



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 12:18 PM UTC

PDB ID : 7W7G / pdb_00007w7g
EMDB ID : EMD-32344
Title : Structure of Mammalian NALCN-FAM155A-UNC79-UNC80 quaternary complex
Authors : Chen, L.; Kang, Y.
Deposited on : 2021-12-04
Resolution : 3.20 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:

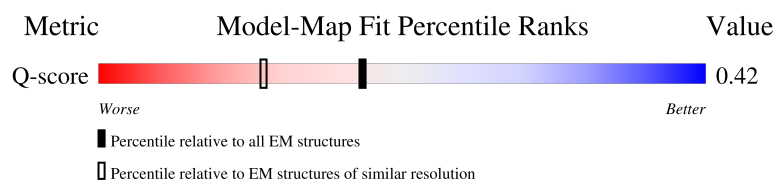
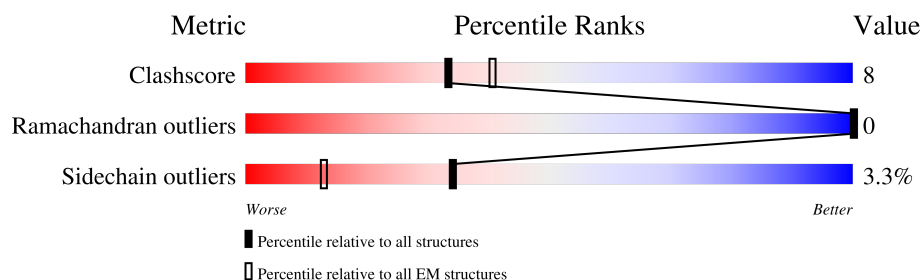
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.20 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	15020 (2.70 - 3.70)

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	2654	11% 43% 13% 42%
2	B	3326	6% 39% 12% 49%
3	C	1738	15% 63% 14% 23%
4	D	467	9% 28% 8% 63%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 38143 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein unc-79 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1528	Total	C	N	O	S	0	0
			12097	7833	1998	2161	105		

- Molecule 2 is a protein called Protein unc-80 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1711	Total	C	N	O	S	0	0
			13777	8900	2351	2430	96		

- Molecule 3 is a protein called Sodium leak channel non-selective protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1346	Total	C	N	O	S	0	0
			10847	7164	1777	1821	85		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	SER	PRO	conflict	UNP Q6Q760
C	748	ALA	THR	conflict	UNP Q6Q760

- Molecule 4 is a protein called Transmembrane protein FAM155A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	173	Total	C	N	O	S	0	0
			1378	875	212	275	16		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

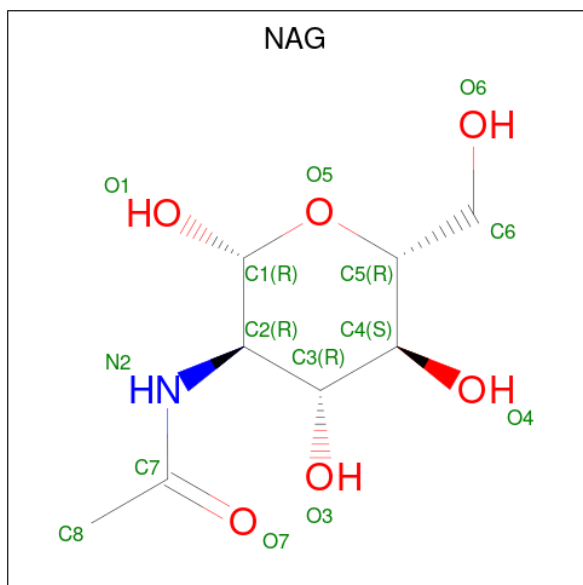
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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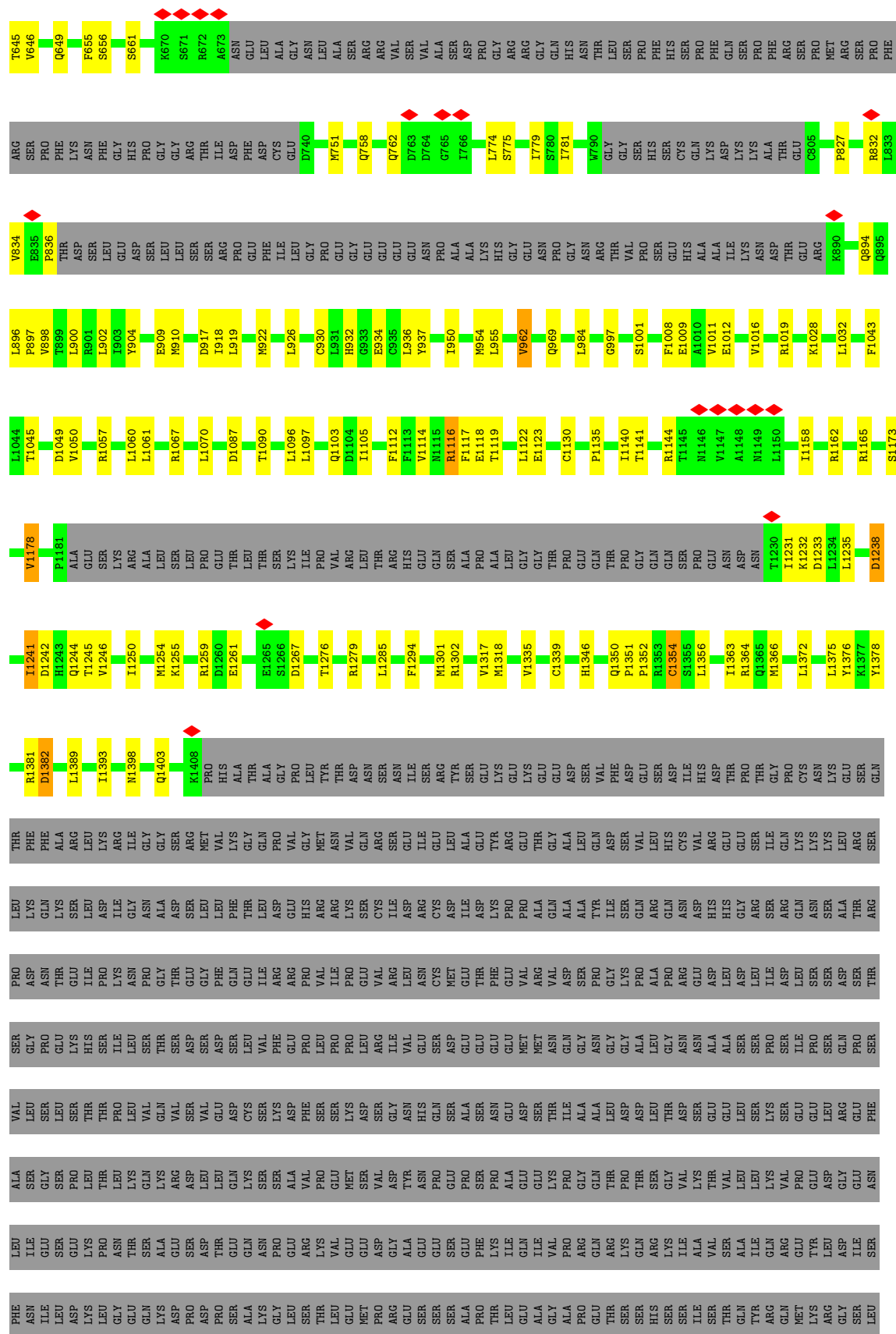
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Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



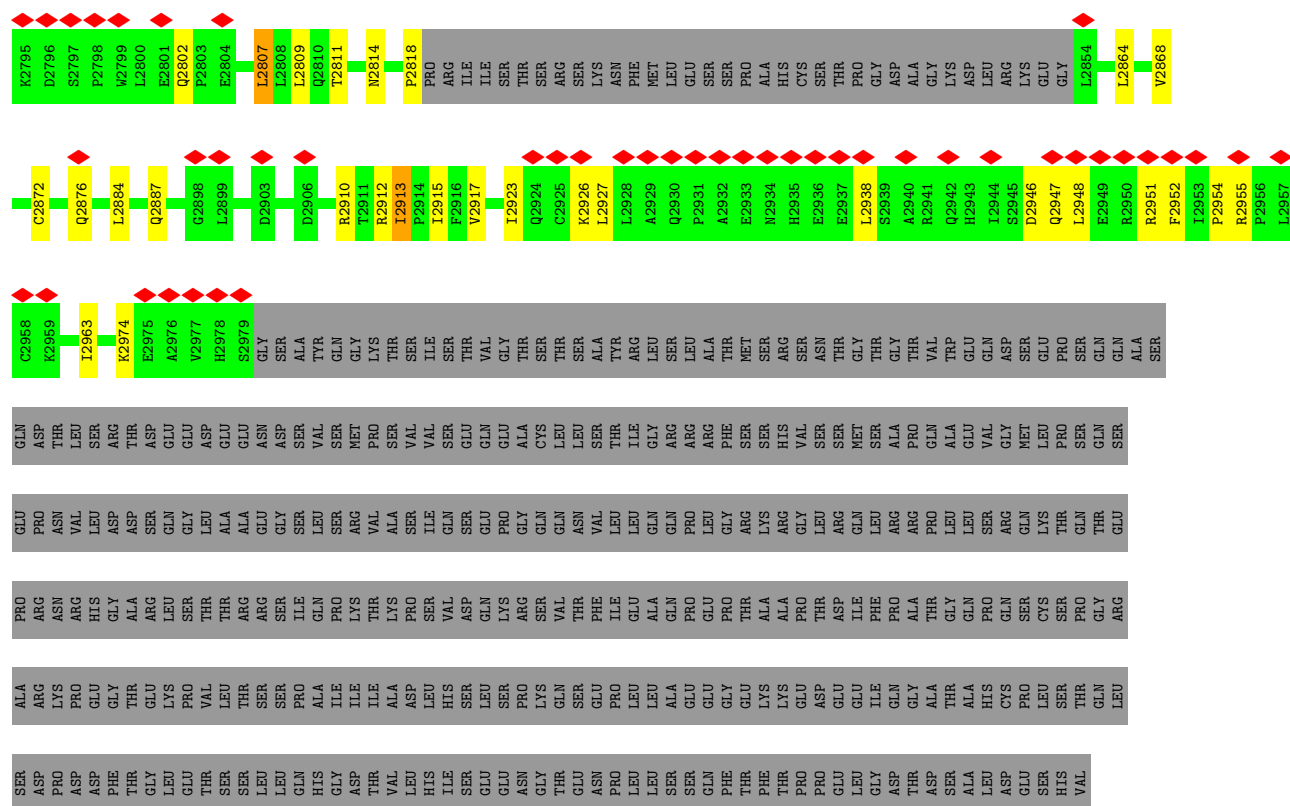
Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	



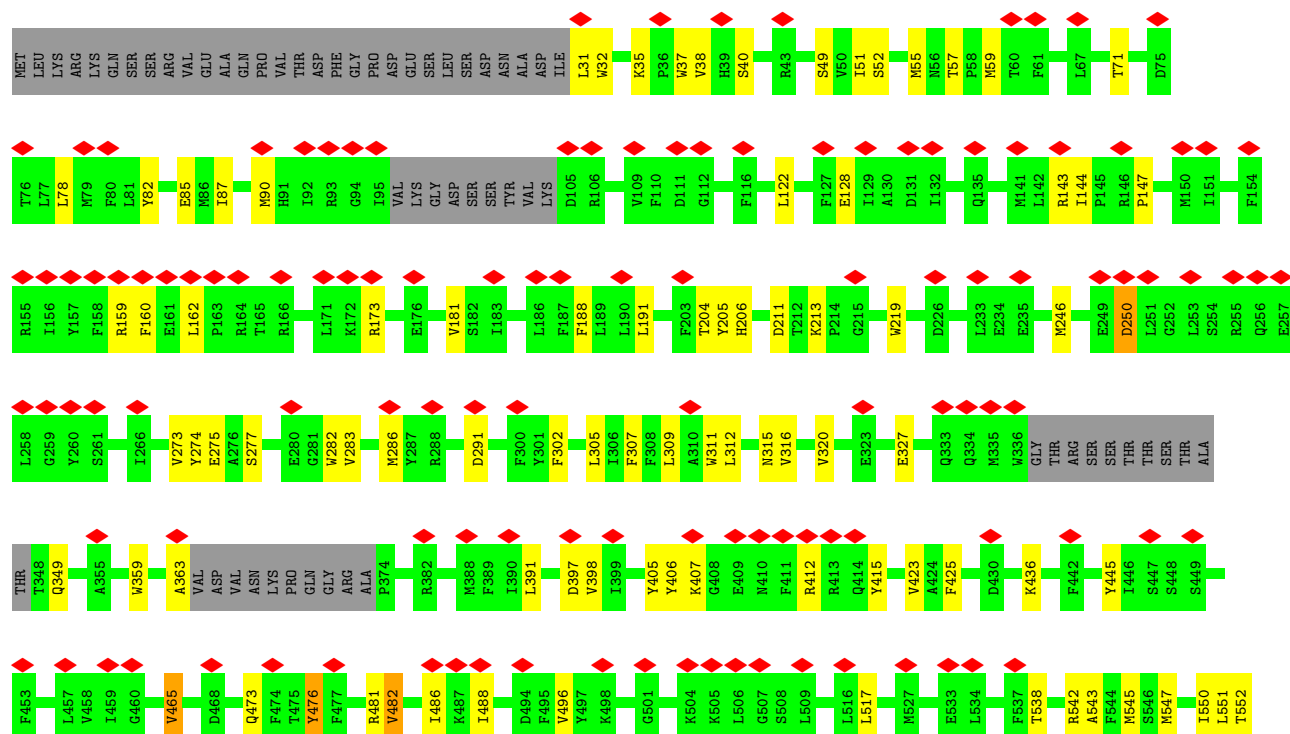




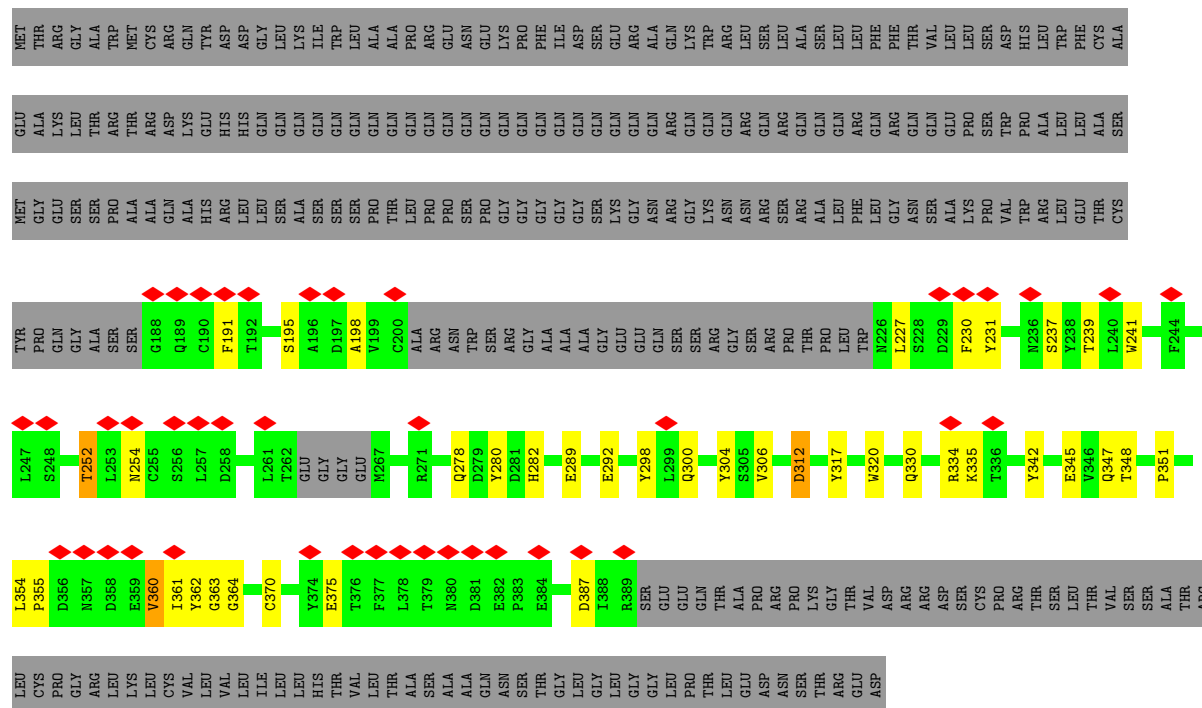




• Molecule 3: Sodium leak channel non-selective protein







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	275170	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	8.606	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.087	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.95	Depositor
Map size ($\text{\AA}$)	370.72, 370.72, 370.72	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.324, 1.324, 1.324	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: NAG, ZN

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	0.17	0/12360	0.27	0/16769
2	B	0.18	0/14084	0.29	0/19082
3	C	0.11	0/11121	0.23	0/15080
4	D	0.10	0/1410	0.21	0/1913
All	All	0.16	0/38975	0.27	0/52844

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12097	0	12285	244	0
2	B	13777	0	14013	252	0
3	C	10847	0	10959	149	0
4	D	1378	0	1253	23	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	C	42	0	39	1	0
All	All	38143	0	38549	633	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 8.

All (633) 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)
2:B:1545:HIS:HE1	2:B:1553:CYS:SG	1.88	0.97
2:B:2421:VAL:HG22	3:C:663:MET:HE1	1.64	0.79
1:A:1162:ARG:HE	1:A:1231:ILE:HG23	1.49	0.77
3:C:173:ARG:HH21	3:C:327:GLU:HB2	1.54	0.73
2:B:1214:ALA:O	2:B:1219:ARG:NH1	2.22	0.72
3:C:205:TYR:HA	3:C:246:MET:O	1.90	0.71
2:B:1224:LEU:HB3	2:B:1626:MET:HE1	1.70	0.71
1:A:218:PRO:HG3	1:A:447:LEU:HD21	1.73	0.70
2:B:2314:SER:HA	3:C:709:LYS:HE2	1.73	0.70
2:B:1732:GLU:HG2	2:B:1734:GLY:H	1.56	0.70
2:B:38:LEU:HB2	2:B:98:LYS:HE3	1.73	0.70
2:B:1926:MET:HE1	2:B:1985:ILE:HG13	1.74	0.69
3:C:398:VAL:HG11	3:C:482:VAL:HG12	1.75	0.69
2:B:2238:GLU:OE2	2:B:2284:ASN:ND2	2.26	0.69
1:A:2344:VAL:HG21	1:A:2391:GLU:HG3	1.73	0.69
3:C:613:GLN:HB3	3:C:1550:LEU:HD21	1.73	0.69
1:A:656:SER:HB3	1:A:781:ILE:HD11	1.75	0.68
1:A:646:VAL:O	1:A:762:GLN:NE2	2.26	0.68
1:A:2258:VAL:HG12	1:A:2306:PHE:HD1	1.56	0.68
1:A:1067:ARG:HG3	1:A:1105:ILE:HG22	1.76	0.67
2:B:2569:THR:HG22	2:B:2635:MET:HB2	1.76	0.67
1:A:2512:THR:HG1	1:A:2521:SER:N	1.92	0.67
2:B:360:LEU:HD12	2:B:680:ILE:HD11	1.76	0.67
1:A:1165:ARG:NH2	1:A:1242:ASP:OD1	2.28	0.67
1:A:1244:GLN:NE2	2:B:1930:GLU:OE1	2.28	0.67
1:A:225:PHE:O	1:A:232:LYS:NZ	2.28	0.66
2:B:2910:ARG:HB3	2:B:2955:ARG:HD3	1.78	0.66
3:C:188:PHE:HB3	3:C:309:LEU:HD21	1.76	0.66
2:B:849:MET:HG3	2:B:907:MET:HE3	1.77	0.66
1:A:834:VAL:HG11	1:A:1032:LEU:HD11	1.77	0.65
2:B:2554:ARG:NH1	2:B:2619:ASP:OD1	2.29	0.65
1:A:233:PRO:HD3	1:A:457:SER:HB3	1.79	0.65
2:B:1746:ILE:HD13	2:B:1959:ARG:HH22	1.62	0.64
2:B:1826:PRO:HB2	2:B:1829:GLN:HB2	1.78	0.64
3:C:906:GLU:HG2	3:C:918:LEU:HD13	1.77	0.64
3:C:1024:LEU:HD21	3:C:1147:GLY:HA3	1.78	0.64
3:C:1054:ARG:NH2	4:D:375:GLU:OE1	2.30	0.64
2:B:669:ILE:HA	2:B:673:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1508:ASP:HB3	3:C:1511:LEU:HB3	1.79	0.64
3:C:1401:GLN:NE2	3:C:1418:GLY:O	2.31	0.64
1:A:2119:GLN:OE1	1:A:2157:LYS:NZ	2.32	0.63
2:B:97:ASN:HA	2:B:102:GLN:HE21	1.62	0.63
2:B:99:LEU:HD12	2:B:101:HIS:H	1.63	0.63
1:A:393:VAL:HG13	1:A:473:LEU:HD23	1.79	0.63
2:B:2432:LEU:HD13	2:B:2559:ARG:HG2	1.80	0.63
2:B:2453:THR:HG21	2:B:2465:GLU:HB2	1.80	0.63
1:A:110:LEU:HD23	1:A:147:SER:HB3	1.81	0.63
2:B:1721:TRP:O	2:B:1724:ARG:NH1	2.32	0.63
3:C:406:TYR:HB2	3:C:1040:ALA:HB1	1.80	0.63
1:A:2530:GLU:OE2	2:B:35:ARG:NH1	2.31	0.62
2:B:2045:MET:HE3	2:B:2054:LEU:HD11	1.80	0.62
3:C:908:PRO:O	3:C:911:ARG:NH1	2.32	0.62
1:A:934:GLU:HB3	1:A:937:TYR:HB2	1.81	0.62
2:B:2295:LEU:O	3:C:665:GLN:NE2	2.31	0.62
2:B:1969:ASN:OD1	2:B:1971:GLN:NE2	2.33	0.62
1:A:1141:THR:O	1:A:1144:ARG:NH2	2.31	0.62
2:B:2105:GLN:HB3	2:B:2108:HIS:HB2	1.82	0.62
3:C:397:ASP:OD2	3:C:481:ARG:NH2	2.33	0.62
2:B:1344:MET:HB3	2:B:1637:LEU:HB3	1.81	0.61
2:B:1710:ARG:NH1	2:B:1928:ASP:OD2	2.33	0.61
3:C:52:SER:HG	3:C:71:THR:HG1	1.48	0.61
1:A:1070:LEU:HB3	1:A:1105:ILE:HD13	1.81	0.61
1:A:1259:ARG:HH21	2:B:1987:ASP:HB2	1.65	0.61
2:B:951:ARG:HD2	2:B:1028:ARG:HD3	1.81	0.61
1:A:175:MET:HE3	2:B:2917:VAL:HG21	1.82	0.61
1:A:445:ARG:HH12	1:A:490:ASP:HB3	1.64	0.61
4:D:237:SER:O	4:D:330:GLN:NE2	2.34	0.61
2:B:1634:VAL:C	2:B:1636:SER:H	2.09	0.60
1:A:2233:ARG:HH21	1:A:2272:ARG:HH22	1.47	0.60
1:A:2409:TRP:HA	1:A:2412:HIS:HB3	1.83	0.60
2:B:357:LEU:HA	2:B:680:ILE:HD13	1.82	0.60
1:A:555:LEU:HD13	1:A:598:MET:HG2	1.83	0.60
1:A:2243:LEU:HD12	1:A:2277:LEU:HD12	1.84	0.60
2:B:361:ARG:NH1	2:B:683:CYS:SG	2.74	0.60
3:C:1045:LYS:HE3	3:C:1127:ARG:HG2	1.84	0.60
2:B:1920:LEU:HD23	2:B:1977:MET:HG3	1.84	0.60
2:B:2453:THR:OG1	2:B:2578:ARG:NH2	2.35	0.60
3:C:1471:GLN:O	3:C:1475:ASN:ND2	2.31	0.60
3:C:1010:LEU:HD13	3:C:1441:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ARG:NH2	1:A:488:MET:SD	2.75	0.59
2:B:1724:ARG:NH2	2:B:1952:GLU:OE2	2.34	0.59
3:C:59:MET:HG3	3:C:538:THR:HB	1.83	0.59
1:A:2439:LEU:HD21	1:A:2634:GLN:HB2	1.84	0.59
1:A:133:PRO:HD2	1:A:136:LEU:HD12	1.84	0.59
1:A:2207:LEU:HD13	1:A:2213:LEU:HD12	1.84	0.59
2:B:2003:LEU:HD22	2:B:2022:THR:HG21	1.85	0.59
2:B:2202:PRO:O	2:B:2206:ILE:HB	2.03	0.59
1:A:394:GLU:HB2	2:B:2952:PHE:HZ	1.68	0.59
1:A:2541:GLN:O	1:A:2545:HIS:ND1	2.36	0.59
2:B:1667:LEU:HD13	2:B:1675:MET:HE1	1.84	0.59
4:D:335:LYS:HB2	4:D:387:ASP:HB3	1.85	0.58
2:B:2644:GLU:OE2	2:B:2647:ARG:NH1	2.37	0.58
3:C:283:VAL:HG13	3:C:1384:ARG:HD2	1.84	0.58
1:A:397:ILE:HG23	1:A:476:MET:HG3	1.86	0.58
2:B:1803:LEU:HD13	2:B:1806:LEU:HD12	1.84	0.58
3:C:1477:VAL:O	3:C:1489:ARG:NH2	2.36	0.58
1:A:1352:PRO:O	1:A:1398:ASN:ND2	2.37	0.58
1:A:624:TYR:O	1:A:629:GLN:NE2	2.37	0.58
3:C:412:ARG:NH2	3:C:415:TYR:O	2.37	0.58
3:C:1539:TYR:HE1	3:C:1548:LEU:HD21	1.68	0.58
4:D:278:GLN:O	4:D:282:HIS:ND1	2.37	0.58
3:C:998:LYS:O	3:C:1004:ARG:NH1	2.37	0.58
3:C:1186:GLN:O	3:C:1471:GLN:NE2	2.36	0.58
1:A:2469:HIS:O	1:A:2472:VAL:HG22	2.04	0.57
3:C:312:LEU:HD22	3:C:1446:ILE:HD11	1.86	0.57
1:A:2396:ASN:ND2	1:A:2457:PRO:O	2.37	0.57
2:B:1178:LEU:HD21	2:B:1326:LEU:HD22	1.86	0.57
1:A:2065:LEU:HA	1:A:2068:MET:HE2	1.85	0.57
2:B:2809:LEU:HD11	2:B:2884:LEU:HD21	1.85	0.57
3:C:1357:PHE:HB2	3:C:1372:PHE:HD2	1.69	0.57
1:A:617:ILE:HG12	1:A:635:TRP:HE1	1.70	0.57
1:A:184:PRO:HA	1:A:187:HIS:CE1	2.39	0.57
2:B:2334:ARG:HH11	2:B:2397:SER:HB3	1.70	0.57
2:B:2791:GLY:HA3	2:B:2872:CYS:HB3	1.84	0.57
3:C:585:PHE:O	3:C:589:ILE:HB	2.04	0.57
2:B:2109:TYR:HB3	2:B:2142:LEU:HD22	1.87	0.57
1:A:1376:TYR:OH	2:B:1763:PHE:O	2.20	0.57
1:A:2223:LEU:HD13	1:A:2235:LEU:HD21	1.86	0.57
1:A:2564:LEU:HB3	1:A:2572:PHE:HB2	1.86	0.57
2:B:2001:VAL:HG11	2:B:2045:MET:HE1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2348:LEU:HD22	1:A:2433:LEU:HD11	1.85	0.57
3:C:311:TRP:O	3:C:315:ASN:ND2	2.38	0.57
2:B:2234:ILE:HG22	2:B:2281:THR:HG21	1.86	0.56
3:C:1287:TRP:NE1	3:C:1299:THR:O	2.38	0.56
2:B:1561:CYS:HB3	2:B:1637:LEU:HB2	1.87	0.56
1:A:576:LEU:HB3	1:A:635:TRP:HB2	1.88	0.56
1:A:2574:LYS:HE2	2:B:191:LEU:HD11	1.86	0.56
2:B:1525:ASN:O	2:B:1525:ASN:ND2	2.39	0.56
2:B:2555:GLU:HG2	2:B:2558:ARG:HH22	1.70	0.56
3:C:181:VAL:HG21	3:C:320:VAL:HG21	1.87	0.56
3:C:552:THR:HG22	3:C:1145:MET:HE1	1.88	0.56
2:B:1320:ASP:O	2:B:1563:ARG:NH1	2.35	0.56
1:A:2431:ILE:HD11	1:A:2469:HIS:HB3	1.88	0.56
1:A:775:SER:O	1:A:779:ILE:HG12	2.06	0.56
1:A:2379:HIS:ND1	1:A:2634:GLN:OE1	2.30	0.56
2:B:359:ARG:O	2:B:362:HIS:ND1	2.38	0.56
2:B:1919:VAL:HB	2:B:1961:PHE:HZ	1.71	0.56
1:A:1119:THR:O	1:A:1123:GLU:HG2	2.06	0.55
2:B:2089:GLU:HB2	2:B:2122:ASN:HB3	1.88	0.55
2:B:2778:MET:HE1	2:B:2811:THR:HG21	1.88	0.55
2:B:2270:GLU:HG2	2:B:2315:ASN:HD22	1.72	0.55
2:B:2946:ASP:HB3	2:B:2951:ARG:HH21	1.70	0.55
1:A:1250:ILE:O	1:A:1254:MET:HG2	2.07	0.55
3:C:275:GLU:HG3	3:C:557:VAL:HG21	1.89	0.55
2:B:2415:ILE:HG23	2:B:2438:LEU:HD21	1.89	0.55
1:A:181:THR:HB	1:A:186:TYR:HD2	1.72	0.55
1:A:2487:HIS:O	1:A:2490:SER:OG	2.24	0.55
2:B:1231:HIS:HE1	2:B:1235:ARG:HE	1.55	0.55
3:C:958:ASP:OD2	3:C:995:ARG:NH2	2.37	0.55
1:A:490:ASP:O	1:A:494:SER:N	2.31	0.55
1:A:1135:PRO:HB2	1:A:1246:VAL:HG21	1.87	0.55
1:A:88:VAL:HG13	1:A:89:PRO:HD3	1.89	0.54
1:A:1302:ARG:NH1	1:A:1339:CYS:O	2.36	0.54
1:A:2403:VAL:HG13	1:A:2410:LEU:HD23	1.88	0.54
3:C:1478:ASP:O	3:C:1481:ARG:NH2	2.39	0.54
1:A:617:ILE:HG21	1:A:636:LEU:HD22	1.89	0.54
2:B:2313:GLU:HG2	3:C:709:LYS:HE3	1.89	0.54
2:B:1201:PRO:HG2	2:B:1206:LEU:HD13	1.88	0.54
3:C:274:TYR:OH	3:C:583:HIS:ND1	2.33	0.54
3:C:391:LEU:HD13	3:C:488:ILE:HG22	1.88	0.54
1:A:1130:CYS:HB3	1:A:1232:LYS:HE2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:665:LEU:HD22	2:B:795:MET:HG3	1.89	0.54
3:C:128:GLU:OE2	3:C:143:ARG:NH2	2.40	0.54
1:A:779:ILE:HG23	1:A:902:LEU:HD22	1.90	0.54
1:A:2174:ALA:O	1:A:2178:GLU:HG2	2.08	0.54
2:B:2477:GLN:HE21	2:B:2597:LEU:H	1.55	0.54
1:A:551:LEU:HB3	1:A:594:VAL:HG11	1.90	0.54
1:A:2574:LYS:HE3	2:B:87:HIS:CE1	2.43	0.54
2:B:2008:VAL:HG21	2:B:2053:LYS:HG3	1.90	0.54
2:B:2781:ASN:OD1	2:B:2974:LYS:NZ	2.35	0.54
3:C:159:ARG:NH1	3:C:162:LEU:O	2.41	0.54
3:C:473:GLN:O	3:C:476:TYR:HB2	2.08	0.54
1:A:39:LEU:HD12	1:A:105:THR:HG21	1.90	0.54
1:A:2526:LEU:HB3	2:B:36:PRO:HB3	1.89	0.54
2:B:2763:SER:HB3	2:B:2807:LEU:HD23	1.88	0.54
1:A:2574:LYS:HZ3	2:B:187:LEU:HD11	1.73	0.53
3:C:1548:LEU:HD23	3:C:1552:GLU:HG2	1.90	0.53
1:A:1114:VAL:O	1:A:1118:GLU:HG2	2.08	0.53
1:A:1285:LEU:HD13	1:A:1335:VAL:HG21	1.89	0.53
1:A:1238:ASP:HB2	1:A:1241:ILE:HG12	1.90	0.53
2:B:1332:ASN:HB3	2:B:1333:PRO:HD3	1.90	0.53
2:B:2313:GLU:HA	2:B:2319:ARG:HD2	1.89	0.53
1:A:43:SER:HB2	1:A:105:THR:HG22	1.91	0.53
2:B:1721:TRP:NE1	2:B:1952:GLU:OE1	2.35	0.53
3:C:305:LEU:HG	3:C:309:LEU:HD12	1.90	0.53
1:A:758:GLN:HE21	1:A:762:GLN:HE21	1.57	0.53
3:C:1464:TYR:OH	3:C:1468:ARG:NH2	2.42	0.53
3:C:1367:ASN:O	3:C:1371:ASN:ND2	2.40	0.53
2:B:2179:ILE:HG13	2:B:2187:HIS:CD2	2.43	0.53
1:A:521:MET:HE2	1:A:526:LYS:HE3	1.90	0.53
1:A:1267:ASP:N	1:A:1267:ASP:OD1	2.41	0.53
1:A:497:GLU:OE2	1:A:560:TYR:OH	2.27	0.53
3:C:903:MET:HE1	3:C:990:CYS:HA	1.89	0.53
1:A:836:PRO:HB3	1:A:1028:LYS:HB3	1.91	0.52
3:C:564:LEU:HD21	3:C:576:ALA:HB2	1.90	0.52
4:D:312:ASP:OD1	4:D:312:ASP:N	2.42	0.52
1:A:2265:TYR:O	1:A:2274:LYS:NZ	2.37	0.52
3:C:1259:LYS:HE3	3:C:1268:PHE:HE1	1.73	0.52
1:A:1356:LEU:O	1:A:1364:ARG:NE	2.42	0.52
1:A:1375:LEU:HD21	1:A:1389:LEU:HD21	1.90	0.52
2:B:2588:GLU:HG3	2:B:2590:ARG:H	1.74	0.52
2:B:332:ASP:O	2:B:356:TYR:OH	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2947:GLN:HA	2:B:2951:ARG:HD2	1.92	0.52
1:A:496:VAL:HG13	1:A:500:LYS:HD3	1.91	0.52
2:B:2297:GLY:HA2	2:B:2300:TRP:HD1	1.74	0.52
3:C:144:ILE:O	3:C:147:PRO:HD2	2.10	0.52
2:B:189:VAL:HG11	2:B:335:VAL:HA	1.92	0.52
1:A:85:LEU:HD13	1:A:128:THR:HG22	1.92	0.52
1:A:997:GLY:O	1:A:1001:SER:OG	2.28	0.52
2:B:1732:GLU:HB3	2:B:1735:ALA:HB2	1.91	0.52
2:B:1961:PHE:HB3	2:B:1974:LEU:HD13	1.91	0.52
2:B:336:LEU:HD12	2:B:339:LEU:HD12	1.91	0.52
2:B:1711:LEU:HD21	2:B:1941:VAL:HG21	1.91	0.52
2:B:2021:ALA:O	2:B:2024:THR:OG1	2.28	0.52
1:A:636:LEU:HD11	1:A:646:VAL:HG21	1.91	0.51
2:B:2366:GLN:NE2	2:B:2370:ASP:OD1	2.43	0.51
4:D:227:LEU:HA	4:D:230:PHE:HE2	1.75	0.51
1:A:2577:PRO:HG2	2:B:187:LEU:HD22	1.93	0.51
2:B:1543:CYS:SG	2:B:1550:HIS:ND1	2.83	0.51
1:A:1381:ARG:NH2	1:A:2058:ASP:OD1	2.42	0.51
2:B:1757:MET:HG2	2:B:2035:GLY:HA3	1.91	0.51
3:C:273:VAL:HG13	3:C:305:LEU:HD11	1.93	0.51
3:C:945:THR:HB	3:C:948:ALA:HB2	1.92	0.51
1:A:2543:MET:SD	1:A:2586:ASN:ND2	2.83	0.51
1:A:918:ILE:O	1:A:922:MET:HG3	2.10	0.51
1:A:1363:ILE:HA	1:A:1366:MET:HE2	1.93	0.51
2:B:2409:PHE:CZ	2:B:2414:ALA:HB2	2.46	0.51
3:C:1522:LEU:HD23	3:C:1532:ASP:HB3	1.93	0.51
1:A:116:ASP:OD1	1:A:116:ASP:N	2.43	0.51
1:A:2594:LEU:H	1:A:2594:LEU:HD12	1.76	0.51
1:A:517:ASP:N	1:A:517:ASP:OD1	2.41	0.51
1:A:1382:ASP:N	1:A:1382:ASP:OD1	2.44	0.51
1:A:2468:ASP:O	1:A:2471:ILE:HG12	2.10	0.51
1:A:2533:SER:HB3	2:B:34:LEU:HD12	1.91	0.51
2:B:1646:ILE:HG22	2:B:1731:MET:HA	1.92	0.51
2:B:2293:PHE:HA	2:B:2296:SER:O	2.11	0.51
1:A:2049:LEU:HD13	1:A:2067:ILE:HG23	1.93	0.50
1:A:2526:LEU:HD23	2:B:36:PRO:HA	1.92	0.50
3:C:1081:LYS:NZ	6:C:2002:NAG:O5	2.38	0.50
1:A:1049:ASP:OD1	1:A:1050:VAL:N	2.44	0.50
2:B:2334:ARG:HH22	2:B:2407:LEU:HD13	1.75	0.50
1:A:1259:ARG:NH2	2:B:1987:ASP:HB2	2.25	0.50
1:A:2389:ALA:O	1:A:2393:SER:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1681:ALA:HA	2:B:1727:VAL:HG22	1.94	0.50
2:B:2596:LEU:H	2:B:2596:LEU:HD23	1.77	0.50
2:B:1811:GLU:OE2	2:B:1814:ARG:NH2	2.44	0.50
3:C:612:LYS:HZ1	3:C:1167:LEU:HB3	1.76	0.50
2:B:677:ALA:HB1	2:B:795:MET:HE3	1.93	0.50
2:B:53:LEU:O	2:B:74:ARG:NH2	2.42	0.50
2:B:841:ASP:HB3	2:B:844:GLN:HB2	1.94	0.50
4:D:227:LEU:HB2	4:D:241:TRP:HE3	1.77	0.50
1:A:2247:ILE:HD13	1:A:2303:LEU:HD21	1.93	0.50
3:C:204:THR:O	3:C:206:HIS:ND1	2.40	0.50
4:D:360:VAL:HG13	4:D:362:TYR:HE1	1.77	0.50
2:B:2145:MET:HE1	2:B:2153:LEU:HD12	1.94	0.50
3:C:644:VAL:HG21	3:C:663:MET:HG3	1.94	0.50
3:C:1223:GLN:OE1	3:C:1310:ARG:NH1	2.45	0.50
1:A:1011:VAL:HG12	1:A:1061:LEU:HD12	1.93	0.49
2:B:216:GLN:HA	2:B:219:TRP:CE3	2.47	0.49
1:A:556:CYS:O	1:A:559:PRO:HD2	2.12	0.49
1:A:2213:LEU:HD21	1:A:2246:VAL:HG13	1.93	0.49
2:B:218:MET:O	2:B:351:TRP:NE1	2.35	0.49
2:B:2313:GLU:HA	2:B:2319:ARG:HH11	1.78	0.49
2:B:2664:ILE:HG12	2:B:2671:ARG:HG3	1.95	0.49
2:B:1985:ILE:HG22	2:B:1987:ASP:H	1.76	0.49
3:C:1485:ILE:HB	3:C:1489:ARG:HB2	1.95	0.49
1:A:2237:GLU:HB3	1:A:2238:PRO:HD3	1.94	0.49
3:C:1473:ILE:HG21	3:C:1497:LEU:HD23	1.95	0.49
1:A:2495:PHE:CG	1:A:2556:HIS:HB3	2.47	0.49
1:A:2558:ILE:O	1:A:2561:MET:HG2	2.13	0.49
2:B:2417:LEU:O	2:B:2421:VAL:HG23	2.12	0.49
2:B:2045:MET:HB3	2:B:2051:GLU:HA	1.93	0.49
3:C:32:TRP:O	3:C:35:LYS:NZ	2.40	0.49
3:C:486:ILE:HD11	3:C:496:VAL:HG21	1.95	0.49
3:C:1253:VAL:HG22	3:C:1281:THR:HB	1.95	0.49
1:A:2275:PHE:HB2	1:A:2278:SER:HB3	1.94	0.49
2:B:2308:VAL:HG12	2:B:2318:LEU:HD21	1.93	0.49
2:B:2802:GLN:NE2	2:B:2876:GLN:O	2.38	0.49
3:C:922:GLU:OE1	3:C:992:ARG:NH1	2.36	0.49
3:C:937:ILE:HG12	3:C:942:LEU:HD13	1.94	0.48
1:A:629:GLN:NE2	1:A:661:SER:OG	2.46	0.48
1:A:2557:VAL:O	1:A:2560:LEU:HB3	2.13	0.48
2:B:2187:HIS:HA	2:B:2190:MET:HE3	1.94	0.48
3:C:405:TYR:CZ	3:C:407:LYS:HE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1273:ARG:H	3:C:1273:ARG:HE	1.61	0.48
2:B:1926:MET:SD	2:B:1946:LEU:HD12	2.53	0.48
2:B:2109:TYR:CE2	2:B:2144:HIS:HB2	2.48	0.48
2:B:2487:THR:O	2:B:2611:SER:OG	2.30	0.48
3:C:159:ARG:NH1	3:C:160:PHE:O	2.45	0.48
3:C:307:PHE:HE2	3:C:1332:MET:HE2	1.78	0.48
1:A:1060:LEU:HD21	2:B:2170:LEU:HD11	1.95	0.48
2:B:2068:VAL:HG22	2:B:2140:LEU:HB2	1.94	0.48
1:A:910:MET:HG3	1:A:919:LEU:HD22	1.95	0.48
1:A:2064:LEU:HD21	1:A:2108:LEU:HD13	1.96	0.48
2:B:2372:LEU:HG	2:B:2409:PHE:HE2	1.79	0.48
1:A:2546:ASN:HB3	1:A:2549:MET:HG2	1.95	0.48
2:B:1185:MET:HE3	2:B:1221:ALA:HB3	1.95	0.48
3:C:211:ASP:OD1	3:C:211:ASP:N	2.42	0.48
3:C:517:LEU:HD21	3:C:551:LEU:HD22	1.96	0.48
2:B:1228:ARG:HD2	2:B:1626:MET:SD	2.53	0.48
2:B:2633:MET:SD	2:B:2681:SER:OG	2.64	0.48
1:A:897:PRO:HG2	1:A:900:LEU:HD13	1.96	0.47
3:C:49:SER:HB2	3:C:78:LEU:HD13	1.96	0.47
1:A:2384:LEU:O	1:A:2387:ILE:HG12	2.13	0.47
2:B:2562:GLU:HG3	2:B:2627:GLY:HA3	1.96	0.47
3:C:82:TYR:HA	3:C:85:GLU:HG3	1.97	0.47
3:C:191:LEU:HB2	3:C:1311:PHE:HE2	1.79	0.47
2:B:2547:GLU:OE2	2:B:2551:ARG:NE	2.47	0.47
4:D:347:GLN:OE1	4:D:370:CYS:N	2.47	0.47
1:A:2246:VAL:HA	1:A:2250:ALA:HB3	1.97	0.47
3:C:1490:VAL:HG11	3:C:1519:MET:HG3	1.96	0.47
2:B:2573:LYS:HD3	2:B:2634:GLU:HB3	1.96	0.47
2:B:2788:LEU:O	2:B:2792:SER:OG	2.23	0.47
3:C:1146:ILE:O	3:C:1150:LEU:N	2.40	0.47
1:A:2087:MET:HE3	1:A:2087:MET:HA	1.95	0.47
2:B:866:HIS:NE2	2:B:872:CYS:HB3	2.29	0.47
3:C:1047:ASN:OD1	3:C:1047:ASN:N	2.46	0.47
3:C:1484:VAL:HA	3:C:1528:VAL:O	2.15	0.47
2:B:2096:LEU:HD23	2:B:2142:LEU:HD11	1.97	0.47
3:C:87:ILE:HA	3:C:90:MET:HG2	1.96	0.47
3:C:979:GLU:N	3:C:983:GLN:OE1	2.42	0.47
3:C:1068:SER:OG	3:C:1070:ASN:OD1	2.31	0.47
3:C:1110:GLU:OE2	3:C:1396:HIS:NE2	2.47	0.47
1:A:2597:ARG:O	1:A:2601:ILE:HG12	2.15	0.47
2:B:1572:TYR:CZ	2:B:1626:MET:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2035:GLU:OE1	1:A:2037:TYR:OH	2.30	0.47
1:A:2058:ASP:OD1	1:A:2058:ASP:N	2.46	0.47
2:B:336:LEU:HB2	2:B:356:TYR:OH	2.14	0.47
2:B:1950:LEU:O	2:B:1954:PRO:HG3	2.15	0.47
3:C:312:LEU:O	3:C:316:VAL:HG23	2.14	0.47
2:B:2738:PRO:HB2	2:B:2740:PRO:HD2	1.97	0.46
1:A:1012:GLU:O	1:A:1016:VAL:HG23	2.15	0.46
2:B:2456:VAL:HG12	2:B:2457:GLU:H	1.80	0.46
1:A:452:ILE:HG13	1:A:500:LYS:HE3	1.98	0.46
1:A:2347:VAL:HG12	1:A:2351:MET:HE2	1.97	0.46
1:A:2396:ASN:O	1:A:2397:HIS:ND1	2.48	0.46
4:D:361:ILE:HG22	4:D:363:GLY:H	1.80	0.46
1:A:904:TYR:CD1	1:A:954:MET:HE1	2.50	0.46
1:A:2353:ASP:HB2	1:A:2356:THR:HG23	1.97	0.46
3:C:37:TRP:O	3:C:40:SER:OG	2.29	0.46
1:A:1165:ARG:HD3	1:A:1165:ARG:HA	1.68	0.46
2:B:96:ARG:NH2	2:B:102:GLN:O	2.49	0.46
2:B:2179:ILE:HG13	2:B:2187:HIS:HD2	1.80	0.46
2:B:2554:ARG:HD3	2:B:2619:ASP:OD2	2.15	0.46
3:C:642:GLN:HG2	3:C:660:GLU:HG3	1.96	0.46
1:A:211:TYR:OH	2:B:2912:ARG:NH1	2.48	0.46
1:A:1276:THR:HG23	1:A:1279:ARG:NH2	2.31	0.46
1:A:2491:LEU:HB3	1:A:2556:HIS:CD2	2.51	0.46
2:B:353:LEU:HD11	2:B:664:VAL:HG11	1.97	0.46
2:B:1316:LEU:HD23	2:B:1548:TYR:HD2	1.81	0.46
3:C:1258:MET:O	3:C:1261:ILE:HG13	2.15	0.46
4:D:342:TYR:O	4:D:345:GLU:HB2	2.16	0.46
2:B:2913:ILE:HG22	2:B:2915:ILE:HG12	1.97	0.46
3:C:1043:LEU:O	3:C:1127:ARG:NH1	2.40	0.46
2:B:2176:THR:HG22	2:B:2187:HIS:NE2	2.31	0.45
2:B:2657:LEU:HA	2:B:2660:MET:HG2	1.98	0.45
4:D:230:PHE:O	4:D:239:THR:HA	2.16	0.45
1:A:1375:LEU:HD11	1:A:1393:ILE:HD11	1.98	0.45
1:A:2468:ASP:O	1:A:2472:VAL:HG13	2.16	0.45
2:B:2626:ARG:CZ	2:B:2630:ARG:HH22	2.30	0.45
1:A:136:LEU:O	1:A:140:ILE:HG12	2.17	0.45
1:A:1158:ILE:HG22	1:A:1162:ARG:HH12	1.81	0.45
1:A:1318:MET:O	1:A:1378:TYR:OH	2.26	0.45
2:B:85:VAL:HG21	2:B:119:MET:SD	2.57	0.45
2:B:2230:LYS:O	2:B:2234:ILE:HG13	2.16	0.45
2:B:2306:LEU:HD21	2:B:2341:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2466:ILE:HD13	2:B:2591:VAL:HG11	1.97	0.45
4:D:354:LEU:HD12	4:D:355:PRO:HD2	1.98	0.45
1:A:2182:MET:O	1:A:2226:ILE:HA	2.16	0.45
1:A:2590:LEU:HD13	1:A:2594:LEU:HB2	1.98	0.45
2:B:690:VAL:HG23	2:B:788:ASN:HB2	1.99	0.45
2:B:1034:LYS:HD3	2:B:1212:LEU:HD23	1.98	0.45
2:B:2041:LEU:HD11	2:B:2171:PHE:HZ	1.82	0.45
2:B:2264:ALA:HB1	2:B:2274:LEU:HD11	1.98	0.45
1:A:456:VAL:HG21	1:A:503:PHE:HB3	1.99	0.45
2:B:2087:GLN:HA	2:B:2125:TYR:HA	1.99	0.45
3:C:1273:ARG:H	3:C:1273:ARG:NE	2.14	0.45
1:A:128:THR:HB	1:A:132:PHE:CE2	2.52	0.45
1:A:2310:ASP:OD2	1:A:2336:ALA:N	2.50	0.45
2:B:1962:LEU:HD13	2:B:1999:TYR:CD1	2.52	0.45
3:C:250:ASP:OD1	3:C:250:ASP:N	2.47	0.45
1:A:149:LEU:HB2	1:A:150:PRO:HD3	1.99	0.45
1:A:2463:GLY:O	1:A:2466:ILE:HG12	2.17	0.45
2:B:799:ILE:O	2:B:802:SER:OG	2.27	0.45
2:B:1340:PHE:CZ	2:B:1344:MET:HE3	2.52	0.45
2:B:2792:SER:HB3	2:B:2963:ILE:HG12	1.98	0.45
3:C:274:TYR:O	3:C:277:SER:OG	2.33	0.45
4:D:195:SER:HB2	4:D:198:ALA:HB2	1.97	0.45
1:A:1087:ASP:OD1	1:A:1173:SER:HB2	2.17	0.45
1:A:2354:MET:SD	1:A:2354:MET:N	2.74	0.45
1:A:2529:LEU:HD21	2:B:87:HIS:CE1	2.52	0.45
1:A:2552:MET:O	1:A:2555:LEU:HB2	2.16	0.45
2:B:1545:HIS:CE1	2:B:1555:LEU:HB2	2.52	0.45
3:C:1516:CYS:SG	3:C:1517:TYR:N	2.90	0.45
1:A:555:LEU:HD21	1:A:597:LYS:HD3	1.98	0.44
1:A:919:LEU:HD13	1:A:962:VAL:HG23	1.99	0.44
1:A:2144:ILE:HD13	1:A:2180:LEU:HD13	1.99	0.44
2:B:2952:PHE:HD2	2:B:2954:PRO:HD3	1.82	0.44
3:C:51:ILE:HG22	3:C:55:MET:HE2	1.99	0.44
3:C:958:ASP:OD2	3:C:998:LYS:NZ	2.44	0.44
1:A:461:PRO:HD3	1:A:507:TRP:HE1	1.82	0.44
1:A:464:ASN:OD1	1:A:464:ASN:N	2.51	0.44
2:B:2066:LEU:HA	2:B:2137:SER:HB2	1.99	0.44
3:C:594:PHE:HB3	3:C:1149:THR:HG21	2.00	0.44
1:A:138:LYS:NZ	1:A:142:GLU:OE2	2.36	0.44
1:A:168:LEU:HD12	1:A:168:LEU:H	1.82	0.44
2:B:93:LEU:HD11	2:B:113:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2339:LEU:HD12	3:C:662:PHE:HE2	1.81	0.44
2:B:2626:ARG:NH1	2:B:2630:ARG:HH22	2.16	0.44
4:D:304:TYR:CG	4:D:351:PRO:HB3	2.52	0.44
1:A:954:MET:HE3	1:A:954:MET:HB2	1.70	0.44
1:A:1103:GLN:NE2	1:A:1261:GLU:OE1	2.50	0.44
2:B:26:LEU:HB3	2:B:84:HIS:CD2	2.53	0.44
2:B:928:LEU:HD13	2:B:929:GLY:H	1.83	0.44
2:B:2335:LYS:HG3	2:B:2417:LEU:HD11	1.99	0.44
2:B:2453:THR:HG22	2:B:2461:ALA:HB1	2.00	0.44
3:C:665:GLN:O	3:C:669:ARG:HG2	2.17	0.44
1:A:80:THR:O	1:A:84:LEU:HG	2.17	0.44
1:A:2409:TRP:CZ3	1:A:2430:HIS:HB3	2.53	0.44
3:C:1311:PHE:O	3:C:1314:ILE:HG22	2.16	0.44
1:A:123:TYR:O	1:A:127:SER:N	2.49	0.44
1:A:2395:GLY:HA3	1:A:2402:ALA:HB2	1.99	0.44
1:A:110:LEU:HB3	1:A:111:PRO:HD3	2.00	0.44
1:A:779:ILE:HG22	1:A:898:VAL:HG12	2.00	0.44
1:A:1008:PHE:CZ	1:A:1057:ARG:HD2	2.53	0.44
1:A:1096:LEU:HD21	1:A:1255:LYS:HD2	1.99	0.44
2:B:2582:LEU:O	2:B:2586:ALA:N	2.51	0.44
3:C:1268:PHE:CE2	3:C:1274:ASN:HB3	2.53	0.44
1:A:2099:GLN:HG2	2:B:1833:TYR:HB3	2.00	0.44
3:C:976:VAL:O	3:C:1412:TYR:N	2.51	0.44
1:A:827:PRO:HD2	1:A:932:HIS:O	2.18	0.43
1:A:1011:VAL:HG13	1:A:1043:PHE:CE1	2.53	0.43
2:B:2020:SER:HA	2:B:2164:GLU:HG2	1.99	0.43
2:B:2267:LEU:HD21	3:C:726:VAL:HG21	2.00	0.43
2:B:2923:ILE:HA	2:B:2927:LEU:HB3	1.99	0.43
1:A:523:LEU:HD22	1:A:554:ILE:HG12	2.00	0.43
1:A:649:GLN:HG3	1:A:774:LEU:HD11	2.00	0.43
2:B:2718:GLY:HA2	2:B:2719:PRO:HD3	1.85	0.43
3:C:1203:MET:HG2	3:C:1261:ILE:HD11	1.99	0.43
2:B:1946:LEU:HD23	2:B:1946:LEU:HA	1.75	0.43
1:A:491:GLU:H	1:A:491:GLU:HG3	1.66	0.43
2:B:1951:ILE:HD13	2:B:1951:ILE:HA	1.81	0.43
2:B:2656:ARG:HD2	2:B:2656:ARG:HA	1.76	0.43
2:B:2923:ILE:HG22	2:B:2948:LEU:HD11	1.98	0.43
3:C:291:ASP:OD1	3:C:1368:ARG:NH2	2.47	0.43
1:A:187:HIS:CD2	1:A:187:HIS:H	2.35	0.43
2:B:1533:ILE:O	2:B:1537:ASN:HB2	2.19	0.43
2:B:2639:THR:HB	2:B:2641:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LEU:O	1:A:459:CYS:HB3	2.18	0.43
1:A:590:GLU:H	1:A:590:GLU:CD	2.27	0.43
1:A:832:ARG:H	1:A:832:ARG:HG3	1.56	0.43
1:A:894:GLN:C	1:A:896:LEU:H	2.25	0.43
2:B:2463:ARG:HH22	2:B:2588:GLU:HB3	1.84	0.43
2:B:2666:LYS:HB3	2:B:2668:PRO:HD2	2.01	0.43
4:D:334:ARG:NH1	4:D:334:ARG:HA	2.34	0.43
2:B:204:LEU:HD11	2:B:215:TRP:HD1	1.83	0.43
1:A:214:SER:C	1:A:216:VAL:H	2.26	0.43
1:A:2150:LEU:HD21	1:A:2173:ILE:HG12	2.00	0.43
1:A:2529:LEU:HD21	2:B:87:HIS:NE2	2.33	0.43
1:A:2564:LEU:HD13	1:A:2572:PHE:HB2	2.01	0.43
2:B:1647:LYS:HA	2:B:1731:MET:O	2.19	0.43
2:B:1687:ALA:HB2	2:B:1694:VAL:HG11	2.01	0.43
1:A:46:LEU:HD23	1:A:109:LEU:HD13	2.01	0.43
1:A:620:ARG:HG3	1:A:632:ALA:HB2	1.99	0.43
1:A:2574:LYS:HE2	2:B:191:LEU:HD21	2.00	0.43
2:B:1920:LEU:HB2	2:B:1921:PRO:HD3	2.01	0.43
2:B:2557:PHE:O	2:B:2561:ARG:NH1	2.52	0.43
3:C:349:GLN:HA	3:C:363:ALA:HA	2.00	0.43
2:B:2051:GLU:HG3	2:B:2055:LEU:HD12	2.00	0.43
2:B:2333:HIS:HE2	2:B:2398:LEU:HD12	1.84	0.43
3:C:895:VAL:HG12	3:C:925:PHE:HD1	1.84	0.43
1:A:2354:MET:HB3	1:A:2432:ARG:NH1	2.33	0.42
2:B:118:TRP:NE1	2:B:122:GLU:OE1	2.52	0.42
2:B:1206:LEU:HD12	2:B:1206:LEU:HA	1.76	0.42
2:B:1912:PRO:HG2	2:B:1915:ILE:HG12	2.01	0.42
2:B:2311:ASP:HA	3:C:712:PHE:HD2	1.84	0.42
2:B:2430:ARG:NH2	3:C:669:ARG:HB2	2.34	0.42
3:C:995:ARG:HH12	3:C:999:LEU:HD11	1.83	0.42
3:C:1087:PRO:HD3	4:D:320:TRP:CZ2	2.54	0.42
3:C:1272:ARG:HB2	3:C:1273:ARG:HH21	1.83	0.42
2:B:2121:TYR:O	2:B:2124:THR:OG1	2.34	0.42
1:A:633:LEU:HD23	1:A:633:LEU:HA	1.85	0.42
1:A:1060:LEU:HD12	2:B:2228:LEU:HD13	2.02	0.42
1:A:2270:LYS:O	1:A:2274:LYS:HG3	2.20	0.42
2:B:2060:MET:HB2	2:B:2131:PRO:HB2	2.01	0.42
2:B:2647:ARG:N	2:B:2648:PRO:HD2	2.34	0.42
3:C:397:ASP:HB2	3:C:425:PHE:CG	2.55	0.42
3:C:1251:ILE:O	3:C:1254:LEU:HG	2.18	0.42
3:C:1524:ASN:OD1	3:C:1524:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2136:MET:HE2	1:A:2181:PRO:HD3	2.01	0.42
2:B:2689:THR:HG22	2:B:2696:ILE:HD13	2.02	0.42
3:C:550:ILE:HA	3:C:556:TRP:HB3	2.00	0.42
1:A:2419:GLN:HB3	1:A:2480:GLN:HE22	1.84	0.42
1:A:2435:SER:HB3	1:A:2497:PHE:HB2	2.02	0.42
2:B:1219:ARG:HE	2:B:1342:LEU:HD21	1.83	0.42
2:B:2158:VAL:HG12	2:B:2222:LEU:HD21	2.01	0.42
1:A:452:ILE:HG21	1:A:500:LYS:NZ	2.34	0.42
1:A:2151:LEU:HD21	1:A:2196:PHE:CD2	2.54	0.42
1:A:2584:GLN:O	1:A:2587:THR:OG1	2.32	0.42
3:C:1156:ILE:HG12	3:C:1444:ALA:HB2	2.02	0.42
2:B:852:TYR:CE2	2:B:861:VAL:HG12	2.55	0.42
2:B:1752:SER:OG	2:B:1753:PRO:HD3	2.20	0.42
3:C:1359:THR:O	3:C:1416:ASP:HA	2.19	0.42
4:D:191:PHE:H	4:D:231:TYR:HD2	1.67	0.42
4:D:252:THR:O	4:D:254:ASN:N	2.45	0.42
1:A:147:SER:O	1:A:150:PRO:HD2	2.19	0.42
1:A:2197:GLN:HG3	1:A:2238:PRO:HG2	2.01	0.42
1:A:2209:LEU:O	1:A:2250:ALA:HA	2.20	0.42
3:C:1074:LYS:HA	3:C:1076:ARG:NH1	2.34	0.42
1:A:1254:MET:HE3	1:A:1317:VAL:HG21	2.01	0.42
1:A:2068:MET:HE1	1:A:2117:LEU:HD13	2.01	0.42
1:A:2646:GLU:O	1:A:2649:SER:OG	2.38	0.42
2:B:1200:ILE:HA	2:B:1201:PRO:HA	1.73	0.42
2:B:1647:LYS:HD3	2:B:1731:MET:O	2.20	0.42
2:B:1918:ALA:C	2:B:1921:PRO:HD2	2.44	0.42
2:B:2064:LYS:HD3	2:B:2133:ARG:HH21	1.84	0.42
1:A:103:PHE:HZ	1:A:128:THR:HG21	1.84	0.42
1:A:461:PRO:HD3	1:A:507:TRP:NE1	2.35	0.42
1:A:1350:GLN:HB2	1:A:1351:PRO:HD3	2.02	0.42
1:A:2463:GLY:HA2	1:A:2466:ILE:HD13	2.02	0.42
2:B:2324:PHE:O	2:B:2328:GLN:HG2	2.20	0.42
2:B:2566:ASN:OD1	2:B:2627:GLY:HA2	2.20	0.42
3:C:542:ARG:HA	3:C:545:MET:HE2	2.02	0.42
3:C:1178:LEU:HD22	3:C:1461:LEU:HG	2.02	0.42
1:A:175:MET:HE2	1:A:208:VAL:HG22	2.02	0.41
1:A:2247:ILE:O	1:A:2299:ASN:ND2	2.38	0.41
2:B:947:ASN:OD1	2:B:1032:TRP:NE1	2.52	0.41
2:B:2399:ASP:HB3	2:B:2402:TYR:HD2	1.85	0.41
3:C:35:LYS:O	3:C:38:VAL:HG12	2.20	0.41
1:A:445:ARG:HG2	1:A:487:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:LEU:HD23	1:A:936:LEU:HA	1.87	0.41
1:A:936:LEU:HB3	1:A:984:LEU:HD11	2.02	0.41
1:A:1112:PHE:O	1:A:1116:ARG:HD2	2.20	0.41
1:A:2065:LEU:HD13	3:C:359:TRP:CZ2	2.55	0.41
1:A:2257:LEU:HD11	1:A:2281:VAL:HG21	2.02	0.41
2:B:33:PHE:HE2	2:B:92:LEU:HD22	1.84	0.41
2:B:1317:ARG:NH1	2:B:1547:ASP:OD1	2.53	0.41
2:B:2342:PHE:CZ	2:B:2414:ALA:HB1	2.55	0.41
4:D:289:GLU:HA	4:D:292:GLU:HG2	2.02	0.41
1:A:751:MET:HE3	1:A:751:MET:HB2	1.92	0.41
1:A:2233:ARG:HH21	1:A:2272:ARG:NH2	2.16	0.41
2:B:1704:HIS:CE1	2:B:1709:GLN:HG3	2.56	0.41
2:B:2195:LEU:HD22	2:B:2201:PHE:CD1	2.55	0.41
3:C:219:TRP:NE1	3:C:1073:LEU:HB3	2.36	0.41
3:C:423:VAL:HG22	3:C:465:VAL:HG22	2.02	0.41
3:C:1085:TRP:O	4:D:317:TYR:OH	2.30	0.41
3:C:1314:ILE:HD12	3:C:1314:ILE:HA	1.85	0.41
3:C:1474:TRP:HZ2	3:C:1483:GLY:HA2	1.85	0.41
1:A:595:LEU:HD23	1:A:598:MET:HE2	2.02	0.41
1:A:2532:TRP:HA	1:A:2535:VAL:HG22	2.02	0.41
2:B:2330:TYR:CZ	2:B:2409:PHE:HB2	2.55	0.41
3:C:1000:VAL:HB	3:C:1003:MET:HG2	2.01	0.41
1:A:74:TYR:HB2	1:A:75:GLN:H	1.75	0.41
1:A:129:LEU:HD12	1:A:137:HIS:CD2	2.55	0.41
1:A:635:TRP:CD1	1:A:635:TRP:C	2.99	0.41
1:A:2564:LEU:O	1:A:2568:ASN:N	2.50	0.41
2:B:2677:GLU:HB2	2:B:2678:PRO:HD3	2.01	0.41
3:C:1227:LEU:HD21	3:C:1307:ILE:HD12	2.03	0.41
1:A:909:GLU:HB2	1:A:922:MET:HE1	2.01	0.41
1:A:2555:LEU:O	1:A:2558:ILE:HG12	2.20	0.41
2:B:1035:MET:HE2	2:B:1035:MET:HB2	1.90	0.41
2:B:2639:THR:O	2:B:2693:GLN:NE2	2.53	0.41
2:B:2687:CYS:SG	2:B:2748:LEU:HB2	2.61	0.41
4:D:298:TYR:CE2	4:D:300:GLN:HB2	2.56	0.41
1:A:926:LEU:O	1:A:930:CYS:N	2.43	0.41
1:A:1241:ILE:O	1:A:1245:THR:HG23	2.20	0.41
1:A:2173:ILE:O	1:A:2177:MET:HG2	2.21	0.41
2:B:1343:LYS:HD3	2:B:1535:LEU:HD21	2.03	0.41
2:B:2783:LEU:O	2:B:2787:VAL:HG23	2.21	0.41
2:B:2864:LEU:O	2:B:2868:VAL:HG23	2.21	0.41
3:C:473:GLN:HE21	3:C:1131:ILE:HG13	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:901:ILE:HA	3:C:904:MET:HE2	2.02	0.41
3:C:1237:VAL:O	3:C:1240:PRO:HD2	2.20	0.41
1:A:567:VAL:HG12	1:A:571:ILE:HD13	2.02	0.41
1:A:1012:GLU:HB2	1:A:1057:ARG:CZ	2.50	0.41
1:A:1117:PHE:HB3	1:A:1140:ILE:HG21	2.03	0.41
2:B:1745:SER:OG	2:B:1963:GLU:OE2	2.38	0.41
2:B:2009:ARG:NH2	2:B:2048:GLU:OE1	2.38	0.41
2:B:2209:GLU:N	2:B:2209:GLU:OE1	2.54	0.41
2:B:2452:GLN:O	2:B:2456:VAL:HG23	2.21	0.41
2:B:2948:LEU:HD23	2:B:2948:LEU:HA	1.94	0.41
3:C:286:MET:HA	3:C:302:PHE:CE2	2.56	0.41
3:C:579:PHE:HD1	3:C:579:PHE:HA	1.76	0.41
3:C:1110:GLU:O	3:C:1113:SER:OG	2.38	0.41
3:C:1439:LEU:O	3:C:1443:VAL:HG23	2.21	0.41
1:A:616:PHE:CE2	1:A:617:ILE:HG13	2.56	0.41
1:A:1045:THR:HG21	1:A:1178:VAL:HG13	2.03	0.41
1:A:1112:PHE:CE1	1:A:1116:ARG:HD3	2.56	0.41
1:A:2355:HIS:O	1:A:2359:LYS:HG2	2.21	0.41
2:B:1763:PHE:HE1	2:B:1813:LYS:HA	1.86	0.41
2:B:2756:LEU:HG	2:B:2759:ASP:HB3	2.02	0.41
1:A:2419:GLN:OE1	1:A:2475:ILE:HG22	2.21	0.40
2:B:1231:HIS:HB2	2:B:1352:GLU:OE1	2.21	0.40
2:B:1922:ILE:O	2:B:1926:MET:HG3	2.21	0.40
2:B:2143:VAL:HG12	2:B:2145:MET:HG3	2.03	0.40
2:B:2157:GLN:O	2:B:2161:ARG:HG3	2.21	0.40
2:B:2302:LEU:N	2:B:2303:PRO:HD2	2.36	0.40
3:C:282:TRP:NE1	3:C:1387:THR:O	2.45	0.40
3:C:1045:LYS:HA	3:C:1090:TRP:CE2	2.56	0.40
1:A:1294:PHE:CD1	1:A:1301:MET:HE1	2.56	0.40
1:A:2157:LYS:HE3	1:A:2157:LYS:HB2	1.87	0.40
1:A:2446:ALA:O	1:A:2627:ARG:NH2	2.53	0.40
2:B:344:TRP:HD1	2:B:345:SER:H	1.69	0.40
2:B:680:ILE:HD12	2:B:680:ILE:HA	1.94	0.40
2:B:2814:ASN:O	2:B:2818:PRO:HD2	2.21	0.40
3:C:543:ALA:O	3:C:547:MET:HG2	2.21	0.40
3:C:1203:MET:HB3	3:C:1262:ALA:HB2	2.03	0.40
3:C:1231:TRP:HE1	3:C:1241:LEU:HD13	1.86	0.40
1:A:633:LEU:HD21	1:A:655:PHE:CE1	2.56	0.40
1:A:1011:VAL:HG13	1:A:1043:PHE:HE1	1.85	0.40
1:A:1346:HIS:HB3	1:A:1354:CYS:SG	2.62	0.40
1:A:2546:ASN:O	1:A:2550:VAL:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1735:ALA:C	2:B:1737:GLN:H	2.29	0.40
2:B:2763:SER:HA	2:B:2766:ILE:HG12	2.03	0.40
3:C:213:LYS:HA	3:C:213:LYS:HD3	1.93	0.40
3:C:607:ASP:OD1	3:C:607:ASP:N	2.53	0.40
3:C:1276:TYR:CE1	3:C:1313:SER:HB2	2.56	0.40
1:A:1019:ARG:NH2	1:A:1061:LEU:HD22	2.37	0.40
1:A:1045:THR:HG21	1:A:1178:VAL:O	2.21	0.40
2:B:216:GLN:HB3	2:B:217:PRO:HD3	2.03	0.40
2:B:793:LEU:HD11	2:B:845:PHE:CD1	2.56	0.40
2:B:2104:SER:OG	2:B:2105:GLN:OE1	2.27	0.40
3:C:312:LEU:HD13	3:C:1328:VAL:HG13	2.03	0.40
3:C:554:GLU:HB3	3:C:1117:TRP:HE1	1.86	0.40
1:A:568:TRP:CH2	1:A:572:MET:HE3	2.57	0.40
1:A:917:ASP:OD1	3:C:717:ARG:NH2	2.53	0.40
1:A:1301:MET:HE3	1:A:1301:MET:HB2	1.87	0.40
1:A:2590:LEU:HD12	1:A:2595:GLN:HG2	2.04	0.40
2:B:2172:LEU:O	2:B:2176:THR:HG23	2.22	0.40
2:B:2409:PHE:HZ	2:B:2414:ALA:HB2	1.87	0.40
3:C:436:LYS:HE3	3:C:445:TYR:HE1	1.86	0.40
3:C:1094:ARG:HD2	4:D:364:GLY:O	2.22	0.40
3:C:1366:ILE:HD11	3:C:1394:ILE:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1492/2654 (56%)	1441 (97%)	51 (3%)	0	100	100
2	B	1671/3326 (50%)	1586 (95%)	85 (5%)	0	100	100
3	C	1330/1738 (76%)	1294 (97%)	36 (3%)	0	100	100
4	D	167/467 (36%)	157 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4660/8185 (57%)	4478 (96%)	182 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1363/2366 (58%)	1313 (96%)	50 (4%)	30	63
2	B	1529/2916 (52%)	1471 (96%)	58 (4%)	29	62
3	C	1174/1572 (75%)	1149 (98%)	25 (2%)	47	71
4	D	157/409 (38%)	151 (96%)	6 (4%)	29	62
All	All	4223/7263 (58%)	4084 (97%)	139 (3%)	34	65

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	85	LEU
1	A	88	VAL
1	A	120	THR
1	A	129	LEU
1	A	187	HIS
1	A	201	VAL
1	A	399	LEU
1	A	447	LEU
1	A	464	ASN
1	A	473	LEU
1	A	481	PHE
1	A	488	MET
1	A	500	LYS
1	A	517	ASP
1	A	602	GLU
1	A	645	THR

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Mol	Chain	Res	Type
1	A	950	ILE
1	A	955	LEU
1	A	962	VAL
1	A	969	GLN
1	A	1009	GLU
1	A	1090	THR
1	A	1097	LEU
1	A	1116	ARG
1	A	1122	LEU
1	A	1178	VAL
1	A	1233	ASP
1	A	1235	LEU
1	A	1238	ASP
1	A	1241	ILE
1	A	1354	CYS
1	A	1372	LEU
1	A	1382	ASP
1	A	1403	GLN
1	A	2196	PHE
1	A	2213	LEU
1	A	2236	LEU
1	A	2243	LEU
1	A	2286	LEU
1	A	2360	LEU
1	A	2394	ARG
1	A	2433	LEU
1	A	2436	TRP
1	A	2466	ILE
1	A	2469	HIS
1	A	2472	VAL
1	A	2477	PHE
1	A	2522	PHE
1	A	2634	GLN
2	B	99	LEU
2	B	107	VAL
2	B	206	PHE
2	B	213	VAL
2	B	689	VAL
2	B	793	LEU
2	B	849	MET
2	B	868	LEU
2	B	928	LEU

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Mol	Chain	Res	Type
2	B	1029	LYS
2	B	1031	PHE
2	B	1034	LYS
2	B	1196	GLU
2	B	1206	LEU
2	B	1210	LEU
2	B	1224	LEU
2	B	1318	LYS
2	B	1331	VAL
2	B	1537	ASN
2	B	1638	SER
2	B	1685	LEU
2	B	1711	LEU
2	B	1736	GLN
2	B	1752	SER
2	B	1914	CYS
2	B	1934	ASP
2	B	1965	LEU
2	B	1971	GLN
2	B	1985	ILE
2	B	1988	PHE
2	B	1991	GLN
2	B	2041	LEU
2	B	2042	LYS
2	B	2052	VAL
2	B	2056	VAL
2	B	2063	THR
2	B	2142	LEU
2	B	2206	ILE
2	B	2207	ASP
2	B	2221	GLU
2	B	2223	PHE
2	B	2256	LEU
2	B	2274	LEU
2	B	2277	GLN
2	B	2320	ARG
2	B	2427	GLU
2	B	2432	LEU
2	B	2456	VAL
2	B	2547	GLU
2	B	2596	LEU
2	B	2601	SER

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Mol	Chain	Res	Type
2	B	2663	LYS
2	B	2674	VAL
2	B	2807	LEU
2	B	2887	GLN
2	B	2913	ILE
2	B	2926	LYS
2	B	2938	LEU
3	C	31	LEU
3	C	57	THR
3	C	122	LEU
3	C	250	ASP
3	C	465	VAL
3	C	476	TYR
3	C	482	VAL
3	C	654	THR
3	C	669	ARG
3	C	712	PHE
3	C	733	CYS
3	C	875	TYR
3	C	932	GLU
3	C	1029	LEU
3	C	1047	ASN
3	C	1151	PHE
3	C	1273	ARG
3	C	1291	HIS
3	C	1488	PHE
3	C	1492	PHE
3	C	1493	LEU
3	C	1509	LYS
3	C	1516	CYS
3	C	1524	ASN
3	C	1559	LEU
4	D	252	THR
4	D	280	TYR
4	D	306	VAL
4	D	312	ASP
4	D	348	THR
4	D	360	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	189	GLN
1	A	758	GLN
1	A	921	ASN
1	A	953	HIS
1	A	1024	HIS
1	A	1115	ASN
1	A	2230	ASN
1	A	2248	GLN
1	A	2541	GLN
1	A	2602	GLN
2	B	84	HIS
2	B	923	HIS
2	B	1709	GLN
2	B	2069	HIS
2	B	2277	GLN
2	B	2291	HIS
2	B	2477	GLN
2	B	2711	ASN
2	B	2764	HIS
3	C	315	ASN
3	C	473	GLN
3	C	914	HIS
3	C	1365	ASN
3	C	1392	ASN
3	C	1449	ASN
3	C	1471	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
6	NAG	C	2001	3	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	C	2002	3	14,14,15	0.22	0	17,19,21	0.48	0
6	NAG	C	2003	3	14,14,15	0.22	0	17,19,21	0.47	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
6	NAG	C	2001	3	-	4/6/23/26	0/1/1/1
6	NAG	C	2002	3	-	0/6/23/26	0/1/1/1
6	NAG	C	2003	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

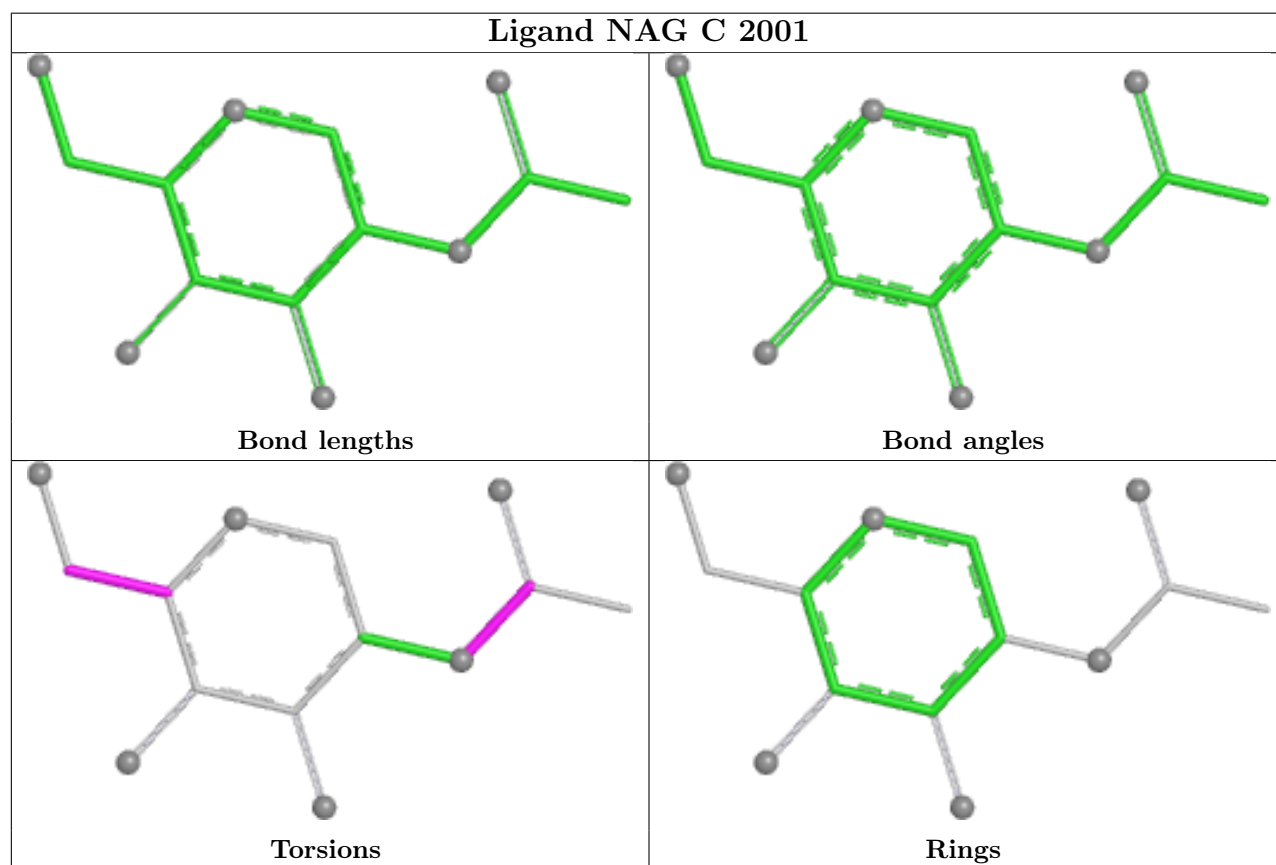
Mol	Chain	Res	Type	Atoms
6	C	2001	NAG	C4-C5-C6-O6
6	C	2001	NAG	O5-C5-C6-O6
6	C	2001	NAG	C8-C7-N2-C2
6	C	2001	NAG	O7-C7-N2-C2

There are no ring outliers.

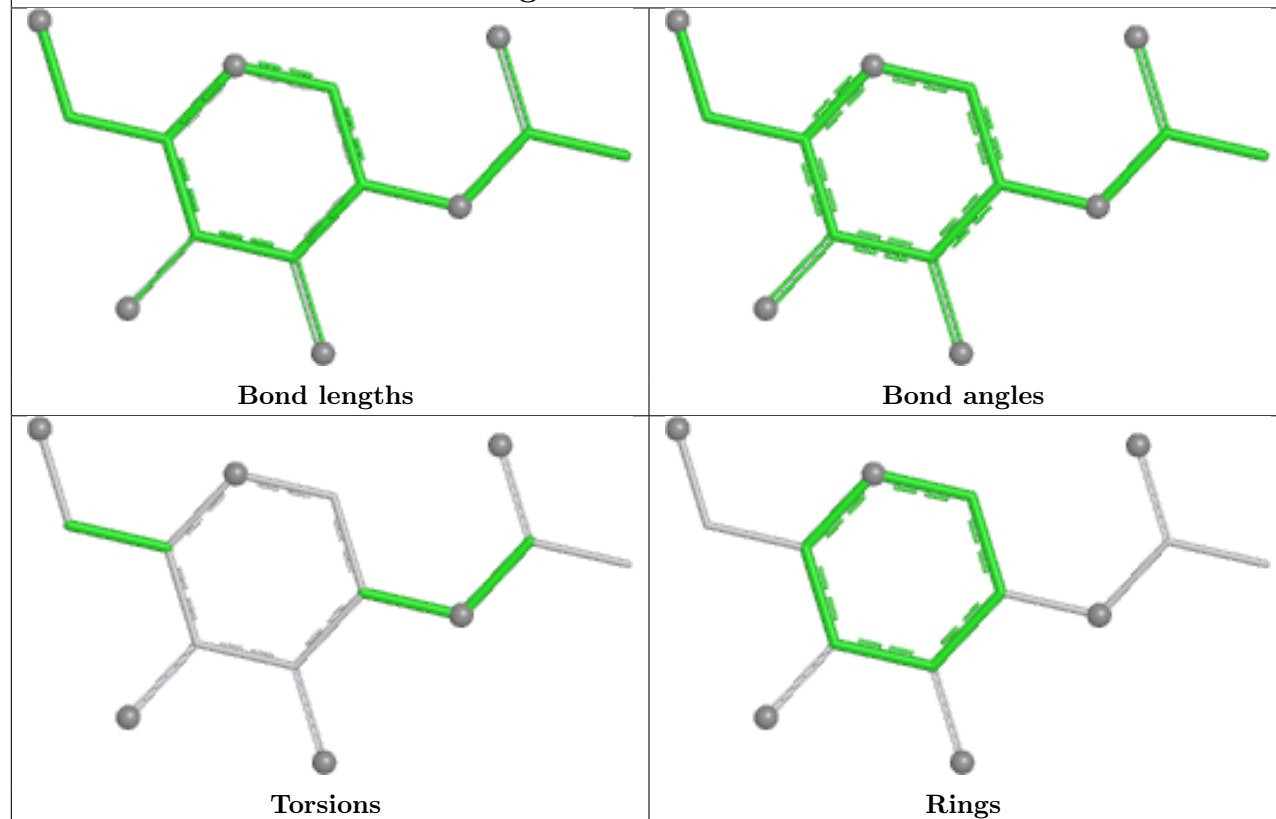
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2002	NAG	1	0

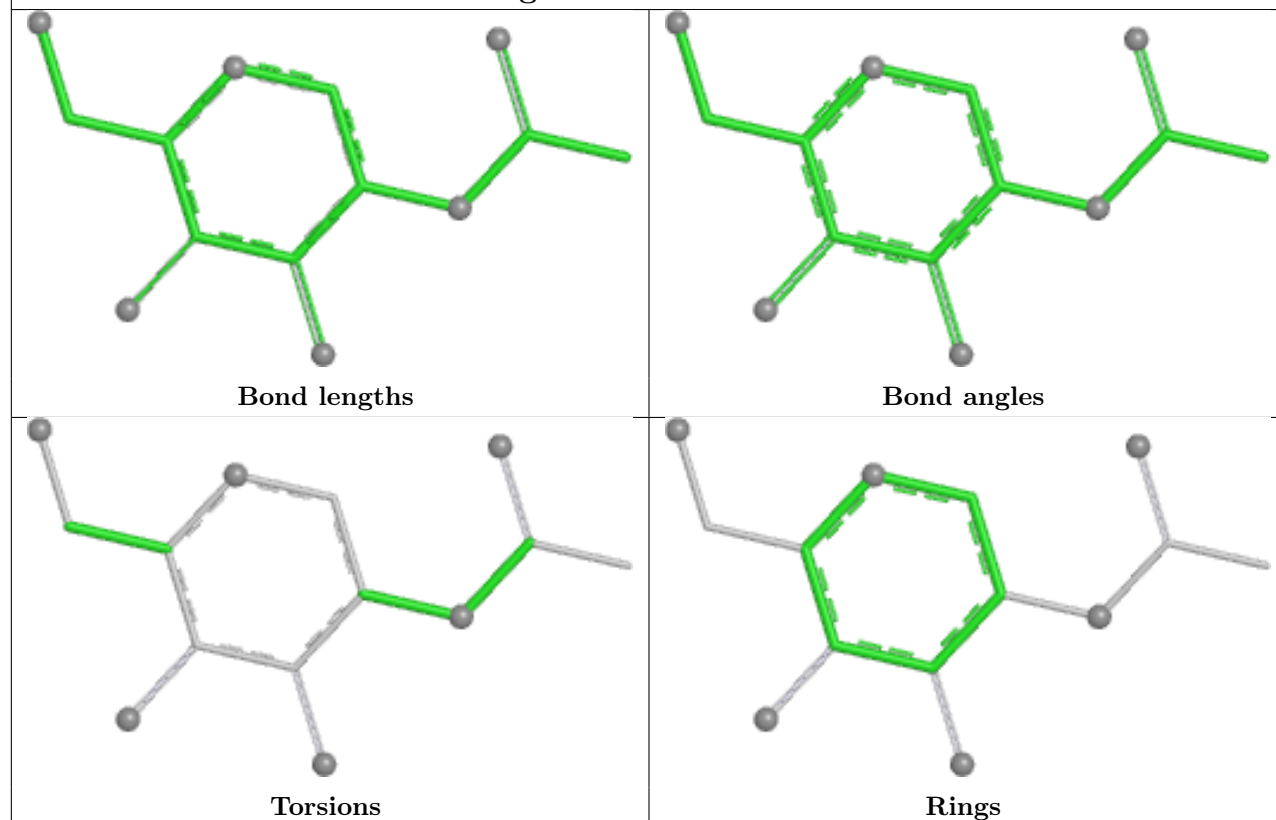
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand NAG C 2002



Ligand NAG C 2003



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.

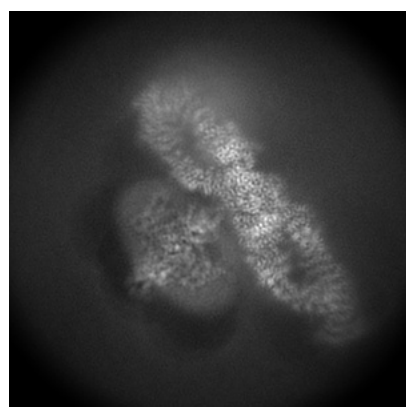
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32344. These allow visual inspection of the internal detail of the map and identification of artifacts.

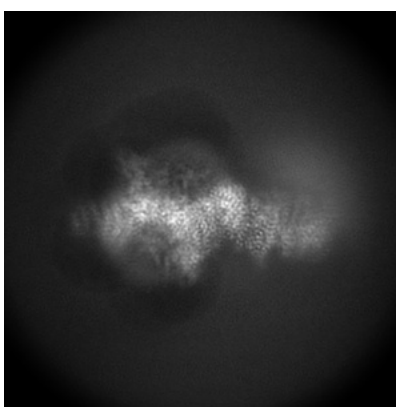
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

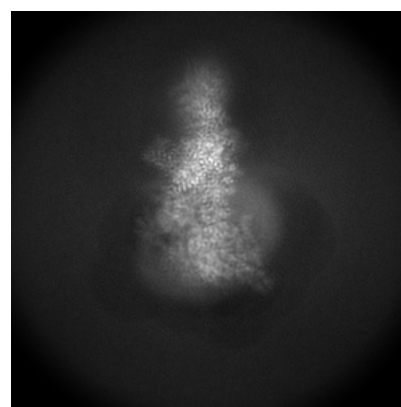
6.1.1 Primary map



X



Y

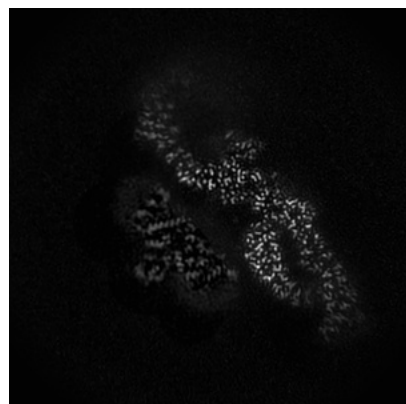


Z

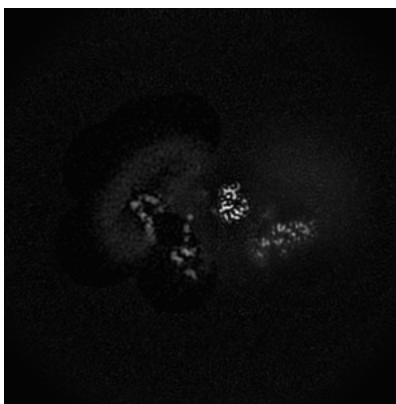
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

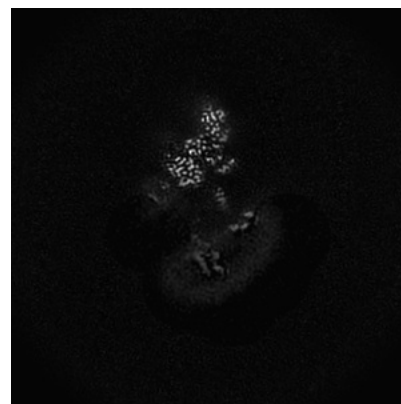
6.2.1 Primary map



X Index: 140



Y Index: 140

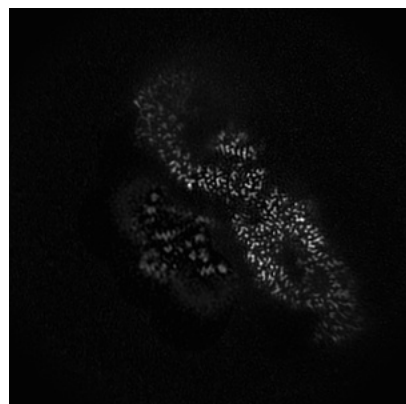


Z Index: 140

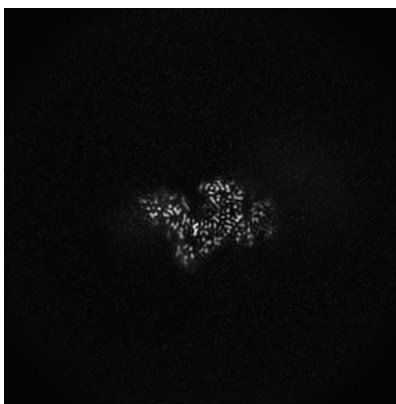
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

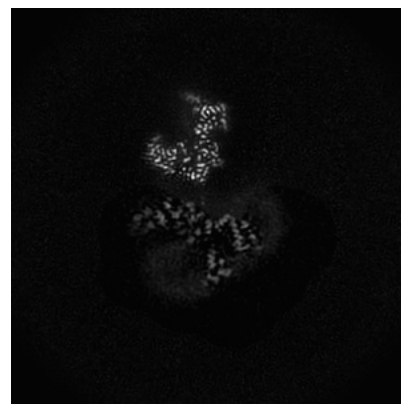
6.3.1 Primary map



X Index: 135



Y Index: 170

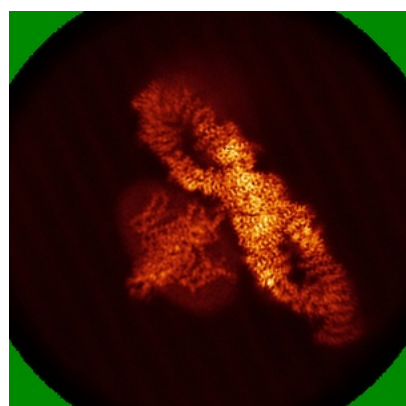


Z Index: 126

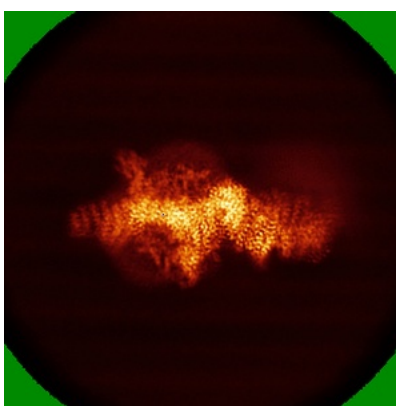
The images above show the largest variance slices of the map in three orthogonal directions.

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

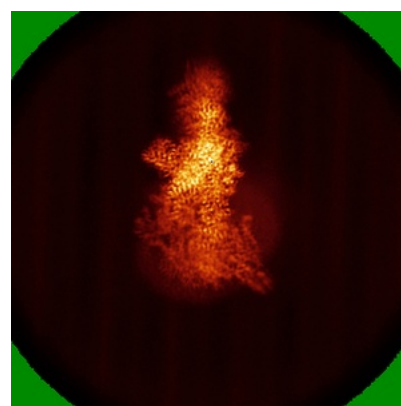
6.4.1 Primary map



X



Y

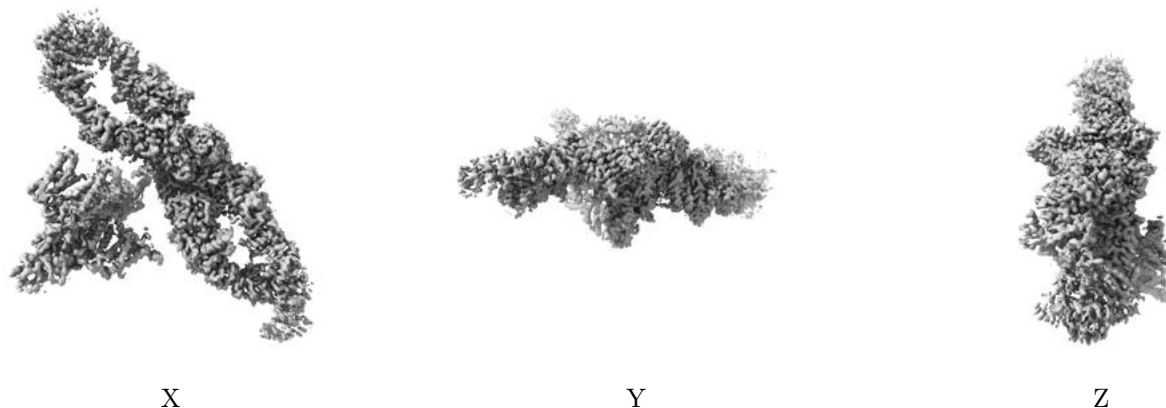


Z

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

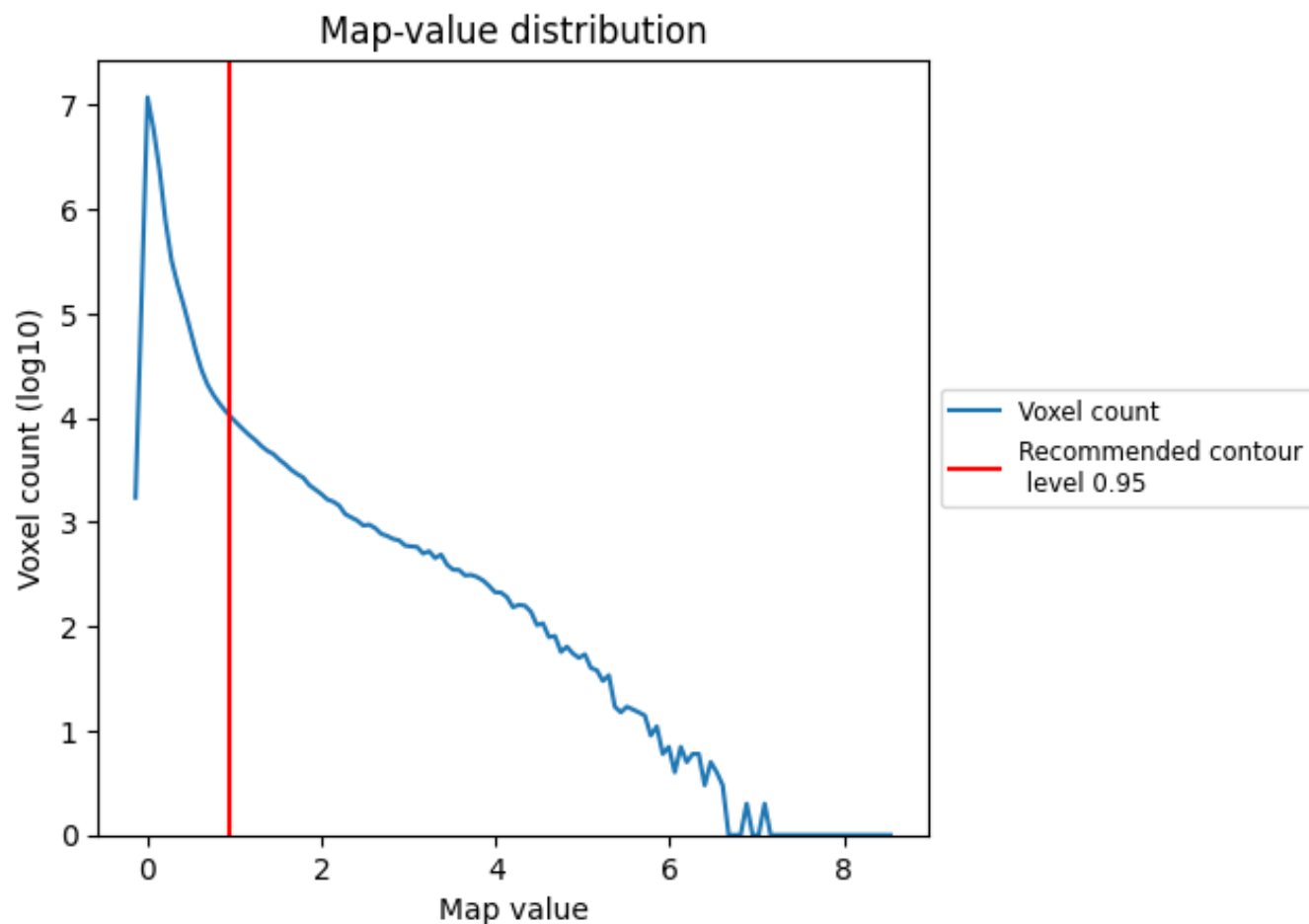
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

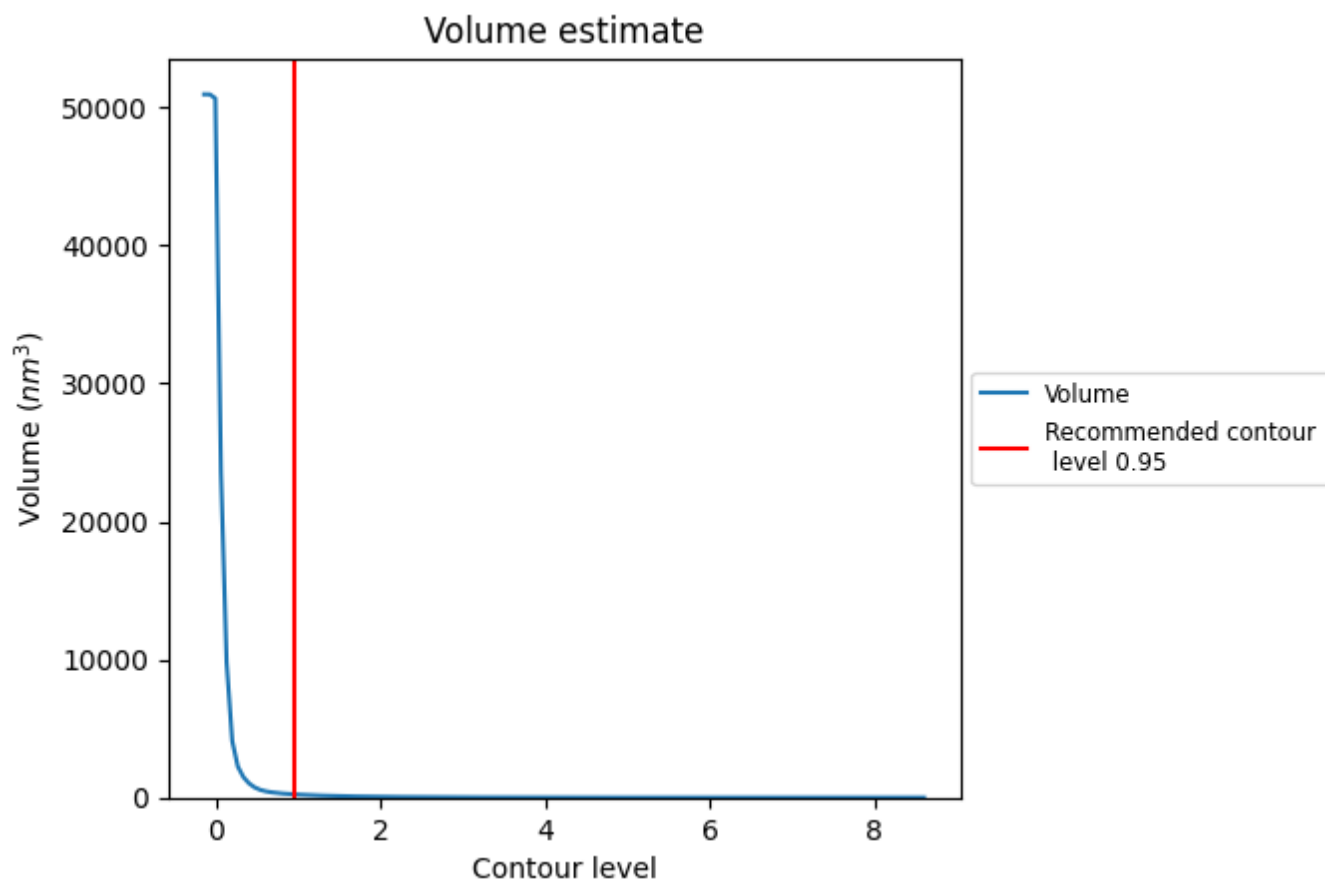
This section contains the results of statistical analysis of the map.

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.

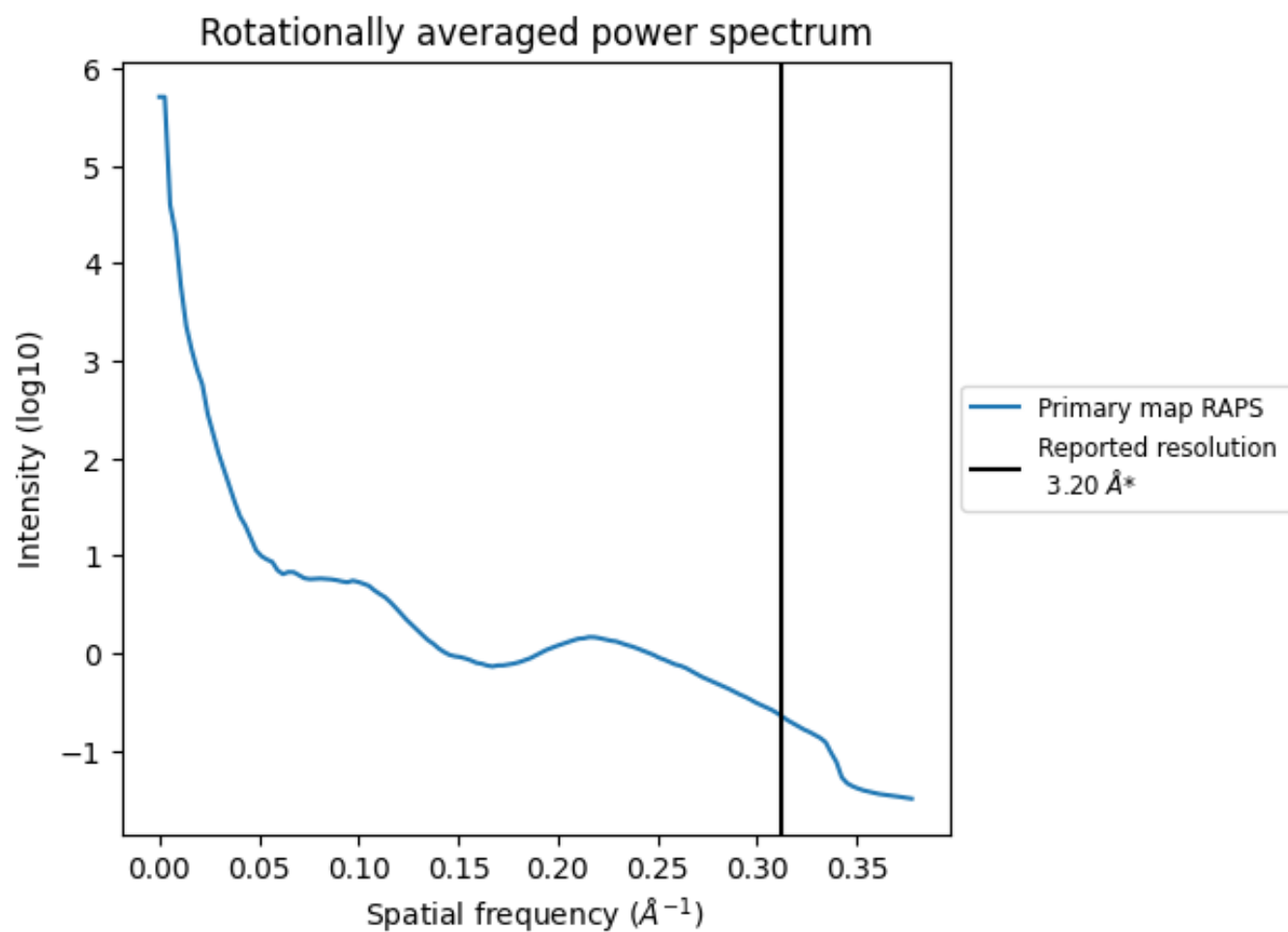
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 234 nm³; this corresponds to an approximate mass of 211 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 0.312 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

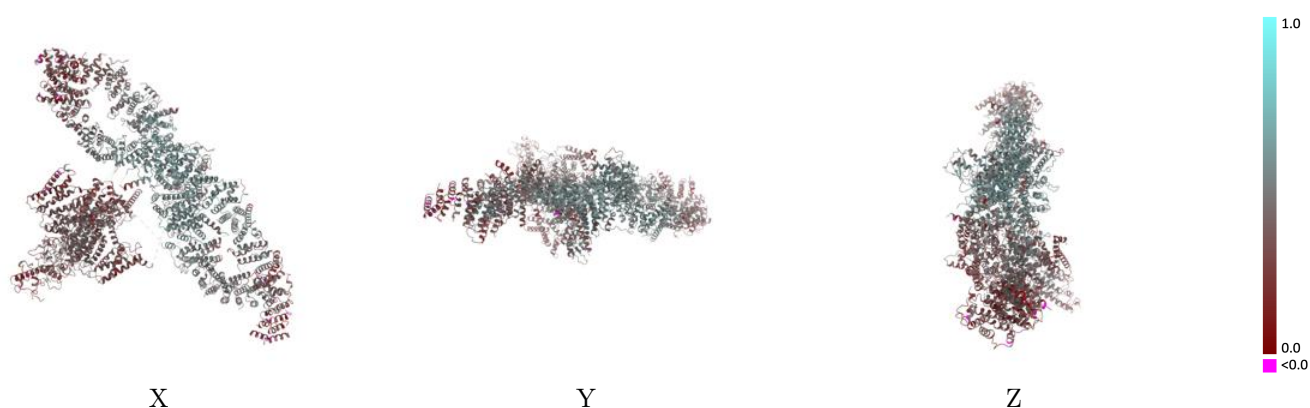
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32344 and PDB model 7W7G. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)

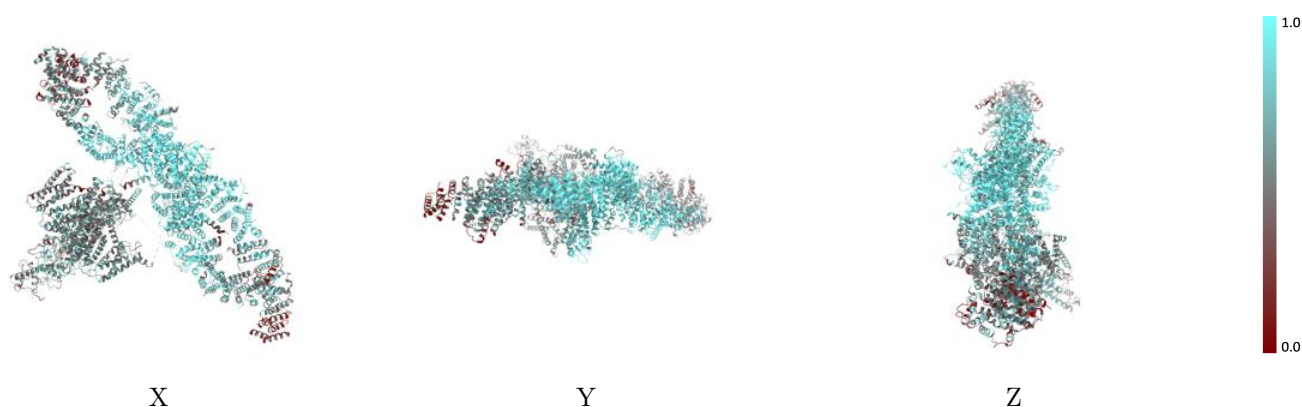
This section was not generated.

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



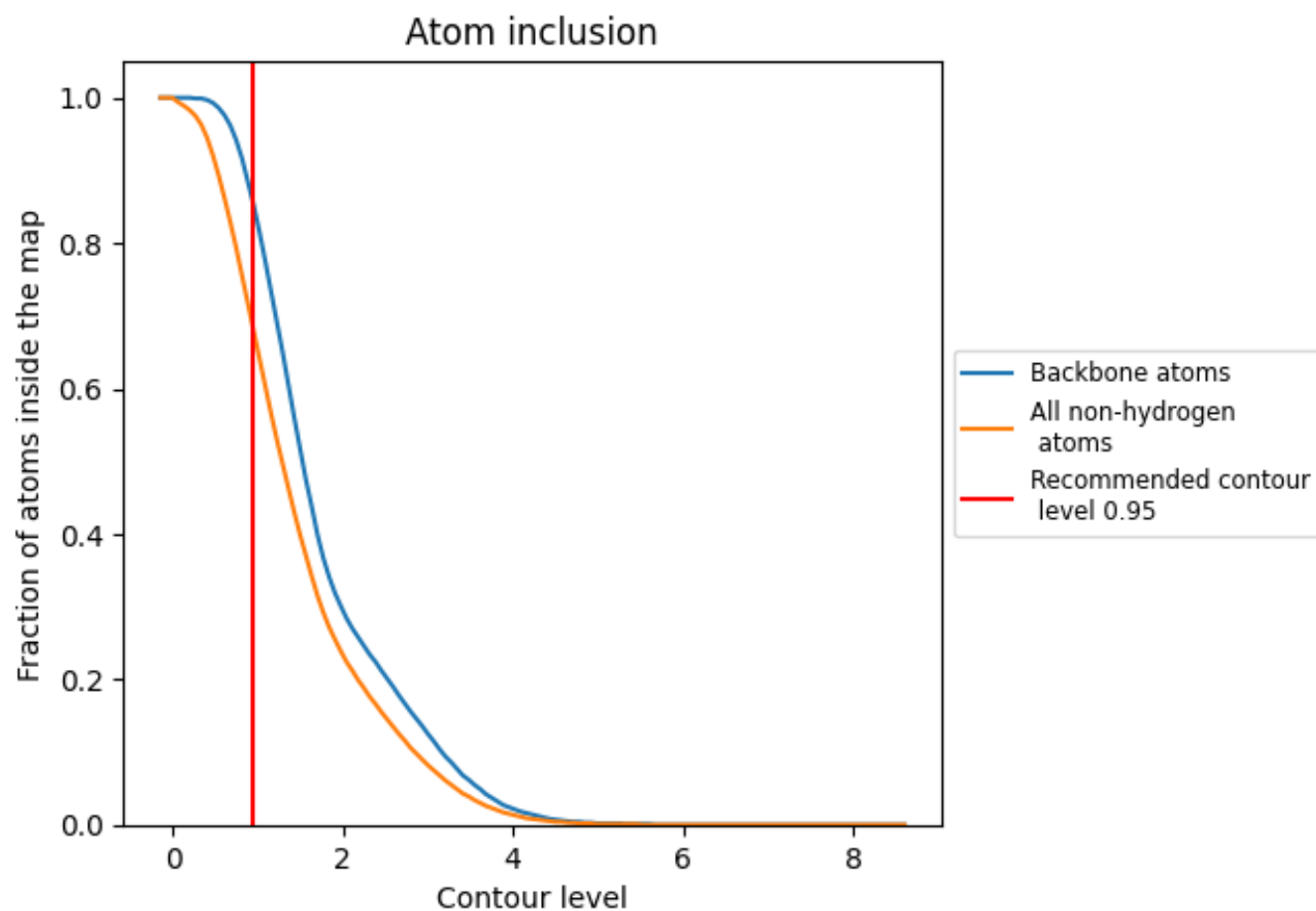
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.95).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 68% 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 (0.95) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6820	0.4200
A	0.7210	0.4400
B	0.7710	0.4660
C	0.5450	0.3520
D	0.5240	0.3220

