



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:04 PM UTC

PDB ID : 6YVU / pdb_00006yvu
EMDB ID : EMD-10951
Title : Condensin complex from S.cerevisiae ATP-free apo non-engaged state
Authors : Lee, B.-G.; Cawood, C.; Gutierrez-Escribano, P.; Nakane, T.; Merkel, F.;
Hassler, M.; Aragon, L.; Haering, C.H.; Lowe, J.
Deposited on : 2020-04-28
Resolution : 7.50 Å(reported)
Based on initial models : 6Q6E, 6QJ2, 4RSI, 6CJ3, 6C63

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
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

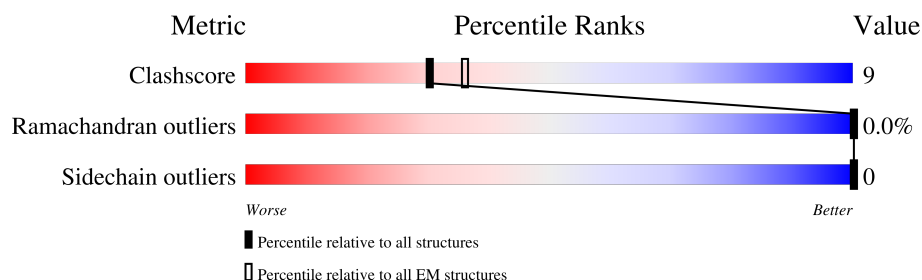
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1178	79% 16% .
2	B	1418	70% 14% 16%
3	C	773	24% 6% 70%
4	D	1185	57% 16% 27%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24216 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 Structural maintenance of chromosomes protein 2,Structural maintenance of chromosomes protein 2,Smc2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1127	Total	C	N	O	S	0	0
			7522	4682	1365	1456	19		

- Molecule 2 is a protein called Structural maintenance of chromosomes protein 4.

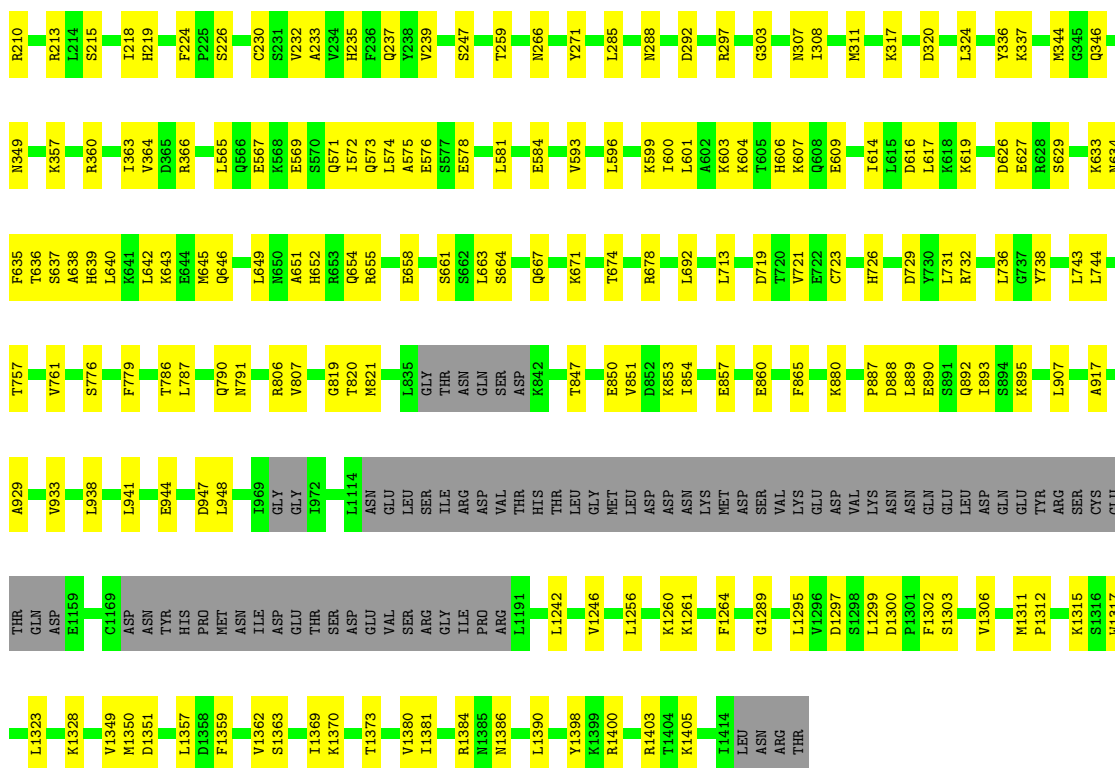
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1191	Total	C	N	O	S	0	0
			8112	5033	1462	1593	24		

- Molecule 3 is a protein called Condensin complex subunit 2,Condensin complex subunit 2,Brn1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	235	Total	C	N	O	S	0	0
			1838	1161	312	358	7		

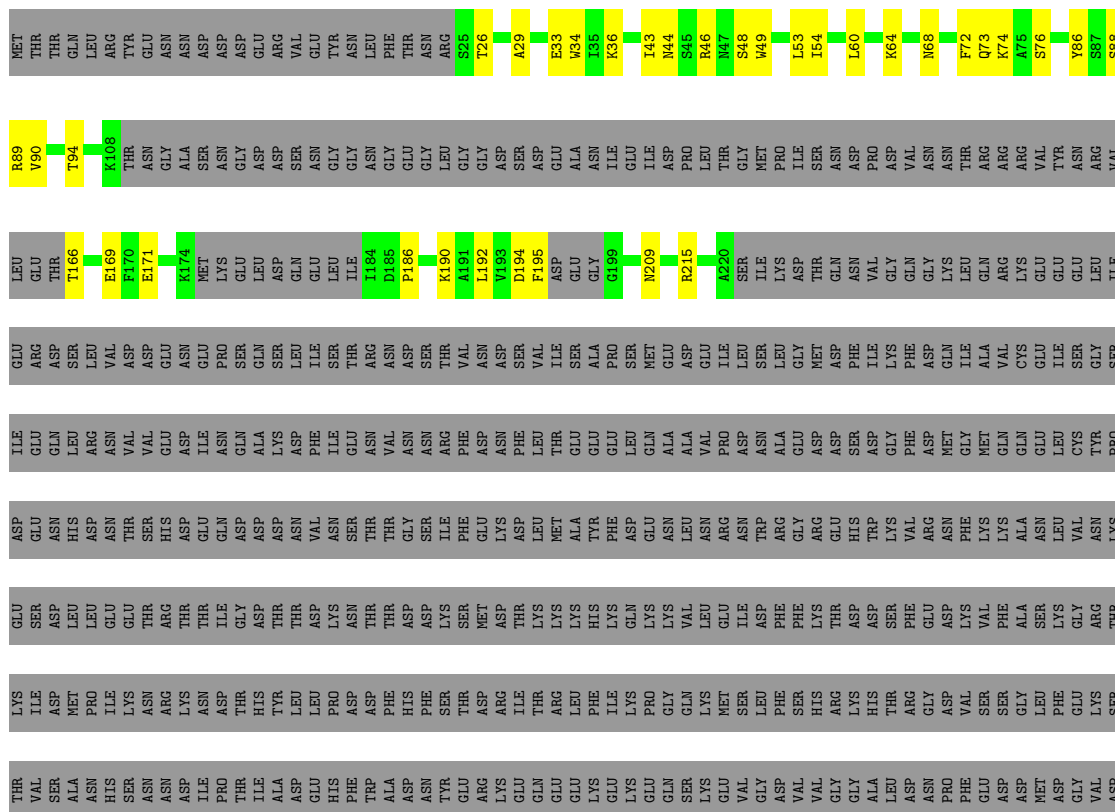
- Molecule 4 is a protein called Condensin complex subunit 1,Condensin complex subunit 1,Ycs4.

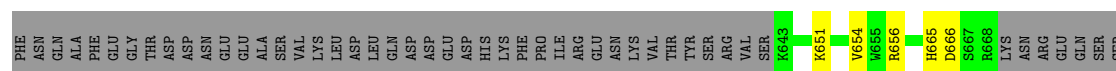
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	866	Total	C	N	O	S	0	0
			6744	4312	1115	1270	47		



● Molecule 3: Condensin complex subunit 2,Condensin complex subunit 2,Brn1

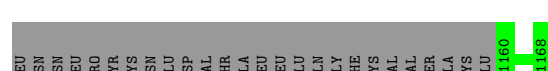
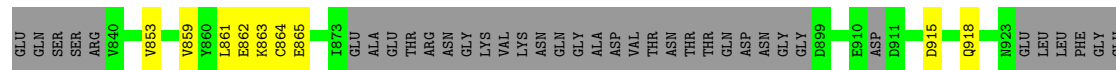
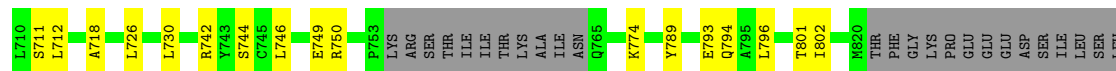
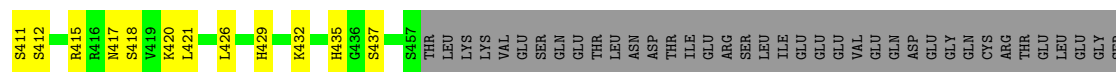
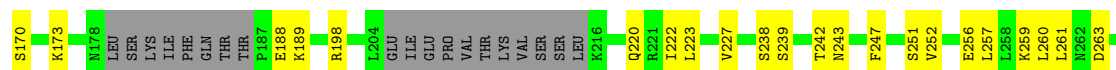
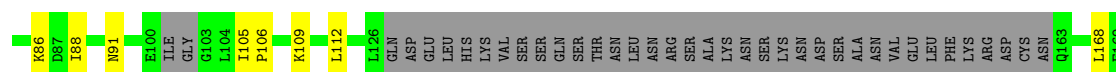
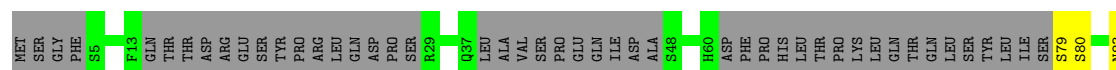
Chain C: 24% 6% 70%





● Molecule 4: Condensin complex subunit 1,Condensin complex subunit 1,Ycs4

Chain D:  57% 16% 27%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	100388	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 ($e^-/\text{\AA}^2$)	45, 1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/7550	0.32	1/10289 (0.0%)
2	B	0.11	0/8189	0.30	0/11128
3	C	0.09	0/1766	0.30	0/2374
4	D	0.11	0/6778	0.31	1/9117 (0.0%)
All	All	0.12	0/24283	0.31	2/32908 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	346	PRO	N-CA-C	-5.37	106.06	113.53
1	A	1162	ASP	N-CA-C	5.34	118.48	111.28

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	7522	0	6296	152	0
2	B	8112	0	6878	133	0
3	C	1838	0	1762	40	0
4	D	6744	0	6799	116	0
All	All	24216	0	21735	413	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 9.

All (413) 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:701:THR:HG22	1:A:705:GLN:HE22	1.40	0.85
4:D:346:PRO:C	4:D:348:THR:H	1.86	0.84
4:D:379:ILE:HG21	4:D:417:ASN:HB3	1.64	0.79
3:C:166:THR:N	4:D:370:SER:HG	1.81	0.79
4:D:632:LEU:HD13	4:D:706:ILE:HG12	1.67	0.74
1:A:20:ILE:HG22	1:A:1167:VAL:HG23	1.71	0.73
1:A:668:GLY:H	2:B:732:ARG:HE	1.36	0.73
4:D:705:ILE:HG22	4:D:709:MET:HE2	1.72	0.72
4:D:981:LEU:HG	4:D:985:MET:HE3	1.73	0.71
1:A:1037:THR:HG22	1:A:1055:LEU:HB3	1.72	0.70
1:A:1016:GLU:HB3	3:C:54:ILE:HD11	1.75	0.69
1:A:49:LEU:HD13	1:A:138:ILE:HB	1.75	0.68
1:A:1043:ILE:HA	1:A:1133:ARG:HH12	1.58	0.68
2:B:160:VAL:HG23	2:B:233:ALA:HB3	1.75	0.68
4:D:609:LYS:HE3	4:D:659:LEU:HD11	1.74	0.67
2:B:168:ALA:HB2	2:B:1403:ARG:HE	1.59	0.67
2:B:721:VAL:HG22	2:B:743:LEU:HD13	1.75	0.67
1:A:29:ALA:HB2	1:A:1152:ALA:HB3	1.76	0.67
4:D:80:SER:HA	4:D:83:ASN:HD22	1.59	0.67
1:A:146:MET:HE3	1:A:147:GLN:HG3	1.75	0.66
1:A:14:TYR:C	1:A:1163:GLY:H	2.04	0.66
1:A:1157:ARG:H	1:A:1167:VAL:HG13	1.59	0.66
3:C:730:GLN:HB3	3:C:743:ASN:HB3	1.78	0.66
4:D:382:CYS:HA	4:D:385:ILE:HG12	1.79	0.65
2:B:719:ASP:HA	2:B:744:LEU:HB2	1.77	0.65
1:A:578:ILE:HB	2:B:821:MET:HB3	1.78	0.65
2:B:317:LYS:HB3	2:B:320:ASP:HB2	1.77	0.65
2:B:790:GLN:HG2	2:B:791:ASN:HD22	1.62	0.65
1:A:80:THR:HG22	1:A:104:THR:HG23	1.78	0.64
4:D:404:VAL:HG23	4:D:543:SER:HB3	1.79	0.64
2:B:292:ASP:H	2:B:297:ARG:HH12	1.45	0.64
2:B:1289:GLY:HA3	2:B:1311:MET:O	1.99	0.63
2:B:1299:LEU:HD12	4:D:1126:GLN:HG2	1.80	0.63
3:C:44:ASN:HB2	3:C:46:ARG:HH21	1.63	0.63
1:A:583:LYS:NZ	2:B:819:GLY:O	2.32	0.63
1:A:653:THR:HB	1:A:657:ASP:HB2	1.79	0.63
4:D:963:LEU:HA	4:D:966:LEU:HD12	1.81	0.63
2:B:731:LEU:HG	2:B:736:LEU:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:712:LEU:HD13	4:D:750:ARG:HG2	1.81	0.63
3:C:43:ILE:O	3:C:88:SER:OG	2.16	0.63
2:B:210:ARG:HE	2:B:213:ARG:HD2	1.62	0.63
2:B:153:ARG:NH2	2:B:178:THR:O	2.31	0.63
4:D:379:ILE:HG12	4:D:421:LEU:HD11	1.80	0.62
4:D:395:SER:HA	4:D:398:LYS:HE2	1.80	0.62
4:D:371:ASN:HB3	4:D:374:VAL:HG22	1.82	0.62
1:A:1116:ALA:HB2	1:A:1145:LYS:HE3	1.81	0.62
4:D:1025:ASP:H	4:D:1031:GLN:HE21	1.46	0.62
2:B:1369:ILE:O	2:B:1373:THR:OG1	2.17	0.61
2:B:629:SER:O	2:B:633:LYS:NZ	2.33	0.61
2:B:218:ILE:HA	2:B:230:CYS:HB3	1.83	0.61
3:C:665:HIS:ND1	3:C:666:ASP:OD1	2.26	0.61
4:D:801:THR:HG23	4:D:802:ILE:HG13	1.83	0.61
2:B:324:LEU:HD21	2:B:1302:PHE:HA	1.82	0.61
1:A:1013:LYS:HD3	3:C:54:ILE:HD12	1.83	0.60
2:B:1261:LYS:HA	2:B:1264:PHE:CE1	2.36	0.60
1:A:129:GLN:HA	1:A:132:GLN:HB2	1.84	0.60
1:A:534:ASP:OD1	1:A:537:ASN:ND2	2.35	0.60
4:D:1139:GLU:HA	4:D:1142:LYS:HG2	1.83	0.60
1:A:14:TYR:O	1:A:1163:GLY:N	2.35	0.60
1:A:18:THR:HB	1:A:1166:VAL:HG11	1.84	0.60
4:D:346:PRO:O	4:D:348:THR:N	2.34	0.59
2:B:617:LEU:HD12	2:B:893:ILE:HD13	1.82	0.59
4:D:368:GLN:OE1	4:D:405:ARG:NH2	2.35	0.59
1:A:633:GLU:HG3	1:A:654:LEU:HD11	1.84	0.59
1:A:1030:VAL:HA	1:A:1033:TRP:CD1	2.37	0.59
2:B:344:MET:HE1	2:B:1260:LYS:HD3	1.84	0.59
1:A:514:PRO:HB3	1:A:569:ARG:HB3	1.83	0.59
4:D:749:GLU:OE1	4:D:794:GLN:NE2	2.36	0.59
4:D:346:PRO:C	4:D:348:THR:N	2.55	0.58
1:A:178:ARG:NH1	3:C:76:SER:O	2.36	0.58
1:A:15:ALA:HB1	1:A:1160:PHE:HA	1.86	0.58
1:A:1055:LEU:HD11	1:A:1067:LEU:HD13	1.85	0.58
1:A:16:THR:OG1	1:A:1162:ASP:O	2.17	0.58
1:A:105:ARG:HD2	1:A:127:VAL:HB	1.86	0.57
1:A:189:GLU:HG2	3:C:90:VAL:HG11	1.86	0.57
4:D:317:ILE:HA	4:D:320:LEU:HD12	1.86	0.57
1:A:1031:LYS:HE3	3:C:68:ASN:HB2	1.87	0.57
2:B:642:LEU:HA	2:B:645:MET:HE2	1.86	0.57
1:A:18:THR:C	1:A:1166:VAL:HG21	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:HD12	1:A:23:TRP:HE1	1.70	0.56
1:A:598:LYS:HA	1:A:605:VAL:HG11	1.88	0.56
1:A:537:ASN:ND2	1:A:611:LEU:O	2.30	0.56
2:B:569:GLU:HG2	2:B:572:ILE:HD12	1.87	0.56
2:B:596:LEU:HA	2:B:599:LYS:HZ3	1.71	0.56
1:A:471:PHE:HB3	1:A:714:THR:HG21	1.87	0.56
2:B:573:GLN:HA	2:B:576:GLU:HB2	1.88	0.56
4:D:79:SER:O	4:D:83:ASN:ND2	2.39	0.56
1:A:195:ASN:HD21	2:B:357:LYS:HE3	1.71	0.56
4:D:645:ALA:O	4:D:648:GLU:HG3	2.06	0.56
1:A:11:PHE:HB3	1:A:1163:GLY:O	2.06	0.55
1:A:196:ARG:NH2	3:C:94:THR:OG1	2.38	0.55
2:B:635:PHE:O	2:B:638:ALA:HB3	2.05	0.55
2:B:1297:ASP:OD2	2:B:1303:SER:OG	2.24	0.55
1:A:20:ILE:HG23	1:A:1166:VAL:HG23	1.87	0.55
2:B:723:CYS:O	2:B:726:HIS:ND1	2.39	0.55
2:B:786:THR:OG1	2:B:806:ARG:NH2	2.39	0.55
4:D:978:LEU:HG	4:D:979:PRO:HD3	1.87	0.55
1:A:488:SER:HA	1:A:491:TYR:CE1	2.42	0.54
1:A:1018:ILE:O	1:A:1022:ASN:ND2	2.40	0.54
1:A:1010:ASP:OD1	3:C:86:TYR:OH	2.24	0.54
2:B:616:ASP:HA	2:B:619:LYS:HE2	1.90	0.54
4:D:223:LEU:HB3	4:D:257:LEU:HD11	1.90	0.54
2:B:723:CYS:HA	2:B:726:HIS:HD1	1.72	0.54
3:C:34:TRP:HE3	3:C:53:LEU:HG	1.72	0.54
1:A:157:LYS:HD2	1:A:161:ILE:HD13	1.90	0.54
2:B:346:GLN:HA	2:B:349:ASN:HD21	1.73	0.54
4:D:711:SER:HB2	4:D:718:ALA:HB2	1.88	0.54
4:D:1129:GLU:HA	4:D:1132:VAL:HG22	1.89	0.54
4:D:545:GLU:O	4:D:549:ASN:ND2	2.40	0.54
2:B:639:HIS:O	2:B:642:LEU:HB3	2.08	0.54
4:D:746:LEU:HD23	4:D:794:GLN:HG2	1.90	0.54
1:A:548:ALA:O	1:A:551:ARG:HB3	2.08	0.53
2:B:663:LEU:HD22	2:B:851:VAL:HG21	1.90	0.53
3:C:654:VAL:HG11	3:C:719:CYS:HB3	1.90	0.53
1:A:1043:ILE:HG12	1:A:1098:MET:HE1	1.90	0.53
2:B:183:VAL:HB	2:B:1381:ILE:HG12	1.90	0.53
4:D:88:ILE:HA	4:D:91:ASN:ND2	2.23	0.53
1:A:992:ASN:OD1	1:A:995:LYS:NZ	2.41	0.53
4:D:360:ILE:O	4:D:364:GLU:HG2	2.08	0.53
2:B:593:VAL:HG22	2:B:917:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:LEU:HD22	1:A:680:ILE:HD13	1.89	0.53
3:C:26:THR:HG23	3:C:29:ALA:H	1.74	0.53
1:A:1017:THR:HA	1:A:1020:LYS:HE3	1.88	0.53
2:B:614:ILE:HG23	2:B:893:ILE:HD11	1.91	0.53
4:D:957:ARG:NE	4:D:990:ASP:OD2	2.42	0.53
4:D:320:LEU:O	4:D:366:ARG:NH1	2.42	0.53
4:D:963:LEU:HD22	4:D:981:LEU:HD13	1.91	0.53
1:A:567:LEU:HD13	2:B:821:MET:HG3	1.90	0.53
1:A:1006:THR:HG23	3:C:49:TRP:HZ2	1.75	0.53
2:B:344:MET:HE2	2:B:1256:LEU:HB3	1.91	0.52
3:C:169:GLU:HG3	3:C:171:GLU:HG2	1.91	0.52
1:A:681:GLN:HA	1:A:684:ASN:HD21	1.74	0.52
2:B:649:LEU:HB2	2:B:865:PHE:HE2	1.74	0.52
2:B:692:LEU:HD23	2:B:713:LEU:HA	1.91	0.52
2:B:787:LEU:HB2	2:B:807:VAL:HG22	1.92	0.52
4:D:705:ILE:O	4:D:709:MET:HG3	2.10	0.52
1:A:36:SER:O	1:A:40:ASN:ND2	2.42	0.52
1:A:1045:ALA:HB2	1:A:1052:PHE:HB3	1.90	0.52
2:B:198:MET:HE1	2:B:1349:VAL:HG11	1.92	0.52
1:A:997:GLU:O	1:A:1001:LYS:HG2	2.10	0.52
2:B:604:LYS:O	2:B:607:LYS:HG3	2.09	0.52
4:D:726:LEU:HD23	4:D:730:LEU:HD12	1.91	0.52
2:B:164:PHE:O	2:B:219:HIS:ND1	2.27	0.52
4:D:630:LYS:O	4:D:634:ASN:ND2	2.43	0.52
3:C:656:ARG:HH12	3:C:702:MET:HG3	1.75	0.51
1:A:14:TYR:HB2	1:A:1163:GLY:O	2.10	0.51
1:A:498:GLU:HA	1:A:501:LYS:HG2	1.91	0.51
1:A:554:ASN:HD22	1:A:579:ILE:HG13	1.75	0.51
1:A:701:THR:O	1:A:705:GLN:NE2	2.43	0.51
1:A:1064:THR:OG1	1:A:1065:GLN:OE1	2.29	0.51
3:C:44:ASN:O	3:C:48:SER:N	2.43	0.51
1:A:42:LEU:HD13	1:A:1110:ILE:HD13	1.93	0.51
4:D:524:LYS:O	4:D:528:VAL:HG23	2.11	0.51
2:B:219:HIS:HD2	2:B:224:PHE:HB2	1.76	0.51
4:D:256:GLU:O	4:D:260:LEU:HG	2.10	0.51
4:D:1147:ILE:HG23	4:D:1148:ALA:H	1.74	0.51
1:A:63:GLN:HB3	1:A:69:ARG:HG3	1.92	0.51
1:A:606:GLU:HB2	1:A:631:ILE:HB	1.93	0.51
2:B:1400:ARG:O	2:B:1403:ARG:HB2	2.11	0.51
4:D:411:SER:O	4:D:415:ARG:NH1	2.43	0.51
4:D:88:ILE:HA	4:D:91:ASN:HD21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:238:SER:O	4:D:242:THR:HG23	2.11	0.51
1:A:1057:PRO:HA	1:A:1067:LEU:HA	1.91	0.51
2:B:651:ALA:O	2:B:654:GLN:HG3	2.11	0.51
2:B:634:ASN:OD1	2:B:635:PHE:N	2.44	0.51
4:D:188:GLU:OE2	4:D:189:LYS:NZ	2.44	0.50
4:D:1025:ASP:O	4:D:1031:GLN:NE2	2.45	0.50
2:B:671:LYS:O	2:B:674:THR:OG1	2.16	0.50
2:B:1370:LYS:NZ	2:B:1390:LEU:O	2.45	0.50
4:D:1143:GLN:HB2	4:D:1149:PHE:C	2.37	0.50
1:A:714:THR:O	1:A:718:GLN:HB2	2.11	0.50
4:D:861:LEU:HA	4:D:864:CYS:SG	2.52	0.50
1:A:808:GLU:O	1:A:812:SER:N	2.37	0.50
4:D:417:ASN:HA	4:D:420:LYS:HE2	1.92	0.50
4:D:749:GLU:HG3	4:D:801:THR:HG21	1.93	0.50
1:A:27:PHE:HB3	1:A:1152:ALA:HB1	1.93	0.50
1:A:513:LYS:NZ	1:A:515:TYR:O	2.40	0.49
2:B:606:HIS:O	2:B:609:GLU:HG2	2.12	0.49
4:D:259:LYS:HG3	4:D:304:LEU:HG	1.93	0.49
1:A:543:ALA:O	1:A:546:THR:OG1	2.21	0.49
1:A:1071:VAL:HG21	1:A:1081:LEU:HB3	1.93	0.49
4:D:918:GLN:HG2	4:D:966:LEU:HD11	1.94	0.49
2:B:308:ILE:HA	2:B:311:MET:HE3	1.95	0.49
2:B:850:GLU:O	2:B:853:LYS:HG3	2.12	0.49
3:C:60:LEU:HB3	3:C:64:LYS:HE3	1.94	0.49
4:D:915:ASP:HB2	4:D:918:GLN:HB2	1.93	0.49
1:A:6:LEU:HB2	1:A:20:ILE:HD11	1.93	0.49
1:A:992:ASN:HA	1:A:995:LYS:HG2	1.94	0.49
2:B:888:ASP:OD1	2:B:889:LEU:N	2.45	0.49
1:A:532:GLN:HG2	1:A:613:ARG:HB2	1.95	0.49
4:D:603:HIS:O	4:D:606:GLU:HG3	2.13	0.49
2:B:658:GLU:O	2:B:661:SER:OG	2.26	0.49
4:D:1143:GLN:HA	4:D:1146:ASP:HB2	1.95	0.49
4:D:564:ASP:N	4:D:564:ASP:OD1	2.44	0.49
1:A:16:THR:HG23	1:A:1164:THR:N	2.27	0.49
4:D:704:ILE:HD11	4:D:744:SER:HB3	1.95	0.49
2:B:944:GLU:HA	2:B:947:ASP:OD2	2.13	0.49
1:A:7:ILE:HB	1:A:19:VAL:HG23	1.94	0.48
4:D:365:GLU:OE1	4:D:366:ARG:NH2	2.43	0.48
2:B:285:LEU:HD13	2:B:288:ASN:HD22	1.79	0.48
2:B:1351:ASP:OD1	2:B:1351:ASP:N	2.46	0.48
4:D:435:HIS:O	4:D:435:HIS:ND1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:661:SER:O	2:B:664:SER:OG	2.26	0.48
1:A:567:LEU:HG	1:A:572:LEU:HD11	1.96	0.48
2:B:569:GLU:O	2:B:572:ILE:HB	2.14	0.48
2:B:637:SER:HA	2:B:640:LEU:HD12	1.96	0.48
4:D:220:GLN:HE21	4:D:260:LEU:HD11	1.78	0.48
4:D:316:VAL:HG13	4:D:319:LEU:HD12	1.95	0.48
4:D:426:LEU:HD21	4:D:540:ILE:HD12	1.94	0.48
2:B:157:ASN:O	2:B:176:PHE:N	2.45	0.48
1:A:172:LYS:HG3	1:A:173:MET:SD	2.53	0.48
2:B:364:VAL:HG22	2:B:366:ARG:H	1.79	0.48
2:B:336:TYR:HD2	2:B:337:LYS:HZ2	1.62	0.48
4:D:437:SER:O	4:D:437:SER:OG	2.30	0.47
4:D:607:CYS:HA	4:D:610:GLN:HG2	1.96	0.47
1:A:668:GLY:HA3	2:B:738:TYR:HA	1.95	0.47
2:B:565:LEU:HB3	2:B:948:LEU:HG	1.97	0.47
1:A:1141:VAL:HG11	1:A:1149:PHE:HD2	1.79	0.47
2:B:636:THR:HA	2:B:639:HIS:CD2	2.49	0.47
4:D:418:SER:HA	4:D:421:LEU:HD12	1.96	0.47
1:A:196:ARG:HH22	3:C:90:VAL:HG13	1.79	0.47
1:A:629:SER:HA	1:A:650:ARG:HB3	1.95	0.47
2:B:215:SER:OG	2:B:266:ASN:ND2	2.47	0.47
2:B:854:ILE:O	2:B:857:GLU:HG3	2.14	0.47
2:B:626:ASP:OD1	2:B:627:GLU:N	2.47	0.47
2:B:239:VAL:HG23	2:B:247:SER:HA	1.97	0.47
4:D:859:VAL:O	4:D:863:LYS:HG2	2.14	0.47
1:A:30:ILE:HG23	1:A:38:LYS:HE3	1.97	0.47
2:B:941:LEU:O	2:B:944:GLU:HG3	2.14	0.47
3:C:209:ASN:HD21	4:D:641:ILE:HD12	1.80	0.47
4:D:105:ILE:N	4:D:106:PRO:HD2	2.30	0.47
4:D:574:ILE:HG23	4:D:576:LEU:H	1.79	0.47
2:B:575:ALA:O	2:B:578:GLU:HG2	2.14	0.47
4:D:83:ASN:O	4:D:86:LYS:HG2	2.13	0.47
1:A:670:ARG:HD3	1:A:674:GLU:HA	1.97	0.47
2:B:1242:LEU:O	2:B:1246:VAL:HG23	2.15	0.47
2:B:929:ALA:O	2:B:933:VAL:HG23	2.15	0.47
1:A:1033:TRP:HA	1:A:1036:VAL:HG22	1.95	0.46
1:A:1113:GLU:HA	1:A:1149:PHE:CE2	2.50	0.46
4:D:1058:LYS:HE3	4:D:1102:LEU:HD12	1.98	0.46
2:B:363:ILE:HG13	2:B:364:VAL:N	2.30	0.46
4:D:168:LEU:HA	4:D:222:ILE:HD11	1.98	0.46
4:D:251:SER:HB3	4:D:297:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1106:SER:H	4:D:1108:LYS:HZ1	1.62	0.46
2:B:643:LYS:O	2:B:646:GLN:HG3	2.16	0.46
1:A:76:LYS:HE2	1:A:78:SER:HB2	1.96	0.46
4:D:412:SER:OG	4:D:555:ASN:ND2	2.46	0.46
4:D:796:LEU:HD12	4:D:853:VAL:HB	1.98	0.46
2:B:664:SER:O	2:B:667:GLN:HG2	2.16	0.46
2:B:1398:TYR:HE1	2:B:1405:LYS:HE2	1.81	0.46
1:A:472:ASP:HB3	1:A:475:ARG:HB3	1.97	0.46
2:B:363:ILE:HG13	2:B:364:VAL:H	1.80	0.46
2:B:633:LYS:O	2:B:636:THR:HB	2.16	0.46
1:A:492:GLN:HE21	1:A:496:ASN:HD21	1.63	0.46
1:A:559:ASP:OD1	1:A:559:ASP:N	2.49	0.46
1:A:1113:GLU:HA	1:A:1149:PHE:HE2	1.81	0.46
4:D:1105:GLU:HA	4:D:1108:LYS:HE2	1.98	0.46
2:B:1357:LEU:O	2:B:1384:ARG:NH1	2.49	0.45
4:D:351:HIS:O	4:D:354:GLN:HG3	2.15	0.45
3:C:33:GLU:O	3:C:36:LYS:HG3	2.16	0.45
1:A:534:ASP:OD1	1:A:534:ASP:N	2.42	0.45
1:A:718:GLN:NE2	1:A:722:ASN:OD1	2.49	0.45
1:A:1107:PRO:HA	1:A:1137:SER:HA	1.98	0.45
2:B:1363:SER:HB3	2:B:1386:ASN:HB3	1.98	0.45
4:D:730:LEU:HB3	4:D:774:LYS:HB3	1.98	0.45
1:A:144:LEU:HD21	1:A:1107:PRO:HG2	1.98	0.45
3:C:73:GLN:HG2	3:C:74:LYS:H	1.80	0.45
4:D:1020:TYR:HD1	4:D:1023:LEU:HD11	1.81	0.45
4:D:604:LEU:HA	4:D:607:CYS:SG	2.57	0.45
1:A:67:TYR:HB3	1:A:74:VAL:HB	1.98	0.45
2:B:360:ARG:HA	2:B:363:ILE:HG23	1.98	0.45
1:A:40:ASN:H	1:A:1165:SER:CB	2.30	0.45
2:B:303:GLY:O	2:B:307:ASN:ND2	2.50	0.45
2:B:757:THR:HB	2:B:761:VAL:HG23	1.99	0.45
4:D:295:SER:HB3	4:D:330:SER:HB2	1.98	0.45
1:A:498:GLU:HG3	1:A:501:LYS:HG3	1.98	0.44
2:B:652:HIS:O	2:B:655:ARG:HG2	2.16	0.44
2:B:887:PRO:O	2:B:890:GLU:HG2	2.17	0.44
1:A:1030:VAL:HA	1:A:1033:TRP:HD1	1.80	0.44
2:B:1311:MET:HB2	2:B:1317:TRP:CD2	2.51	0.44
3:C:732:THR:HB	3:C:741:ILE:HB	1.97	0.44
4:D:537:ILE:HA	4:D:540:ILE:HG22	1.99	0.44
1:A:127:VAL:O	1:A:130:LEU:HB3	2.18	0.44
1:A:144:LEU:HD23	1:A:1108:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:ILE:O	1:A:684:ASN:ND2	2.50	0.44
1:A:718:GLN:HA	1:A:721:LEU:HB3	2.00	0.44
1:A:913:GLN:O	1:A:917:HIS:N	2.44	0.44
2:B:567:GLU:O	2:B:571:GLN:NE2	2.50	0.44
1:A:49:LEU:HD23	1:A:51:ILE:HD11	1.99	0.44
1:A:462:LEU:O	1:A:466:LEU:HD23	2.18	0.44
2:B:601:LEU:O	2:B:604:LYS:HB2	2.17	0.44
2:B:604:LYS:HG2	2:B:907:LEU:HD21	1.99	0.44
2:B:776:SER:O	2:B:779:PHE:HB2	2.18	0.44
2:B:1312:PRO:HB2	2:B:1315:LYS:HD3	2.00	0.44
3:C:64:LYS:NZ	3:C:68:ASN:OD1	2.51	0.44
1:A:1110:ILE:HG12	1:A:1140:ILE:HG13	1.99	0.44
2:B:857:GLU:O	2:B:860:GLU:HG3	2.18	0.44
3:C:192:LEU:HD11	4:D:1043:LEU:HD12	2.00	0.44
4:D:967:MET:HB3	4:D:974:CYS:SG	2.58	0.44
1:A:87:ASP:OD2	1:A:89:SER:OG	2.36	0.44
1:A:454:GLN:O	1:A:457:GLU:HG3	2.18	0.44
2:B:572:ILE:HA	2:B:941:LEU:HD13	1.99	0.44
2:B:938:LEU:HA	2:B:941:LEU:HD12	2.00	0.44
3:C:215:ARG:NH1	4:D:1029:MET:SD	2.91	0.44
2:B:726:HIS:HA	2:B:729:ASP:OD2	2.17	0.43
4:D:252:VAL:HG23	4:D:300:LYS:HG3	2.00	0.43
2:B:166:SER:O	2:B:166:SER:OG	2.33	0.43
2:B:571:GLN:HA	2:B:574:LEU:HB2	2.00	0.43
2:B:637:SER:O	2:B:640:LEU:HB2	2.18	0.43
2:B:847:THR:HG23	2:B:850:GLU:H	1.83	0.43
2:B:1300:ASP:H	4:D:1126:GLN:NE2	2.16	0.43
3:C:194:ASP:OD1	3:C:195:PHE:N	2.51	0.43
4:D:243:ASN:HA	4:D:247:PHE:HD2	1.82	0.43
1:A:1073:LEU:HB2	1:A:1078:LYS:HD3	2.00	0.43
3:C:64:LYS:HG2	3:C:68:ASN:HA	2.00	0.43
4:D:280:THR:HG23	4:D:315:LEU:HD21	2.00	0.43
4:D:566:LEU:HD11	4:D:584:MET:HG2	1.99	0.43
4:D:631:ASN:HA	4:D:634:ASN:HD21	1.84	0.43
4:D:1127:LEU:O	4:D:1131:LEU:HG	2.19	0.43
2:B:196:ASP:HB2	2:B:208:LYS:NZ	2.33	0.43
2:B:1359:PHE:HA	2:B:1362:VAL:HB	2.00	0.43
1:A:578:ILE:O	2:B:820:THR:OG1	2.33	0.43
1:A:1001:LYS:HA	1:A:1001:LYS:HD3	1.93	0.43
1:A:991:GLU:OE1	1:A:995:LYS:NZ	2.52	0.43
1:A:1018:ILE:HG13	1:A:1022:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1350:MET:HE2	2:B:1380:VAL:HG12	2.00	0.43
4:D:742:ARG:O	4:D:746:LEU:HG	2.18	0.43
1:A:594:LEU:HD11	1:A:607:LEU:HD13	2.01	0.43
2:B:232:VAL:O	2:B:259:THR:HA	2.19	0.43
1:A:491:TYR:HA	1:A:494:CYS:SG	2.58	0.43
1:A:1091:LEU:HD23	1:A:1094:LEU:HD21	2.00	0.43
1:A:30:ILE:HB	1:A:1141:VAL:HB	2.00	0.43
1:A:1112:ASP:HA	1:A:1142:VAL:HG12	2.01	0.43
2:B:344:MET:HG3	2:B:1256:LEU:HD13	2.01	0.43
2:B:346:GLN:HA	2:B:349:ASN:ND2	2.32	0.43
2:B:880:LYS:HE3	2:B:880:LYS:HB3	1.91	0.43
2:B:581:LEU:O	2:B:584:GLU:HB2	2.20	0.42
1:A:40:ASN:H	1:A:1165:SER:HB3	1.85	0.42
1:A:537:ASN:HB3	1:A:544:LEU:HD11	2.00	0.42
4:D:1016:THR:HG23	4:D:1017:ASP:OD1	2.19	0.42
1:A:16:THR:N	1:A:1161:GLN:O	2.52	0.42
1:A:805:LYS:O	1:A:809:GLU:N	2.44	0.42
2:B:235:HIS:CE1	2:B:237:GLN:HB3	2.55	0.42
4:D:1027:ASN:HD22	4:D:1030:VAL:HG23	1.84	0.42
1:A:681:GLN:HA	1:A:684:ASN:ND2	2.34	0.42
2:B:892:GLN:O	2:B:895:LYS:HG3	2.20	0.42
4:D:429:HIS:O	4:D:432:LYS:NZ	2.53	0.42
1:A:452:VAL:O	1:A:456:GLN:HG2	2.20	0.42
4:D:170:SER:HA	4:D:173:LYS:HD2	2.02	0.42
4:D:394:LYS:HA	4:D:394:LYS:HD2	1.87	0.42
1:A:198:LEU:O	1:A:201:GLU:HG3	2.19	0.42
2:B:151:GLN:HB3	2:B:152:SER:H	1.64	0.42
2:B:157:ASN:HB2	2:B:237:GLN:HE22	1.85	0.42
4:D:522:LYS:O	4:D:525:LEU:HG	2.20	0.42
1:A:81:ILE:HB	1:A:130:LEU:HG	2.01	0.42
1:A:770:LYS:O	1:A:774:GLU:N	2.41	0.42
2:B:640:LEU:O	2:B:643:LYS:HG2	2.20	0.42
2:B:678:ARG:HA	2:B:678:ARG:HD2	1.90	0.42
2:B:1295:LEU:HD13	2:B:1306:VAL:HG22	2.02	0.42
3:C:186:PRO:O	3:C:190:LYS:HG2	2.20	0.41
1:A:21:THR:O	1:A:1154:ARG:NH2	2.53	0.41
1:A:40:ASN:ND2	1:A:1165:SER:HB2	2.35	0.41
1:A:173:MET:SD	1:A:173:MET:N	2.93	0.41
1:A:1098:MET:HE3	1:A:1098:MET:HB3	1.86	0.41
1:A:144:LEU:HD11	1:A:1107:PRO:HD2	2.01	0.41
1:A:466:LEU:HG	1:A:721:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:LYS:HZ1	1:A:518:PHE:HB3	1.85	0.41
4:D:263:ASP:O	4:D:266:ASN:ND2	2.54	0.41
4:D:672:TYR:HB2	4:D:707:LEU:HD11	2.01	0.41
4:D:789:TYR:O	4:D:793:GLU:HG2	2.20	0.41
1:A:40:ASN:HB2	1:A:1165:SER:H	1.85	0.41
1:A:1005:LYS:O	1:A:1008:GLU:HG3	2.21	0.41
4:D:862:GLU:O	4:D:865:GLU:HG3	2.20	0.41
4:D:1104:LYS:HA	4:D:1104:LYS:HD2	1.93	0.41
1:A:38:LYS:NZ	1:A:1156:PHE:O	2.48	0.41
1:A:1013:LYS:HE2	3:C:54:ILE:HB	2.01	0.41
2:B:1400:ARG:NH2	3:C:729:LEU:O	2.52	0.41
1:A:668:GLY:H	2:B:732:ARG:NE	2.10	0.41
1:A:1104:ARG:HA	1:A:1104:ARG:HD2	1.88	0.41
4:D:534:ILE:O	4:D:537:ILE:HG22	2.21	0.41
1:A:3:VAL:HG23	1:A:83:PHE:CE1	2.55	0.41
1:A:144:LEU:HG	1:A:1106:ALA:HB1	2.02	0.41
1:A:1028:THR:HG21	3:C:72:PHE:HE2	1.85	0.41
2:B:1323:LEU:O	2:B:1328:LYS:NZ	2.52	0.41
1:A:116:LEU:HA	1:A:120:HIS:O	2.21	0.41
1:A:1009:LYS:HD2	1:A:1009:LYS:HA	1.92	0.41
1:A:1091:LEU:O	1:A:1094:LEU:HG	2.21	0.41
2:B:185:GLY:HA2	3:C:721:LEU:HD13	2.03	0.41
3:C:712:SER:OG	3:C:713:THR:N	2.54	0.41
1:A:472:ASP:H	1:A:475:ARG:HH21	1.67	0.41
1:A:1006:THR:HG23	3:C:49:TRP:CZ2	2.56	0.41
4:D:109:LYS:O	4:D:112:LEU:HG	2.21	0.41
4:D:227:VAL:HG21	4:D:261:LEU:HD21	2.03	0.41
1:A:1128:HIS:O	1:A:1132:THR:HG23	2.22	0.40
2:B:226:SER:O	2:B:226:SER:OG	2.36	0.40
2:B:887:PRO:HA	2:B:890:GLU:HG2	2.03	0.40
1:A:149:LYS:HA	1:A:149:LYS:HD3	1.91	0.40
2:B:667:GLN:HG3	2:B:671:LYS:NZ	2.36	0.40
4:D:706:ILE:HD12	4:D:709:MET:HE3	2.03	0.40
4:D:1054:GLY:O	4:D:1058:LYS:HG2	2.21	0.40
2:B:162:GLU:OE2	2:B:163:ASN:ND2	2.54	0.40
3:C:710:ASP:OD1	3:C:710:ASP:N	2.53	0.40
3:C:48:SER:HB3	3:C:89:ARG:HE	1.86	0.40
4:D:1124:GLN:O	4:D:1128:ASN:ND2	2.54	0.40
1:A:15:ALA:HB1	1:A:1160:PHE:CA	2.51	0.40
1:A:715:LYS:HA	1:A:715:LYS:HD3	1.94	0.40
2:B:259:THR:OG1	2:B:271:TYR:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:LYS:HE2	2:B:1302:PHE:CZ	2.57	0.40
2:B:600:ILE:HA	2:B:603:LYS:HE2	2.04	0.40
3:C:651:LYS:NZ	3:C:719:CYS:O	2.54	0.40
4:D:198:ARG:HE	4:D:239:SER:HB3	1.87	0.40
4:D:310:LEU:HD13	4:D:338:ILE:HG21	2.04	0.40
4:D:1121:GLU:OE2	4:D:1123:HIS:HB2	2.22	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	1105/1178 (94%)	1050 (95%)	55 (5%)	0	100	100
2	B	1181/1418 (83%)	1154 (98%)	27 (2%)	0	100	100
3	C	204/773 (26%)	197 (97%)	7 (3%)	0	100	100
4	D	819/1185 (69%)	791 (97%)	27 (3%)	1 (0%)	48	83
All	All	3309/4554 (73%)	3192 (96%)	116 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	347	GLN

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	579/1071 (54%)	579 (100%)	0	100	100
2	B	655/1301 (50%)	655 (100%)	0	100	100
3	C	198/688 (29%)	198 (100%)	0	100	100
4	D	745/1072 (70%)	745 (100%)	0	100	100
All	All	2177/4132 (53%)	2177 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	40	ASN
1	A	63	GLN
1	A	100	GLN
1	A	129	GLN
1	A	489	HIS
1	A	496	ASN
1	A	558	GLN
1	A	610	ASN
1	A	684	ASN
1	A	694	GLN
1	A	705	GLN
1	A	1022	ASN
1	A	1075	ASN
1	A	1124	GLN
2	B	163	ASN
2	B	266	ASN
2	B	288	ASN
2	B	307	ASN
2	B	571	GLN
2	B	586	GLN
2	B	608	GLN
2	B	622	ASN
2	B	725	GLN
2	B	749	GLN
2	B	791	ASN
2	B	873	HIS
2	B	930	GLN
2	B	937	ASN

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Mol	Chain	Res	Type
3	C	725	ASN
3	C	730	GLN
4	D	83	ASN
4	D	91	ASN
4	D	97	ASN
4	D	220	GLN
4	D	269	GLN
4	D	312	GLN
4	D	351	HIS
4	D	380	GLN
4	D	454	GLN
4	D	549	ASN
4	D	586	HIS
4	D	634	ASN
4	D	649	GLN
4	D	666	ASN
4	D	673	ASN
4	D	786	ASN
4	D	909	ASN
4	D	1027	ASN
4	D	1031	GLN
4	D	1046	GLN
4	D	1124	GLN
4	D	1126	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 ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2264:UNK	C	2266:UNK	N	11.43

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10951. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.