37	0.45
1:C:30:SER:O	1:C:33:GLU:N	2.50	0.45
1:D:136:PHE:O	1:D:136:PHE:CG	2.68	0.45
1:D:367:ILE:O	1:D:371:ALA:CB	2.64	0.45
1:A:29:LEU:CD1	1:A:68:PRO:HD3	2.47	0.45
1:A:136:PHE:O	1:A:136:PHE:CG	2.68	0.45
1:B:302:ALA:H	1:B:307:GLN:HE21	1.64	0.45
1:D:528:LEU:HD23	1:D:528:LEU:HA	1.78	0.45
1:D:556:LYS:O	1:D:556:LYS:HD3	2.16	0.45
1:D:612:LEU:HD23	1:D:612:LEU:HA	1.79	0.45
1:A:579:ILE:HG23	1:A:583:VAL:HG21	1.99	0.45
1:A:22:ILE:HG23	1:B:211:LEU:HD22	1.98	0.45
1:A:32:SER:HB2	1:A:61:ILE:HD11	1.98	0.45
1:B:367:ILE:O	1:B:371:ALA:CB	2.64	0.45
1:C:67:ASP:HB2	1:C:70:GLY:O	2.17	0.45
1:A:168:VAL:O	1:D:18:ILE:CG2	2.64	0.45
1:C:561:PHE:HD1	1:C:567:THR:HG23	1.81	0.45
1:D:136:PHE:O	1:D:136:PHE:CD2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:LEU:HA	1:D:256:LEU:HD23	1.71	0.45
1:D:723:ARG:NH1	1:D:727:THR:CG2	2.80	0.45
1:B:519:PHE:CD2	1:B:619:MET:SD	3.10	0.44
1:C:495:LEU:HD23	2:C:801:Y01:CAD	2.46	0.44
1:D:466:GLU:C	1:D:466:GLU:CD	2.85	0.44
1:B:561:PHE:HD1	1:B:567:THR:HG23	1.82	0.44
1:C:136:PHE:O	1:C:136:PHE:CD2	2.70	0.44
1:D:413:PHE:O	1:D:417:GLU:HG2	2.17	0.44
1:B:32:SER:C	1:B:61:ILE:HD11	2.42	0.44
1:C:519:PHE:CZ	1:C:612:LEU:HD22	2.52	0.44
1:D:579:ILE:HG23	1:D:583:VAL:HG21	1.99	0.44
1:C:302:ALA:H	1:C:307:GLN:HE21	1.64	0.44
1:A:136:PHE:O	1:A:136:PHE:CD2	2.70	0.44
1:C:343:PHE:CE1	1:C:358:PHE:CE2	3.06	0.44
1:C:723:ARG:HH12	1:C:727:THR:HG21	1.82	0.44
2:C:801:Y01:HBE	2:C:801:Y01:HAJ1	1.88	0.44
1:A:621:ASN:ND2	1:A:621:ASN:N	2.65	0.44
1:B:29:LEU:O	1:B:34:LYS:HE3	2.16	0.44
1:B:136:PHE:O	1:B:136:PHE:CD2	2.70	0.44
1:C:723:ARG:NH1	1:C:727:THR:CG2	2.81	0.44
1:C:313:ARG:CG	1:C:313:ARG:NH2	2.80	0.44
1:A:630:HIS:O	1:A:634:GLU:HB2	2.17	0.44
1:C:350:ALA:O	1:C:353:SER:OG	2.35	0.44
1:C:607:ILE:O	1:C:612:LEU:HB2	2.17	0.44
1:A:66:ILE:HG12	1:A:72:THR:HB	2.00	0.44
1:A:136:PHE:CE1	1:B:715:LYS:HG3	2.52	0.44
1:A:581:LEU:HD22	1:B:553:ARG:HG3	1.99	0.44
1:B:579:ILE:HG23	1:B:583:VAL:HG21	1.99	0.44
1:C:466:GLU:C	1:C:466:GLU:CD	2.85	0.44
1:A:534:LEU:HD21	1:A:600:MET:HB3	2.00	0.43
1:A:572:PHE:CE2	3:A:802:LPP:HC62	2.53	0.43
1:B:33:GLU:HG2	1:B:61:ILE:CG2	2.41	0.43
1:C:579:ILE:HG23	1:C:583:VAL:HG21	1.99	0.43
1:A:605:ASN:HB3	1:B:576:PHE:CZ	2.52	0.43
1:A:621:ASN:OD1	1:B:621:ASN:OD1	2.37	0.43
1:B:24:ARG:NH2	1:C:214:GLU:O	2.51	0.43
1:B:37:LEU:CD2	1:B:73:ALA:HB2	2.45	0.43
1:B:723:ARG:HH12	1:B:727:THR:HG21	1.83	0.43
1:A:723:ARG:NH1	1:A:727:THR:HG21	2.33	0.43
1:B:210:ALA:HB1	1:B:714:VAL:HG13	2.01	0.43
1:A:598:ALA:HB2	1:B:553:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ALA:HB1	1:D:63:ILE:CD1	2.48	0.43
1:D:723:ARG:HH12	1:D:727:THR:HG21	1.83	0.43
3:A:802:LPP:H311	1:D:603:THR:HG22	2.01	0.43
1:B:466:GLU:C	1:B:466:GLU:CD	2.85	0.43
1:D:67:ASP:OD2	1:D:71:ARG:CB	2.67	0.43
1:A:44:ASP:OD1	1:A:748:PHE:CG	2.71	0.43
1:A:561:PHE:HD1	1:A:567:THR:HG23	1.84	0.43
1:A:611:VAL:HG11	3:A:803:LPP:H412	2.01	0.43
1:C:210:ALA:HB1	1:C:714:VAL:HG13	2.01	0.43
1:C:607:ILE:CG2	3:D:802:LPP:H422	2.49	0.43
1:A:214:GLU:O	1:D:24:ARG:NH2	2.51	0.43
1:A:415:TRP:CD1	1:A:659:VAL:CG2	3.02	0.43
1:B:599:THR:HA	3:C:802:LPP:HC81	1.99	0.43
1:A:314:TRP:HA	1:A:362:PRO:HG2	2.00	0.43
1:B:314:TRP:HA	1:B:362:PRO:HG2	2.00	0.43
1:B:381:LEU:HD23	1:B:381:LEU:HA	1.92	0.43
1:B:206:PRO:HB3	1:B:251:PHE:CD1	2.54	0.43
1:D:210:ALA:HB1	1:D:714:VAL:HG13	2.01	0.43
3:A:802:LPP:H422	1:D:607:ILE:CG2	2.49	0.42
1:B:438:ASP:OD1	1:B:491:ARG:NH2	2.53	0.42
1:B:525:LEU:HD23	2:C:801:Y01:CAN	2.42	0.42
1:C:314:TRP:HA	1:C:362:PRO:HG2	2.00	0.42
1:D:263:ARG:HG3	1:D:264:GLU:N	2.33	0.42
1:A:24:ARG:NH2	1:B:213:SER:O	2.51	0.42
1:B:519:PHE:HE2	1:B:619:MET:CE	2.28	0.42
1:C:438:ASP:OD1	1:C:491:ARG:NH2	2.53	0.42
1:D:314:TRP:HA	1:D:362:PRO:HG2	2.00	0.42
1:A:552:ILE:HG21	1:A:579:ILE:HD11	2.01	0.42
1:B:307:GLN:HE22	1:B:640:THR:HG21	1.85	0.42
1:C:60:LYS:C	1:C:61:ILE:HG13	2.43	0.42
1:A:33:GLU:HG2	1:A:61:ILE:HG23	2.01	0.42
1:B:723:ARG:NH1	1:B:727:THR:HG21	2.34	0.42
1:D:438:ASP:OD1	1:D:491:ARG:NH2	2.53	0.42
1:D:495:LEU:HD23	2:D:801:Y01:CAD	2.48	0.42
1:A:318:PHE:CE2	1:A:363:PHE:HD2	2.38	0.42
1:B:92:PHE:N	1:B:92:PHE:HD1	2.16	0.42
1:B:150:ALA:HA	1:B:158:ILE:HD11	2.02	0.42
1:C:451:LEU:O	1:C:455:ALA:HB2	2.20	0.42
1:D:513:LEU:HD21	3:D:802:LPP:H402	2.02	0.42
1:A:61:ILE:HG22	1:A:62:ASN:N	2.33	0.42
1:A:746:PHE:CE1	1:D:747:ARG:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:ILE:HG22	1:B:694:ARG:H	1.84	0.42
1:C:376:PHE:HB2	1:C:409:TRP:NE1	2.35	0.42
1:C:556:LYS:O	1:C:556:LYS:HD3	2.19	0.42
1:A:210:ALA:HB1	1:A:714:VAL:HG13	2.01	0.42
1:A:313:ARG:CG	1:A:313:ARG:NH2	2.80	0.42
1:A:511:ARG:HD2	1:A:634:GLU:OE1	2.19	0.42
1:B:378:PHE:CE1	2:B:801:Y01:HAB2	1.87	0.42
1:C:92:PHE:N	1:C:92:PHE:HD1	2.16	0.42
1:D:519:PHE:CD2	1:D:619:MET:SD	3.12	0.42
1:C:209:ILE:O	1:C:213:SER:OG	2.34	0.42
1:C:307:GLN:HE22	1:C:640:THR:HG21	1.85	0.42
1:C:374:LEU:HD21	2:C:801:Y01:CAE	2.49	0.42
1:A:692:ILE:HG22	1:A:694:ARG:H	1.84	0.42
1:C:692:ILE:HG22	1:C:694:ARG:H	1.84	0.42
1:D:150:ALA:HA	1:D:158:ILE:HD11	2.02	0.42
1:D:633:ILE:C	1:D:633:ILE:CD1	2.85	0.42
1:A:619:MET:HB2	1:A:619:MET:HE3	1.69	0.41
1:B:403:GLU:HA	1:B:406:ILE:HB	2.02	0.41
1:B:415:TRP:HA	1:B:415:TRP:CE3	2.55	0.41
1:C:444:LEU:HD22	1:C:480:LEU:HD22	2.02	0.41
1:D:444:LEU:HD22	1:D:480:LEU:HD22	2.02	0.41
1:D:513:LEU:CD2	3:D:802:LPP:H402	2.50	0.41
1:D:633:ILE:HD12	1:D:633:ILE:O	2.20	0.41
1:A:466:GLU:CD	1:A:467:SER:N	2.78	0.41
1:A:555:GLU:HG3	1:D:582:TYR:CG	2.56	0.41
1:B:444:LEU:HD22	1:B:480:LEU:HD22	2.02	0.41
2:C:801:Y01:HAC1	2:C:801:Y01:CAU	2.46	0.41
1:A:24:ARG:HD3	1:B:711:ARG:HA	2.02	0.41
1:A:537:LEU:CD1	1:A:596:VAL:HG12	2.50	0.41
1:B:451:LEU:O	1:B:455:ALA:HB2	2.20	0.41
2:B:801:Y01:HAC3	2:B:801:Y01:HAJ2	1.87	0.41
2:B:801:Y01:HAS1	2:B:801:Y01:HAT1	1.87	0.41
1:C:150:ALA:HA	1:C:158:ILE:HD11	2.02	0.41
1:A:444:LEU:HD22	1:A:480:LEU:HD22	2.02	0.41
1:B:209:ILE:O	1:B:213:SER:OG	2.34	0.41
1:C:100:LEU:C	1:C:100:LEU:CD2	2.94	0.41
1:C:403:GLU:HA	1:C:406:ILE:HB	2.02	0.41
1:D:373:TYR:OH	1:D:488:SER:O	2.28	0.41
1:D:451:LEU:O	1:D:455:ALA:HB2	2.20	0.41
1:A:373:TYR:OH	1:A:488:SER:O	2.28	0.41
1:B:45:TYR:CE1	1:B:88:LEU:HD22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:692:ILE:HG22	1:D:694:ARG:H	1.84	0.41
1:A:288:ARG:HA	1:A:288:ARG:HD3	1.80	0.41
1:A:438:ASP:OD1	1:A:491:ARG:NH2	2.53	0.41
1:A:451:LEU:O	1:A:455:ALA:HB2	2.20	0.41
1:A:572:PHE:CD2	3:A:802:LPP:C6	3.00	0.41
1:A:700:LEU:HD22	1:A:700:LEU:HA	1.83	0.41
1:B:522:ILE:HG12	1:C:496:PHE:CE2	2.53	0.41
1:C:136:PHE:O	1:C:137:SER:C	2.60	0.41
1:A:466:GLU:CD	1:A:466:GLU:C	2.88	0.41
1:A:556:LYS:HD2	1:A:556:LYS:HA	1.74	0.41
1:C:519:PHE:CZ	1:C:612:LEU:O	2.74	0.41
1:D:69:LEU:O	1:D:71:ARG:HG2	2.20	0.41
1:A:372:SER:O	1:A:409:TRP:CH2	2.72	0.41
1:B:148:LEU:O	1:B:152:THR:HG23	2.20	0.41
1:B:633:ILE:C	1:B:633:ILE:CD1	2.85	0.41
1:C:83:LEU:HD23	1:C:86:ILE:HD12	2.02	0.41
1:D:307:GLN:HE22	1:D:640:THR:HG21	1.85	0.41
2:D:801:Y01:HAJ2	2:D:801:Y01:HAC3	1.79	0.41
1:A:226:GLU:O	1:A:230:LEU:CB	2.69	0.41
1:A:399:PRO:O	1:A:400:THR:CG2	2.69	0.41
2:A:801:Y01:HAP2	1:D:521:PHE:CZ	2.55	0.41
1:C:429:TYR:CZ	1:C:435:ASN:HB3	2.56	0.41
1:C:492:LEU:HA	1:C:495:LEU:HD13	2.03	0.41
1:D:44:ASP:OD1	1:D:748:PHE:CD1	2.72	0.41
1:D:64:ASN:OD1	1:D:64:ASN:N	2.54	0.41
1:D:260:ARG:O	1:D:261:SER:CB	2.69	0.41
1:A:150:ALA:HA	1:A:158:ILE:HD11	2.02	0.41
1:A:492:LEU:HD13	2:A:801:Y01:HAO2	2.02	0.41
1:B:83:LEU:HD23	1:B:86:ILE:HD12	2.03	0.41
1:B:423:ASP:N	1:B:423:ASP:OD1	2.54	0.41
1:D:492:LEU:HA	1:D:495:LEU:HD13	2.03	0.41
1:A:83:LEU:HD23	1:A:86:ILE:HD12	2.02	0.40
1:A:200:TYR:HB3	1:A:227:LEU:HD21	2.03	0.40
1:D:544:THR:HG22	1:D:559:ASN:HD21	1.86	0.40
1:D:723:ARG:NH1	1:D:727:THR:HG21	2.36	0.40
1:A:534:LEU:HD23	1:A:600:MET:CE	2.36	0.40
1:A:537:LEU:HD11	1:A:596:VAL:CG1	2.51	0.40
2:A:801:Y01:CAQ	1:D:525:LEU:HD11	2.51	0.40
2:A:801:Y01:HAS1	2:A:801:Y01:HAT1	1.92	0.40
1:D:100:LEU:O	1:D:100:LEU:HD23	2.22	0.40
1:D:318:PHE:HB3	1:D:321:TRP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:HG12	1:A:116:LEU:HD12	2.03	0.40
1:B:373:TYR:OH	1:B:488:SER:O	2.28	0.40
1:C:543:GLU:O	1:C:545:LYS:N	2.55	0.40
1:B:18:ILE:HG13	1:C:170:ARG:HG3	2.04	0.40
1:C:226:GLU:O	1:C:230:LEU:CB	2.69	0.40
1:D:83:LEU:HD23	1:D:86:ILE:HD12	2.02	0.40
2:D:801:Y01:HAS2	2:D:801:Y01:HAE1	1.91	0.40
3:A:802:LPP:H302	1:D:603:THR:CG2	2.51	0.40
1:C:190:LEU:HD11	1:D:265:LEU:HD22	2.02	0.40
1:C:521:PHE:HE2	2:D:801:Y01:HAQ2	1.85	0.40
1:C:723:ARG:NH1	1:C:727:THR:HG21	2.36	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	654/755 (87%)	632 (97%)	19 (3%)	3 (0%)	24	55
1	B	649/755 (86%)	629 (97%)	17 (3%)	3 (0%)	24	55
1	C	649/755 (86%)	628 (97%)	18 (3%)	3 (0%)	24	55
1	D	649/755 (86%)	631 (97%)	15 (2%)	3 (0%)	24	55
All	All	2601/3020 (86%)	2520 (97%)	69 (3%)	12 (0%)	26	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	PRO
1	C	543	GLU
1	C	544	THR
1	D	544	THR

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Mol	Chain	Res	Type
1	D	261	SER
1	A	262	SER
1	A	319	PRO
1	B	262	SER
1	B	549	CYS
1	C	262	SER
1	B	73	ALA
1	D	654	PRO

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	555/677 (82%)	529 (95%)	26 (5%)	23	52
1	B	552/677 (82%)	533 (97%)	19 (3%)	32	59
1	C	552/677 (82%)	540 (98%)	12 (2%)	45	66
1	D	549/677 (81%)	534 (97%)	15 (3%)	39	63
All	All	2208/2708 (82%)	2136 (97%)	72 (3%)	34	59

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	29	LEU
1	A	41	GLU
1	A	74	LEU
1	A	288	ARG
1	A	313	ARG
1	A	422	TRP
1	A	505	LEU
1	A	506	GLN
1	A	548	SER
1	A	580	ASN
1	A	621	ASN
1	A	633	ILE

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Mol	Chain	Res	Type
1	A	634	GLU
1	A	640	THR
1	A	642	LEU
1	A	652	THR
1	A	700	LEU
1	A	701	ARG
1	A	702	ARG
1	A	708	GLU
1	A	726	LYS
1	A	733	GLU
1	A	737	LYS
1	A	740	LYS
1	A	742	ASP
1	B	15	ARG
1	B	44	ASP
1	B	50	LYS
1	B	63	ILE
1	B	74	LEU
1	B	92	PHE
1	B	100	LEU
1	B	105	ARG
1	B	190	LEU
1	B	288	ARG
1	B	313	ARG
1	B	340	PHE
1	B	409	TRP
1	B	466	GLU
1	B	505	LEU
1	B	580	ASN
1	B	621	ASN
1	B	632	ASP
1	B	633	ILE
1	C	74	LEU
1	C	92	PHE
1	C	100	LEU
1	C	313	ARG
1	C	409	TRP
1	C	466	GLU
1	C	505	LEU
1	C	552	ILE
1	C	559	ASN
1	C	580	ASN

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Mol	Chain	Res	Type
1	C	632	ASP
1	C	633	ILE
1	D	18	ILE
1	D	29	LEU
1	D	63	ILE
1	D	74	LEU
1	D	76	ILE
1	D	92	PHE
1	D	100	LEU
1	D	313	ARG
1	D	353	SER
1	D	466	GLU
1	D	505	LEU
1	D	552	ILE
1	D	580	ASN
1	D	621	ASN
1	D	633	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	80	ASN
1	A	102	HIS
1	A	154	ASN
1	A	369	HIS
1	A	506	GLN
1	A	535	ASN
1	A	536	GLN
1	A	557	GLN
1	A	559	ASN
1	A	585	ASN
1	A	622	ASN
1	A	625	GLN
1	A	704	HIS
1	A	735	ASN
1	B	80	ASN
1	B	118	HIS
1	B	308	GLN
1	B	369	HIS
1	B	535	ASN
1	B	558	ASN

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Mol	Chain	Res	Type
1	B	559	ASN
1	B	580	ASN
1	B	585	ASN
1	B	622	ASN
1	B	625	GLN
1	C	80	ASN
1	C	102	HIS
1	C	308	GLN
1	C	535	ASN
1	C	558	ASN
1	C	559	ASN
1	C	580	ASN
1	C	585	ASN
1	C	622	ASN
1	C	625	GLN
1	D	64	ASN
1	D	102	HIS
1	D	308	GLN
1	D	386	HIS
1	D	442	ASN
1	D	559	ASN
1	D	580	ASN
1	D	585	ASN
1	D	622	ASN
1	D	625	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

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	LPP	D	802	-	43,43,43	0.97	2 (4%)	46,48,48	1.19	2 (4%)
2	Y01	A	801	-	38,38,38	1.85	5 (13%)	57,57,57	1.76	12 (21%)
2	Y01	C	801	-	38,38,38	1.87	6 (15%)	57,57,57	1.86	13 (22%)
2	Y01	D	801	-	38,38,38	1.85	6 (15%)	57,57,57	1.84	12 (21%)
2	Y01	B	801	-	38,38,38	1.84	5 (13%)	57,57,57	1.85	11 (19%)
3	LPP	A	803	-	43,43,43	0.97	2 (4%)	46,48,48	1.19	2 (4%)
3	LPP	A	802	-	43,43,43	0.97	2 (4%)	46,48,48	1.19	2 (4%)
3	LPP	C	802	-	43,43,43	0.97	2 (4%)	46,48,48	1.19	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LPP	D	802	-	-	25/45/45/45	-
2	Y01	A	801	-	-	9/19/77/77	0/4/4/4
2	Y01	C	801	-	-	8/19/77/77	0/4/4/4
2	Y01	D	801	-	-	8/19/77/77	0/4/4/4
2	Y01	B	801	-	-	7/19/77/77	0/4/4/4
3	LPP	A	803	-	-	25/45/45/45	-
3	LPP	A	802	-	-	25/45/45/45	-
3	LPP	C	802	-	-	25/45/45/45	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	Y01	CAV-CAZ	-5.95	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	Y01	CAV-CAZ	-5.91	1.39	1.51
2	D	801	Y01	CAV-CAZ	-5.91	1.39	1.51
2	A	801	Y01	CAV-CAZ	-5.83	1.40	1.51
2	A	801	Y01	CBH-CAZ	-5.45	1.42	1.52
2	D	801	Y01	CBH-CAZ	-5.39	1.42	1.52
2	C	801	Y01	CBH-CAZ	-5.38	1.42	1.52
2	B	801	Y01	CBH-CAZ	-5.26	1.42	1.52
2	A	801	Y01	CAK-CAI	-4.39	1.41	1.50
2	C	801	Y01	CAK-CAI	-4.34	1.41	1.50
2	D	801	Y01	CAK-CAI	-4.31	1.41	1.50
2	B	801	Y01	CAK-CAI	-4.31	1.41	1.50
3	A	802	LPP	O9-C11	4.14	1.46	1.34
3	A	803	LPP	O9-C11	4.14	1.46	1.34
3	C	802	LPP	O9-C11	4.14	1.46	1.34
3	D	802	LPP	O9-C11	4.14	1.46	1.34
3	A	802	LPP	O27-C29	4.00	1.45	1.33
3	A	803	LPP	O27-C29	4.00	1.45	1.33
3	C	802	LPP	O27-C29	4.00	1.45	1.33
3	D	802	LPP	O27-C29	4.00	1.45	1.33
2	D	801	Y01	CAI-CAZ	3.64	1.40	1.33
2	B	801	Y01	CAI-CAZ	3.64	1.40	1.33
2	C	801	Y01	CAI-CAZ	3.62	1.40	1.33
2	A	801	Y01	CAI-CAZ	3.59	1.40	1.33
2	C	801	Y01	CBI-CBG	-2.52	1.50	1.55
2	B	801	Y01	CBI-CBG	-2.50	1.50	1.55
2	A	801	Y01	CBI-CBG	-2.49	1.50	1.55
2	D	801	Y01	CBI-CBG	-2.45	1.50	1.55
2	C	801	Y01	CBI-CBE	-2.18	1.51	1.55
2	D	801	Y01	CBI-CBE	-2.05	1.51	1.55

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	Y01	CBI-CBE-CBB	-5.62	110.82	119.50
2	C	801	Y01	CBI-CBE-CBB	-5.60	110.85	119.50
2	D	801	Y01	CBI-CBE-CBB	-5.48	111.03	119.50
2	C	801	Y01	CAD-CBH-CBF	-4.32	106.81	111.66
2	A	801	Y01	CBI-CBE-CBB	-4.28	112.88	119.50
3	A	802	LPP	O9-C11-C12	4.24	120.66	111.48
3	A	803	LPP	O9-C11-C12	4.24	120.66	111.48
3	C	802	LPP	O9-C11-C12	4.24	120.66	111.48
3	D	802	LPP	O9-C11-C12	4.24	120.66	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	Y01	CAD-CBH-CBF	-4.24	106.90	111.66
2	B	801	Y01	CBI-CBG-CBD	-4.18	108.47	114.41
2	B	801	Y01	CAD-CBH-CBF	-4.18	106.97	111.66
2	D	801	Y01	CBI-CBG-CBD	-4.15	108.52	114.41
2	C	801	Y01	CBI-CBG-CBD	-4.14	108.53	114.41
2	A	801	Y01	CAD-CBH-CBF	-4.09	107.07	111.66
2	B	801	Y01	CAQ-CBG-CBD	-4.02	112.69	119.10
2	A	801	Y01	CBI-CBG-CBD	-4.01	108.72	114.41
2	A	801	Y01	CAQ-CBG-CBD	-3.80	113.03	119.10
2	C	801	Y01	CAQ-CBG-CBD	-3.80	113.05	119.10
2	D	801	Y01	CAQ-CBG-CBD	-3.79	113.05	119.10
2	B	801	Y01	CAR-CBC-CAV	3.55	115.91	110.97
2	A	801	Y01	CAC-CBB-CBE	-3.35	107.86	112.88
2	D	801	Y01	CAR-CBC-CAV	3.33	115.60	110.97
2	C	801	Y01	CAR-CBC-CAV	3.32	115.59	110.97
2	A	801	Y01	CAR-CBC-CAV	3.32	115.58	110.97
2	B	801	Y01	CAT-CBH-CAZ	3.23	114.32	108.74
2	B	801	Y01	CBH-CBF-CBD	-3.15	108.11	112.71
2	C	801	Y01	CAT-CBH-CAZ	3.09	114.07	108.74
3	A	802	LPP	O27-C29-C30	3.08	121.23	111.83
3	A	803	LPP	O27-C29-C30	3.08	121.23	111.83
3	C	802	LPP	O27-C29-C30	3.08	121.23	111.83
3	D	802	LPP	O27-C29-C30	3.08	121.23	111.83
2	A	801	Y01	CAT-CBH-CAZ	3.08	114.05	108.74
2	D	801	Y01	CAT-CBH-CAZ	3.05	114.01	108.74
2	D	801	Y01	CBH-CBF-CBD	-2.96	108.38	112.71
2	C	801	Y01	CBH-CBF-CBD	-2.93	108.43	112.71
2	C	801	Y01	CAS-CAU-CBI	-2.85	107.94	112.74
2	D	801	Y01	CAS-CAU-CBI	-2.83	107.97	112.74
2	B	801	Y01	CAS-CAU-CBI	-2.70	108.18	112.74
2	A	801	Y01	CBH-CBF-CBD	-2.69	108.78	112.71
2	B	801	Y01	CAC-CBB-CBE	-2.54	109.07	112.88
2	D	801	Y01	CAC-CBB-CBE	-2.53	109.09	112.88
2	A	801	Y01	CBC-OAW-CAY	-2.48	111.87	117.80
2	D	801	Y01	CBC-OAW-CAY	-2.47	111.88	117.80
2	A	801	Y01	CAS-CAU-CBI	-2.47	108.58	112.74
2	C	801	Y01	CBC-OAW-CAY	-2.44	111.95	117.80
2	C	801	Y01	CAC-CBB-CBE	-2.41	109.26	112.88
2	D	801	Y01	CBF-CBH-CAZ	2.37	113.12	109.65
2	A	801	Y01	CBF-CBH-CAZ	2.34	113.08	109.65
2	B	801	Y01	CBF-CBH-CAZ	2.34	113.07	109.65
2	C	801	Y01	CBF-CBH-CAZ	2.30	113.02	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	Y01	CAP-CBE-CBI	-2.25	101.19	103.84
2	B	801	Y01	CAP-CBE-CBI	-2.25	101.19	103.84
2	D	801	Y01	CAP-CBE-CBI	-2.17	101.28	103.84
2	C	801	Y01	CBD-CAK-CAI	2.14	115.73	112.76
2	A	801	Y01	CBD-CAK-CAI	2.08	115.64	112.76

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	LPP	C7-C6-O5-P1
3	A	803	LPP	C7-C6-O5-P1
3	C	802	LPP	C7-C6-O5-P1
3	D	802	LPP	C7-C6-O5-P1
3	A	802	LPP	O10-C11-O9-C7
3	A	803	LPP	O10-C11-O9-C7
3	C	802	LPP	O10-C11-O9-C7
3	D	802	LPP	O10-C11-O9-C7
3	A	802	LPP	C12-C11-O9-C7
3	A	803	LPP	C12-C11-O9-C7
3	C	802	LPP	C12-C11-O9-C7
3	D	802	LPP	C12-C11-O9-C7
2	A	801	Y01	CAC-CBB-CBE-CBI
2	A	801	Y01	CAO-CBB-CBE-CBI
3	A	802	LPP	C29-C30-C31-C32
3	A	803	LPP	C29-C30-C31-C32
3	C	802	LPP	C29-C30-C31-C32
3	D	802	LPP	C29-C30-C31-C32
3	A	802	LPP	C30-C29-O27-C8
3	A	803	LPP	C30-C29-O27-C8
3	C	802	LPP	C30-C29-O27-C8
3	D	802	LPP	C30-C29-O27-C8
2	C	801	Y01	CAN-CAJ-CAO-CBB
2	A	801	Y01	CAC-CBB-CBE-CAP
2	A	801	Y01	CAO-CAJ-CAN-CBA
3	A	802	LPP	O28-C29-O27-C8
3	A	803	LPP	O28-C29-O27-C8
3	C	802	LPP	O28-C29-O27-C8
3	D	802	LPP	O28-C29-O27-C8
3	A	802	LPP	C16-C17-C18-C19
3	A	803	LPP	C16-C17-C18-C19
3	C	802	LPP	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
3	D	802	LPP	C16-C17-C18-C19
2	A	801	Y01	CAJ-CAO-CBB-CAC
3	A	802	LPP	C12-C13-C14-C15
3	A	803	LPP	C12-C13-C14-C15
3	C	802	LPP	C12-C13-C14-C15
3	D	802	LPP	C12-C13-C14-C15
3	A	802	LPP	C37-C38-C39-C40
3	A	803	LPP	C37-C38-C39-C40
3	C	802	LPP	C37-C38-C39-C40
3	D	802	LPP	C37-C38-C39-C40
3	A	802	LPP	C17-C18-C19-C20
3	A	803	LPP	C17-C18-C19-C20
3	C	802	LPP	C17-C18-C19-C20
3	D	802	LPP	C17-C18-C19-C20
3	A	802	LPP	C32-C33-C34-C35
3	A	803	LPP	C32-C33-C34-C35
3	C	802	LPP	C32-C33-C34-C35
3	D	802	LPP	C32-C33-C34-C35
2	A	801	Y01	CAM-CAY-OAW-CBC
2	C	801	Y01	CAM-CAY-OAW-CBC
2	D	801	Y01	CAM-CAY-OAW-CBC
3	A	802	LPP	C33-C34-C35-C36
3	A	803	LPP	C33-C34-C35-C36
3	C	802	LPP	C33-C34-C35-C36
3	D	802	LPP	C33-C34-C35-C36
3	A	802	LPP	C34-C35-C36-C37
3	A	803	LPP	C34-C35-C36-C37
3	C	802	LPP	C34-C35-C36-C37
3	D	802	LPP	C34-C35-C36-C37
2	B	801	Y01	CAJ-CAN-CBA-CAB
3	A	802	LPP	C14-C15-C16-C17
3	A	803	LPP	C14-C15-C16-C17
3	C	802	LPP	C14-C15-C16-C17
3	D	802	LPP	C14-C15-C16-C17
2	B	801	Y01	CAJ-CAN-CBA-CAA
3	A	802	LPP	C39-C40-C41-C42
3	A	803	LPP	C39-C40-C41-C42
3	C	802	LPP	C39-C40-C41-C42
3	D	802	LPP	C39-C40-C41-C42
2	A	801	Y01	OAG-CAY-OAW-CBC
2	C	801	Y01	OAG-CAY-OAW-CBC
2	D	801	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
2	B	801	Y01	CAC-CBB-CBE-CBI
2	D	801	Y01	CAJ-CAN-CBA-CAB
3	A	802	LPP	O5-C6-C7-C8
3	A	803	LPP	O5-C6-C7-C8
3	C	802	LPP	O5-C6-C7-C8
3	D	802	LPP	O5-C6-C7-C8
3	A	802	LPP	C23-C24-C25-C26
3	A	803	LPP	C23-C24-C25-C26
3	C	802	LPP	C23-C24-C25-C26
3	D	802	LPP	C23-C24-C25-C26
2	D	801	Y01	CAJ-CAN-CBA-CAA
3	A	802	LPP	C35-C36-C37-C38
3	A	803	LPP	C35-C36-C37-C38
3	C	802	LPP	C35-C36-C37-C38
3	D	802	LPP	C35-C36-C37-C38
2	B	801	Y01	CAX-CAL-CAM-CAY
3	A	802	LPP	C18-C19-C20-C21
3	A	803	LPP	C18-C19-C20-C21
3	C	802	LPP	C18-C19-C20-C21
3	D	802	LPP	C18-C19-C20-C21
2	B	801	Y01	CAO-CBB-CBE-CBI
2	C	801	Y01	CAC-CBB-CBE-CBI
2	D	801	Y01	CAC-CBB-CBE-CBI
2	A	801	Y01	CAX-CAL-CAM-CAY
3	A	802	LPP	O5-C6-C7-O9
3	A	803	LPP	O5-C6-C7-O9
3	C	802	LPP	O5-C6-C7-O9
3	D	802	LPP	O5-C6-C7-O9
3	A	802	LPP	C22-C23-C24-C25
3	A	803	LPP	C22-C23-C24-C25
3	C	802	LPP	C22-C23-C24-C25
3	D	802	LPP	C22-C23-C24-C25
2	D	801	Y01	CAX-CAL-CAM-CAY
3	A	802	LPP	C31-C32-C33-C34
3	A	803	LPP	C31-C32-C33-C34
3	C	802	LPP	C31-C32-C33-C34
3	D	802	LPP	C31-C32-C33-C34
2	C	801	Y01	CAX-CAL-CAM-CAY
3	A	802	LPP	C38-C39-C40-C41
3	A	803	LPP	C38-C39-C40-C41
3	C	802	LPP	C38-C39-C40-C41
3	D	802	LPP	C38-C39-C40-C41

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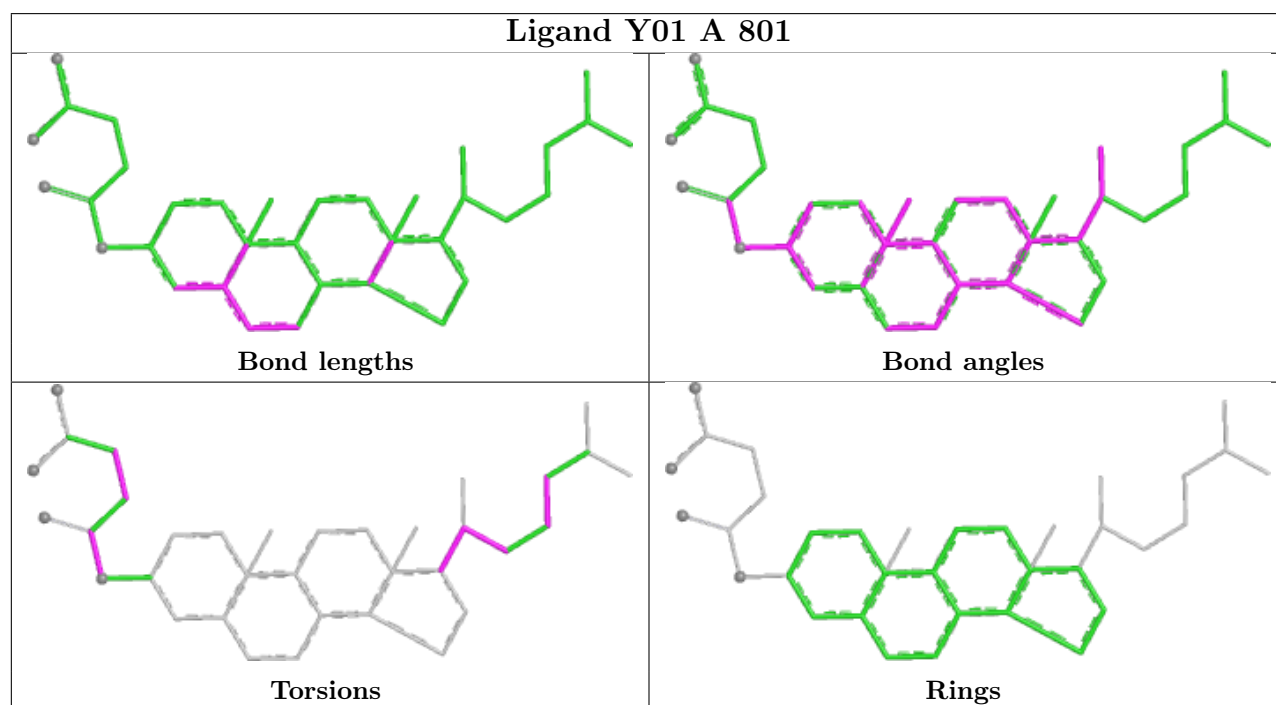
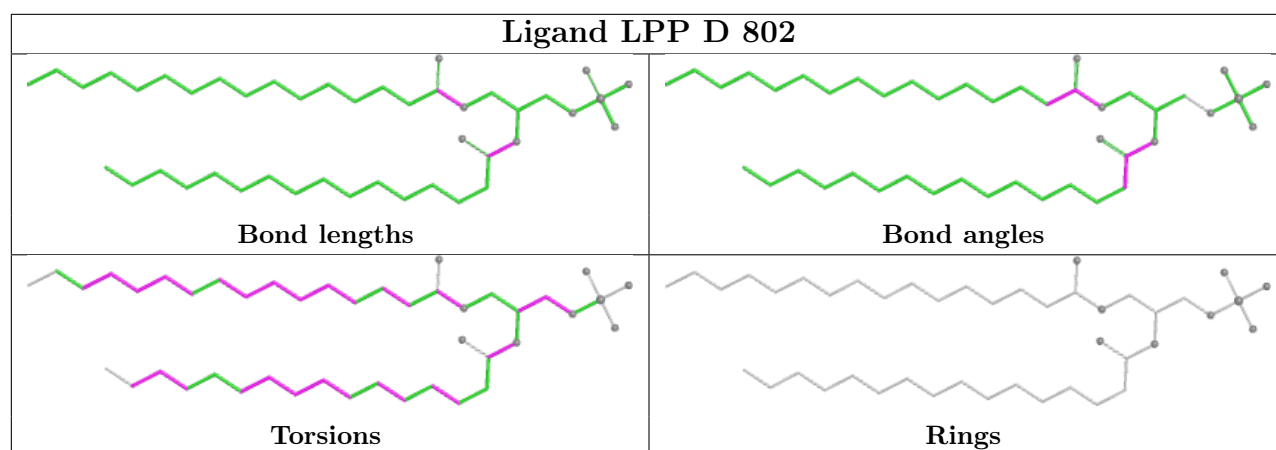
Mol	Chain	Res	Type	Atoms
3	A	802	LPP	C19-C20-C21-C22
3	A	803	LPP	C19-C20-C21-C22
3	C	802	LPP	C19-C20-C21-C22
3	D	802	LPP	C19-C20-C21-C22
2	B	801	Y01	CAM-CAL-CAX-OAH
2	B	801	Y01	CAM-CAL-CAX-OAF
2	D	801	Y01	CAO-CBB-CBE-CBI
2	C	801	Y01	CAO-CBB-CBE-CBI
2	A	801	Y01	CAO-CBB-CBE-CAP
2	C	801	Y01	CAO-CAJ-CAN-CBA
2	C	801	Y01	CAJ-CAO-CBB-CBE
3	A	802	LPP	C40-C41-C42-C43
3	A	803	LPP	C40-C41-C42-C43
3	C	802	LPP	C40-C41-C42-C43
3	D	802	LPP	C40-C41-C42-C43
2	D	801	Y01	CAN-CAJ-CAO-CBB

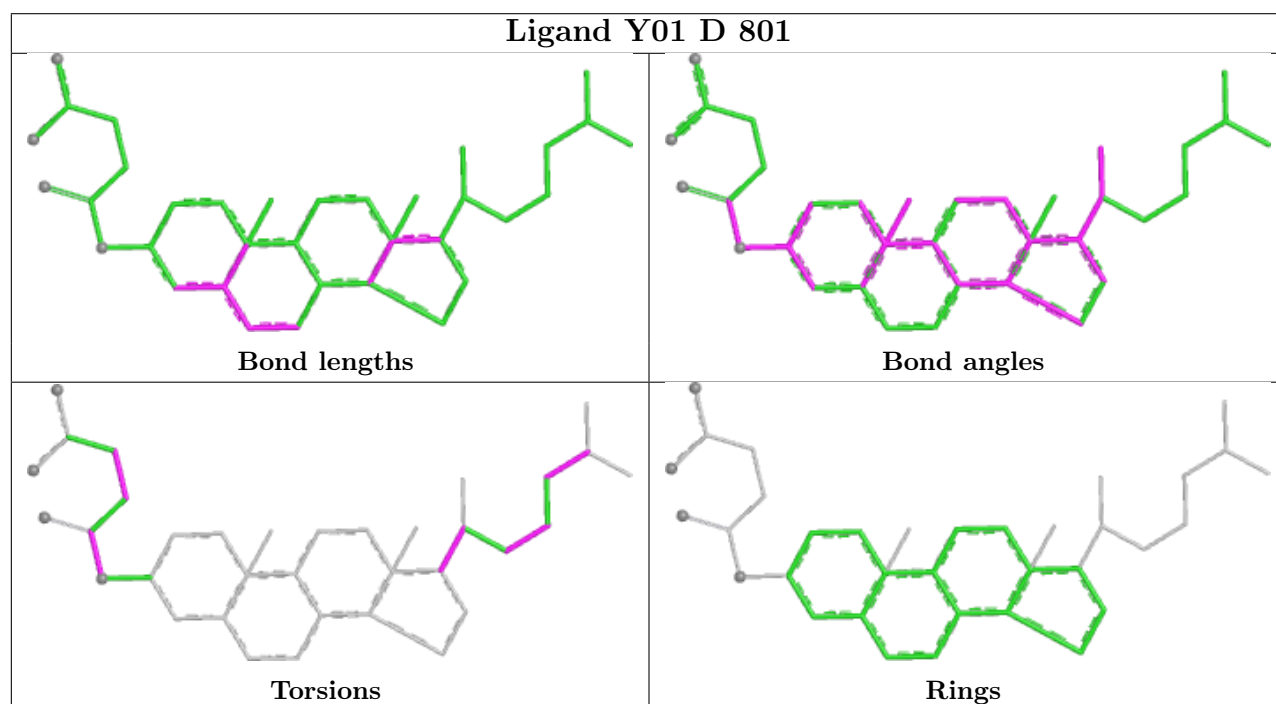
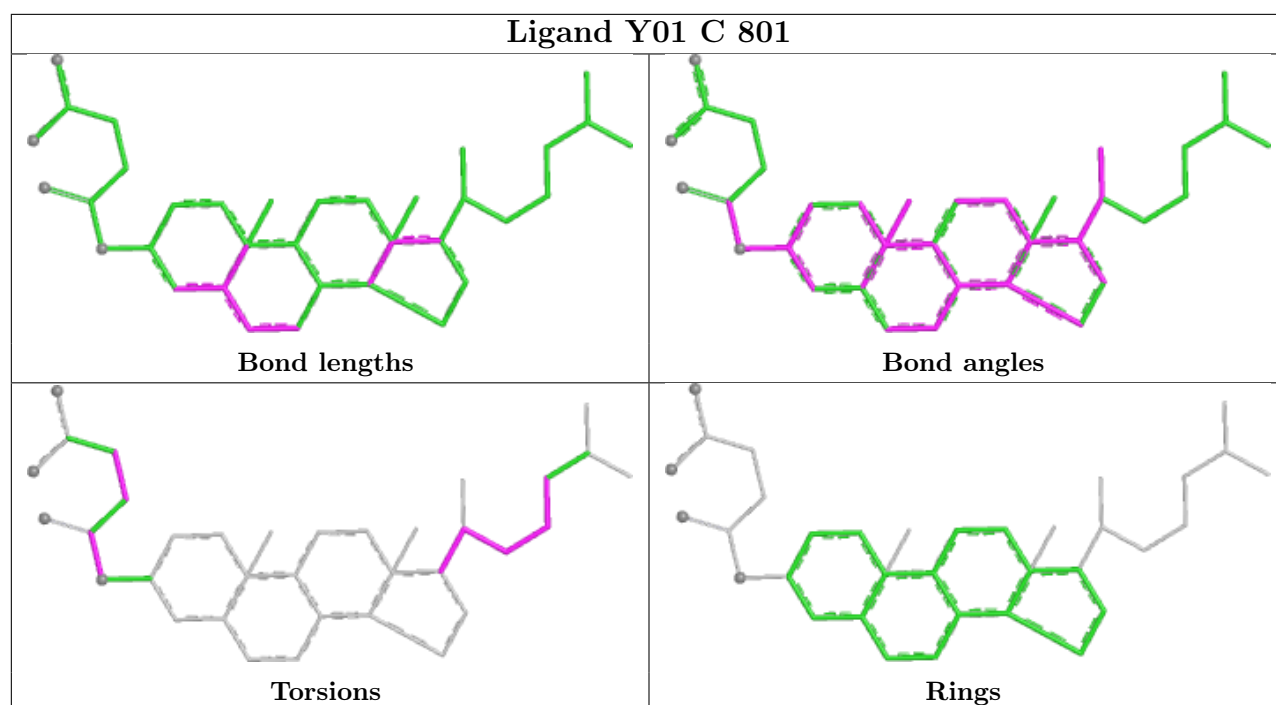
There are no ring outliers.

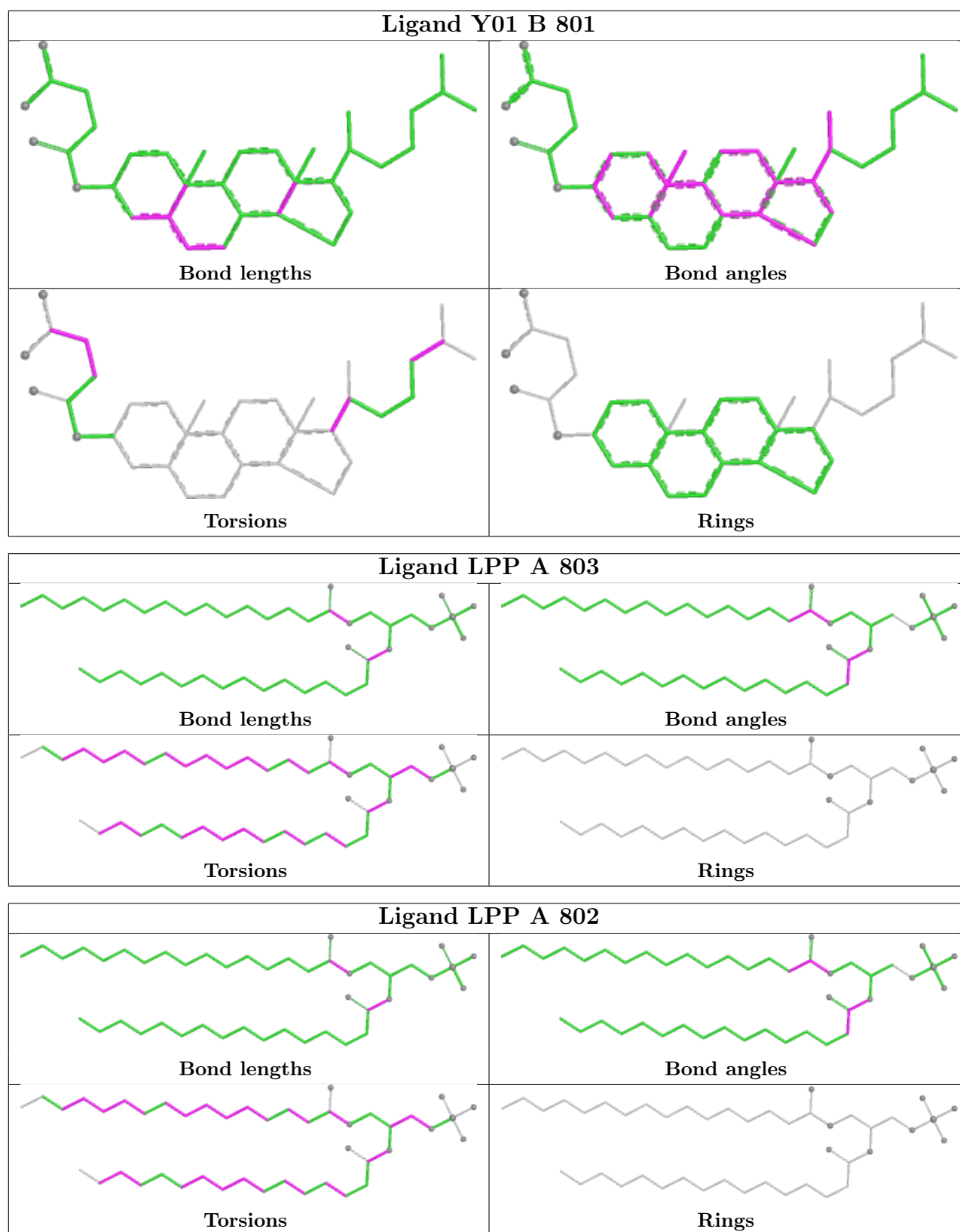
8 monomers are involved in 185 short contacts:

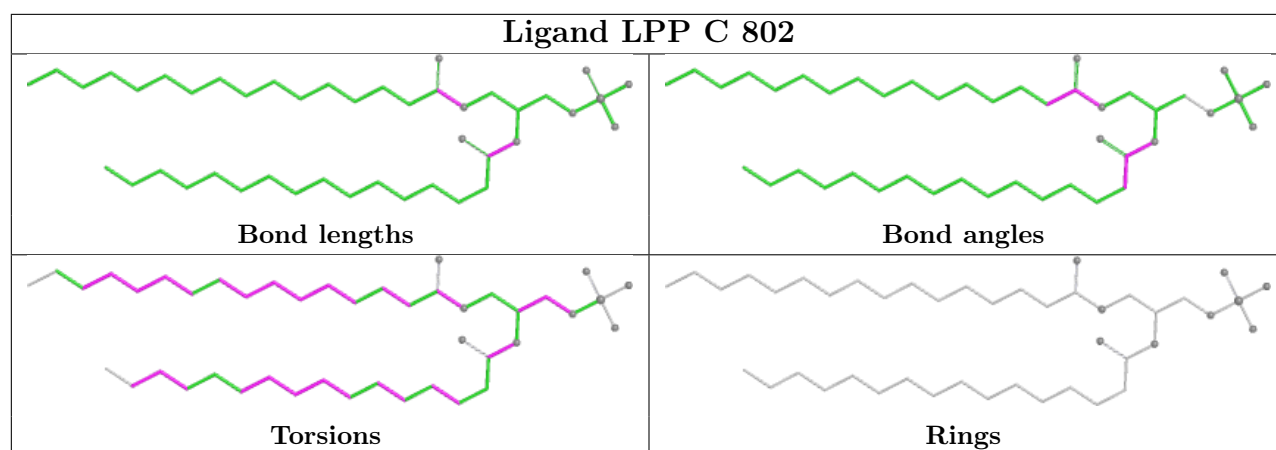
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	802	LPP	25	0
2	A	801	Y01	19	0
2	C	801	Y01	21	0
2	D	801	Y01	22	0
2	B	801	Y01	26	0
3	A	803	LPP	28	0
3	A	802	LPP	23	0
3	C	802	LPP	21	0

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.

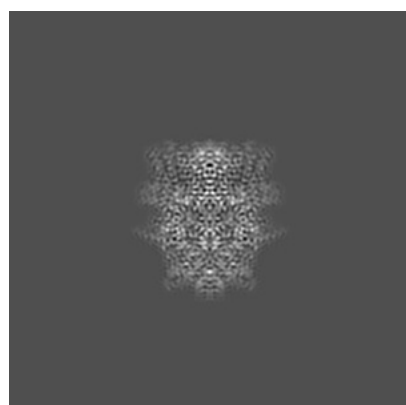
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9898. These allow visual inspection of the internal detail of the map and identification of artifacts.

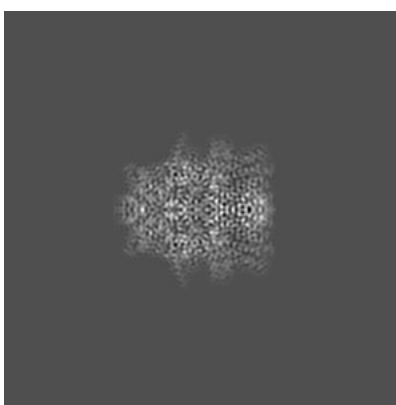
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

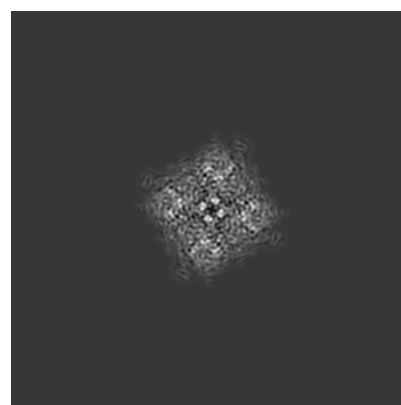
6.1.1 Primary map



X



Y



Z

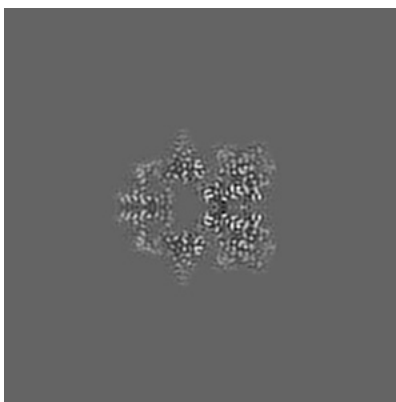
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

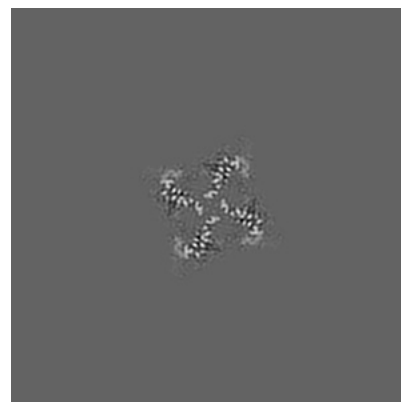
6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

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: 131



Y Index: 131

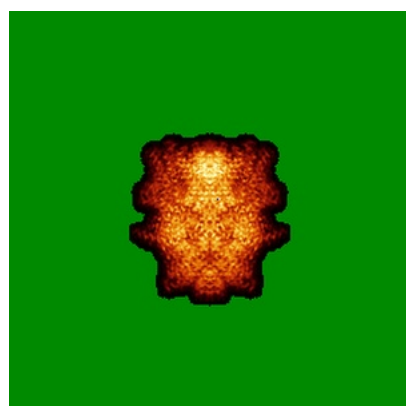


Z Index: 135

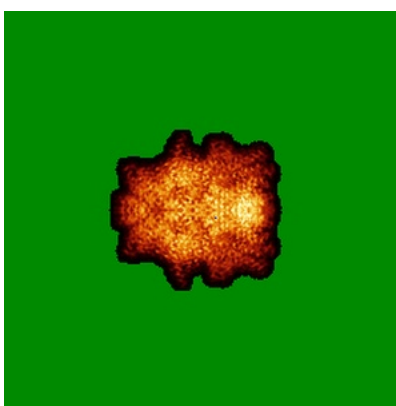
The images above show the largest variance slices of the map in three orthogonal directions.

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

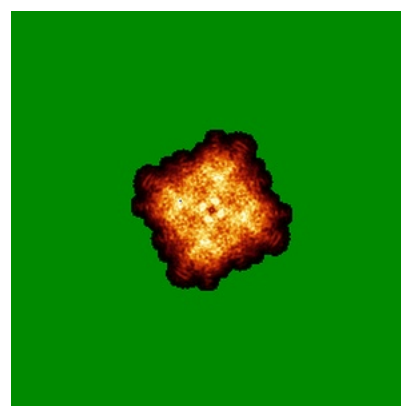
6.4.1 Primary map



X



Y

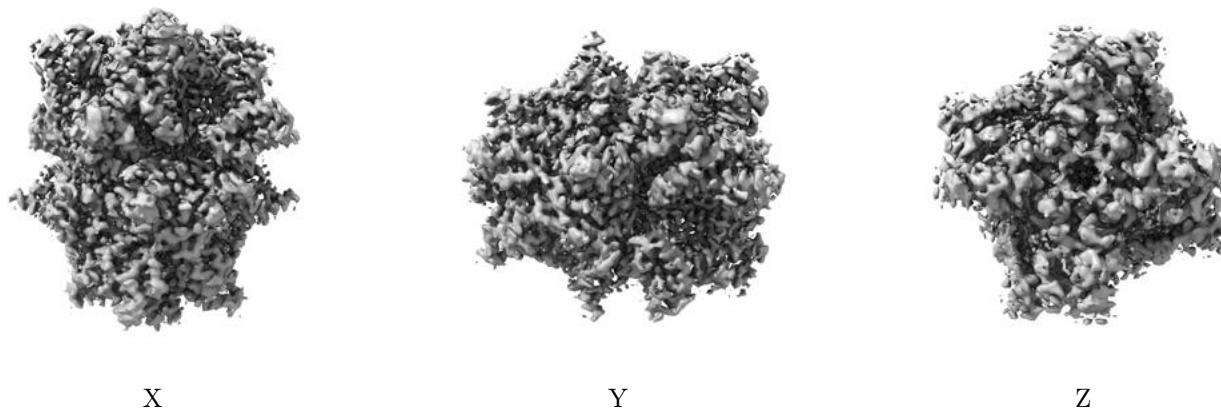


Z

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 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

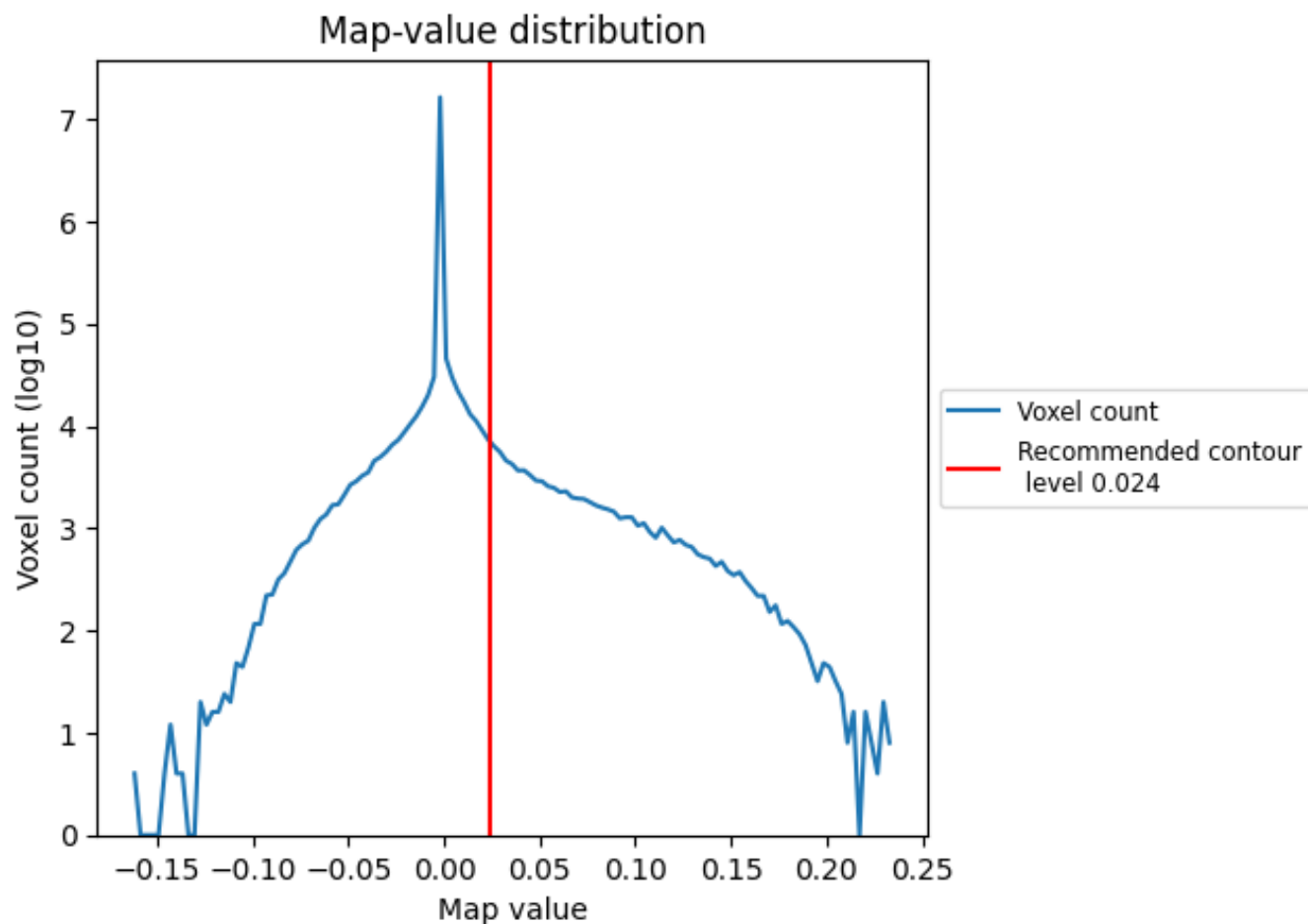
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

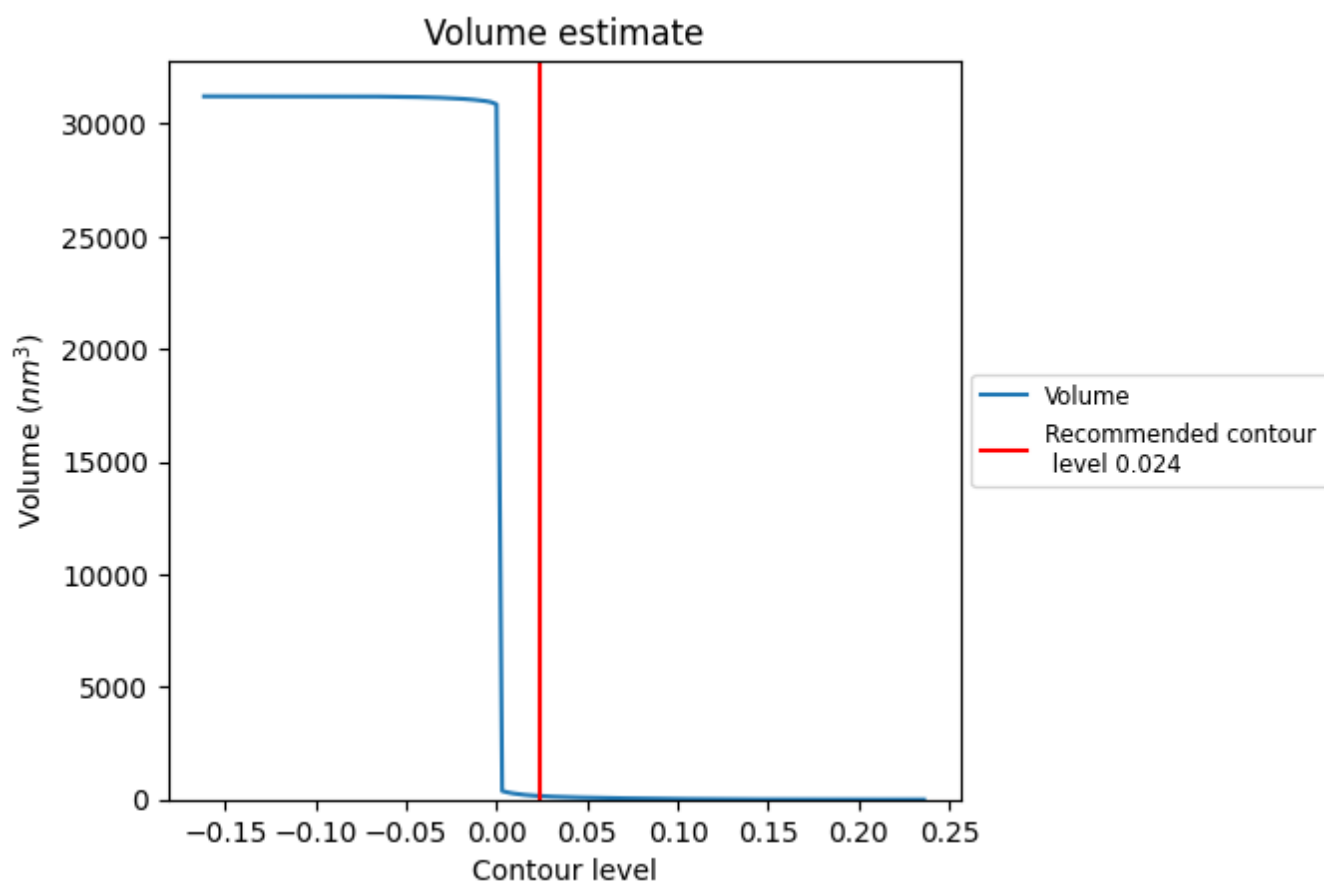
This section contains the results of statistical analysis of the map.

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.

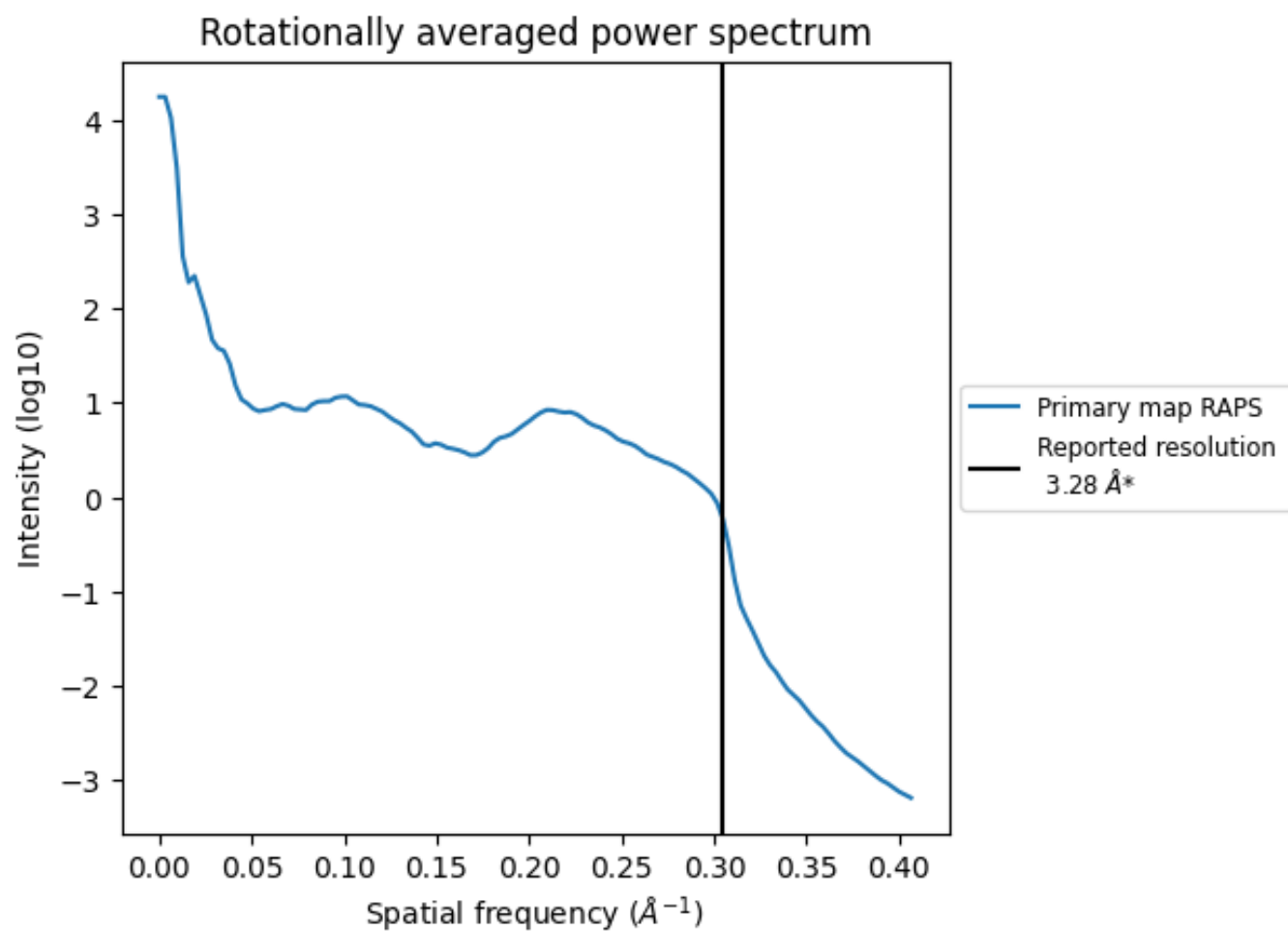
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 157 nm³; this corresponds to an approximate mass of 142 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 ⓘ

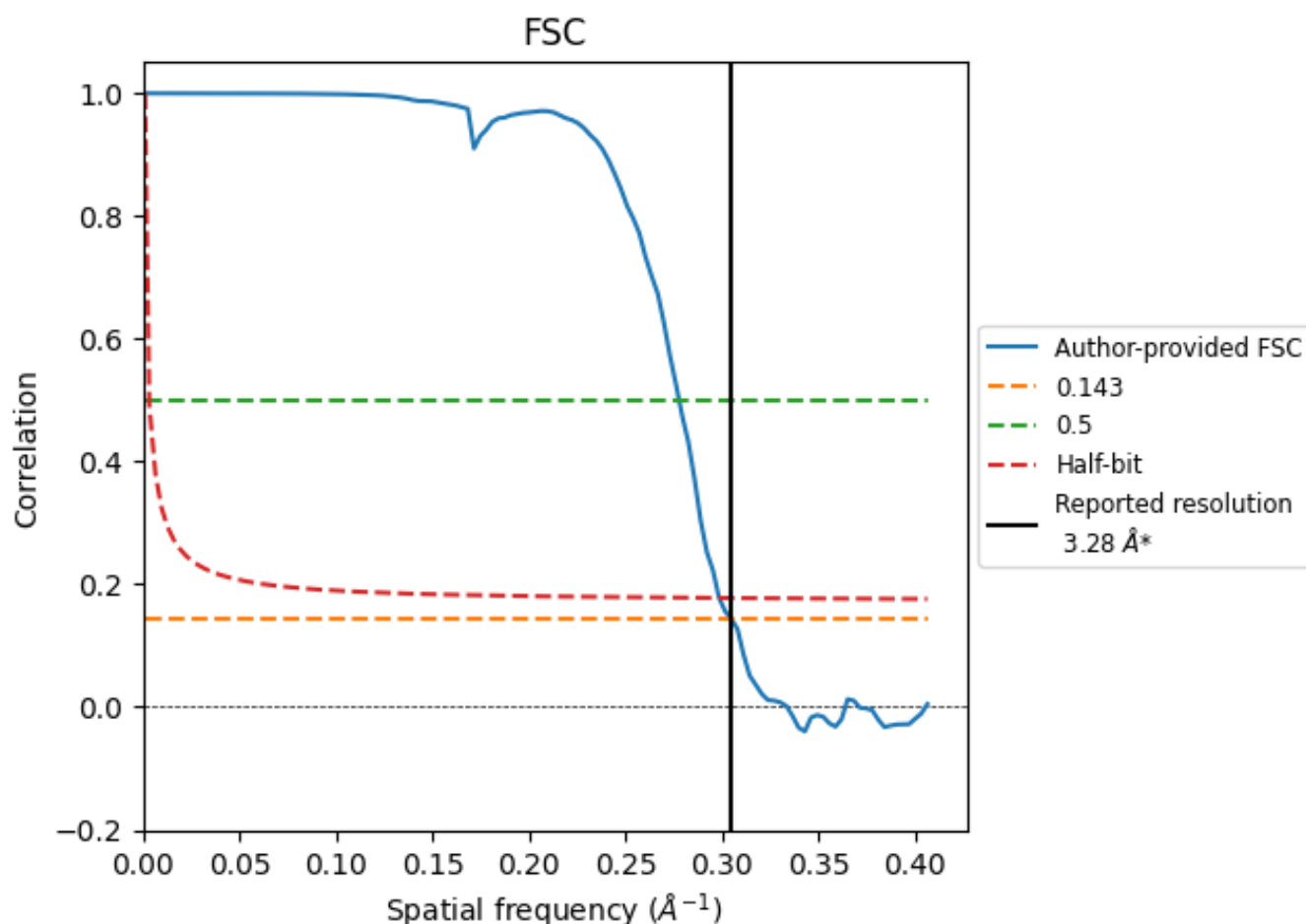


*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.305 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

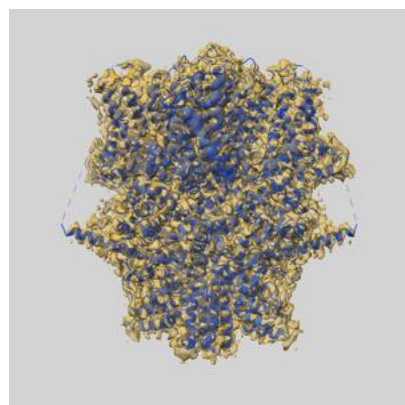
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.28	3.60	3.35
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

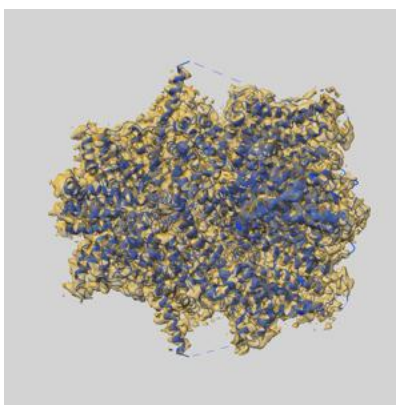
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9898 and PDB model 6JZO. Per-residue inclusion information can be found in section [3](#) on page [7](#).

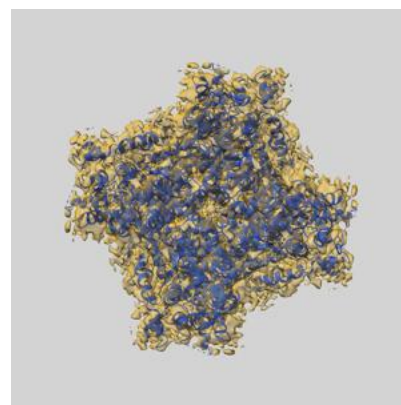
9.1 Map-model overlay [i](#)



X



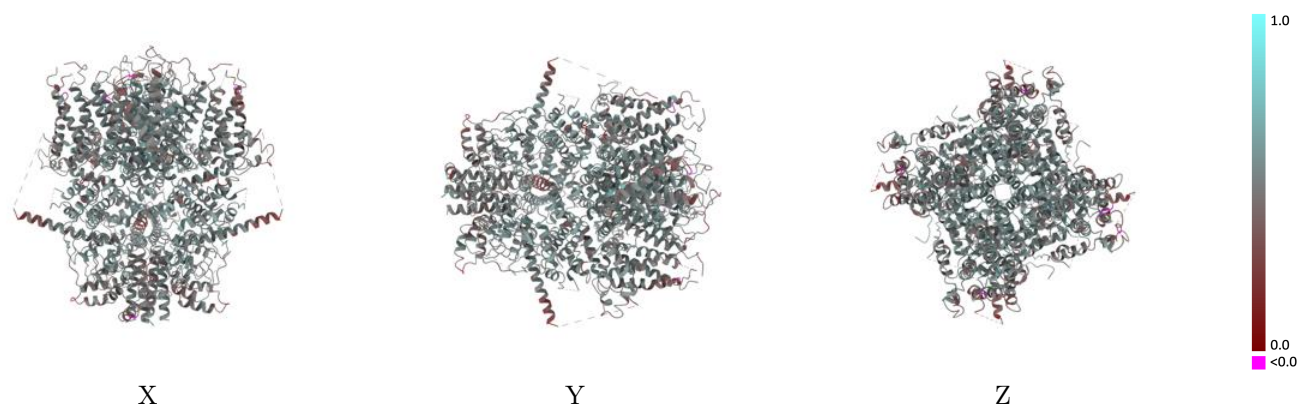
Y



Z

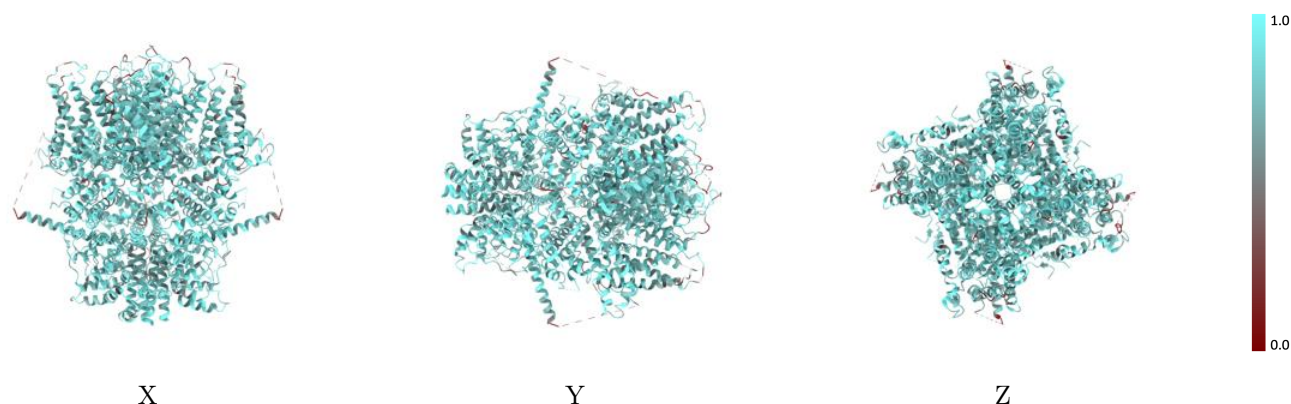
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



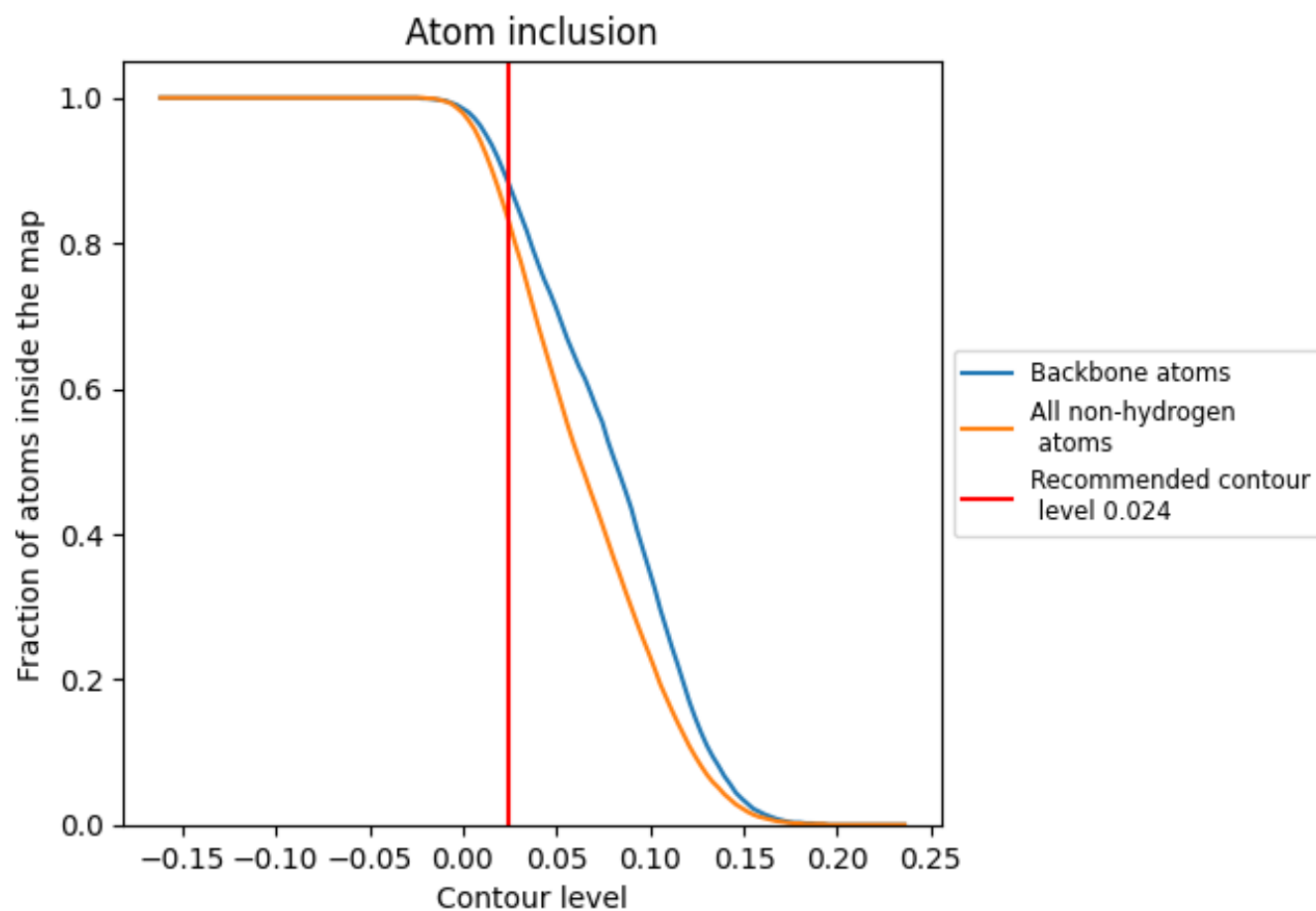
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.024).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.4990
A	0.8320	0.5040
B	0.8360	0.4970
C	0.8350	0.4980
D	0.8380	0.4970

