



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:53 AM UTC

PDB ID : 7QTQ / pdb_00007qtq
EMDB ID : EMD-14145
Title : Structure of Native, iodinated bovine thyroglobulin solved on strepavidin affinity grids.
Authors : Marechal, N.; Weitz, J.C.; Serrano, B.P.; Zhang, X.
Deposited on : 2022-01-15
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
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

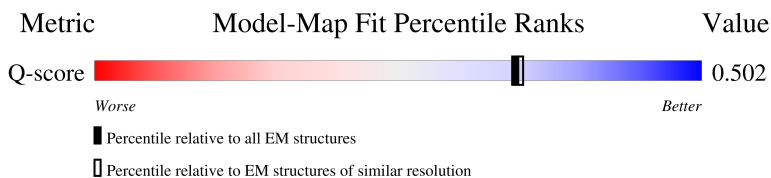
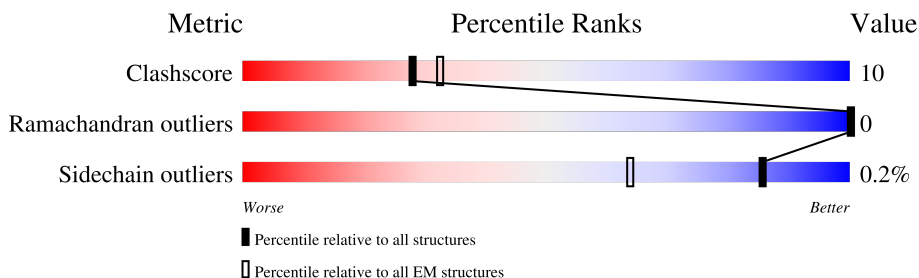
1 Overall quality at a glance

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	2769	
1	B	2769	
2	C	3	
2	E	3	

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Mol	Chain	Length	Quality of chain
3	D	2	50% 50%
3	F	2	100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 55234 atoms, of which 27101 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.

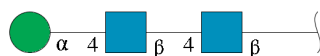
- Molecule 1 is a protein called Thyroglobulin.

Mol	Chain	Residues	Atoms							AltConf	Trace
1	A	1790	Total	C	H	I	N	O	S	0	0
			27329	8768	13410	4	2459	2587	101		
1	B	1789	Total	C	H	I	N	O	S	0	0
			27329	8768	13417	4	2455	2584	101		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	PHE	LEU	variant	UNP P01267
A	2540	DHA	TYR	modified residue	UNP P01267
A	2573	T44	TYR	modified residue	UNP P01267
B	196	PHE	LEU	variant	UNP P01267
B	2540	DHA	TYR	modified residue	UNP P01267
B	2573	T44	TYR	modified residue	UNP P01267

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
2	E	3	Total	C	H	N	O	0	0
			73	22	34	2	15		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	F	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	

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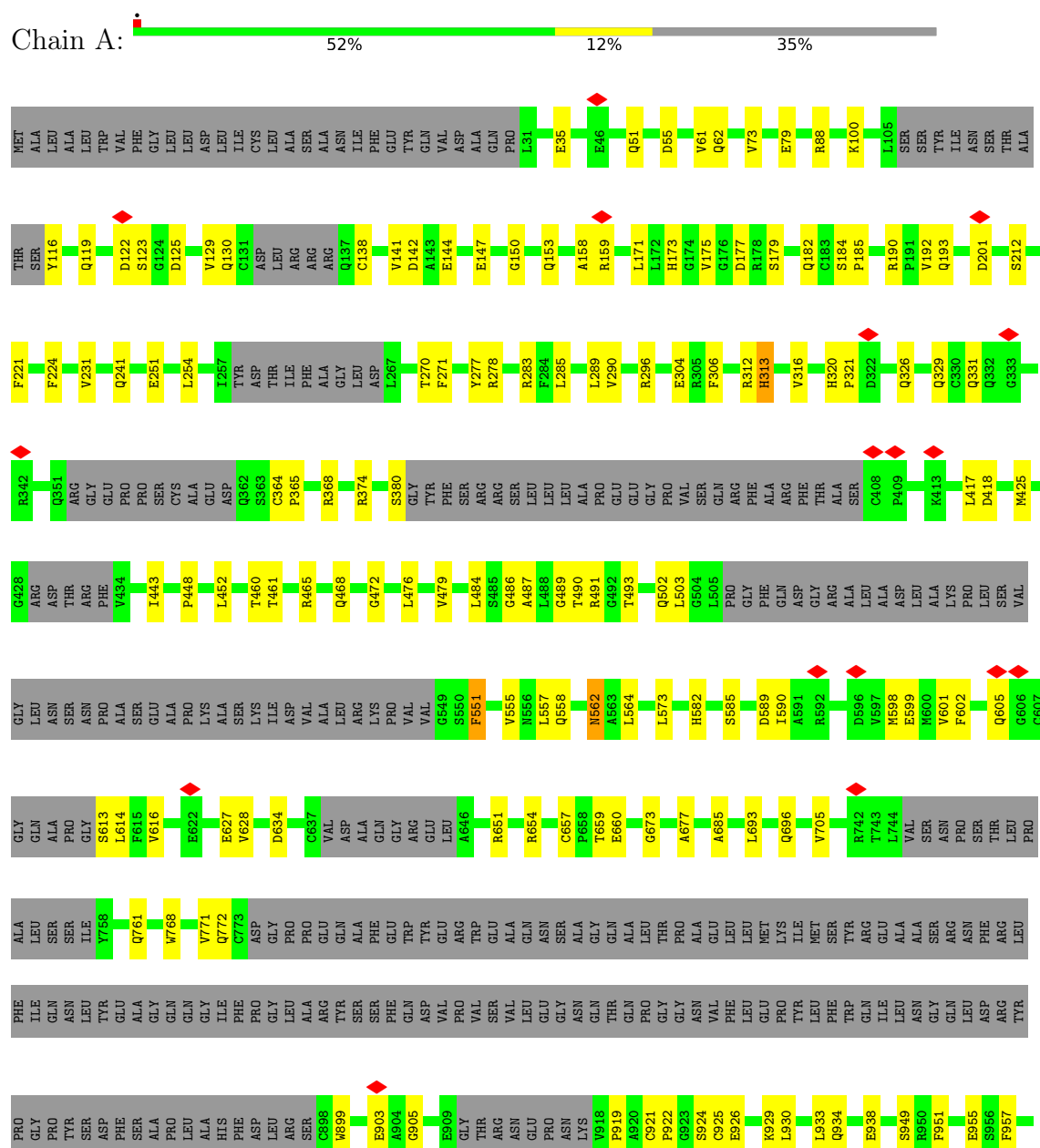
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Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	

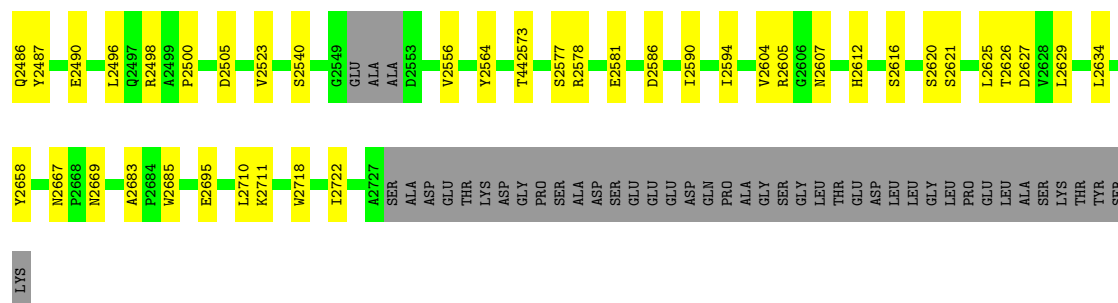
3 Residue-property plots

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.

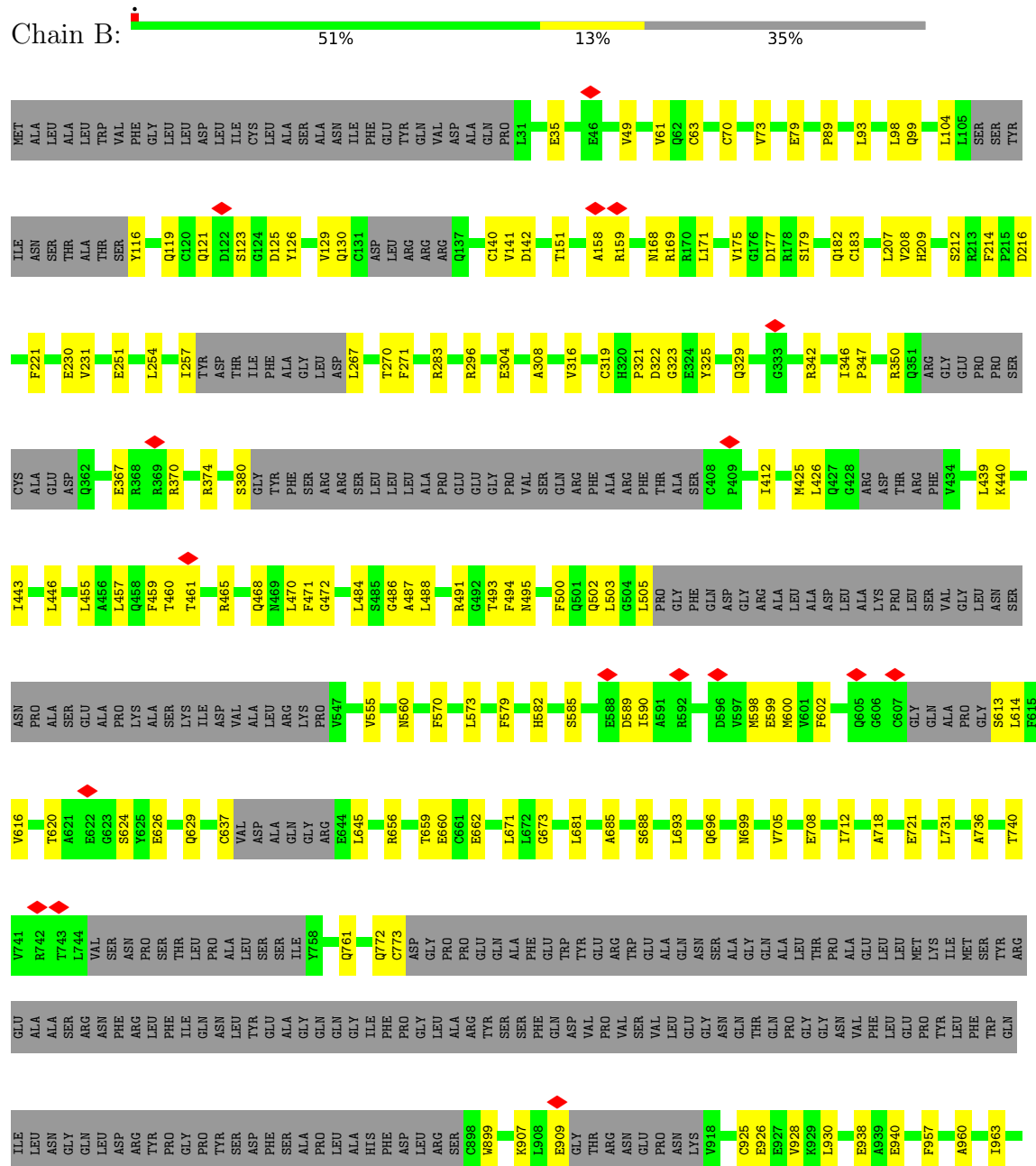
• Molecule 1: Thyroglobulin



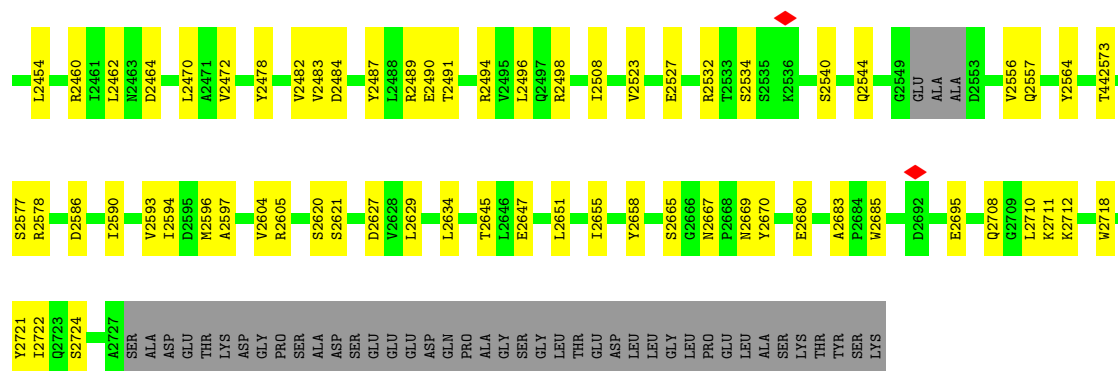




• Molecule 1: Thyroglobulin







- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 33% 67%



- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 33% 67%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	242813	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	70.827	Depositor
Minimum map value	-46.451	Depositor
Average map value	-0.014	Depositor
Map value standard deviation	1.031	Depositor
Recommended contour level	6	Depositor
Map size (Å)	422.4, 422.4, 422.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: T44, MAN, DHA, 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	0.36	0/14211	0.52	5/19249 (0.0%)
1	B	0.34	0/14204	0.45	4/19241 (0.0%)
All	All	0.35	0/28415	0.48	9/38490 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2250	ASN	CB-CA-C	-7.21	101.64	111.89
1	B	494	PHE	O-C-N	-6.65	114.84	122.09
1	A	313	HIS	CA-CB-CG	6.45	120.25	113.80
1	A	313	HIS	CB-CA-C	5.98	121.05	110.47
1	A	2121	GLY	CA-C-O	-5.57	117.78	122.29
1	A	964	ARG	N-CA-C	-5.55	101.69	109.96
1	B	2011	GLY	O-C-N	-5.24	115.88	122.70
1	B	216	ASP	CA-C-N	5.08	128.72	120.60
1	B	216	ASP	C-N-CA	5.08	128.72	120.60

There are no chirality outliers.

There are no planarity outliers.

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	13919	13410	13428	256	0
1	B	13912	13417	13430	277	0
2	C	39	34	34	3	0
2	E	39	34	34	3	0
3	D	28	25	25	0	0
3	F	28	25	25	0	0
4	A	84	78	78	3	0
4	B	84	78	78	5	0
All	All	28133	27101	27132	532	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 10.

All (532) 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:924:SER:HG	1:A:1037:TRP:CD1	2.01	0.78
2:C:2:NAG:O7	2:C:2:NAG:O3	2.05	0.74
1:B:296:ARG:NH1	1:B:321:PRO:O	2.20	0.74
1:A:1977:ILE:HD12	1:A:1979:ILE:HD11	1.70	0.74
4:B:2804:NAG:O7	4:B:2804:NAG:O3	2.05	0.74
4:A:2802:NAG:O7	4:A:2802:NAG:O3	2.05	0.73
1:A:921:CYS:SG	1:A:922:PRO:HD2	2.28	0.73
1:A:73:VAL:HG12	1:A:79:GLU:HA	1.70	0.72
1:A:182:GLN:N	1:A:182:GLN:OE1	2.23	0.72
1:B:938:GLU:OE1	1:B:992:TYR:OH	2.06	0.72
1:A:2586:ASP:OD1	1:A:2711:LYS:NZ	2.21	0.71
1:B:2249:LEU:HD12	1:B:2249:LEU:O	1.90	0.71
1:A:374:ARG:O	1:B:995:ARG:NH1	2.24	0.71
1:B:251:GLU:OE1	1:B:491:ARG:NH1	2.24	0.70
1:A:201:ASP:OD1	1:A:201:ASP:O	2.09	0.70
1:A:1282:GLN:NE2	1:A:1463:LYS:O	2.26	0.69
1:B:1891:ASN:ND2	1:B:1910:VAL:HG21	2.08	0.69
2:E:2:NAG:O7	2:E:2:NAG:O3	2.08	0.69
1:B:616:VAL:HG21	1:B:963:ILE:HG23	1.74	0.69
1:A:2470:LEU:HD22	1:A:2523:VAL:HG21	1.73	0.68
1:A:1979:ILE:HD12	1:A:2026:LEU:HD13	1.74	0.68
1:B:925:CYS:SG	1:B:926:GLU:N	2.66	0.68
1:B:308:ALA:HB1	1:B:316:VAL:HG12	1.76	0.67
1:A:88:ARG:HD3	1:A:331:GLN:OE1	1.94	0.67
1:B:140:CYS:SG	1:B:151:THR:HG21	2.34	0.67
1:A:2347:SER:O	1:A:2351:SER:OG	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2801:NAG:O7	4:B:2801:NAG:O3	2.05	0.67
1:B:171:LEU:HD11	1:B:177:ASP:O	1.95	0.67
4:A:2805:NAG:O7	4:A:2805:NAG:O3	2.11	0.67
1:A:2216:ILE:HD11	1:A:2324:ALA:CB	2.24	0.66
1:B:230:GLU:OE1	1:B:230:GLU:N	2.29	0.66
1:B:1972:GLN:HG3	1:B:2056:VAL:HG23	1.78	0.66
1:B:2146:GLN:OE1	1:B:2181:THR:OG1	2.12	0.66
1:A:2233:TYR:OH	1:A:2334:SER:O	2.10	0.65
1:B:2470:LEU:HD22	1:B:2523:VAL:HG21	1.76	0.65
1:A:2249:LEU:HD12	1:A:2249:LEU:O	1.97	0.65
1:A:144:GLU:OE2	1:A:241:GLN:NE2	2.29	0.64
1:A:465:ARG:NH1	1:A:468:GLN:OE1	2.31	0.64
1:B:1979:ILE:HD12	1:B:2026:LEU:HD13	1.79	0.64
1:A:1758:LEU:HD12	1:A:1758:LEU:O	1.98	0.64
1:B:2353:ASN:OD1	1:B:2353:ASN:N	2.31	0.64
1:A:1285:GLN:O	1:A:1460:GLY:N	2.31	0.64
1:A:476:LEU:HB2	1:A:564:LEU:HD11	1.79	0.64
1:B:2216:ILE:HD11	1:B:2324:ALA:CB	2.28	0.64
1:B:620:THR:OG1	1:B:624:SER:O	2.17	0.63
1:A:903:GLU:OE2	1:A:903:GLU:HA	1.99	0.63
1:A:955:GLU:OE2	1:B:1005:TYR:OH	2.10	0.63
1:A:1926:ALA:O	1:A:1942:LEU:HD13	1.98	0.63
1:A:2360:VAL:O	1:A:2364:THR:HG23	1.99	0.63
1:B:207:LEU:HD21	1:B:271:PHE:CD2	2.34	0.63
1:B:1877:GLN:O	1:B:1878:HIS:ND1	2.31	0.63
1:B:2028:LEU:HD12	1:B:2031:LEU:HD23	1.80	0.62
1:B:2432:GLN:NE2	1:B:2478:TYR:O	2.33	0.62
1:B:304:GLU:OE2	1:B:325:TYR:OH	2.18	0.62
1:B:2556:VAL:HG13	1:B:2722:ILE:HD12	1.80	0.62
1:A:171:LEU:HD11	1:A:177:ASP:O	2.00	0.62
1:A:2490:GLU:OE1	1:A:2498:ARG:NH2	2.31	0.62
1:B:671:LEU:HD22	1:B:681:LEU:HD11	1.80	0.62
1:B:940:GLU:OE2	1:B:1007:ARG:NH2	2.33	0.62
4:B:2806:NAG:O7	4:B:2806:NAG:O3	2.15	0.62
1:B:2454:LEU:HD22	1:B:2462:LEU:HD11	1.80	0.62
1:A:2573:T44:O	1:A:2577:SER:HB3	1.98	0.62
1:A:2281:CYS:O	1:A:2334:SER:OG	2.17	0.62
1:B:637:CYS:SG	1:B:645:LEU:HD21	2.40	0.61
1:B:2586:ASP:OD1	1:B:2711:LYS:NZ	2.27	0.61
1:A:417:LEU:HD12	1:A:605:GLN:NE2	2.16	0.61
1:B:99:GLN:OE1	1:B:126:TYR:OH	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2490:GLU:OE1	1:B:2498:ARG:NH2	2.33	0.61
1:B:2460:ARG:NH2	1:B:2464:ASP:OD1	2.34	0.61
1:A:2658:TYR:OH	1:A:2683:ALA:O	2.18	0.61
1:B:443:ILE:HD12	1:B:598:MET:CE	2.30	0.61
1:A:2113:VAL:HG22	1:A:2155:MET:HG2	1.81	0.60
1:B:693:LEU:HD21	1:B:2645:THR:HG22	1.82	0.60
1:B:963:ILE:HG22	1:B:963:ILE:O	2.01	0.60
1:A:2216:ILE:HD11	1:A:2324:ALA:HB2	1.84	0.60
1:B:1926:ALA:O	1:B:1942:LEU:HD13	2.00	0.60
1:A:1856:LEU:HD23	1:A:1856:LEU:O	2.01	0.60
1:A:1910:VAL:HG12	1:A:1920:CYS:HB2	1.82	0.60
1:B:1891:ASN:O	1:B:1895:LEU:HD13	2.01	0.60
1:A:418:ASP:O	1:B:2708:GLN:NE2	2.35	0.59
1:B:2013:LEU:HD23	1:B:2013:LEU:H	1.66	0.59
1:A:173:HIS:NE2	1:B:1998:GLU:OE1	2.35	0.59
1:A:306:PHE:CD2	1:A:551:PHE:CE2	2.90	0.59
1:B:2396:LEU:HD12	1:B:2596:MET:HE1	1.84	0.59
4:B:2801:NAG:HO3	4:B:2801:NAG:C7	2.07	0.59
1:A:979:ARG:O	1:A:983:LEU:HD13	2.03	0.58
1:B:688:SER:OG	1:B:2647:GLU:OE1	2.16	0.58
1:B:2594:ILE:HD11	1:B:2710:LEU:HD23	1.83	0.58
1:B:2721:TYR:O	1:B:2724:SER:OG	2.13	0.58
1:B:182:GLN:N	1:B:182:GLN:OE1	2.36	0.58
1:B:1891:ASN:HD22	1:B:1910:VAL:HG21	1.68	0.58
1:B:2233:TYR:OH	1:B:2334:SER:O	2.17	0.58
1:A:192:VAL:O	1:A:277:TYR:OH	2.20	0.58
1:B:2472:VAL:HG13	1:B:2472:VAL:O	2.03	0.58
1:A:2586:ASP:HA	1:A:2590:ILE:HG22	1.84	0.58
1:A:35:GLU:OE1	1:A:35:GLU:N	2.37	0.58
1:A:417:LEU:CD1	1:A:605:GLN:NE2	2.67	0.58
1:A:589:ASP:OD1	1:A:590:ILE:N	2.36	0.58
1:B:2496:LEU:O	1:B:2605:ARG:NH1	2.37	0.58
1:B:589:ASP:OD1	1:B:590:ILE:N	2.37	0.58
1:B:2292:MET:HE3	1:B:2296:ALA:CB	2.34	0.58
1:B:2284:LEU:HD13	1:B:2331:VAL:CG1	2.33	0.58
1:A:1277:GLN:OE1	1:A:1279:ARG:N	2.37	0.58
1:B:439:LEU:HG	1:B:598:MET:HE3	1.85	0.58
1:A:2629:LEU:HA	1:A:2634:LEU:HD23	1.86	0.57
1:B:2620:SER:O	1:B:2621:SER:OG	2.13	0.57
1:A:119:GLN:OE1	1:A:119:GLN:N	2.36	0.57
1:A:2505:ASP:OD2	1:A:2607:ASN:ND2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1932:ILE:O	1:B:1982:LYS:NZ	2.35	0.57
1:A:1910:VAL:HG12	1:A:1920:CYS:CB	2.35	0.57
1:B:123:SER:HB3	1:B:342:ARG:HH22	1.70	0.57
1:B:123:SER:OG	1:B:125:ASP:OD1	2.20	0.57
1:B:613:SER:OG	1:B:614:LEU:N	2.34	0.57
1:A:2667:ASN:OD1	1:A:2669:ASN:ND2	2.38	0.57
1:A:2472:VAL:HG13	1:A:2472:VAL:O	2.05	0.57
1:A:555:VAL:O	1:A:555:VAL:HG13	2.05	0.57
1:B:2242:ARG:O	1:B:2336:ARG:NH1	2.38	0.56
1:A:1932:ILE:O	1:A:1982:LYS:NZ	2.36	0.56
1:A:2454:LEU:HD22	1:A:2462:LEU:HD11	1.86	0.56
1:B:89:PRO:O	1:B:350:ARG:NH2	2.37	0.56
1:B:439:LEU:HD23	1:B:602:PHE:HZ	1.71	0.56
1:B:2234:ALA:HB3	1:B:2282:LEU:HD23	1.87	0.56
1:A:448:PRO:HD2	1:A:452:LEU:HD13	1.88	0.56
1:B:2586:ASP:HA	1:B:2590:ILE:HG22	1.87	0.56
1:A:2284:LEU:HD13	1:A:2331:VAL:HG13	1.87	0.56
1:B:2658:TYR:OH	1:B:2683:ALA:O	2.21	0.56
1:A:963:ILE:HG22	1:A:963:ILE:O	2.05	0.56
1:B:1150:GLU:N	1:B:1150:GLU:OE1	2.38	0.56
1:A:1968:ARG:NH2	1:A:2061:PHE:O	2.39	0.56
1:B:2281:CYS:O	1:B:2334:SER:OG	2.24	0.55
1:A:329:GLN:N	1:A:329:GLN:OE1	2.39	0.55
1:A:1758:LEU:HD11	1:A:1879:TRP:HB2	1.87	0.55
1:A:2339:ILE:HD11	1:A:2462:LEU:HG	1.88	0.55
1:A:138:CYS:N	1:A:153:GLN:O	2.38	0.55
1:B:177:ASP:OD2	1:B:179:SER:OG	2.25	0.55
1:B:1895:LEU:HD11	1:B:1952:TYR:CD2	2.41	0.55
1:A:2284:LEU:HD13	1:A:2331:VAL:CG1	2.37	0.55
1:A:2037:SER:OG	1:A:2038:GLU:N	2.40	0.55
1:B:626:GLU:O	1:B:629:GLN:NE2	2.40	0.55
1:A:2028:LEU:HD12	1:A:2031:LEU:HD23	1.89	0.55
1:A:761:GLN:OE1	1:A:761:GLN:N	2.41	0.54
1:A:771:VAL:HG23	1:A:899:TRP:O	2.07	0.54
1:B:73:VAL:HG12	1:B:79:GLU:HA	1.89	0.54
1:B:772:GLN:N	1:B:899:TRP:O	2.39	0.54
1:B:1873:LEU:HD23	1:B:1923:TYR:CD2	2.43	0.54
1:B:2284:LEU:HD13	1:B:2331:VAL:HG13	1.88	0.54
1:A:493:THR:HG23	1:A:493:THR:O	2.08	0.54
1:B:2667:ASN:OD1	1:B:2669:ASN:ND2	2.39	0.54
1:A:2234:ALA:HB3	1:A:2282:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:LEU:O	1:B:486:GLY:N	2.39	0.54
1:B:2344:SER:HB3	1:B:2482:VAL:HG21	1.90	0.54
1:A:88:ARG:CD	1:A:331:GLN:OE1	2.56	0.53
1:A:251:GLU:OE2	1:A:491:ARG:NH1	2.41	0.53
1:A:1977:ILE:CD1	1:A:1979:ILE:HD11	2.37	0.53
1:A:925:CYS:SG	1:A:926:GLU:N	2.81	0.53
1:A:2103:ILE:HB	1:A:2175:LEU:HD23	1.90	0.53
1:B:1959:GLN:O	1:B:1999:ARG:NH2	2.39	0.53
1:B:119:GLN:N	1:B:119:GLN:OE1	2.41	0.53
1:A:190:ARG:O	1:A:193:GLN:NE2	2.38	0.53
1:B:2112:ASP:OD1	1:B:2113:VAL:N	2.40	0.53
1:B:2573:T44:O	1:B:2577:SER:HB3	2.08	0.53
1:B:1910:VAL:HG12	1:B:1920:CYS:HB2	1.90	0.53
1:A:2594:ILE:HD11	1:A:2710:LEU:HD23	1.91	0.53
1:B:1763:ARG:O	1:B:1763:ARG:HG3	2.08	0.53
1:B:2349:GLU:OE1	1:B:2349:GLU:N	2.42	0.53
1:A:2223:LYS:NZ	1:A:2327:ASN:OD1	2.40	0.53
1:B:1910:VAL:HG12	1:B:1920:CYS:CB	2.39	0.53
1:B:1977:ILE:HD12	1:B:1979:ILE:HD11	1.90	0.53
1:A:2203:ILE:HD11	1:A:2251:TRP:CZ2	2.44	0.52
1:B:685:ALA:HB3	1:B:693:LEU:HD12	1.90	0.52
1:A:2344:SER:HB3	1:A:2482:VAL:HG21	1.91	0.52
1:A:2620:SER:O	1:A:2621:SER:OG	2.16	0.52
1:A:589:ASP:OD1	1:A:590:ILE:HG23	2.10	0.52
1:B:443:ILE:HD12	1:B:598:MET:HE1	1.90	0.52
1:B:1371:GLN:NE2	1:B:1372:LEU:O	2.41	0.52
1:B:2695:GLU:O	1:B:2695:GLU:HG2	2.09	0.52
1:B:1027:TYR:CE1	1:B:1043:HIS:HA	2.44	0.52
1:B:2484:ASP:OD1	1:B:2484:ASP:N	2.42	0.52
1:A:613:SER:OG	1:A:614:LEU:N	2.43	0.52
1:A:685:ALA:HB3	1:A:693:LEU:HD12	1.89	0.52
1:A:924:SER:OG	1:A:1037:TRP:NE1	2.43	0.52
1:B:2103:ILE:HB	1:B:2175:LEU:HD23	1.90	0.52
1:A:1973:LYS:O	1:A:1974:LEU:HD12	2.09	0.52
1:B:696:GLN:HG3	1:B:705:VAL:HG11	1.90	0.52
1:A:1116:ARG:NE	1:A:1147:SER:OG	2.42	0.52
1:A:425:MET:CE	1:A:573:LEU:HD23	2.40	0.52
1:A:761:GLN:O	1:A:772:GLN:NE2	2.39	0.52
1:B:2216:ILE:HD11	1:B:2324:ALA:HB2	1.92	0.51
1:A:2104:VAL:HG12	1:A:2104:VAL:O	2.10	0.51
1:B:1281:CYS:O	1:B:1282:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ALA:CB	1:B:316:VAL:HG12	2.40	0.51
1:A:158:ALA:O	1:A:159:ARG:CG	2.59	0.51
1:B:1987:ASP:N	1:B:1987:ASP:OD1	2.43	0.51
1:A:951:PHE:CE1	1:A:979:ARG:HA	2.45	0.51
1:B:1956:VAL:O	1:B:1956:VAL:HG13	2.11	0.51
1:A:116:TYR:OH	1:A:130:GLN:OE1	2.28	0.51
1:A:1866:ILE:HD12	1:A:1941:ARG:HB3	1.93	0.51
1:B:1906:GLN:O	1:B:1907:LEU:HD22	2.12	0.51
1:B:2116:ILE:O	1:B:2117:SER:OG	2.25	0.51
1:A:2057:ARG:NH2	1:B:267:LEU:O	2.44	0.50
1:B:761:GLN:NE2	1:B:773:CYS:SG	2.79	0.50
1:B:1758:LEU:O	1:B:1758:LEU:HD23	2.10	0.50
1:B:1925:GLU:OE1	1:B:1953:ARG:NH1	2.44	0.50
1:B:2203:ILE:HD11	1:B:2251:TRP:CZ2	2.46	0.50
1:B:500:PHE:CD2	1:B:505:LEU:HD13	2.46	0.50
1:B:1873:LEU:HD21	1:B:1926:ALA:HB2	1.94	0.50
1:A:61:VAL:O	1:A:61:VAL:HG13	2.11	0.50
1:A:582:HIS:O	1:A:585:SER:OG	2.28	0.50
1:A:1030:GLN:NE2	1:A:1042:CYS:O	2.43	0.50
1:A:1283:ARG:O	1:A:1462:VAL:HG12	2.11	0.50
1:B:2284:LEU:HD12	1:B:2284:LEU:O	2.12	0.50
1:B:673:GLY:O	1:B:2578:ARG:NE	2.45	0.50
1:B:616:VAL:CG2	1:B:963:ILE:HG23	2.40	0.50
1:B:2116:ILE:HD11	1:B:2130:CYS:SG	2.51	0.50
1:A:2472:VAL:HG12	1:A:2573:T44:I5'	2.82	0.50
1:B:2344:SER:CB	1:B:2482:VAL:HG21	2.42	0.50
1:A:929:LYS:O	1:A:933:LEU:HD23	2.12	0.49
1:B:645:LEU:HD23	1:B:645:LEU:H	1.77	0.49
1:B:2470:LEU:HD23	1:B:2470:LEU:O	2.12	0.49
1:A:924:SER:HG	1:A:1037:TRP:HD1	1.55	0.49
1:A:955:GLU:CD	1:A:983:LEU:HD21	2.37	0.49
1:A:2496:LEU:O	1:A:2605:ARG:NH1	2.46	0.49
1:B:2508:ILE:HG21	1:B:2597:ALA:HB2	1.94	0.49
1:A:926:GLU:O	1:A:930:LEU:HD23	2.12	0.49
1:A:951:PHE:CZ	1:A:979:ARG:HA	2.47	0.49
1:A:1861:ASP:OD1	1:A:1861:ASP:N	2.45	0.49
1:A:1873:LEU:HD21	1:A:1926:ALA:HB2	1.94	0.49
1:A:2344:SER:CB	1:A:2482:VAL:HG21	2.42	0.49
1:A:212:SER:HA	1:B:2058:THR:HG21	1.94	0.49
1:A:1262:LEU:HD11	1:A:1273:SER:HB3	1.93	0.49
1:A:1906:GLN:O	1:A:1907:LEU:HD22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1996:GLU:OE2	1:A:1999:ARG:NH1	2.45	0.49
1:B:1764:ASP:CG	1:B:1766:ARG:HH12	2.21	0.49
1:A:490:THR:HG22	1:A:491:ARG:N	2.28	0.49
1:B:2030:SER:HB2	1:B:2080:VAL:HG11	1.95	0.49
1:B:2556:VAL:HG13	1:B:2722:ILE:HG23	1.94	0.49
1:A:290:VAL:HG21	1:A:479:VAL:HG12	1.95	0.49
1:B:231:VAL:O	1:B:254:LEU:HD12	2.13	0.48
1:B:460:THR:HG23	1:B:461:THR:H	1.78	0.48
1:A:479:VAL:HB	1:A:564:LEU:HD21	1.95	0.48
1:A:634:ASP:OD1	1:A:651:ARG:NE	2.46	0.48
1:A:2058:THR:HG21	1:B:212:SER:HA	1.96	0.48
1:B:151:THR:O	1:B:151:THR:HG22	2.13	0.48
1:B:2227:GLN:OE1	1:B:2320:SER:OG	2.30	0.48
1:A:158:ALA:O	1:A:159:ARG:HG3	2.13	0.48
1:B:2398:THR:HG23	1:B:2487:TYR:O	2.13	0.48
1:A:484:LEU:O	1:A:487:ALA:N	2.46	0.48
1:A:924:SER:OG	1:A:1037:TRP:CD1	2.63	0.48
1:A:479:VAL:HG13	1:A:484:LEU:CD2	2.44	0.48
1:A:1088:SER:O	1:A:1088:SER:OG	2.31	0.48
1:A:1956:VAL:O	1:A:1956:VAL:HG13	2.14	0.48
1:B:329:GLN:N	1:B:329:GLN:OE1	2.46	0.48
1:A:696:GLN:HG3	1:A:705:VAL:HG11	1.94	0.48
1:A:2242:ARG:O	1:A:2336:ARG:NH1	2.46	0.48
1:B:2350:LEU:HD12	1:B:2350:LEU:O	2.14	0.48
1:A:2204:ALA:O	1:A:2205:THR:HG22	2.14	0.47
1:B:2086:THR:OG1	1:B:2087:GLU:OE1	2.30	0.47
1:B:2350:LEU:HD12	1:B:2354:TRP:HZ2	1.77	0.47
1:A:1873:LEU:HD23	1:A:1923:TYR:CD1	2.49	0.47
1:B:502:GLN:O	1:B:503:LEU:HD12	2.13	0.47
1:B:1448:VAL:HG12	1:B:1449:VAL:N	2.29	0.47
1:B:2527:GLU:OE1	1:B:2532:ARG:NH2	2.47	0.47
1:B:2680:GLU:N	1:B:2680:GLU:OE1	2.46	0.47
1:A:1987:ASP:OD1	1:A:1987:ASP:N	2.47	0.47
1:B:1284:PRO:HA	1:B:1462:VAL:HG12	1.95	0.47
1:A:425:MET:HE1	1:A:573:LEU:HD23	1.96	0.47
1:A:598:MET:HG3	1:A:602:PHE:CE2	2.49	0.47
1:A:965:LEU:HD12	1:A:965:LEU:C	2.39	0.47
1:B:158:ALA:O	1:B:159:ARG:CG	2.62	0.47
1:A:177:ASP:OD2	1:A:179:SER:OG	2.32	0.47
1:A:2030:SER:HB2	1:A:2080:VAL:HG11	1.96	0.47
1:A:2339:ILE:HG22	1:A:2479:TRP:NE1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:ASN:O	1:B:699:ASN:OD1	2.32	0.47
1:B:2651:LEU:HD11	1:B:2655:ILE:HD11	1.96	0.47
1:A:768:TRP:CE2	1:A:905:GLY:HA3	2.50	0.47
1:A:2235:ALA:HA	1:A:2249:LEU:HD13	1.96	0.47
1:B:1087:SER:OG	1:B:2172:CYS:SG	2.68	0.47
1:A:628:VAL:HG13	1:A:628:VAL:O	2.15	0.47
1:A:2398:THR:HG23	1:A:2487:TYR:O	2.15	0.47
1:B:439:LEU:HD11	1:B:570:PHE:CE2	2.50	0.47
1:B:991:ASP:OD1	1:B:992:TYR:N	2.48	0.47
1:B:2056:VAL:HG23	1:B:2056:VAL:O	2.14	0.47
1:A:484:LEU:O	1:A:486:GLY:N	2.48	0.46
1:B:1027:TYR:OH	1:B:1041:GLN:HB3	2.15	0.46
1:B:582:HIS:O	1:B:585:SER:OG	2.29	0.46
1:B:439:LEU:HD11	1:B:570:PHE:CZ	2.51	0.46
1:B:2236:PRO:O	1:B:2238:LEU:N	2.49	0.46
1:B:116:TYR:OH	1:B:130:GLN:OE1	2.33	0.46
1:B:2604:VAL:HG13	1:B:2604:VAL:O	2.14	0.46
1:A:150:GLY:O	1:B:1965:PHE:N	2.48	0.46
1:A:685:ALA:CB	1:A:693:LEU:HD12	2.46	0.46
1:A:1273:SER:OG	1:A:1274:ARG:N	2.47	0.46
1:A:2564:TYR:OH	1:A:2718:TRP:NE1	2.42	0.46
1:B:49:VAL:HG13	1:B:49:VAL:O	2.15	0.46
1:B:129:VAL:HG13	1:B:129:VAL:O	2.15	0.46
1:B:493:THR:HG23	1:B:493:THR:O	2.16	0.46
1:B:1030:GLN:NE2	1:B:1042:CYS:O	2.48	0.46
1:B:2564:TYR:OH	1:B:2718:TRP:NE1	2.44	0.46
1:B:1958:LEU:HD13	1:B:2003:MET:HE1	1.96	0.46
1:A:2069:SER:O	1:A:2071:SER:N	2.44	0.46
1:A:2360:VAL:O	1:A:2360:VAL:HG22	2.16	0.46
1:A:2484:ASP:N	1:A:2484:ASP:OD1	2.46	0.46
1:B:2113:VAL:HG12	1:B:2114:ALA:N	2.31	0.46
1:A:270:THR:HG22	1:A:270:THR:O	2.14	0.46
1:A:654:ARG:HH21	1:A:654:ARG:HG3	1.81	0.46
1:B:221:PHE:CD2	1:B:257:ILE:HG21	2.51	0.46
1:B:283:ARG:NH2	1:B:472:GLY:O	2.49	0.46
1:A:659:THR:HG22	1:A:660:GLU:N	2.31	0.46
1:A:1127:VAL:HG21	1:A:1132:GLY:HA2	1.98	0.46
1:A:2482:VAL:HG12	1:A:2483:VAL:N	2.30	0.46
1:B:460:THR:HG23	1:B:461:THR:N	2.31	0.46
1:B:2087:GLU:OE1	1:B:2087:GLU:N	2.49	0.46
1:A:175:VAL:HG13	1:A:175:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:HD23	1:A:289:LEU:O	2.16	0.46
1:B:1092:ALA:HB2	1:B:2222:TRP:NE1	2.30	0.46
1:A:677:ALA:HB1	1:A:2581:GLU:OE1	2.16	0.45
1:A:949:SER:O	1:B:1008:ARG:NH2	2.48	0.45
1:B:158:ALA:O	1:B:159:ARG:HG3	2.16	0.45
1:B:656:ARG:NH1	1:B:662:GLU:OE1	2.43	0.45
1:B:1861:ASP:N	1:B:1861:ASP:OD1	2.48	0.45
1:B:2665:SER:OG	1:B:2670:TYR:O	2.23	0.45
1:A:2040:TYR:O	1:A:2045:ARG:NH2	2.49	0.45
1:B:370:ARG:HB3	1:B:370:ARG:HH21	1.81	0.45
1:B:899:TRP:CG	1:B:907:LYS:HZ2	2.33	0.45
1:B:2482:VAL:HG12	1:B:2483:VAL:N	2.32	0.45
1:A:123:SER:OG	1:A:125:ASP:OD1	2.35	0.45
1:A:285:LEU:HD22	1:A:296:ARG:HA	1.98	0.45
1:A:460:THR:HG23	1:A:461:THR:H	1.81	0.45
1:A:2590:ILE:HD11	1:A:2612:HIS:CE1	2.51	0.45
1:B:61:VAL:HG23	1:B:61:VAL:O	2.16	0.45
1:B:1116:ARG:NH2	1:B:1147:SER:OG	2.49	0.45
1:B:2069:SER:O	1:B:2071:SER:N	2.41	0.45
1:B:2344:SER:OG	1:B:2345:SER:N	2.49	0.45
1:B:761:GLN:O	1:B:772:GLN:NE2	2.45	0.45
1:B:2058:THR:HG22	1:B:2059:TYR:H	1.82	0.45
1:A:326:GLN:O	1:A:329:GLN:NE2	2.45	0.45
1:A:460:THR:HG23	1:A:461:THR:N	2.32	0.45
1:B:1092:ALA:HB2	1:B:2222:TRP:CD1	2.52	0.45
1:B:2028:LEU:CD1	1:B:2031:LEU:HD23	2.45	0.45
1:B:2204:ALA:O	1:B:2205:THR:HG22	2.16	0.45
1:A:2695:GLU:O	1:A:2695:GLU:HG2	2.16	0.45
1:B:367:GLU:HA	1:B:370:ARG:NH2	2.31	0.45
1:B:1957:VAL:O	1:B:1957:VAL:HG13	2.15	0.45
1:A:2604:VAL:HG13	1:A:2604:VAL:O	2.16	0.45
1:B:2669:ASN:OD1	1:B:2685:TRP:N	2.43	0.45
1:B:2386:ARG:O	1:B:2388:GLY:N	2.47	0.45
1:B:2386:ARG:NH1	1:B:2627:ASP:OD2	2.45	0.45
1:A:2203:ILE:HD11	1:A:2251:TRP:CH2	2.51	0.45
1:B:270:THR:O	1:B:270:THR:HG22	2.17	0.45
1:B:465:ARG:NH1	1:B:468:GLN:OE1	2.49	0.45
1:B:909:GLU:OE1	1:B:909:GLU:N	2.44	0.45
1:A:1319:VAL:HG11	1:B:104:LEU:HD11	1.99	0.45
1:A:2349:GLU:N	1:A:2349:GLU:OE1	2.50	0.45
1:A:2590:ILE:HD13	1:A:2711:LYS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2470:LEU:CD2	1:B:2523:VAL:HG21	2.47	0.45
1:B:2223:LYS:NZ	1:B:2327:ASN:OD1	2.41	0.44
1:B:426:LEU:HD21	1:B:602:PHE:CE1	2.53	0.44
1:A:100:LYS:NZ	1:B:1323:ASP:OD1	2.40	0.44
1:A:278:ARG:NE	1:A:452:LEU:HD11	2.32	0.44
1:A:1461:CYS:O	1:A:1461:CYS:SG	2.75	0.44
1:B:175:VAL:HG13	1:B:175:VAL:O	2.18	0.44
1:A:443:ILE:O	1:A:443:ILE:CG2	2.65	0.44
1:A:503:LEU:CD2	1:A:557:LEU:HD22	2.47	0.44
1:A:979:ARG:C	1:A:979:ARG:CD	2.90	0.44
1:B:2235:ALA:HA	1:B:2249:LEU:HD13	2.00	0.44
1:A:957:PHE:CD2	1:B:960:ALA:HB2	2.52	0.44
1:A:2341:GLY:O	1:A:2354:TRP:N	2.51	0.44
1:B:1281:CYS:C	1:B:1282:GLN:HG3	2.42	0.44
1:B:1283:ARG:CZ	1:B:1283:ARG:HA	2.47	0.44
1:B:208:VAL:HG23	1:B:209:HIS:N	2.33	0.44
1:B:2380:VAL:HG12	1:B:2381:THR:N	2.32	0.44
1:A:1966:TYR:O	1:B:169:ARG:NH1	2.41	0.44
1:B:718:ALA:N	1:B:721:GLU:OE2	2.50	0.44
1:B:2695:GLU:OE2	1:B:2712:LYS:HD3	2.17	0.44
1:A:925:CYS:HB3	1:A:1037:TRP:CD2	2.53	0.44
1:A:2386:ARG:O	1:A:2388:GLY:N	2.48	0.44
1:A:2386:ARG:NH1	1:A:2627:ASP:OD2	2.49	0.44
1:B:367:GLU:OE1	1:B:370:ARG:NH2	2.51	0.44
1:A:425:MET:HA	1:A:425:MET:HE2	1.99	0.43
1:A:673:GLY:O	1:A:2578:ARG:NE	2.51	0.43
1:A:1032:ASP:OD1	1:A:1036:GLY:N	2.51	0.43
1:B:925:CYS:O	1:B:928:VAL:N	2.51	0.43
1:B:63:CYS:HA	1:B:70:CYS:HA	2.00	0.43
1:A:1092:ALA:HB2	1:A:2222:TRP:NE1	2.33	0.43
1:A:2398:THR:HG21	1:A:2487:TYR:CZ	2.54	0.43
1:B:659:THR:HG22	1:B:660:GLU:N	2.33	0.43
1:B:957:PHE:O	1:B:960:ALA:HB3	2.18	0.43
1:B:1868:ASP:O	1:B:1871:VAL:HG12	2.18	0.43
1:B:2104:VAL:HG12	1:B:2104:VAL:O	2.18	0.43
1:A:2142:VAL:HG23	1:A:2184:TYR:O	2.18	0.43
1:B:2026:LEU:HD12	1:B:2026:LEU:O	2.19	0.43
1:A:141:VAL:HG23	1:A:147:GLU:HA	1.99	0.43
1:A:558:GLN:NE2	1:A:562:ASN:OD1	2.50	0.43
1:A:2055:GLU:HG2	2:C:1:NAG:C8	2.48	0.43
1:B:283:ARG:NH2	1:B:471:PHE:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ARG:HH11	1:B:488:LEU:HD22	1.82	0.43
1:A:278:ARG:CD	1:A:452:LEU:HD11	2.49	0.43
1:A:320:HIS:HB2	1:A:321:PRO:HD2	2.01	0.43
1:A:2087:GLU:OE1	1:A:2132:TRP:NE1	2.46	0.43
1:A:2321:PHE:O	1:A:2325:VAL:HG22	2.19	0.43
1:A:2339:ILE:HG22	1:A:2479:TRP:CD1	2.53	0.43
1:A:2344:SER:OG	1:A:2345:SER:N	2.52	0.43
1:B:443:ILE:HG22	1:B:443:ILE:O	2.17	0.43
1:B:1765:TRP:O	1:B:1766:ARG:NH2	2.52	0.43
1:B:2590:ILE:HD13	1:B:2711:LYS:HD2	2.00	0.43
1:A:2123:PHE:CD1	1:A:2123:PHE:C	2.97	0.43
1:B:2037:SER:OG	1:B:2038:GLU:N	2.51	0.43
1:B:2360:VAL:O	1:B:2364:THR:HG23	2.19	0.43
1:B:2363:LEU:HD11	1:B:2382:LEU:HD12	2.00	0.43
1:A:934:GLN:O	1:A:938:GLU:HG2	2.19	0.43
1:A:2026:LEU:HD12	1:A:2026:LEU:O	2.19	0.43
1:B:35:GLU:OE2	1:B:35:GLU:N	2.51	0.43
1:B:446:LEU:HD22	1:B:470:LEU:HD23	2.01	0.43
1:B:1027:TYR:CD1	1:B:1043:HIS:HA	2.53	0.43
1:B:2629:LEU:HA	1:B:2634:LEU:HD23	2.01	0.43
1:A:221:PHE:CE1	1:A:254:LEU:HD22	2.53	0.43
1:A:312:ARG:O	1:A:312:ARG:HG3	2.19	0.43
1:A:364:CYS:N	1:A:365:PRO:CD	2.82	0.43
1:A:479:VAL:HG13	1:A:484:LEU:HD23	2.01	0.43
1:A:616:VAL:HG22	1:A:963:ILE:HD13	2.00	0.43
1:A:1092:ALA:HB2	1:A:2222:TRP:CD1	2.54	0.43
1:B:322:ASP:OD1	1:B:323:GLY:N	2.52	0.43
2:C:2:NAG:HO3	2:C:2:NAG:C7	2.18	0.43
1:A:122:ASP:OD1	1:A:123:SER:N	2.51	0.42
1:A:316:VAL:HG23	1:A:316:VAL:O	2.19	0.42
1:A:1905:CYS:SG	1:A:1922:LEU:HD22	2.59	0.42
1:A:2256:GLU:HG3	1:A:2258:THR:HG22	2.01	0.42
1:B:439:LEU:HD23	1:B:602:PHE:CZ	2.53	0.42
1:B:1283:ARG:O	1:B:1462:VAL:HG12	2.19	0.42
1:A:51:GLN:O	1:A:62:GLN:NE2	2.46	0.42
1:A:1284:PRO:HA	1:A:1462:VAL:HG12	2.01	0.42
1:A:2484:ASP:OD2	1:A:2486:GLN:NE2	2.52	0.42
1:B:712:ILE:HD11	1:B:731:LEU:HD21	2.02	0.42
2:E:2:NAG:HO3	2:E:2:NAG:C7	2.22	0.42
1:A:2108:ILE:HD11	1:A:2160:THR:HG21	2.01	0.42
1:B:659:THR:HG22	1:B:660:GLU:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2544:GLN:OE1	1:B:2557:GLN:NE2	2.52	0.42
1:B:2695:GLU:N	1:B:2695:GLU:OE1	2.52	0.42
1:A:2122:ASN:O	1:A:2122:ASN:OD1	2.38	0.42
1:A:2556:VAL:HG13	1:A:2722:ILE:HD12	2.01	0.42
1:B:2382:LEU:HD21	1:B:2392:ALA:HB1	2.00	0.42
1:A:995:ARG:NH2	1:B:374:ARG:O	2.49	0.42
1:A:1081:ARG:NH1	1:A:1106:PRO:O	2.46	0.42
4:A:2805:NAG:HO3	4:A:2805:NAG:C7	2.24	0.42
1:B:2013:LEU:HD23	1:B:2013:LEU:N	2.34	0.42
1:B:598:MET:HG3	1:B:602:PHE:CE2	2.53	0.42
1:B:708:GLU:O	1:B:708:GLU:HG2	2.20	0.42
1:B:2210:LEU:HD12	1:B:2210:LEU:O	2.19	0.42
1:A:919:PRO:O	1:A:919:PRO:HG2	2.19	0.42
1:A:1857:PHE:CD1	1:A:1954:LYS:HA	2.54	0.42
1:B:380:SER:OG	1:B:380:SER:O	2.34	0.42
1:B:2358:ASP:OD1	1:B:2358:ASP:C	2.63	0.42
1:B:2491:THR:HG23	1:B:2494:ARG:H	1.84	0.42
1:A:2210:LEU:HD12	1:A:2210:LEU:O	2.20	0.42
1:B:2347:SER:HG	1:B:2348:SER:H	1.67	0.42
1:A:129:VAL:HG13	1:A:129:VAL:O	2.20	0.42
1:A:289:LEU:HD23	1:A:289:LEU:C	2.45	0.42
1:A:1448:VAL:HG23	1:A:1450:ALA:H	1.85	0.42
1:B:141:VAL:HG22	1:B:142:ASP:N	2.35	0.42
1:B:316:VAL:O	1:B:316:VAL:HG23	2.20	0.42
1:B:2394:ILE:HG22	1:B:2394:ILE:O	2.18	0.42
1:A:502:GLN:O	1:A:503:LEU:HD12	2.20	0.41
1:B:121:GLN:N	1:B:125:ASP:O	2.50	0.41
4:B:2806:NAG:HO3	4:B:2806:NAG:C7	2.28	0.41
1:A:278:ARG:HD2	1:A:452:LEU:HD11	2.02	0.41
1:B:457:LEU:HD12	1:B:457:LEU:C	2.45	0.41
1:B:2008:THR:O	1:B:2008:THR:HG23	2.20	0.41
1:B:2246:PRO:O	1:B:2247:GLU:CD	2.62	0.41
2:E:3:MAN:O6	2:E:3:MAN:O4	2.21	0.41
1:A:184:SER:OG	1:A:185:PRO:HD2	2.20	0.41
1:A:224:PHE:HZ	1:A:231:VAL:HG11	1.84	0.41
1:B:1027:TYR:HE1	1:B:1042:CYS:O	2.03	0.41
1:A:289:LEU:HD22	1:A:564:LEU:HB2	2.01	0.41
1:B:412:ILE:HG13	1:B:600:MET:HE1	2.02	0.41
1:B:455:LEU:HD11	1:B:459:PHE:CE2	2.55	0.41
1:B:555:VAL:HG23	1:B:560:ASN:HD21	1.84	0.41
1:B:2298:VAL:HG12	1:B:2299:LEU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2196:THR:OG1	1:B:2197:SER:N	2.53	0.41
1:B:2400:ARG:NH2	1:B:2406:LEU:HD11	2.35	0.41
1:A:627:GLU:HG3	1:A:657:CYS:SG	2.61	0.41
1:A:768:TRP:CD2	1:A:905:GLY:HA3	2.55	0.41
1:A:2189:ILE:O	1:A:2189:ILE:HG23	2.21	0.41
1:A:2629:LEU:HD12	1:A:2629:LEU:O	2.21	0.41
1:B:425:MET:CE	1:B:573:LEU:HD23	2.50	0.41
1:B:2350:LEU:O	1:B:2350:LEU:CG	2.67	0.41
1:A:271:PHE:O	1:A:271:PHE:CG	2.74	0.41
1:A:2386:ARG:HD2	1:A:2625:LEU:HD12	2.03	0.41
1:B:579:PHE:CZ	1:B:598:MET:SD	3.14	0.41
1:B:926:GLU:O	1:B:930:LEU:HD23	2.20	0.41
1:B:1090:LYS:N	1:B:2222:TRP:O	2.54	0.41
1:B:1972:GLN:NE2	1:B:2038:GLU:OE2	2.47	0.41
1:A:368:ARG:NH2	1:A:966:THR:HG23	2.36	0.41
1:A:1109:LEU:CD1	1:A:1111:THR:HG22	2.51	0.41
1:A:2669:ASN:OD1	1:A:2685:TRP:N	2.45	0.41
1:B:93:LEU:HD23	1:B:98:LEU:HD23	2.02	0.41
1:B:129:VAL:HG23	1:B:140:CYS:HB3	2.02	0.41
1:B:346:ILE:O	1:B:347:PRO:C	2.63	0.41
1:B:2590:ILE:HA	1:B:2593:VAL:HG22	2.03	0.41
1:A:141:VAL:HG22	1:A:142:ASP:N	2.35	0.41
1:A:380:SER:O	1:A:380:SER:OG	2.39	0.41
1:A:1043:HIS:O	1:A:1043:HIS:ND1	2.51	0.41
1:A:1957:VAL:O	1:A:1957:VAL:HG13	2.21	0.41
1:A:1979:ILE:HG21	1:A:1982:LYS:CG	2.51	0.41
1:A:2353:ASN:OD1	1:A:2353:ASN:O	2.39	0.41
1:A:2616:SER:HB3	1:A:2626:THR:HG21	2.03	0.41
1:B:319:CYS:SG	1:B:325:TYR:HA	2.61	0.41
1:B:1759:LEU:H	1:B:1759:LEU:HD23	1.86	0.41
1:B:2332:THR:O	1:B:2332:THR:HG22	2.20	0.41
1:A:304:GLU:OE1	1:A:304:GLU:HA	2.21	0.40
1:A:1069:GLN:O	1:A:1070:ILE:C	2.65	0.40
1:A:2357:LEU:O	1:A:2361:VAL:HG23	2.22	0.40
1:B:168:ASN:ND2	1:B:183:CYS:SG	2.94	0.40
1:B:736:ALA:O	1:B:740:THR:HG22	2.21	0.40
1:B:2108:ILE:O	1:B:2108:ILE:HG23	2.21	0.40
1:B:2534:SER:HA	1:B:2573:T44:I3'	2.91	0.40
1:A:283:ARG:NH2	1:A:472:GLY:O	2.54	0.40
1:A:489:GLY:O	1:A:490:THR:OG1	2.37	0.40
1:A:599:GLU:HA	1:A:602:PHE:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2073:ALA:O	1:A:2074:PRO:C	2.63	0.40
1:A:2500:PRO:HB3	1:A:2605:ARG:HD3	2.03	0.40
1:B:440:LYS:HD2	1:B:599:GLU:OE1	2.22	0.40
1:B:484:LEU:O	1:B:487:ALA:N	2.54	0.40
1:B:2350:LEU:O	1:B:2350:LEU:HG	2.21	0.40
1:A:55:ASP:OD1	1:A:55:ASP:O	2.39	0.40
1:A:2339:ILE:HG13	1:A:2340:PHE:N	2.36	0.40
1:B:271:PHE:O	1:B:271:PHE:CG	2.74	0.40
1:B:2073:ALA:O	1:B:2074:PRO:C	2.64	0.40
1:A:598:MET:HA	1:A:601:VAL:HG12	2.03	0.40
1:A:2112:ASP:OD1	1:A:2113:VAL:N	2.55	0.40
1:A:2336:ARG:NE	1:A:2358:ASP:OD2	2.52	0.40
1:B:2360:VAL:O	1:B:2360:VAL:HG22	2.21	0.40
1:B:2399:THR:OG1	1:B:2489:ARG:NH1	2.54	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	1726/2769 (62%)	1548 (90%)	178 (10%)	0	100	100
1	B	1725/2769 (62%)	1539 (89%)	186 (11%)	0	100	100
All	All	3451/5538 (62%)	3087 (90%)	364 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1509/2312 (65%)	1506 (100%)	3 (0%)	87	88
1	B	1509/2312 (65%)	1506 (100%)	3 (0%)	87	88
All	All	3018/4624 (65%)	3012 (100%)	6 (0%)	85	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	A	551	PHE
1	A	562	ASN
1	B	214	PHE
1	B	495	ASN
1	B	2353	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	423	GLN
1	A	427	GLN
1	A	498	HIS
1	A	502	GLN
1	A	605	GLN
1	A	2137	HIS
1	A	2369	HIS
1	B	121	GLN
1	B	288	GLN
1	B	427	GLN
1	B	562	ASN
1	B	605	GLN
1	B	1091	GLN
1	B	1877	GLN
1	B	2369	HIS
1	B	2512	GLN
1	B	2612	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	DHA	B	2540	1	3,4,5	4.24	1 (33%)	2,4,6	3.34	1 (50%)
1	DHA	A	2540	1	3,4,5	4.35	1 (33%)	2,4,6	3.28	1 (50%)

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
1	DHA	B	2540	1	-	0/0/2/4	-
1	DHA	A	2540	1	-	0/0/2/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2540	DHA	C-CA	7.31	1.57	1.45
1	B	2540	DHA	C-CA	7.15	1.57	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2540	DHA	O-C-CA	-4.66	116.78	125.53
1	A	2540	DHA	O-C-CA	-4.43	117.22	125.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2,1	14,14,15	0.61	0	17,19,21	2.74	7 (41%)
2	NAG	C	2	2	14,14,15	0.39	0	17,19,21	0.97	1 (5%)
2	MAN	C	3	2	11,11,12	0.26	0	15,15,17	0.85	0
3	NAG	D	1	3,1	14,14,15	0.55	0	17,19,21	0.78	0
3	NAG	D	2	3	14,14,15	0.36	0	17,19,21	1.16	1 (5%)
2	NAG	E	1	2,1	14,14,15	1.01	1 (7%)	17,19,21	1.10	1 (5%)
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	1.34	3 (17%)
2	MAN	E	3	2	11,11,12	0.36	0	15,15,17	1.15	1 (6%)
3	NAG	F	1	3,1	14,14,15	0.30	0	17,19,21	0.68	0
3	NAG	F	2	3	14,14,15	0.29	0	17,19,21	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	MAN	C	3	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	MAN	E	3	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	C1-C2	3.49	1.57	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	-7.74	99.31	111.29
2	C	1	NAG	C1-O5-C5	-3.98	106.85	112.19
2	C	1	NAG	C2-N2-C7	-3.70	117.94	122.90
2	E	2	NAG	O5-C1-C2	-3.62	105.69	111.29
2	C	1	NAG	C4-C3-C2	2.89	115.26	111.02
2	C	2	NAG	C1-O5-C5	2.76	115.89	112.19
2	C	1	NAG	O5-C5-C4	-2.74	104.16	110.83
2	C	1	NAG	C3-C4-C5	-2.69	105.35	110.23
2	E	2	NAG	C4-C3-C2	-2.53	107.30	111.02
2	E	3	MAN	O5-C5-C6	2.51	112.54	107.66
2	E	1	NAG	C3-C4-C5	-2.41	105.86	110.23
3	D	2	NAG	C1-C2-N2	2.24	113.96	110.43
2	E	2	NAG	C1-O5-C5	2.19	115.13	112.19
2	C	1	NAG	O5-C5-C6	2.16	111.87	107.66

There are no chirality outliers.

All (17) torsion outliers are listed below:

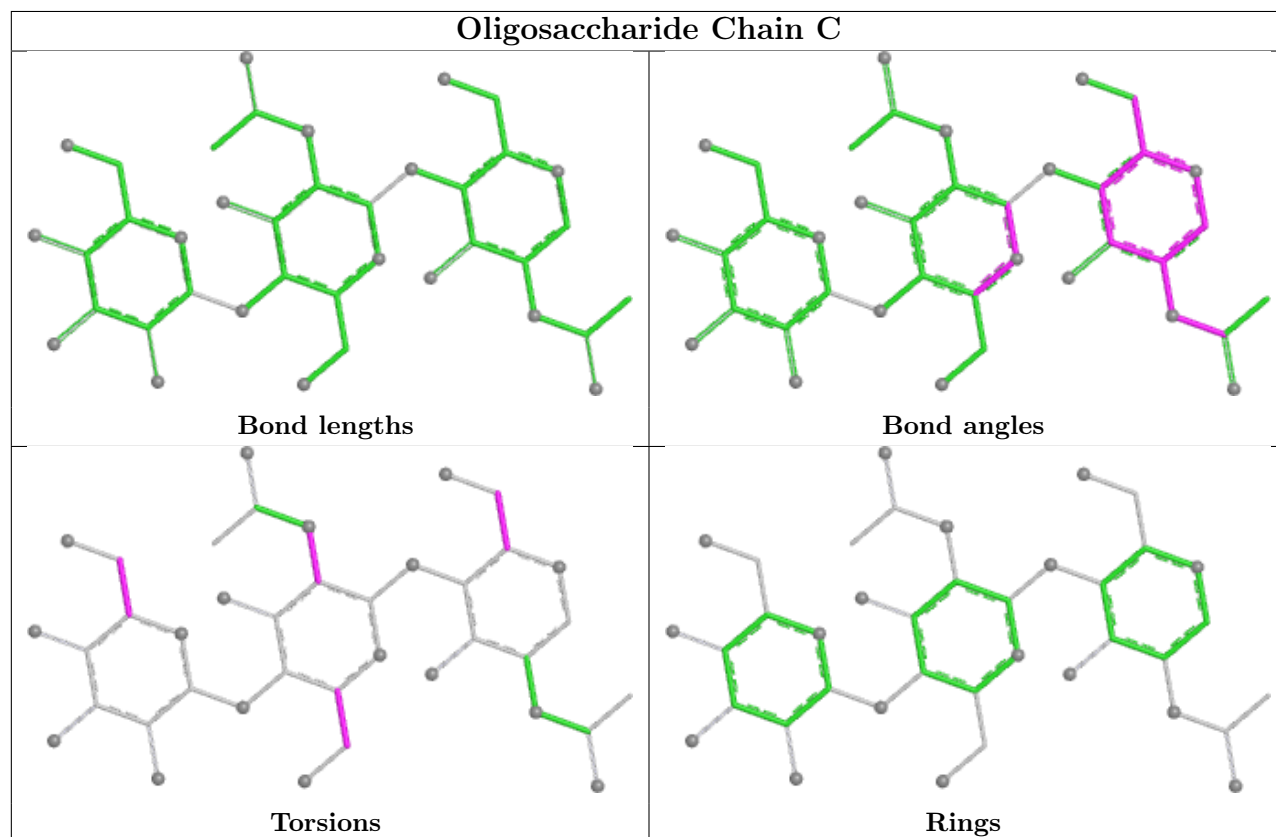
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C1-C2-N2-C7
3	D	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	E	3	MAN	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	C	3	MAN	O5-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	E	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C1-C2-N2-C7
3	D	1	NAG	C3-C2-N2-C7

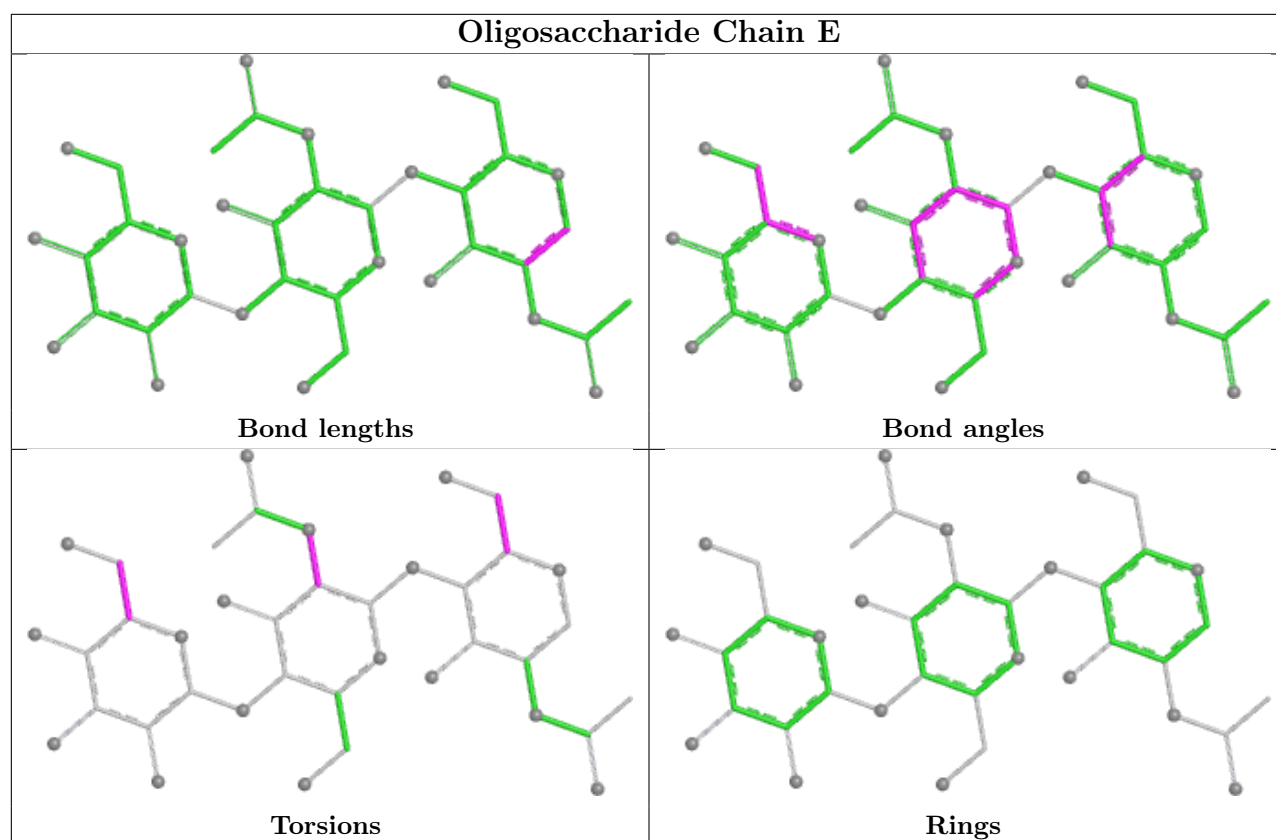
There are no ring outliers.

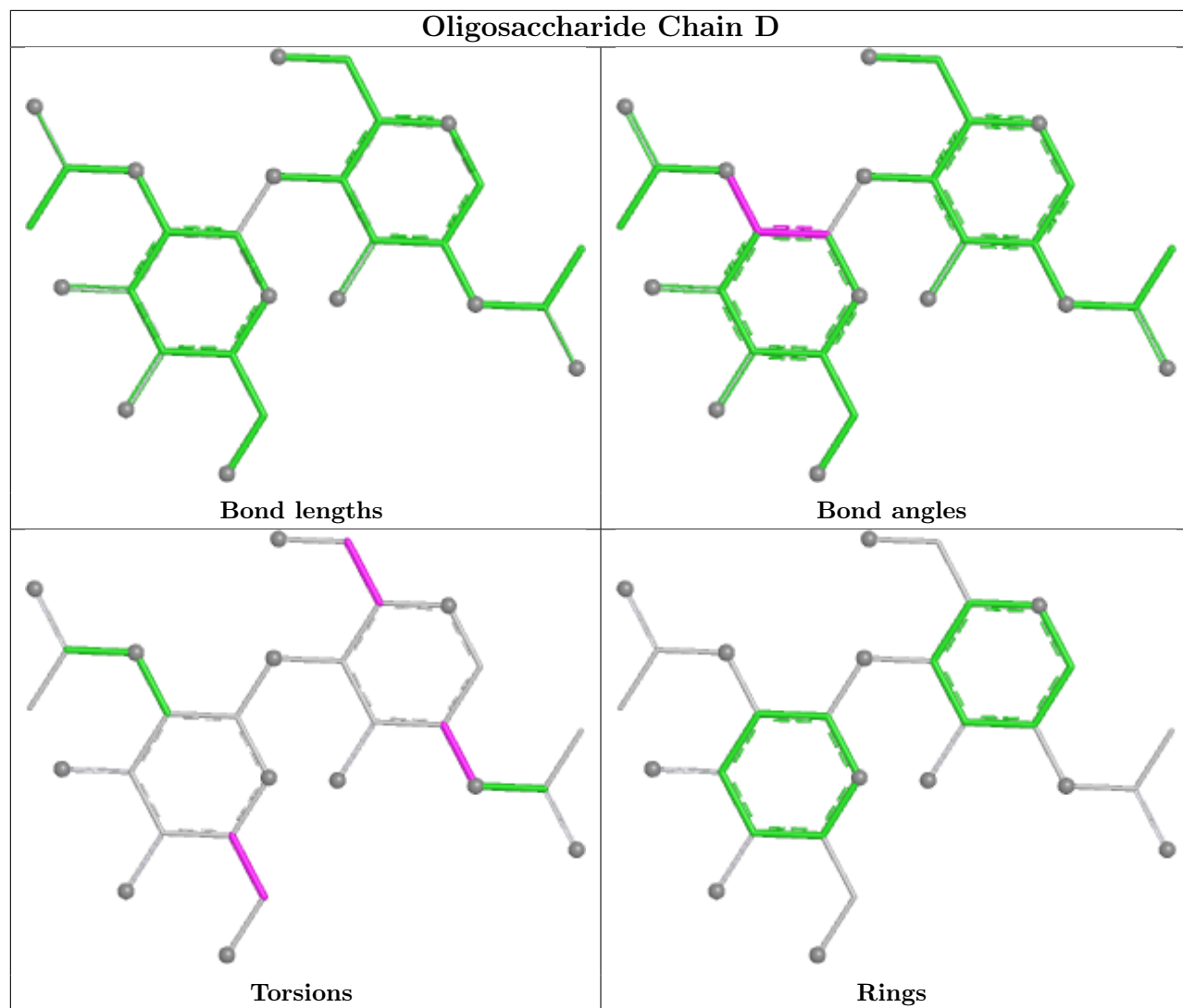
4 monomers are involved in 6 short contacts:

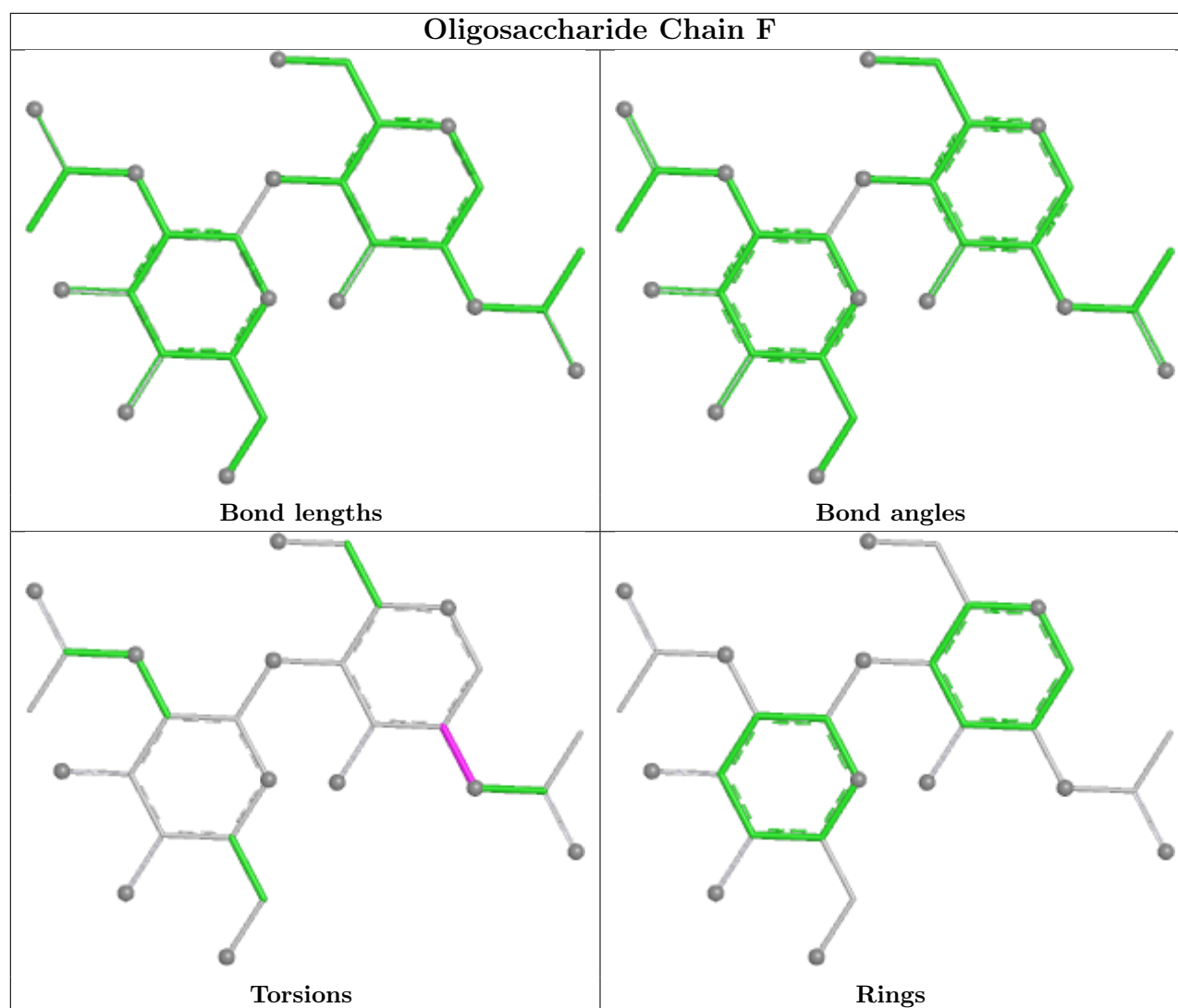
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	2	0
2	E	2	NAG	2	0
2	E	3	MAN	1	0
2	C	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	2802	1	14,14,15	0.65	0	17,19,21	2.01	5 (29%)
4	NAG	B	2806	1	14,14,15	0.42	0	17,19,21	1.19	1 (5%)
4	NAG	A	2805	1	14,14,15	0.42	0	17,19,21	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	2806	1	14,14,15	0.43	0	17,19,21	1.37	1 (5%)
4	NAG	B	2805	1	14,14,15	0.64	0	17,19,21	1.13	1 (5%)
4	NAG	A	2803	1	14,14,15	0.51	0	17,19,21	1.18	2 (11%)
4	NAG	B	2803	1	14,14,15	0.42	0	17,19,21	1.28	3 (17%)
4	NAG	B	2802	1	14,14,15	0.45	0	17,19,21	0.66	0
4	NAG	B	2804	1	14,14,15	0.63	0	17,19,21	1.96	4 (23%)
4	NAG	A	2804	1	14,14,15	0.35	0	17,19,21	1.30	1 (5%)
4	NAG	B	2801	1	14,14,15	0.46	0	17,19,21	1.02	1 (5%)
4	NAG	A	2801	1	14,14,15	0.44	0	17,19,21	0.71	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	NAG	A	2802	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2806	1	-	1/6/23/26	0/1/1/1
4	NAG	A	2805	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2806	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2805	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2803	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2803	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2802	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2804	1	-	1/6/23/26	0/1/1/1
4	NAG	A	2804	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2801	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2801	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2802	NAG	C1-O5-C5	5.39	119.41	112.19
4	B	2804	NAG	C1-O5-C5	5.29	119.27	112.19
4	A	2806	NAG	C1-O5-C5	4.88	118.72	112.19
4	A	2804	NAG	C1-O5-C5	4.50	118.22	112.19
4	A	2805	NAG	C1-O5-C5	3.95	117.48	112.19
4	B	2804	NAG	O5-C1-C2	3.77	117.13	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2802	NAG	O5-C1-C2	3.63	116.90	111.29
4	B	2801	NAG	C1-O5-C5	3.54	116.93	112.19
4	B	2806	NAG	C2-N2-C7	-3.13	118.70	122.90
4	B	2803	NAG	C4-C3-C2	-3.13	106.44	111.02
4	B	2803	NAG	C2-N2-C7	-3.01	118.86	122.90
4	A	2802	NAG	C2-N2-C7	-2.85	119.08	122.90
4	B	2804	NAG	C2-N2-C7	-2.84	119.10	122.90
4	A	2802	NAG	C4-C3-C2	-2.83	106.87	111.02
4	A	2803	NAG	C1-O5-C5	2.81	115.95	112.19
4	B	2804	NAG	C4-C3-C2	-2.77	106.97	111.02
4	B	2805	NAG	C1-O5-C5	-2.67	108.61	112.19
4	A	2803	NAG	C2-N2-C7	-2.37	119.72	122.90
4	B	2803	NAG	O5-C1-C2	-2.07	108.09	111.29
4	A	2802	NAG	C1-C2-N2	-2.01	107.26	110.43

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2806	NAG	O5-C5-C6-O6
4	A	2803	NAG	O5-C5-C6-O6
4	B	2801	NAG	O5-C5-C6-O6
4	B	2801	NAG	C4-C5-C6-O6
4	A	2806	NAG	C4-C5-C6-O6
4	A	2805	NAG	O5-C5-C6-O6
4	A	2803	NAG	C4-C5-C6-O6
4	B	2801	NAG	C1-C2-N2-C7
4	A	2804	NAG	O5-C5-C6-O6
4	A	2802	NAG	C3-C2-N2-C7
4	A	2805	NAG	C3-C2-N2-C7
4	B	2801	NAG	C3-C2-N2-C7
4	B	2804	NAG	C3-C2-N2-C7
4	A	2804	NAG	C1-C2-N2-C7
4	A	2805	NAG	C1-C2-N2-C7
4	B	2806	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2802	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2806	NAG	2	0
4	A	2805	NAG	2	0
4	B	2804	NAG	1	0
4	B	2801	NAG	2	0

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.

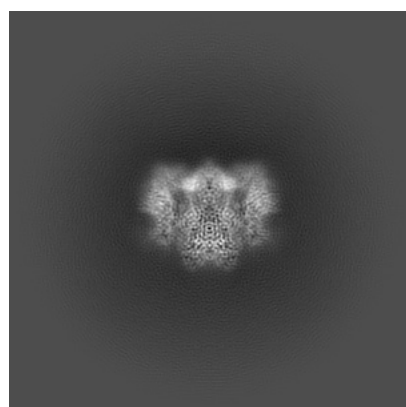
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14145. These allow visual inspection of the internal detail of the map and identification of artifacts.

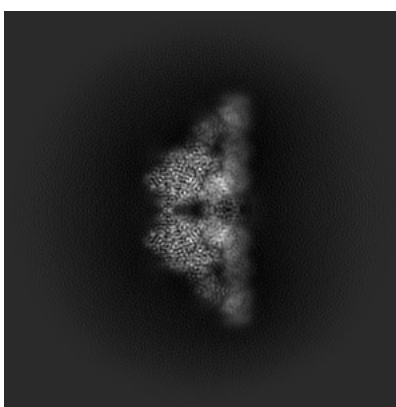
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

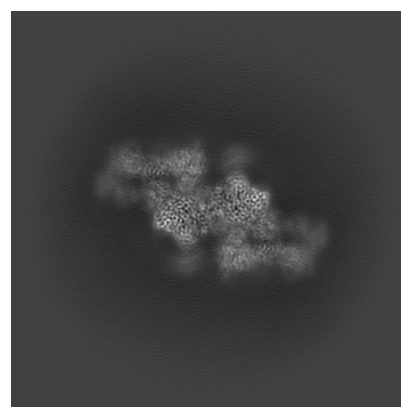
6.1.1 Primary map



X



Y

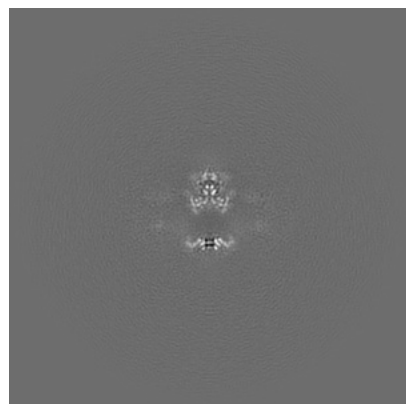


Z

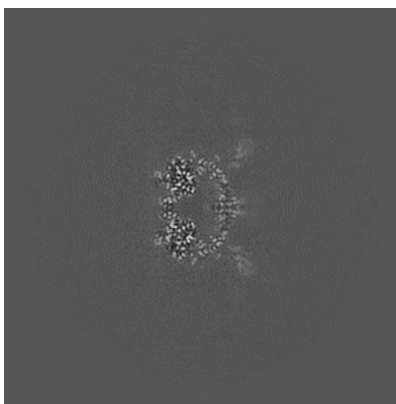
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

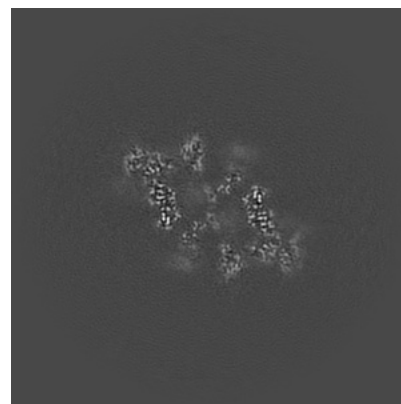
6.2.1 Primary map



X Index: 256



Y Index: 256

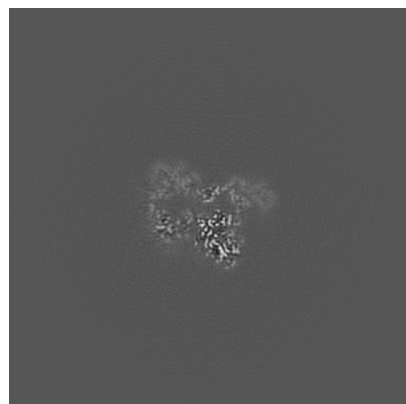


Z Index: 256

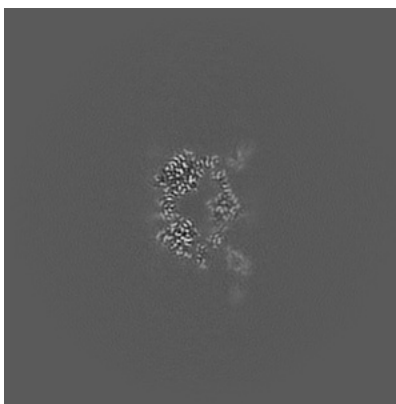
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

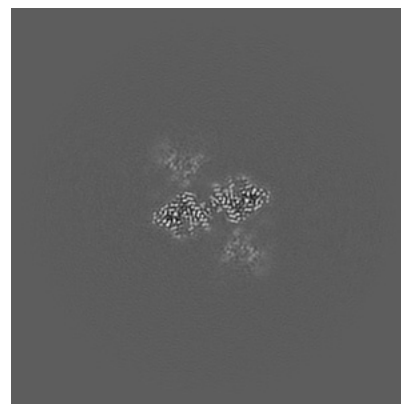
6.3.1 Primary map



X Index: 294



Y Index: 261

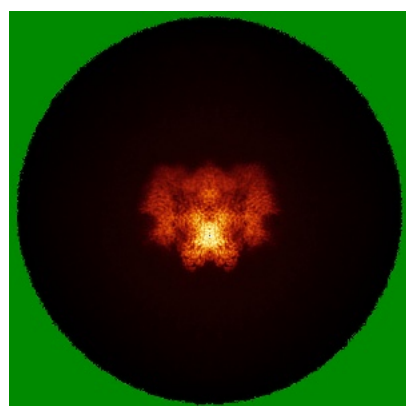


Z Index: 216

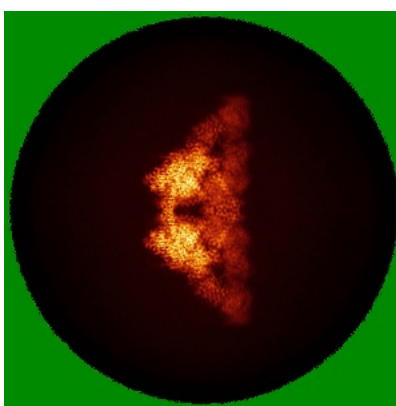
The images above show the largest variance slices of the map in three orthogonal directions.

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

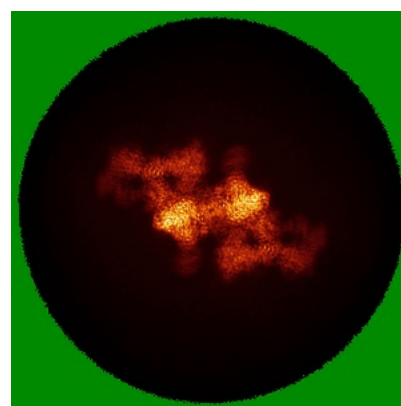
6.4.1 Primary map



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

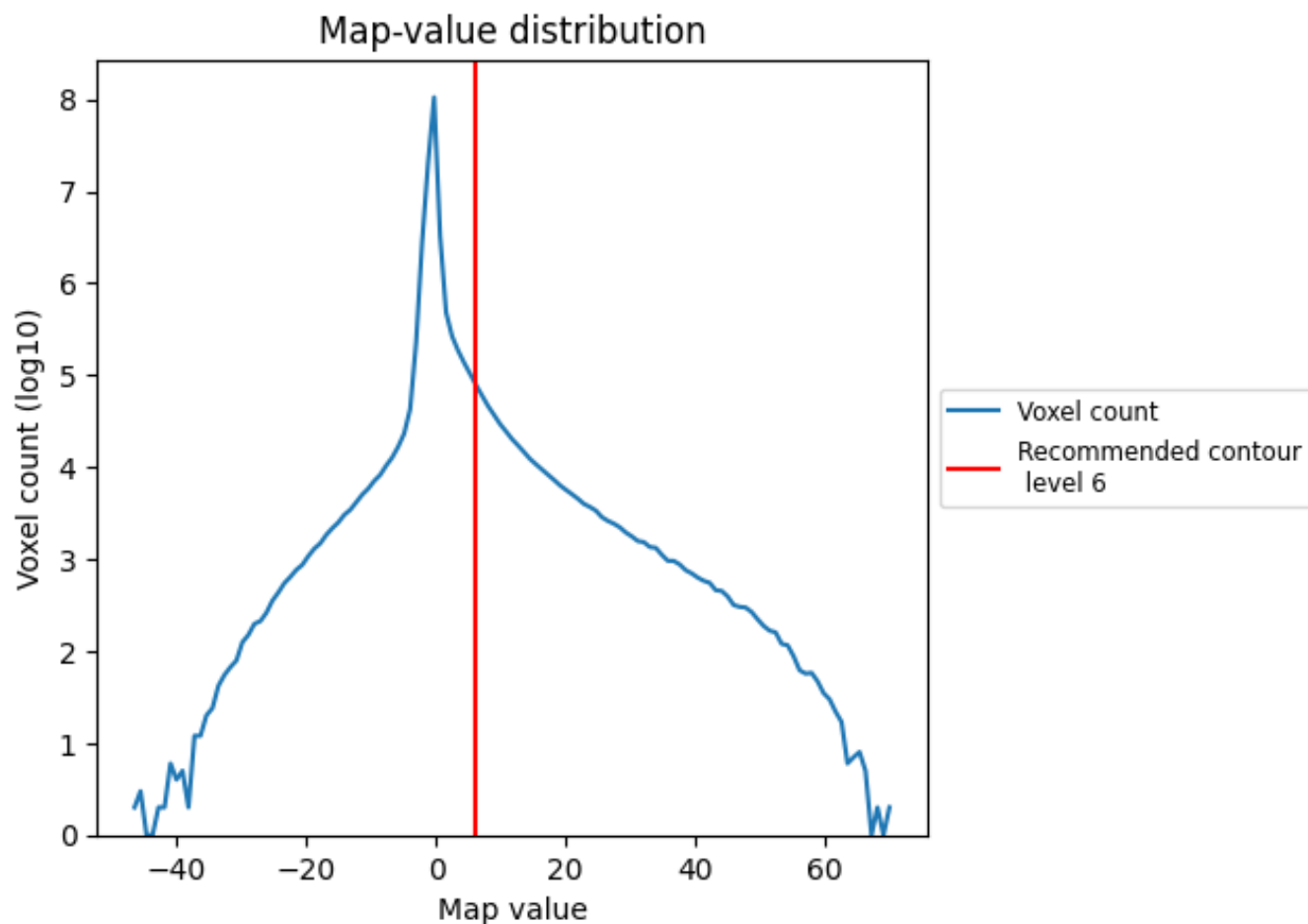
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

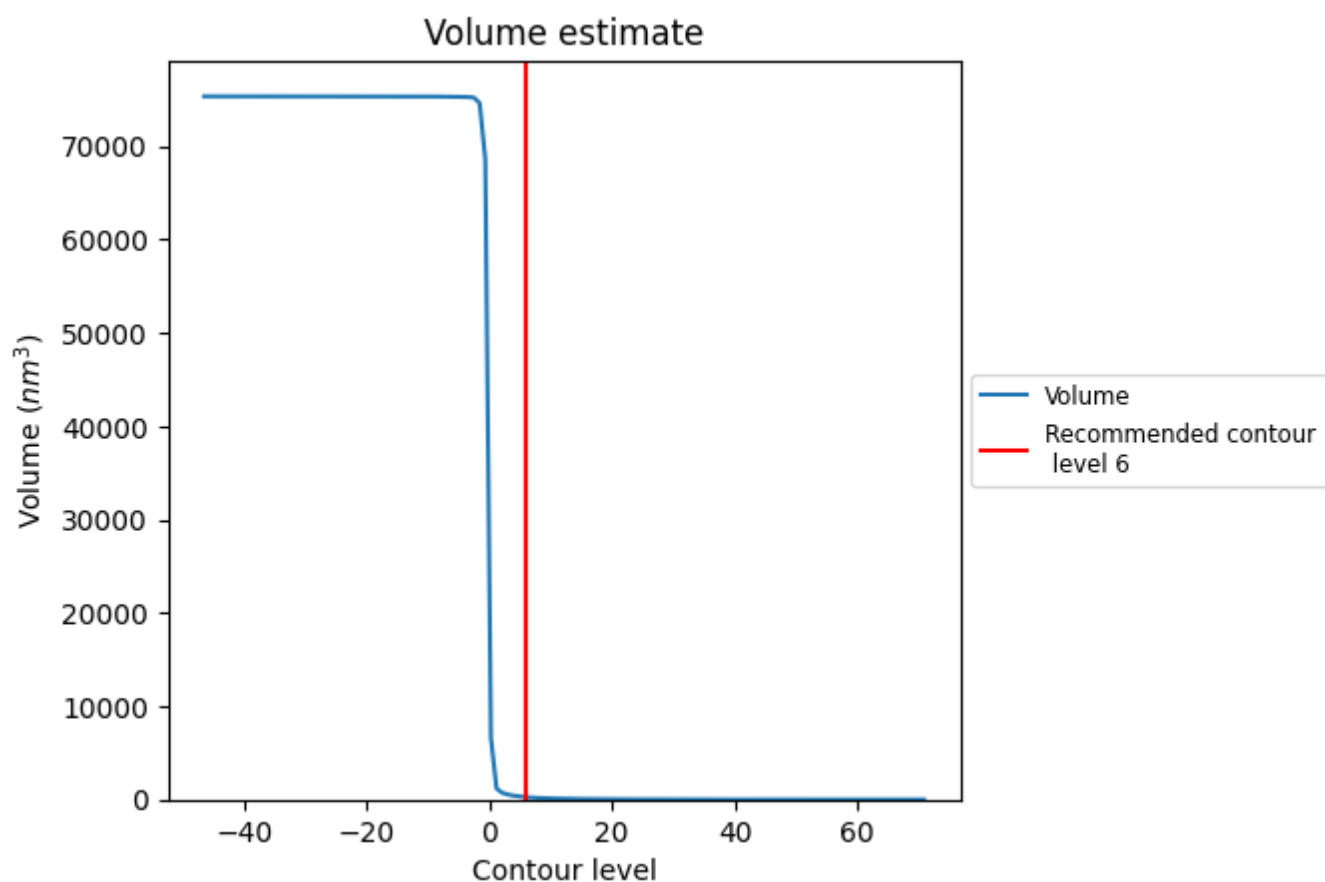
This section contains the results of statistical analysis of the map.

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.

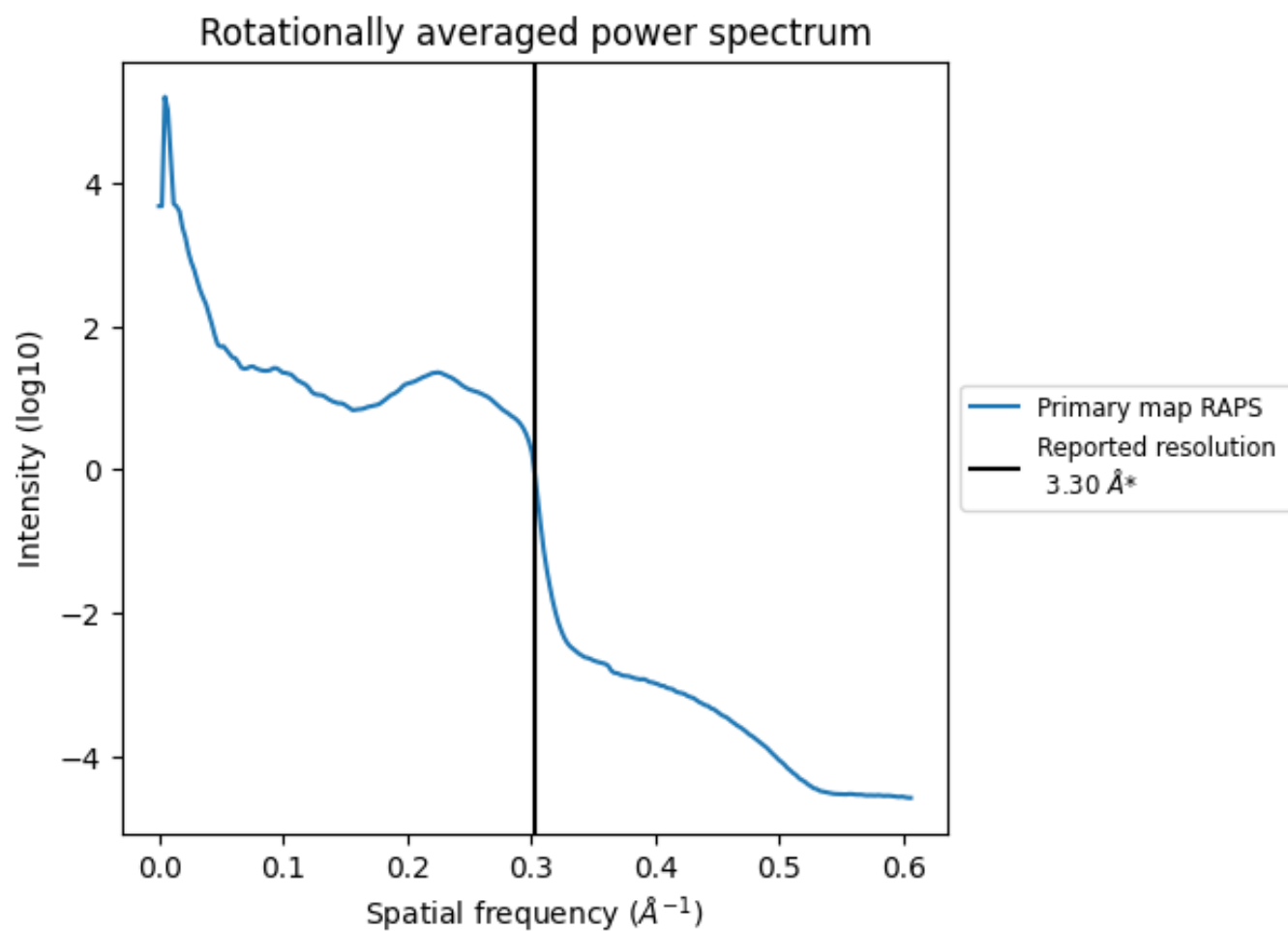
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 258 nm³; this corresponds to an approximate mass of 233 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 ⓘ

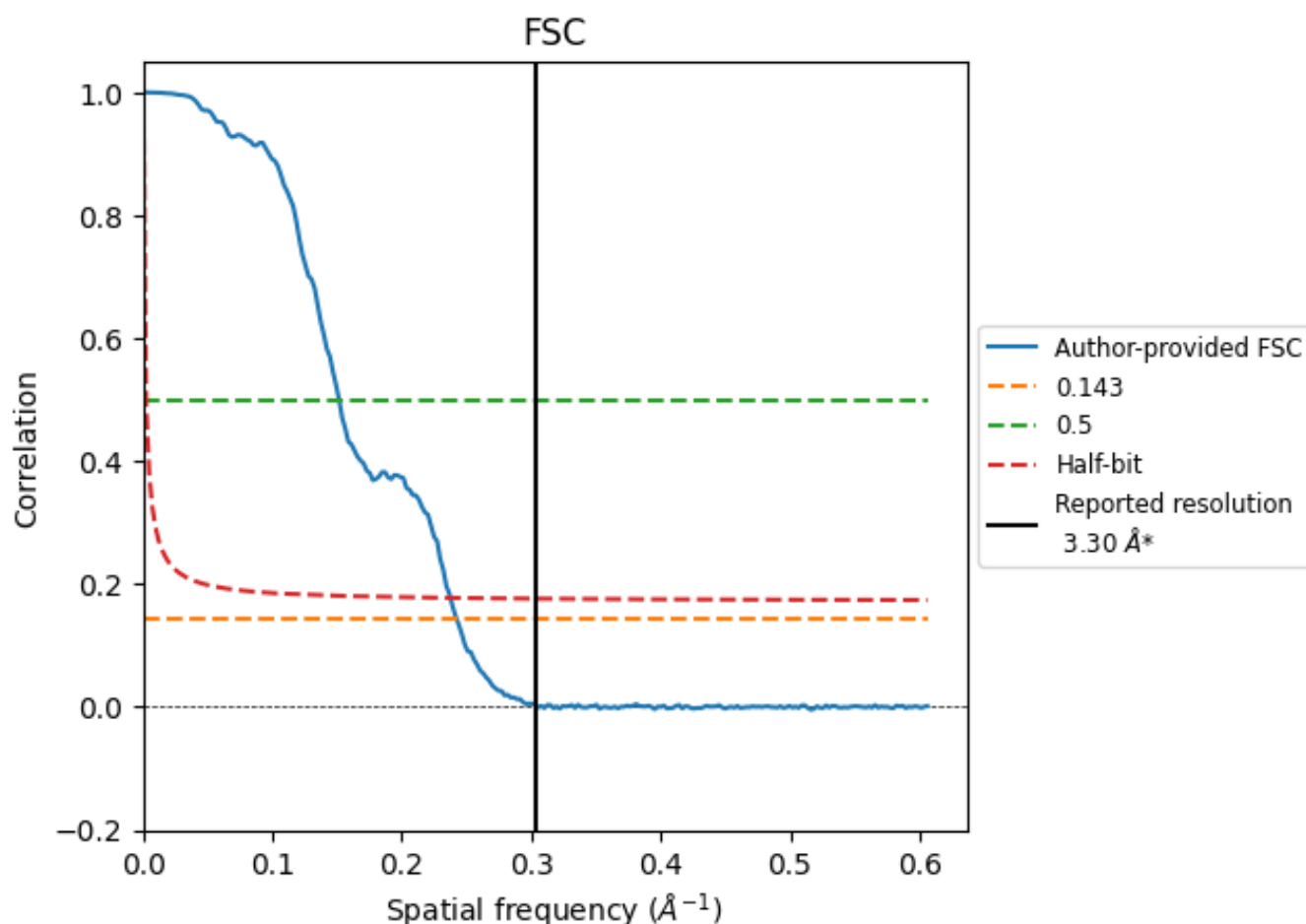


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

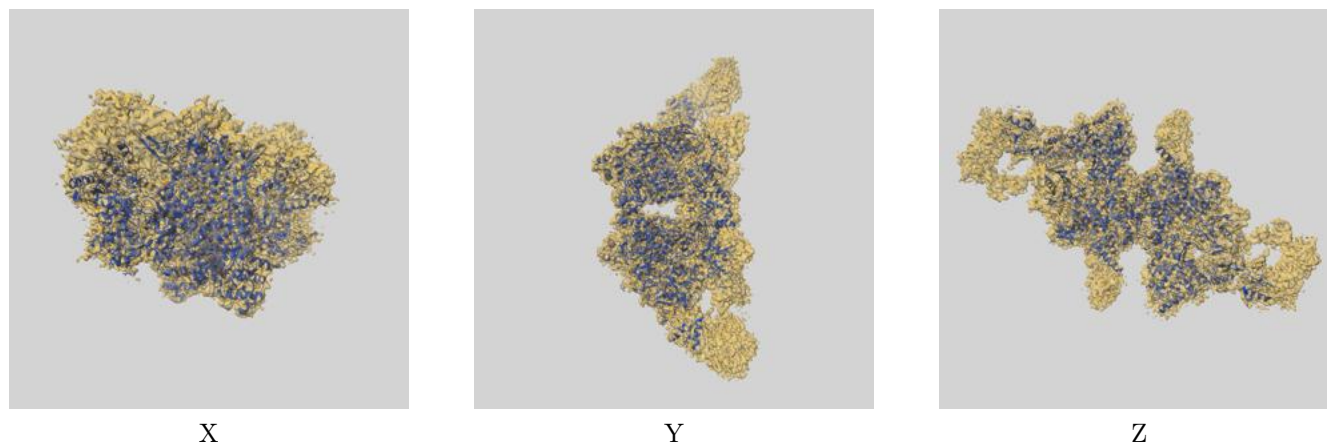
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	4.13	6.61	4.21
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.13 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14145 and PDB model 7QTQ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



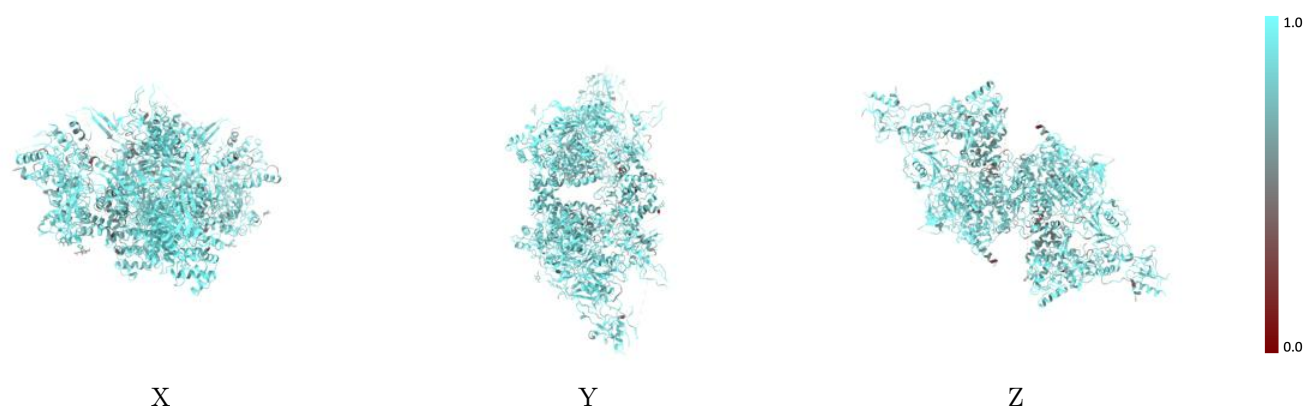
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



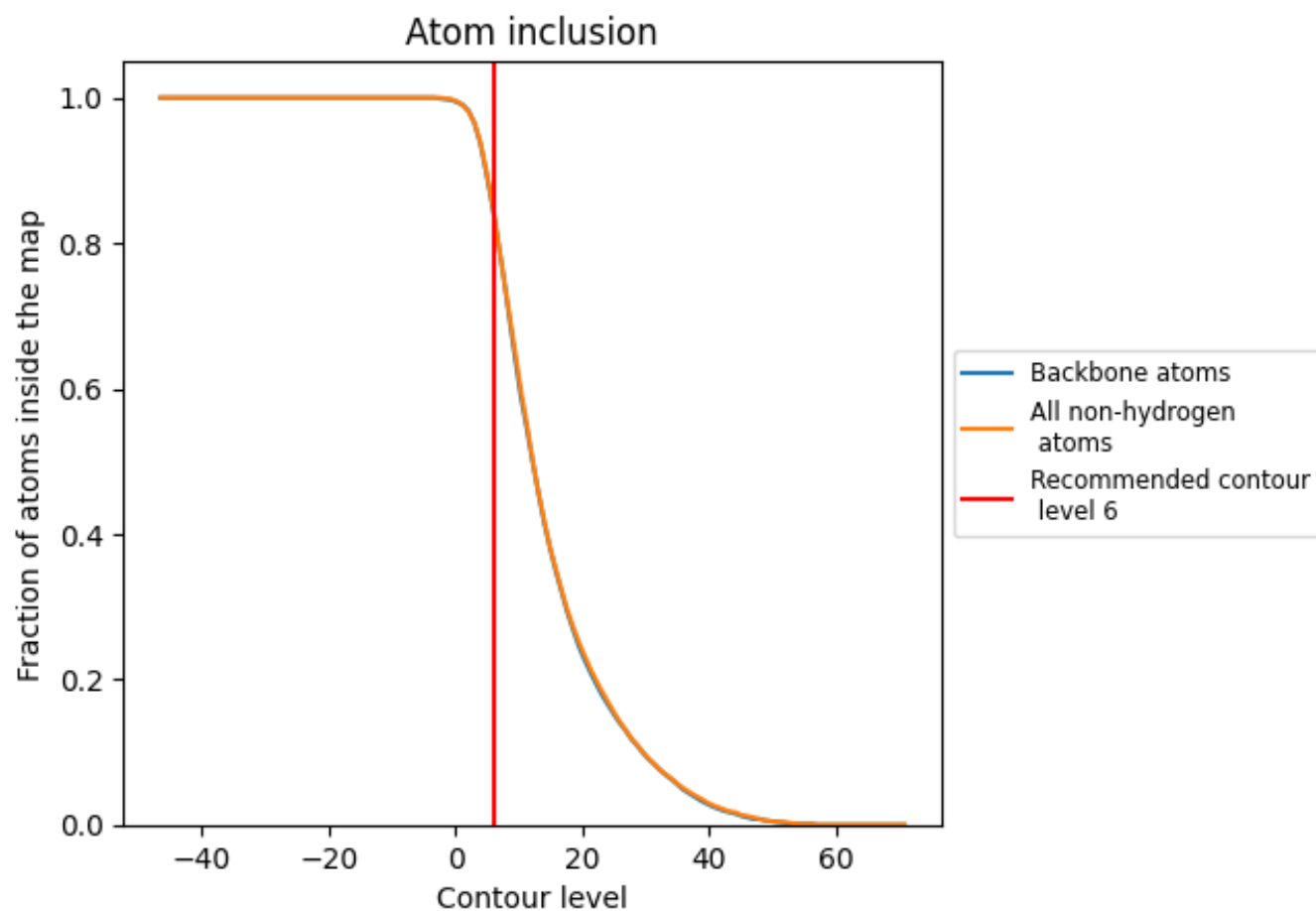
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 85% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.5020
A	0.8600	0.5010
B	0.8550	0.5020
C	0.7440	0.4780
D	0.7140	0.4670
E	0.8210	0.5330
F	0.6070	0.4400

1.0

0.0

<0.0