



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 11:21 AM UTC

PDB ID : 7D7C / pdb_00007d7c
EMDB ID : EMD-30604
Title : CryoEM structure of gp55-dependent RNA polymerase-promoter open complex
Authors : Shi, J.; Wen, A.; Jin, S.; Feng, Y.
Deposited on : 2020-10-03
Resolution : 3.60 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
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

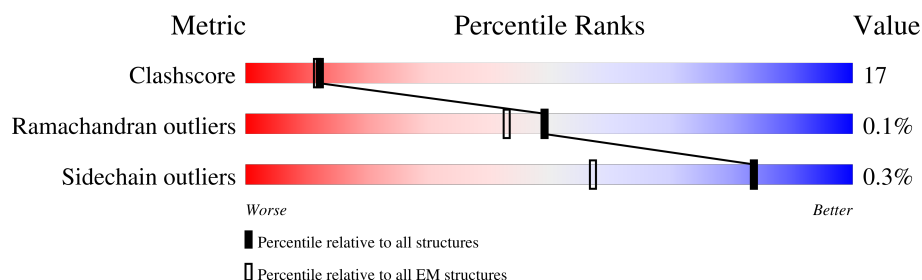
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	329	41% 26% 33%
1	B	329	40% 26% 34%
2	C	1342	63% 35% .
3	D	1407	60% 34% 5%
4	T	59	8% 31% 61%
5	F	185	43% 30% . 26%
6	N	59	8% 34% 58%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26249 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	219	Total	C	N	O	S	0	0
			1686	1056	298	326	6		
1	B	218	Total	C	N	O	S	0	0
			1681	1050	297	328	6		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1316	Total	C	N	O	S	0	0
			10381	6514	1810	2014	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1335	Total	C	N	O	S	0	0
			10384	6524	1851	1959	50		

- Molecule 4 is a DNA chain called DNA (template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	23	Total	C	N	O	P	0	0
			467	225	75	144	23		

- Molecule 5 is a protein called gp55.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	137	Total	C	N	O	S	0	0
			1128	720	189	214	5		

- Molecule 6 is a DNA chain called DNA (nontemplate strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	25	Total	C	N	O	P	0	0
			519	246	105	143	25		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total	Mg	0
			1	1	

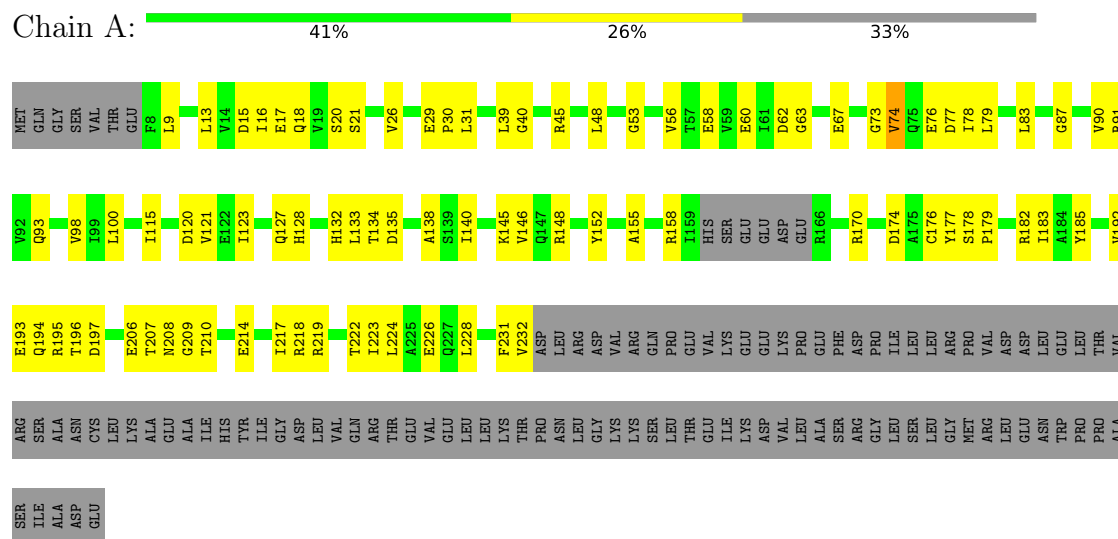
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	D	2	Total	Zn	0
			2	2	

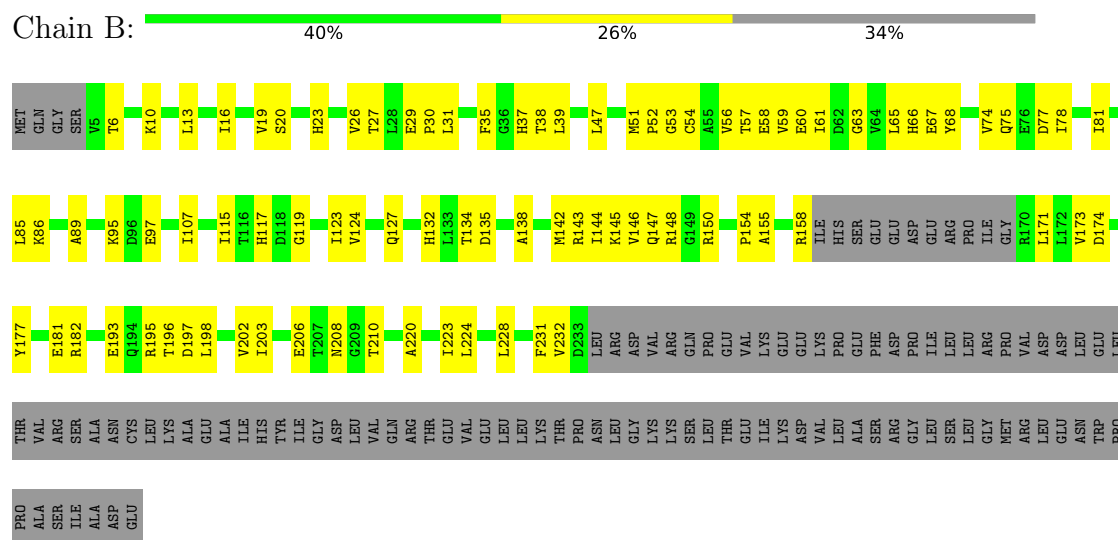
3 Residue-property plots

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. 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. 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: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

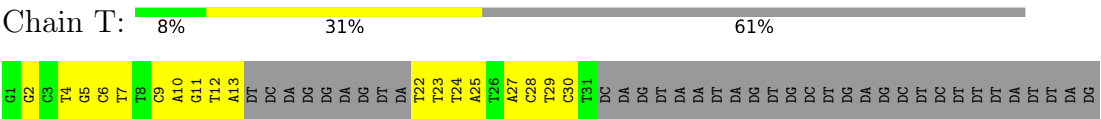


- Molecule 2: DNA-directed RNA polymerase subunit beta

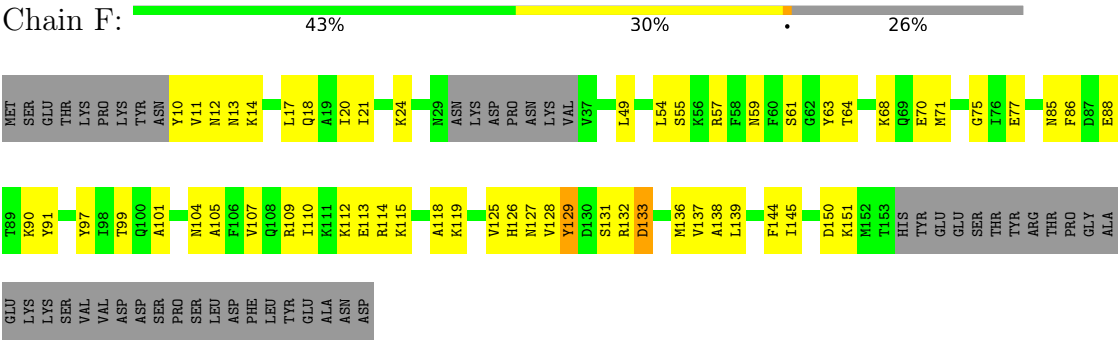




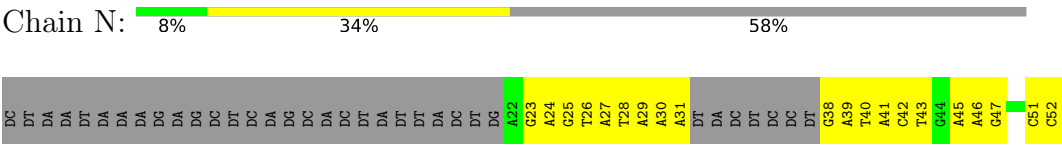
- Molecule 4: DNA (template strand)



• Molecule 5: gp55



• Molecule 6: DNA (nontemplate strand)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57776	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.37	0/1706	0.50	0/2312
1	B	0.30	0/1700	0.46	0/2304
2	C	0.36	0/10547	0.49	1/14232 (0.0%)
3	D	0.33	0/10541	0.48	3/14232 (0.0%)
4	T	0.30	0/519	0.48	0/796
5	F	0.30	0/1149	0.50	0/1546
6	N	0.30	0/584	0.41	0/897
All	All	0.34	0/26746	0.48	4/36319 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	503	SER	CA-C-N	-5.86	111.32	121.52
3	D	503	SER	C-N-CA	-5.86	111.32	121.52
2	C	162	GLY	N-CA-C	5.34	116.59	111.67
3	D	839	VAL	N-CA-C	-5.12	108.29	113.20

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	1686	0	1726	58	0
1	B	1681	0	1714	68	0
2	C	10381	0	10392	366	0
3	D	10384	0	10608	373	0
4	T	467	0	265	14	0
5	F	1128	0	1105	62	0
6	N	519	0	281	28	0
7	D	1	0	0	0	0
8	D	2	0	0	0	0
All	All	26249	0	26091	892	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 17.

All (892) 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)
3:D:1161:GLY:HA3	3:D:1178:THR:O	1.43	1.15
3:D:556:GLU:O	3:D:563:LEU:HA	1.64	0.98
3:D:1087:ASP:HB3	3:D:1096:PRO:HG2	1.50	0.93
2:C:589:THR:HG23	2:C:591:TYR:CE2	2.07	0.90
2:C:105:TYR:HA	2:C:114:VAL:HA	1.62	0.82
3:D:201:LEU:HD22	3:D:217:LEU:HD11	1.61	0.82
3:D:1344:LEU:HD23	3:D:1349:GLU:HB2	1.64	0.80
1:A:155:ALA:HA	1:A:158:ARG:HH21	1.47	0.78
2:C:183:TRP:H	6:N:38:DG:H1	1.33	0.77
3:D:1287:ILE:HG22	3:D:1290:ARG:HH21	1.49	0.76
2:C:267:ARG:NH1	2:C:268:ARG:O	2.18	0.76
3:D:126:LEU:HD11	3:D:223:LEU:HD13	1.69	0.76
3:D:848:VAL:HG12	3:D:858:VAL:HG12	1.69	0.75
3:D:702:GLN:HG3	3:D:703:THR:HG23	1.68	0.75
2:C:250:THR:HA	2:C:268:ARG:HA	1.68	0.74
2:C:595:THR:HG22	2:C:596:ASP:H	1.51	0.74
3:D:44:ILE:HB	5:F:119:LYS:HD2	1.68	0.74
2:C:1214:ASP:OD1	2:C:1215:GLY:N	2.20	0.73
5:F:125:VAL:HG13	5:F:126:HIS:HD2	1.51	0.73
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.69	0.73
3:D:741:ALA:O	3:D:762:ASN:ND2	2.20	0.73
2:C:57:PHE:HD2	2:C:70:TYR:HB2	1.52	0.73
3:D:1040:MET:HB3	3:D:1046:ILE:HD13	1.70	0.73
5:F:63:TYR:OH	5:F:71:MET:SD	2.46	0.73
1:B:16:ILE:HG12	1:B:26:VAL:HG23	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1039:ASP:OD1	3:D:1079:LYS:NZ	2.21	0.73
3:D:1093:THR:HG22	3:D:1095:MET:H	1.53	0.73
1:B:195:ARG:HD2	1:B:198:LEU:HD21	1.71	0.72
2:C:199:ASP:HA	6:N:38:DG:H21	1.54	0.72
2:C:211:ARG:HH22	2:C:217:THR:HG1	1.37	0.72
2:C:731:ARG:HH12	2:C:958:LYS:HD2	1.54	0.72
3:D:871:LEU:O	3:D:875:ASN:ND2	2.22	0.72
2:C:699:LEU:HB2	2:C:799:ASN:HD22	1.54	0.72
2:C:1005:GLU:HB3	2:C:1007:LYS:HG2	1.72	0.72
1:A:196:THR:HG22	1:A:197:ASP:H	1.55	0.71
2:C:211:ARG:NH2	2:C:217:THR:OG1	2.22	0.71
1:B:95:LYS:HZ2	1:B:97:GLU:H	1.37	0.71
2:C:811:ASN:ND2	2:C:1098:LEU:O	2.24	0.71
2:C:667:LEU:HA	2:C:702:THR:HG21	1.72	0.71
3:D:527:LEU:HD21	3:D:536:LEU:HD12	1.73	0.71
2:C:685:MET:SD	2:C:1073:LYS:NZ	2.61	0.70
2:C:1269:ARG:NH1	3:D:344:GLY:O	2.23	0.70
3:D:274:ASN:ND2	5:F:70:GLU:OE1	2.24	0.70
1:B:61:ILE:HD13	1:B:142:MET:HB3	1.74	0.70
2:C:1080:ASN:ND2	2:C:1085:MET:SD	2.59	0.70
5:F:125:VAL:HG13	5:F:126:HIS:CD2	2.26	0.70
2:C:589:THR:CG2	2:C:591:TYR:CE2	2.75	0.69
2:C:823:VAL:HG22	2:C:1059:ARG:HH21	1.55	0.69
2:C:104:ILE:O	2:C:115:LYS:N	2.26	0.69
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.24	0.69
3:D:1034:PHE:N	3:D:1081:VAL:O	2.24	0.69
2:C:60:GLN:HG2	2:C:67:GLU:HG3	1.72	0.69
2:C:1246:ARG:NH1	2:C:1265:PHE:O	2.25	0.69
3:D:137:ARG:NH1	3:D:143:SER:OG	2.26	0.69
3:D:1153:PRO:O	3:D:1194:ARG:NH2	2.26	0.69
2:C:721:GLY:N	2:C:740:GLU:OE1	2.24	0.69
2:C:1072:ASN:ND2	2:C:1111:GLN:OE1	2.25	0.69
3:D:805:GLN:HE21	3:D:1348:LYS:H	1.40	0.68
3:D:1163:VAL:HB	3:D:1200:GLU:HA	1.75	0.68
2:C:1005:GLU:HG2	2:C:1006:GLU:HG3	1.75	0.68
4:T:12:DT:H2'	4:T:13:DA:C8	2.29	0.68
3:D:68:TYR:HA	3:D:92:VAL:HG13	1.76	0.68
2:C:633:LEU:HB3	2:C:644:LEU:HD22	1.76	0.68
2:C:772:SER:N	2:C:775:GLU:OE2	2.24	0.67
3:D:596:LEU:HD22	3:D:601:ILE:HG22	1.75	0.67
1:B:23:HIS:HB2	1:B:206:GLU:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:393:THR:HG23	3:D:396:ALA:H	1.60	0.67
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.76	0.66
2:C:349:GLU:N	2:C:349:GLU:OE1	2.27	0.66
3:D:30:ILE:HD13	3:D:243:PRO:HD3	1.76	0.66
2:C:91:THR:O	2:C:91:THR:HG23	1.93	0.66
3:D:1176:VAL:HG23	3:D:1187:GLU:HG3	1.77	0.66
2:C:36:GLN:NE2	2:C:40:GLU:OE2	2.28	0.66
2:C:3:TYR:O	2:C:8:LYS:NZ	2.29	0.65
2:C:122:VAL:HG11	2:C:493:ILE:HG21	1.78	0.65
1:A:15:ASP:OD1	1:A:16:ILE:N	2.29	0.65
3:D:270:ARG:NH2	5:F:113:GLU:OE1	2.30	0.65
1:B:154:PRO:O	1:B:158:ARG:NH1	2.30	0.65
3:D:62:PHE:O	3:D:101:ARG:NE	2.29	0.64
3:D:413:ASP:O	3:D:417:ARG:NH2	2.30	0.64
2:C:620:ASN:HD21	3:D:768:ASN:HB2	1.62	0.64
2:C:106:GLU:HA	2:C:115:LYS:HE3	1.80	0.64
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.30	0.64
1:B:77:ASP:OD1	1:B:78:ILE:N	2.31	0.64
1:B:75:GLN:OE1	1:B:132:HIS:ND1	2.31	0.64
3:D:144:TYR:HB2	3:D:160:LEU:HB2	1.80	0.64
3:D:1035:VAL:O	3:D:1036:ARG:NH1	2.28	0.64
1:A:193:GLU:HG3	1:A:194:GLN:H	1.63	0.64
3:D:1071:GLY:HA2	3:D:1074:LEU:HB3	1.79	0.64
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.80	0.64
2:C:233:ARG:HG3	2:C:238:GLN:HB2	1.80	0.64
3:D:825:VAL:HG13	3:D:832:LYS:HB2	1.80	0.64
2:C:290:GLU:OE1	2:C:290:GLU:N	2.31	0.63
3:D:495:ASN:ND2	3:D:1247:LYS:O	2.30	0.63
3:D:1075:ARG:NH2	3:D:1168:GLU:OE1	2.31	0.63
3:D:1090:ILE:HG12	3:D:1096:PRO:HA	1.80	0.63
3:D:1175:LEU:HD13	3:D:1190:ILE:HD12	1.81	0.63
4:T:22:DT:H2"	4:T:23:DT:C2	2.34	0.63
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.80	0.63
2:C:675:ASP:OD2	2:C:676:ALA:N	2.30	0.63
2:C:84:GLU:OE1	2:C:84:GLU:N	2.25	0.62
2:C:1119:MET:HE2	2:C:1204:LEU:HD13	1.80	0.62
3:D:812:ASP:O	3:D:897:HIS:ND1	2.32	0.62
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.81	0.62
2:C:165:HIS:ND1	2:C:167:SER:OG	2.28	0.62
2:C:618:GLN:HE21	3:D:769:VAL:HB	1.64	0.62
3:D:235:GLU:OE1	3:D:235:GLU:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:874:GLU:OE2	3:D:875:ASN:ND2	2.32	0.62
3:D:1237:VAL:HG11	3:D:1253:ILE:HG21	1.80	0.62
2:C:560:PRO:HB2	3:D:776:THR:HG21	1.81	0.62
3:D:1219:ASP:HA	3:D:1222:ARG:HE	1.65	0.62
2:C:937:ASP:HB2	2:C:1039:GLY:HA3	1.81	0.62
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.82	0.62
3:D:638:SER:OG	3:D:639:VAL:N	2.32	0.62
1:A:53:GLY:HA3	1:A:177:TYR:HB3	1.82	0.62
2:C:528:ARG:HH21	2:C:577:VAL:HA	1.65	0.62
3:D:964:LYS:HG2	3:D:977:SER:HB2	1.80	0.61
2:C:576:SER:OG	2:C:577:VAL:N	2.33	0.61
3:D:826:ILE:HG22	3:D:828:GLY:H	1.65	0.61
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.80	0.61
2:C:183:TRP:N	6:N:38:DG:H22	1.98	0.61
2:C:365:GLU:HA	2:C:368:ARG:HH11	1.64	0.61
3:D:111:THR:O	3:D:239:LEU:N	2.30	0.61
3:D:44:ILE:O	5:F:119:LYS:NZ	2.34	0.61
3:D:1293:GLU:OE2	3:D:1299:GLY:N	2.33	0.61
2:C:213:LEU:O	2:C:422:LYS:NZ	2.25	0.61
3:D:804:ALA:O	3:D:806:ASP:N	2.32	0.61
3:D:450:HIS:HD2	3:D:452:LEU:H	1.47	0.60
3:D:1034:PHE:HB3	3:D:1036:ARG:NH1	2.16	0.60
2:C:674:ASP:OD1	2:C:675:ASP:N	2.32	0.60
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.34	0.60
2:C:975:ILE:HG21	2:C:997:TRP:HB3	1.83	0.60
3:D:515:ARG:HH22	3:D:717:VAL:HG22	1.67	0.60
5:F:24:LYS:NZ	5:F:88:GLU:OE1	2.33	0.60
2:C:735:LYS:HA	2:C:748:ILE:HG22	1.82	0.60
3:D:1177:ILE:HD13	3:D:1186:TYR:HD2	1.67	0.60
3:D:1305:ASP:OD1	3:D:1306:LEU:N	2.35	0.60
1:B:19:VAL:HB	1:B:23:HIS:HD2	1.67	0.60
5:F:14:LYS:NZ	5:F:18:GLN:OE1	2.29	0.60
2:C:1168:GLU:N	2:C:1168:GLU:OE1	2.35	0.60
3:D:233:LYS:NZ	3:D:235:GLU:OE2	2.33	0.60
1:B:155:ALA:N	1:B:174:ASP:OD1	2.32	0.60
3:D:883:ARG:NH2	3:D:898:CYS:SG	2.70	0.60
3:D:1061:VAL:HG11	3:D:1076:PRO:HG3	1.84	0.60
2:C:988:LYS:O	2:C:988:LYS:NZ	2.29	0.59
3:D:950:ILE:HB	3:D:1017:VAL:HG22	1.84	0.59
3:D:275:ARG:HH11	3:D:302:ALA:HB2	1.67	0.59
2:C:947:GLU:O	2:C:951:MET:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:297:ARG:NH1	3:D:298:MET:SD	2.75	0.59
2:C:728:ASP:OD1	2:C:729:ALA:N	2.35	0.59
2:C:618:GLN:HE22	3:D:770:LEU:H	1.50	0.59
3:D:108:ALA:HB3	3:D:279:LEU:HD23	1.83	0.59
2:C:1032:LYS:O	2:C:1036:ILE:HG12	2.03	0.59
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.84	0.59
2:C:1103:VAL:HG21	2:C:1112:ILE:HD11	1.85	0.59
1:B:95:LYS:O	1:B:148:ARG:NH2	2.36	0.59
2:C:840:SER:HA	2:C:886:LYS:NZ	2.18	0.59
1:A:45:ARG:HE	1:B:38:THR:HB	1.68	0.59
1:A:91:ARG:HG2	1:A:93:GLN:HE21	1.66	0.59
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.35	0.59
2:C:1035:LYS:HA	2:C:1038:GLN:HE21	1.67	0.59
3:D:1180:VAL:HG11	3:D:1203:ARG:HH11	1.67	0.59
2:C:1340:GLU:HG2	2:C:1341:ASP:H	1.67	0.58
3:D:746:LEU:HG	3:D:758:PRO:HB3	1.85	0.58
2:C:575:LEU:HD21	2:C:579:ALA:HB3	1.85	0.58
2:C:672:GLU:N	2:C:672:GLU:OE1	2.35	0.58
1:A:58:GLU:HG2	1:A:145:LYS:HB3	1.85	0.58
2:C:189:ASP:OD1	2:C:190:PRO:HD2	2.04	0.58
2:C:207:THR:HA	2:C:210:LEU:HD12	1.85	0.58
2:C:1222:GLU:OE1	2:C:1222:GLU:N	2.25	0.58
1:A:214:GLU:OE1	1:A:218:ARG:NE	2.37	0.58
2:C:18:ARG:HE	2:C:620:ASN:HA	1.69	0.58
2:C:596:ASP:OD1	2:C:596:ASP:N	2.35	0.58
2:C:1137:GLU:N	2:C:1137:GLU:OE1	2.36	0.58
3:D:515:ARG:NH2	3:D:718:SER:O	2.36	0.58
2:C:159:SER:HB2	2:C:442:VAL:HG11	1.86	0.58
2:C:980:VAL:HA	2:C:984:VAL:HB	1.84	0.58
5:F:101:ALA:HA	6:N:26:DT:H3	1.68	0.58
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.86	0.58
3:D:51:PRO:HB2	3:D:58:CYS:HA	1.85	0.58
3:D:980:THR:OG1	3:D:997:VAL:O	2.22	0.58
3:D:1004:ALA:N	3:D:1017:VAL:O	2.26	0.58
3:D:1321:SER:OG	3:D:1349:GLU:OE1	2.22	0.58
1:A:60:GLU:HG2	1:A:170:ARG:HA	1.86	0.57
2:C:245:ARG:HD3	2:C:337:PHE:CG	2.39	0.57
3:D:1080:ILE:HD11	3:D:1097:ALA:H	1.69	0.57
2:C:188:PHE:HE2	2:C:436:ARG:HB2	1.69	0.57
3:D:425:ARG:NH2	3:D:464:ASP:OD2	2.27	0.57
3:D:1080:ILE:HD12	3:D:1088:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:254:PRO:HG2	3:D:261:ALA:HB3	1.86	0.57
1:A:155:ALA:N	1:A:174:ASP:OD1	2.38	0.57
2:C:301:TYR:OH	2:C:334:GLU:N	2.33	0.57
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.86	0.57
3:D:975:ILE:O	3:D:1000:GLY:HA2	2.05	0.57
3:D:1205:GLU:N	3:D:1208:ASP:OD2	2.31	0.57
1:A:226:GLU:HG2	1:B:10:LYS:HE3	1.86	0.57
1:B:181:GLU:OE1	3:D:535:ARG:NH1	2.36	0.57
2:C:601:ASP:OD1	2:C:601:ASP:N	2.37	0.57
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.86	0.57
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.33	0.57
3:D:132:LEU:HB3	3:D:133:ARG:NH2	2.19	0.57
3:D:414:GLU:HA	3:D:417:ARG:HH21	1.70	0.57
3:D:516:ASP:OD1	3:D:516:ASP:N	2.36	0.57
1:A:182:ARG:NH2	1:A:206:GLU:OE1	2.38	0.56
2:C:258:ASN:ND2	2:C:262:TYR:OH	2.38	0.56
5:F:129:TYR:N	5:F:129:TYR:CD2	2.73	0.56
1:B:19:VAL:HB	1:B:23:HIS:CD2	2.40	0.56
2:C:884:VAL:HG11	2:C:1050:VAL:HG11	1.87	0.56
2:C:232:ILE:HB	2:C:331:LYS:HD3	1.87	0.56
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.87	0.56
2:C:1240:ASP:OD1	2:C:1240:ASP:O	2.22	0.56
3:D:475:GLU:N	3:D:475:GLU:OE1	2.38	0.56
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.88	0.56
3:D:312:ARG:HD3	3:D:313:GLY:H	1.70	0.56
4:T:25:DA:OP2	5:F:114:ARG:NH2	2.38	0.56
2:C:1106:ARG:O	2:C:1108:ASN:N	2.37	0.56
3:D:129:ASP:OD1	3:D:220:ARG:NH1	2.38	0.56
3:D:816:THR:OG1	3:D:818:GLU:OE1	2.20	0.56
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.86	0.56
1:A:13:LEU:HG	1:B:231:PHE:CE1	2.41	0.56
3:D:511:TYR:OH	3:D:515:ARG:NH1	2.39	0.56
2:C:350:THR:HA	2:C:353:VAL:HG12	1.88	0.55
3:D:512:TYR:HD1	3:D:724:MET:HE1	1.71	0.55
3:D:1079:LYS:HA	3:D:1098:GLN:HG3	1.88	0.55
3:D:1238:GLN:O	3:D:1242:ARG:HB2	2.06	0.55
2:C:247:ARG:HA	2:C:274:ILE:HG13	1.88	0.55
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.87	0.55
5:F:57:ARG:HD3	5:F:59:ASN:HD21	1.72	0.55
5:F:63:TYR:HD2	5:F:64:THR:HG22	1.71	0.55
2:C:813:GLU:HB2	3:D:461:PHE:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1070:HIS:NE2	2:C:1114:GLU:OE1	2.35	0.55
2:C:949:GLU:O	2:C:953:LEU:HG	2.06	0.55
5:F:14:LYS:HZ3	5:F:17:LEU:HB2	1.71	0.55
1:B:26:VAL:HG12	1:B:203:ILE:HB	1.87	0.55
5:F:10:TYR:OH	6:N:31:DA:N7	2.39	0.55
2:C:64:GLY:HA2	2:C:107:ARG:HH12	1.72	0.55
3:D:425:ARG:HG2	3:D:426:ALA:H	1.72	0.55
3:D:1358:PRO:HB3	3:D:1366:HIS:ND1	2.21	0.55
2:C:253:PHE:HZ	2:C:285:ILE:HD12	1.72	0.54
3:D:201:LEU:HB2	3:D:221:ILE:HD13	1.89	0.54
1:A:77:ASP:OD1	1:A:78:ILE:N	2.40	0.54
2:C:224:PHE:CD1	2:C:347:ILE:HG13	2.42	0.54
3:D:1049:GLN:HB3	3:D:1058:SER:O	2.07	0.54
3:D:1156:LEU:HD22	3:D:1223:LEU:HD12	1.90	0.54
2:C:106:GLU:N	2:C:113:THR:O	2.40	0.54
1:B:97:GLU:HB2	1:B:147:GLN:HA	1.89	0.54
2:C:932:GLN:HB2	2:C:1051:LYS:HB2	1.89	0.54
1:B:107:ILE:HG23	1:B:134:THR:HA	1.90	0.54
2:C:618:GLN:NE2	3:D:770:LEU:H	2.05	0.54
1:B:56:VAL:HG22	1:B:146:VAL:HG12	1.89	0.54
3:D:712:GLN:N	3:D:712:GLN:OE1	2.40	0.54
1:B:31:LEU:HD23	1:B:35:PHE:HB3	1.89	0.54
2:C:189:ASP:HB2	2:C:195:PHE:HE2	1.73	0.54
2:C:517:GLN:OE1	2:C:760:ASN:ND2	2.39	0.54
3:D:644:MET:HB2	3:D:764:ARG:HD2	1.90	0.54
5:F:144:PHE:HD1	5:F:145:ILE:HD13	1.73	0.54
3:D:974:VAL:HB	3:D:1002:VAL:HG12	1.89	0.53
1:A:67:GLU:HB3	1:A:79:LEU:HD13	1.89	0.53
2:C:545:PHE:HZ	3:D:781:LYS:HG3	1.73	0.53
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.08	0.53
1:B:31:LEU:HD21	1:B:39:LEU:HD12	1.90	0.53
2:C:72:SER:OG	2:C:73:TYR:N	2.41	0.53
1:A:83:LEU:HD23	2:C:694:ARG:HH22	1.72	0.53
2:C:615:VAL:HG23	2:C:650:VAL:HA	1.89	0.53
3:D:1089:LEU:HA	3:D:1096:PRO:HG3	1.90	0.53
2:C:229:ILE:HD12	2:C:334:GLU:HG3	1.91	0.53
2:C:1237:HIS:HB3	2:C:1242:LYS:NZ	2.24	0.53
3:D:515:ARG:HG2	3:D:516:ASP:H	1.72	0.53
3:D:839:VAL:HG22	3:D:864:LEU:HD12	1.90	0.53
3:D:1321:SER:O	3:D:1324:SER:OG	2.26	0.53
1:B:61:ILE:HG22	1:B:63:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:232:ILE:HG12	2:C:331:LYS:HA	1.90	0.53
3:D:309:ASN:OD1	3:D:310:GLY:N	2.41	0.53
3:D:516:ASP:HB3	3:D:573:THR:HG21	1.91	0.53
3:D:741:ALA:C	3:D:762:ASN:HD22	2.17	0.53
3:D:767:LEU:H	3:D:767:LEU:HD12	1.74	0.53
1:A:17:GLU:N	1:A:17:GLU:OE2	2.42	0.53
2:C:915:ASP:OD1	2:C:916:SER:N	2.42	0.52
2:C:180:ARG:NH1	2:C:393:ASP:O	2.42	0.52
2:C:347:ILE:O	2:C:350:THR:OG1	2.26	0.52
2:C:272:ARG:HH21	2:C:273:HIS:CE1	2.26	0.52
2:C:815:SER:HB3	2:C:1077:SER:HB3	1.90	0.52
3:D:975:ILE:O	3:D:1000:GLY:CA	2.57	0.52
5:F:61:SER:HA	5:F:68:LYS:NZ	2.25	0.52
3:D:554:GLU:OE2	3:D:570:LYS:NZ	2.35	0.52
3:D:1327:GLU:OE2	3:D:1330:ARG:NH1	2.42	0.52
2:C:158:ASP:OD2	2:C:159:SER:N	2.43	0.52
2:C:148:GLN:O	2:C:453:ILE:HA	2.10	0.52
2:C:808:ASN:H	3:D:633:ALA:HB2	1.74	0.52
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.10	0.52
3:D:543:SER:OG	3:D:544:LEU:N	2.42	0.52
3:D:705:THR:CG2	3:D:718:SER:HA	2.39	0.52
3:D:1272:SER:OG	3:D:1273:ASP:N	2.41	0.52
1:A:26:VAL:HG11	1:A:217:ILE:HD12	1.90	0.52
2:C:573:ASN:OD1	2:C:573:ASN:N	2.42	0.52
2:C:236:LYS:HZ2	2:C:289:VAL:H	1.55	0.52
3:D:342:LEU:HB3	3:D:1352:ILE:HD12	1.92	0.52
3:D:514:THR:HG21	3:D:596:LEU:HD12	1.91	0.52
3:D:1263:LYS:NZ	3:D:1281:GLU:OE1	2.29	0.52
2:C:83:GLN:H	2:C:83:GLN:CD	2.18	0.52
3:D:850:LYS:C	3:D:852:GLY:H	2.17	0.52
3:D:1178:THR:HA	3:D:1184:ASP:HB3	1.90	0.52
4:T:11:DG:H2'	4:T:12:DT:C6	2.45	0.52
1:B:78:ILE:HA	1:B:81:ILE:HD12	1.92	0.51
3:D:394:ILE:O	3:D:398:LYS:HG3	2.09	0.51
3:D:786:THR:O	3:D:790:THR:HG23	2.10	0.51
3:D:1031:VAL:HG22	3:D:1032:SER:H	1.75	0.51
5:F:57:ARG:HD3	5:F:59:ASN:ND2	2.25	0.51
3:D:520:ALA:HB3	3:D:546:ALA:HB2	1.91	0.51
4:T:27:DA:N6	5:F:104:ASN:HB3	2.25	0.51
1:A:219:ARG:O	1:A:222:THR:OG1	2.24	0.51
2:C:348:SER:OG	2:C:349:GLU:OE1	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:992:LEU:HD23	2:C:996:ARG:HG2	1.93	0.51
2:C:1257:GLN:HG2	2:C:1296:ASP:OD1	2.11	0.51
2:C:175:ARG:HH22	2:C:200:ARG:HD3	1.76	0.51
2:C:207:THR:HG21	2:C:354:ASP:HB2	1.92	0.51
2:C:921:PRO:HA	5:F:133:ASP:HB2	1.93	0.51
2:C:1006:GLU:O	2:C:1010:GLN:HG2	2.09	0.51
3:D:665:GLN:NE2	3:D:678:ARG:HD2	2.26	0.51
1:A:179:PRO:O	1:A:207:THR:OG1	2.20	0.51
1:B:115:ILE:HD11	1:B:144:ILE:HD11	1.92	0.51
2:C:1297:ASP:OD2	2:C:1319:MET:N	2.44	0.51
3:D:1145:PHE:CE1	3:D:1256:ILE:HG21	2.46	0.51
1:A:48:LEU:HG	1:A:183:ILE:HD12	1.93	0.51
2:C:183:TRP:H	6:N:38:DG:H22	1.56	0.51
2:C:232:ILE:HD13	2:C:237:LEU:HD11	1.92	0.51
2:C:818:VAL:HG22	2:C:1096:ILE:HG12	1.92	0.51
2:C:1066:MET:HE3	2:C:1076:ILE:HB	1.92	0.51
3:D:362:ARG:O	3:D:450:HIS:ND1	2.32	0.51
2:C:177:ILE:HG12	2:C:183:TRP:CD1	2.46	0.51
1:B:52:PRO:HG3	1:B:150:ARG:NE	2.26	0.51
3:D:1048:ARG:HA	3:D:1059:LEU:HG	1.93	0.51
3:D:1222:ARG:HG3	3:D:1223:LEU:HG	1.92	0.51
5:F:88:GLU:OE1	5:F:88:GLU:N	2.44	0.51
2:C:628:HIS:HB3	2:C:647:ARG:HH21	1.76	0.50
2:C:964:LEU:HD13	2:C:1025:PHE:HD2	1.75	0.50
1:A:74:VAL:HG23	1:A:76:GLU:H	1.77	0.50
2:C:358:ASP:OD1	2:C:361:SER:OG	2.21	0.50
3:D:156:ARG:NH2	3:D:191:SER:OG	2.44	0.50
3:D:166:LEU:O	3:D:170:GLU:HG3	2.11	0.50
3:D:85:CYS:HB3	3:D:89:GLY:H	1.75	0.50
3:D:515:ARG:NH2	3:D:717:VAL:HG13	2.26	0.50
1:B:89:ALA:HB3	1:B:124:VAL:HG21	1.92	0.50
2:C:255:ILE:HG13	2:C:269:ILE:HD11	1.94	0.50
2:C:301:TYR:HD2	2:C:311:CYS:HB3	1.76	0.50
3:D:452:LEU:HD13	3:D:500:ILE:HG22	1.92	0.50
1:A:231:PHE:HD2	1:A:232:VAL:HG23	1.76	0.50
2:C:49:LEU:O	2:C:52:ALA:N	2.45	0.50
3:D:432:LEU:HB3	3:D:456:ALA:HB1	1.92	0.50
5:F:17:LEU:O	5:F:21:ILE:HG12	2.12	0.50
1:B:220:ALA:HA	1:B:223:ILE:HD12	1.93	0.50
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.27	0.50
2:C:28:LEU:HD21	2:C:527:LYS:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1001:GLY:O	2:C:1002:LEU:HD23	2.12	0.50
2:C:1278:LEU:HD23	2:C:1287:LEU:HD13	1.93	0.50
2:C:515:MET:HE1	2:C:527:LYS:HE2	1.94	0.50
3:D:205:LEU:HD11	3:D:214:ARG:HG3	1.94	0.50
3:D:288:PRO:HG2	3:D:291:ILE:HD12	1.94	0.50
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.94	0.50
3:D:891:ASP:OD1	3:D:891:ASP:N	2.39	0.50
3:D:901:ARG:HG3	3:D:907:HIS:O	2.12	0.50
5:F:118:ALA:HB2	5:F:150:ASP:OD2	2.12	0.50
2:C:509:SER:OG	2:C:510:GLN:N	2.44	0.50
2:C:539:THR:HB	2:C:542:ARG:HB3	1.94	0.50
2:C:764:CYS:SG	2:C:831:ILE:HB	2.52	0.50
3:D:75:TYR:HA	3:D:80:HIS:ND1	2.27	0.50
5:F:91:TYR:CD1	6:N:27:DA:H2'	2.46	0.50
2:C:242:VAL:HG12	2:C:245:ARG:HH12	1.77	0.49
2:C:491:ASP:OD1	2:C:491:ASP:N	2.43	0.49
2:C:810:TYR:CE1	3:D:359:PRO:HD2	2.47	0.49
2:C:1089:GLU:OE2	2:C:1089:GLU:N	2.37	0.49
3:D:70:CYS:SG	3:D:71:LEU:N	2.85	0.49
3:D:727:ASP:OD1	3:D:728:SER:N	2.45	0.49
3:D:1164:SER:HB2	3:D:1176:VAL:HG13	1.93	0.49
3:D:1316:THR:OG1	3:D:1317:GLU:N	2.45	0.49
3:D:117:LEU:HD23	3:D:118:LYS:HG3	1.94	0.49
3:D:510:LEU:HD11	3:D:624:ILE:HG23	1.93	0.49
3:D:705:THR:HG23	3:D:718:SER:HA	1.93	0.49
2:C:516:ASP:HA	2:C:761:GLN:HE22	1.76	0.49
2:C:1059:ARG:HG3	2:C:1060:ILE:H	1.77	0.49
3:D:275:ARG:NE	5:F:70:GLU:OE2	2.45	0.49
1:A:219:ARG:O	1:A:223:ILE:HG13	2.12	0.49
2:C:104:ILE:HB	2:C:116:ASP:OD1	2.13	0.49
2:C:615:VAL:HG12	2:C:638:SER:HB3	1.94	0.49
3:D:568:SER:OG	3:D:569:LEU:N	2.45	0.49
3:D:1028:ILE:HA	3:D:1121:LEU:HD23	1.95	0.49
4:T:4:DT:H2''	4:T:5:DG:C8	2.47	0.49
3:D:964:LYS:HE3	3:D:976:THR:O	2.12	0.49
3:D:1282:TYR:CZ	3:D:1286:LYS:HD3	2.47	0.49
1:A:208:ASN:OD1	1:A:210:THR:HG22	2.12	0.49
2:C:364:VAL:HG13	2:C:376:PRO:HB3	1.95	0.49
3:D:334:LYS:HG2	3:D:339:ARG:NH2	2.28	0.49
5:F:55:SER:O	5:F:61:SER:HB3	2.11	0.49
2:C:277:LEU:HD22	2:C:282:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:310:ILE:HD12	2:C:325:LEU:HD13	1.94	0.49
3:D:282:LEU:HD21	5:F:77:GLU:HG3	1.95	0.49
3:D:647:PRO:HG3	3:D:697:MET:HA	1.93	0.49
1:A:9:LEU:HD22	1:A:30:PRO:HG2	1.95	0.49
2:C:1281:TYR:C	2:C:1283:ALA:H	2.20	0.49
3:D:342:LEU:HD12	3:D:1352:ILE:HG23	1.94	0.49
1:B:65:LEU:HD12	1:B:66:HIS:HB2	1.95	0.49
3:D:114:ILE:HD13	3:D:311:ARG:HB3	1.95	0.49
2:C:91:THR:O	2:C:91:THR:CG2	2.60	0.49
2:C:276:GLN:HA	2:C:279:LYS:HE3	1.94	0.49
2:C:699:LEU:HB2	2:C:799:ASN:ND2	2.24	0.49
2:C:1281:TYR:HE1	3:D:489:ASN:HD21	1.60	0.49
3:D:233:LYS:HB3	3:D:235:GLU:OE1	2.13	0.49
3:D:714:GLU:HG2	3:D:715:LYS:H	1.78	0.49
3:D:1261:LEU:HD12	3:D:1304:ARG:HH21	1.78	0.49
5:F:125:VAL:CG1	5:F:126:HIS:CD2	2.96	0.49
1:A:192:VAL:HG11	1:A:195:ARG:HB3	1.94	0.48
2:C:60:GLN:HA	2:C:67:GLU:HA	1.93	0.48
2:C:67:GLU:HB3	2:C:103:VAL:HG23	1.94	0.48
2:C:624:ASP:O	2:C:626:GLU:N	2.46	0.48
1:A:152:TYR:CE1	2:C:824:GLN:HG2	2.48	0.48
2:C:988:LYS:HE2	2:C:991:LYS:HD2	1.95	0.48
3:D:951:GLN:N	3:D:951:GLN:OE1	2.45	0.48
3:D:1236:GLU:O	3:D:1240:VAL:HG23	2.13	0.48
2:C:44:GLU:O	2:C:46:GLN:HG2	2.12	0.48
2:C:56:VAL:HG12	2:C:57:PHE:CD1	2.49	0.48
2:C:49:LEU:O	2:C:50:GLU:C	2.57	0.48
2:C:116:ASP:OD1	2:C:116:ASP:N	2.44	0.48
2:C:705:GLU:OE1	2:C:705:GLU:N	2.46	0.48
3:D:930:LEU:HD11	3:D:1241:TYR:HE1	1.79	0.48
3:D:1087:ASP:OD1	3:D:1098:GLN:NE2	2.46	0.48
2:C:318:SER:OG	2:C:320:ASP:OD1	2.32	0.48
3:D:926:PRO:HA	3:D:929:GLN:HE21	1.78	0.48
3:D:977:SER:OG	3:D:978:ARG:N	2.45	0.48
3:D:1172:LYS:NZ	4:T:5:DG:OP1	2.46	0.48
2:C:921:PRO:HA	5:F:133:ASP:CB	2.43	0.48
2:C:1237:HIS:HB3	2:C:1242:LYS:HZ1	1.79	0.48
3:D:337:ARG:HB3	3:D:342:LEU:HD23	1.95	0.48
2:C:176:ILE:CG2	2:C:184:LEU:HB3	2.43	0.48
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.46	0.48
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD11	1:A:39:LEU:HD12	1.96	0.48
1:B:196:THR:OG1	1:B:197:ASP:OD1	2.28	0.48
3:D:353:SER:OG	3:D:372:MET:SD	2.71	0.48
3:D:812:ASP:OD1	3:D:812:ASP:N	2.46	0.48
5:F:11:VAL:HB	5:F:49:LEU:HD23	1.95	0.48
1:A:87:GLY:O	1:A:128:HIS:NE2	2.47	0.48
2:C:164:THR:HG21	2:C:171:LEU:HG	1.95	0.47
2:C:202:ARG:HH22	2:C:369:MET:HA	1.79	0.47
2:C:840:SER:HG	2:C:1048:LYS:H	1.59	0.47
3:D:114:ILE:HB	3:D:304:ASP:OD1	2.14	0.47
1:B:193:GLU:OE1	1:B:193:GLU:N	2.47	0.47
2:C:542:ARG:HH22	6:N:40:DT:H72	1.79	0.47
2:C:930:ASP:OD1	2:C:931:VAL:N	2.47	0.47
2:C:950:GLU:O	2:C:954:LYS:HG2	2.15	0.47
2:C:964:LEU:O	2:C:968:GLU:HG3	2.14	0.47
2:C:183:TRP:H	6:N:38:DG:N2	2.12	0.47
3:D:193:ASP:OD1	3:D:196:GLN:HB3	2.13	0.47
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.96	0.47
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.49	0.47
2:C:1332:SER:OG	3:D:327:LEU:HD11	2.14	0.47
3:D:250:ARG:O	3:D:250:ARG:HG2	2.14	0.47
3:D:210:SER:OG	4:T:2:DG:H3'	2.15	0.47
3:D:1219:ASP:HA	3:D:1222:ARG:HG2	1.97	0.47
5:F:85:ASN:O	5:F:97:TYR:OH	2.25	0.47
5:F:101:ALA:HA	6:N:26:DT:N3	2.30	0.47
1:B:135:ASP:HB2	1:B:138:ALA:HB2	1.95	0.47
2:C:230:PHE:CD1	2:C:239:MET:HB3	2.49	0.47
2:C:992:LEU:HD12	2:C:993:PRO:HD2	1.96	0.47
2:C:1203:ASP:N	2:C:1203:ASP:OD1	2.47	0.47
5:F:14:LYS:HD2	5:F:17:LEU:HD12	1.96	0.47
5:F:24:LYS:NZ	5:F:86:PHE:O	2.47	0.47
2:C:129:LEU:HD23	2:C:129:LEU:HA	1.75	0.47
2:C:256:GLU:HG2	2:C:261:VAL:HA	1.96	0.47
2:C:925:SER:OG	2:C:926:GLY:N	2.47	0.47
2:C:1288:GLN:O	2:C:1292:THR:HG22	2.15	0.47
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.49	0.47
3:D:712:GLN:HG2	3:D:713:GLU:H	1.79	0.47
3:D:807:LEU:HA	3:D:807:LEU:HD23	1.61	0.47
3:D:884:SER:OG	3:D:885:VAL:N	2.47	0.47
2:C:698:PRO:HA	2:C:1231:TYR:CE1	2.50	0.47
2:C:823:VAL:O	2:C:1059:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:66:LYS:HG3	3:D:69:GLU:HB2	1.97	0.47
3:D:255:LEU:HD21	5:F:127:ASN:CB	2.44	0.47
3:D:876:SER:HA	3:D:990:ARG:NH2	2.29	0.47
3:D:1090:ILE:HB	3:D:1093:THR:HB	1.96	0.47
6:N:51:DC:H1'	6:N:52:DC:C2	2.50	0.47
1:B:95:LYS:NZ	1:B:97:GLU:H	2.07	0.47
2:C:1085:MET:HE3	2:C:1085:MET:HB3	1.79	0.47
3:D:1003:LEU:HA	3:D:1018:ALA:HB2	1.96	0.47
2:C:183:TRP:N	6:N:38:DG:H1	2.07	0.47
2:C:303:ASP:HB2	2:C:310:ILE:HG23	1.97	0.47
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.95	0.47
3:D:44:ILE:H	5:F:119:LYS:NZ	2.13	0.47
3:D:259:ARG:HG2	5:F:139:LEU:HD22	1.97	0.47
3:D:572:THR:HG21	3:D:589:TYR:OH	2.15	0.47
2:C:801:ARG:HB3	2:C:1095:ASP:OD1	2.16	0.46
2:C:720:ARG:HB2	2:C:740:GLU:OE1	2.15	0.46
3:D:899:TYR:CE1	3:D:1251:LYS:HD2	2.50	0.46
3:D:961:SER:HB3	3:D:983:LYS:NZ	2.30	0.46
2:C:297:VAL:HG11	2:C:311:CYS:SG	2.55	0.46
2:C:731:ARG:HH21	2:C:733:VAL:HG21	1.78	0.46
2:C:943:LYS:O	2:C:947:GLU:HG3	2.15	0.46
2:C:1010:GLN:O	2:C:1014:LEU:HG	2.15	0.46
2:C:1060:ILE:HD11	2:C:1066:MET:HE2	1.98	0.46
3:D:903:LEU:HD23	3:D:903:LEU:HA	1.79	0.46
1:B:67:GLU:N	1:B:67:GLU:OE1	2.46	0.46
2:C:255:ILE:HG22	2:C:262:TYR:HB2	1.97	0.46
2:C:575:LEU:HD23	2:C:576:SER:O	2.15	0.46
2:C:947:GLU:O	2:C:950:GLU:HG2	2.14	0.46
2:C:952:GLN:O	2:C:955:GLN:NE2	2.47	0.46
2:C:1083:GLU:OE1	2:C:1083:GLU:N	2.36	0.46
3:D:1044:GLN:C	3:D:1067:ARG:HH21	2.24	0.46
2:C:180:ARG:O	2:C:396:ASP:N	2.36	0.46
2:C:602:GLU:OE1	2:C:604:HIS:NE2	2.48	0.46
3:D:209:ASN:O	3:D:214:ARG:NH2	2.49	0.46
3:D:357:VAL:HG23	3:D:358:GLY:H	1.80	0.46
3:D:681:LYS:HA	3:D:681:LYS:HD3	1.49	0.46
2:C:605:TYR:O	2:C:606:LEU:HD23	2.16	0.46
2:C:1315:MET:HG2	3:D:473:THR:HG21	1.98	0.46
3:D:363:LEU:HA	3:D:450:HIS:ND1	2.31	0.46
2:C:213:LEU:HD13	2:C:422:LYS:HG2	1.98	0.46
3:D:40:LYS:HB3	3:D:40:LYS:HE2	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:172:PHE:C	3:D:174:ASP:H	2.24	0.46
3:D:1146:GLU:HB2	3:D:1148:ARG:HD2	1.97	0.46
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.97	0.46
3:D:707:ILE:O	3:D:714:GLU:N	2.49	0.46
3:D:949:SER:HB3	3:D:1019:ASN:ND2	2.31	0.46
3:D:1193:TRP:O	3:D:1195:GLN:NE2	2.49	0.46
2:C:38:PHE:CD2	2:C:39:ILE:HG23	2.51	0.46
2:C:183:TRP:CE2	6:N:38:DG:C6	3.03	0.46
2:C:309:LEU:HD23	2:C:309:LEU:H	1.81	0.46
2:C:365:GLU:HA	2:C:368:ARG:NH1	2.31	0.46
2:C:844:LYS:HB3	2:C:844:LYS:HE2	1.71	0.46
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.16	0.46
3:D:46:TYR:OH	5:F:151:LYS:HD3	2.16	0.46
3:D:244:VAL:HG12	3:D:269:TYR:HE1	1.81	0.46
3:D:1143:ASP:HA	3:D:1148:ARG:HD3	1.98	0.46
5:F:57:ARG:O	5:F:61:SER:OG	2.31	0.46
5:F:137:VAL:HG13	5:F:138:ALA:N	2.31	0.46
1:A:208:ASN:OD1	1:A:209:GLY:N	2.49	0.46
2:C:672:GLU:HG2	2:C:673:HIS:CD2	2.51	0.46
3:D:423:LEU:HB3	3:D:466:MET:HE1	1.98	0.46
6:N:42:DC:H2'	6:N:43:DT:H71	1.97	0.46
2:C:263:VAL:HG11	2:C:269:ILE:HG13	1.97	0.45
3:D:699:ASP:OD1	3:D:700:ASN:N	2.49	0.45
3:D:1095:MET:HE3	3:D:1096:PRO:HD2	1.98	0.45
6:N:24:DA:H2''	6:N:25:DG:H8	1.81	0.45
2:C:812:PHE:CD2	3:D:451:PRO:HB3	2.50	0.45
2:C:1232:MET:HE3	2:C:1232:MET:HB3	1.75	0.45
3:D:151:MET:H	3:D:151:MET:HG2	1.57	0.45
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.98	0.45
2:C:68:LEU:HD13	2:C:102:LEU:HB3	1.98	0.45
2:C:862:LEU:HD13	2:C:865:LEU:HD12	1.98	0.45
2:C:1264:GLN:N	2:C:1264:GLN:OE1	2.49	0.45
3:D:1174:ARG:HE	3:D:1174:ARG:HB2	1.54	0.45
2:C:1279:GLU:HG3	3:D:1357:ILE:HD12	1.98	0.45
3:D:363:LEU:HD12	3:D:450:HIS:CE1	2.52	0.45
3:D:430:HIS:CD2	3:D:432:LEU:H	2.35	0.45
3:D:709:ARG:HD2	3:D:714:GLU:OE1	2.17	0.45
1:B:54:CYS:HB3	1:B:148:ARG:HD3	1.99	0.45
2:C:1035:LYS:HB2	2:C:1035:LYS:HE3	1.83	0.45
3:D:325:LYS:HB3	3:D:325:LYS:HE2	1.66	0.45
1:A:73:GLY:O	1:A:134:THR:OG1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:358:ASP:OD1	2:C:358:ASP:N	2.44	0.45
3:D:244:VAL:HA	3:D:269:TYR:OH	2.15	0.45
3:D:485:MET:HE3	3:D:486:SER:H	1.81	0.45
6:N:25:DG:C8	6:N:26:DT:H72	2.52	0.45
1:A:193:GLU:HG3	1:A:194:GLN:N	2.30	0.45
2:C:184:LEU:CD1	2:C:198:ILE:HG12	2.47	0.45
3:D:515:ARG:NH2	3:D:717:VAL:O	2.50	0.45
5:F:99:THR:HG21	6:N:29:DA:N7	2.32	0.45
1:A:20:SER:OG	1:A:21:SER:N	2.50	0.45
1:A:53:GLY:O	1:A:148:ARG:HD2	2.17	0.45
2:C:532:ALA:O	2:C:533:LEU:HD23	2.17	0.45
3:D:950:ILE:HG22	3:D:952:VAL:HG23	1.98	0.45
6:N:28:DT:H5'	6:N:28:DT:C6	2.51	0.45
1:A:56:VAL:HA	1:A:146:VAL:HG22	1.99	0.45
1:A:133:LEU:HD11	1:A:140:ILE:HG22	1.99	0.45
3:D:1179:PRO:HG2	3:D:1182:GLY:C	2.42	0.45
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.17	0.45
4:T:29:DT:H2''	4:T:30:DC:O4'	2.16	0.45
2:C:840:SER:OG	2:C:1048:LYS:N	2.36	0.45
2:C:849:GLU:O	2:C:886:LYS:HA	2.16	0.45
3:D:975:ILE:O	3:D:1000:GLY:N	2.49	0.45
1:A:196:THR:HG22	1:A:197:ASP:N	2.28	0.44
1:B:60:GLU:HG3	1:B:143:ARG:HB2	1.99	0.44
1:B:123:ILE:HD13	1:B:123:ILE:HA	1.80	0.44
2:C:915:ASP:OD1	2:C:917:SER:N	2.48	0.44
2:C:130:MET:SD	2:C:134:GLY:HA2	2.58	0.44
3:D:799:ARG:NH1	3:D:1146:GLU:OE2	2.49	0.44
2:C:742:TYR:HB3	2:C:743:PRO:HD2	1.99	0.44
2:C:950:GLU:HB2	2:C:954:LYS:NZ	2.33	0.44
3:D:46:TYR:HD1	5:F:119:LYS:HB2	1.82	0.44
3:D:227:PHE:HZ	3:D:237:MET:HE2	1.83	0.44
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.30	0.44
6:N:24:DA:H2''	6:N:25:DG:C8	2.51	0.44
2:C:557:ARG:NH2	2:C:611:GLU:OE1	2.31	0.44
3:D:218:THR:HA	3:D:221:ILE:HG22	1.98	0.44
4:T:6:DC:H1'	4:T:7:DT:H5'	2.00	0.44
1:A:98:VAL:HG11	1:A:121:VAL:HG21	1.99	0.44
1:B:127:GLN:CD	1:B:127:GLN:H	2.26	0.44
2:C:71:VAL:HB	2:C:99:LYS:O	2.18	0.44
3:D:965:SER:HG	3:D:974:VAL:C	2.16	0.44
1:A:228:LEU:HD11	1:B:224:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:813:GLU:HB2	3:D:461:PHE:CD2	2.52	0.44
3:D:858:VAL:HG22	3:D:862:THR:HG21	1.99	0.44
3:D:1046:ILE:HG22	3:D:1061:VAL:HG22	1.98	0.44
1:A:179:PRO:HB3	1:A:210:THR:HG23	2.00	0.44
1:B:58:GLU:HG3	1:B:145:LYS:HB3	2.00	0.44
2:C:9:LYS:O	2:C:1175:ASN:ND2	2.45	0.44
2:C:28:LEU:HD23	2:C:28:LEU:HA	1.71	0.44
2:C:41:GLN:HG2	2:C:73:TYR:CE1	2.53	0.44
2:C:970:GLY:O	2:C:974:ARG:NE	2.38	0.44
2:C:1272:GLU:O	2:C:1275:VAL:N	2.50	0.44
3:D:716:GLN:N	3:D:716:GLN:OE1	2.50	0.44
1:A:18:GLN:NE2	1:A:20:SER:O	2.50	0.44
1:B:19:VAL:HG12	1:B:20:SER:N	2.32	0.44
2:C:936:ARG:O	2:C:939:VAL:HG23	2.18	0.44
3:D:450:HIS:NE2	3:D:625:MET:SD	2.91	0.44
3:D:701:LEU:HD21	3:D:723:TYR:HB2	2.00	0.44
3:D:708:ASN:HA	3:D:713:GLU:HA	2.00	0.44
3:D:1037:PHE:CG	3:D:1111:ASP:HB3	2.53	0.44
3:D:1049:GLN:OE1	3:D:1058:SER:OG	2.36	0.44
5:F:10:TYR:CD2	6:N:30:DA:H1'	2.53	0.44
5:F:136:MET:HE3	5:F:137:VAL:H	1.83	0.44
6:N:45:DA:H2''	6:N:46:DA:C8	2.53	0.44
2:C:1007:LYS:O	2:C:1011:LEU:HD23	2.18	0.44
2:C:1082:ILE:HD11	2:C:1093:PRO:HG2	2.00	0.44
2:C:1279:GLU:HG3	3:D:1357:ILE:CD1	2.47	0.44
3:D:1159:ILE:HG13	3:D:1160:SER:H	1.83	0.44
3:D:1167:LYS:HD3	3:D:1174:ARG:NH2	2.33	0.44
3:D:1200:GLU:CD	3:D:1200:GLU:H	2.26	0.44
2:C:180:ARG:HG2	2:C:396:ASP:HB3	1.99	0.43
2:C:314:ASN:OD1	2:C:352:ARG:NE	2.51	0.43
2:C:453:ILE:HD11	2:C:581:THR:OG1	2.18	0.43
2:C:977:ALA:O	2:C:980:VAL:HG12	2.18	0.43
3:D:849:LEU:HA	3:D:856:ILE:HA	2.00	0.43
3:D:883:ARG:NH2	3:D:895:CYS:SG	2.91	0.43
1:A:224:LEU:HD23	1:B:228:LEU:HD11	2.00	0.43
1:B:155:ALA:HA	1:B:158:ARG:NH1	2.33	0.43
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.52	0.43
3:D:144:TYR:HA	3:D:180:MET:HB3	1.99	0.43
3:D:352:ARG:HE	3:D:465:GLN:NE2	2.16	0.43
2:C:178:PRO:HD2	2:C:183:TRP:HD1	1.84	0.43
2:C:1022:LYS:HG2	2:C:1026:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1149:TYR:CZ	2:C:1180:MET:HE2	2.53	0.43
3:D:169:LEU:HD12	3:D:173:GLY:HA2	2.00	0.43
3:D:215:LYS:O	3:D:218:THR:HG22	2.18	0.43
3:D:844:THR:HG23	3:D:860:ARG:O	2.18	0.43
3:D:845:ALA:HB3	3:D:881:LYS:HG2	2.00	0.43
3:D:965:SER:OG	3:D:966:VAL:N	2.50	0.43
3:D:1357:ILE:O	3:D:1362:GLY:HA3	2.18	0.43
2:C:25:PRO:O	2:C:27:LEU:HD12	2.19	0.43
2:C:49:LEU:O	2:C:51:ALA:N	2.51	0.43
2:C:1176:LEU:O	2:C:1178:LYS:N	2.51	0.43
3:D:97:VAL:HG22	3:D:101:ARG:HD2	2.00	0.43
3:D:225:GLU:HA	3:D:228:VAL:HG12	2.01	0.43
3:D:485:MET:HE3	3:D:486:SER:N	2.33	0.43
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.83	0.43
3:D:139:LEU:HA	3:D:139:LEU:HD23	1.67	0.43
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	2.00	0.43
5:F:107:VAL:O	5:F:110:ILE:HG22	2.19	0.43
3:D:1035:VAL:C	3:D:1036:ARG:HH11	2.24	0.43
3:D:1088:VAL:O	3:D:1096:PRO:HB3	2.19	0.43
5:F:131:SER:OG	5:F:132:ARG:N	2.50	0.43
2:C:678:ARG:HA	2:C:678:ARG:HD3	1.81	0.43
2:C:716:ALA:HB3	2:C:784:ALA:HB3	2.00	0.43
3:D:876:SER:HA	3:D:990:ARG:HH21	1.83	0.43
3:D:1046:ILE:HG22	3:D:1061:VAL:HG13	2.00	0.43
3:D:1164:SER:HB2	3:D:1176:VAL:CG1	2.49	0.43
4:T:24:DT:O2	5:F:63:TYR:HB2	2.19	0.43
2:C:157:PHE:CE2	2:C:431:LYS:HG2	2.53	0.43
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	2.01	0.43
2:C:764:CYS:HB3	2:C:833:ILE:HD11	2.01	0.43
3:D:107:LEU:HD22	3:D:299:LEU:HD21	2.00	0.43
3:D:384:LYS:HA	3:D:384:LYS:HD2	1.79	0.43
3:D:495:ASN:O	3:D:497:GLU:N	2.52	0.43
3:D:824:PRO:HD3	3:D:835:LEU:HB2	2.00	0.43
3:D:1058:SER:HA	3:D:1108:GLN:HA	2.01	0.43
5:F:12:ASN:OD1	5:F:13:ASN:N	2.51	0.43
1:B:117:HIS:HD2	1:B:119:GLY:H	1.66	0.43
2:C:159:SER:HB2	2:C:442:VAL:HG21	2.00	0.43
2:C:1142:ARG:NH1	2:C:1161:LEU:O	2.52	0.43
3:D:499:ILE:HD12	3:D:499:ILE:HA	1.89	0.43
2:C:151:ARG:HD2	6:N:39:DA:C6	2.54	0.43
3:D:1077:ALA:HB2	3:D:1100:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:VAL:O	1:B:171:LEU:N	2.37	0.42
1:B:59:VAL:HG13	1:B:171:LEU:HB2	2.01	0.42
1:B:74:VAL:HA	1:B:132:HIS:O	2.18	0.42
1:B:208:ASN:OD1	1:B:210:THR:HG22	2.19	0.42
2:C:696:ASP:OD2	2:C:697:LYS:HG2	2.19	0.42
2:C:1005:GLU:HG2	2:C:1006:GLU:N	2.34	0.42
2:C:1138:VAL:HG11	2:C:1166:ASP:OD1	2.19	0.42
2:C:1151:LEU:HD11	2:C:1197:GLU:HG3	2.00	0.42
2:C:1278:LEU:HD21	2:C:1286:THR:HG23	2.01	0.42
2:C:1321:GLU:OE2	3:D:99:ARG:NE	2.46	0.42
3:D:1034:PHE:HB3	3:D:1036:ARG:HH12	1.84	0.42
3:D:1049:GLN:NE2	3:D:1052:GLU:OE1	2.52	0.42
1:A:62:ASP:OD1	1:A:63:GLY:N	2.52	0.42
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.54	0.42
2:C:515:MET:CE	2:C:527:LYS:HE2	2.49	0.42
2:C:799:ASN:HA	2:C:1231:TYR:HA	2.00	0.42
3:D:44:ILE:H	5:F:119:LYS:HZ2	1.66	0.42
3:D:743:MET:HE3	3:D:760:THR:HA	2.01	0.42
5:F:90:LYS:HZ1	6:N:27:DA:N6	2.17	0.42
5:F:109:ARG:HD2	5:F:109:ARG:HA	1.80	0.42
1:A:219:ARG:NH2	1:B:6:THR:OG1	2.52	0.42
2:C:66:SER:HA	2:C:104:ILE:HA	2.02	0.42
2:C:410:LEU:HD23	2:C:410:LEU:HA	1.90	0.42
2:C:528:ARG:NH2	2:C:577:VAL:O	2.50	0.42
3:D:103:GLY:C	3:D:244:VAL:HG22	2.44	0.42
3:D:103:GLY:CA	3:D:244:VAL:HG22	2.49	0.42
3:D:514:THR:OG1	3:D:596:LEU:HB2	2.19	0.42
3:D:1287:ILE:HG13	3:D:1288:ALA:N	2.34	0.42
1:B:53:GLY:C	1:B:177:TYR:HB3	2.44	0.42
1:B:197:ASP:OD1	1:B:197:ASP:N	2.52	0.42
2:C:107:ARG:HD2	2:C:107:ARG:HA	1.77	0.42
2:C:805:MET:HE1	2:C:1221:PHE:CE2	2.54	0.42
3:D:658:GLU:O	3:D:661:VAL:HG12	2.20	0.42
3:D:998:PRO:HG2	3:D:1020:TRP:CE2	2.54	0.42
1:B:35:PHE:HA	1:B:38:THR:HG22	2.01	0.42
1:B:57:THR:HG23	1:B:58:GLU:HG2	2.02	0.42
1:B:67:GLU:HA	1:B:78:ILE:HD11	2.01	0.42
2:C:384:LEU:O	2:C:388:LEU:HB2	2.20	0.42
2:C:971:LEU:O	2:C:975:ILE:HG12	2.19	0.42
3:D:133:ARG:H	3:D:133:ARG:HG2	1.66	0.42
1:A:120:ASP:OD1	1:A:121:VAL:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:VAL:HG12	1:B:20:SER:H	1.83	0.42
2:C:97:ARG:NH1	2:C:123:TYR:HD1	2.17	0.42
2:C:245:ARG:HD3	2:C:337:PHE:CD1	2.54	0.42
2:C:1292:THR:HG23	2:C:1293:VAL:N	2.34	0.42
3:D:217:LEU:HD12	3:D:217:LEU:HA	1.80	0.42
3:D:610:ARG:HA	3:D:610:ARG:HD3	1.81	0.42
5:F:115:LYS:HD2	5:F:115:LYS:HA	1.75	0.42
6:N:51:DC:H6	6:N:51:DC:H2'	1.67	0.42
6:N:51:DC:H2''	6:N:52:DC:C5	2.54	0.42
1:A:222:THR:HG22	1:B:232:VAL:O	2.20	0.42
2:C:165:HIS:C	2:C:167:SER:H	2.27	0.42
2:C:562:GLU:OE1	2:C:662:SER:OG	2.25	0.42
2:C:564:PRO:HA	2:C:684:ASN:HD21	1.84	0.42
3:D:813:ASP:OD1	3:D:883:ARG:NH1	2.37	0.42
3:D:1042:ASP:OD2	3:D:1043:GLY:N	2.50	0.42
2:C:118:LYS:HD3	2:C:118:LYS:HA	1.89	0.42
2:C:268:ARG:NH2	2:C:270:THR:HA	2.35	0.42
2:C:671:LEU:HB3	2:C:1186:VAL:HG13	2.02	0.42
3:D:238:ILE:HD13	3:D:238:ILE:HA	1.86	0.42
3:D:651:HIS:CE1	3:D:652:GLU:HG2	2.55	0.42
6:N:23:DG:H2''	6:N:24:DA:H8	1.84	0.42
2:C:45:GLY:H	2:C:54:ARG:NH1	2.17	0.42
2:C:211:ARG:O	2:C:214:ASN:N	2.53	0.42
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	2.02	0.42
2:C:1275:VAL:HG22	2:C:1287:LEU:HD11	2.00	0.42
3:D:255:LEU:HD21	5:F:127:ASN:HB3	2.01	0.42
3:D:420:PRO:HA	3:D:437:PHE:O	2.20	0.42
3:D:581:MET:HE2	3:D:581:MET:HB3	1.76	0.42
3:D:1056:LEU:HD23	3:D:1056:LEU:HA	1.95	0.42
3:D:1057:SER:OG	3:D:1110:GLU:OE1	2.37	0.42
1:A:62:ASP:OD1	1:A:62:ASP:N	2.52	0.42
2:C:169:LYS:NZ	2:C:192:ASP:OD1	2.52	0.42
2:C:365:GLU:CD	2:C:368:ARG:HH12	2.27	0.42
2:C:367:TYR:HD1	2:C:381:ALA:HA	1.85	0.42
3:D:382:TYR:HE1	3:D:401:VAL:HG21	1.85	0.42
3:D:491:LEU:HD22	3:D:496:GLY:O	2.20	0.42
3:D:605:LEU:HD21	3:D:621:ALA:HB2	2.01	0.42
6:N:46:DA:H2''	6:N:47:DG:H8	1.84	0.42
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.83	0.41
1:B:29:GLU:HA	1:B:30:PRO:HA	1.79	0.41
2:C:253:PHE:CZ	2:C:285:ILE:HD12	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:526:HIS:O	2:C:526:HIS:ND1	2.50	0.41
2:C:638:SER:OG	2:C:639:LYS:N	2.53	0.41
3:D:1143:ASP:OD1	3:D:1144:LEU:N	2.53	0.41
2:C:253:PHE:HA	2:C:265:LYS:HD3	2.02	0.41
2:C:706:ARG:HD3	2:C:793:GLU:HG2	2.01	0.41
2:C:842:ASP:N	2:C:842:ASP:OD1	2.52	0.41
2:C:1282:GLY:O	3:D:1360:GLY:HA3	2.20	0.41
3:D:528:THR:O	3:D:528:THR:OG1	2.36	0.41
1:B:181:GLU:CD	3:D:535:ARG:HH11	2.27	0.41
2:C:716:ALA:HB2	2:C:767:GLN:OE1	2.21	0.41
2:C:798:GLN:HB2	2:C:828:PHE:CE1	2.55	0.41
2:C:883:LEU:HD13	2:C:1052:VAL:HG11	2.02	0.41
3:D:156:ARG:NH1	3:D:157:GLN:OE1	2.53	0.41
3:D:525:MET:HE2	3:D:525:MET:HB3	1.96	0.41
3:D:1081:VAL:HG12	3:D:1087:ASP:HA	2.02	0.41
1:A:29:GLU:HA	1:A:30:PRO:HA	1.72	0.41
1:A:127:GLN:OE1	1:A:127:GLN:N	2.54	0.41
1:B:47:LEU:HD23	1:B:51:MET:SD	2.60	0.41
2:C:801:ARG:HB2	2:C:1229:TYR:CZ	2.55	0.41
2:C:1045:GLY:HA3	5:F:144:PHE:HZ	1.85	0.41
2:C:1192:GLU:HA	2:C:1195:ILE:HD12	2.03	0.41
3:D:362:ARG:H	3:D:365:GLN:HE21	1.68	0.41
3:D:641:ILE:HD12	3:D:641:ILE:HA	1.82	0.41
3:D:961:SER:OG	3:D:981:GLU:HB3	2.20	0.41
3:D:1226:VAL:HG13	3:D:1227:HIS:CD2	2.55	0.41
3:D:1329:THR:O	3:D:1333:THR:HG22	2.20	0.41
5:F:112:LYS:HB2	5:F:112:LYS:HE3	1.72	0.41
1:B:10:LYS:HA	1:B:10:LYS:HD3	1.91	0.41
1:B:13:LEU:HD21	1:B:16:ILE:HG13	2.01	0.41
1:B:27:THR:HG22	1:B:202:VAL:HG13	2.01	0.41
2:C:22:LEU:HB3	2:C:655:VAL:HG11	2.02	0.41
2:C:23:ASP:OD1	2:C:23:ASP:N	2.53	0.41
2:C:120:GLN:HE22	2:C:490:GLN:HB2	1.84	0.41
2:C:186:PHE:CD1	2:C:196:VAL:HG22	2.55	0.41
2:C:398:SER:O	2:C:401:GLY:N	2.53	0.41
2:C:959:ASP:OD1	2:C:959:ASP:N	2.53	0.41
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	2.02	0.41
2:C:623:LEU:HA	2:C:630:VAL:HG13	2.01	0.41
2:C:1005:GLU:HG2	2:C:1006:GLU:H	1.85	0.41
3:D:93:THR:OG1	3:D:94:GLN:N	2.53	0.41
3:D:858:VAL:HG22	3:D:859:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:961:SER:HB3	3:D:983:LYS:HZ2	1.84	0.41
3:D:961:SER:O	3:D:980:THR:HA	2.20	0.41
3:D:1183:SER:O	3:D:1185:PRO:HD3	2.21	0.41
3:D:1226:VAL:O	3:D:1229:VAL:HG12	2.20	0.41
6:N:40:DT:C2	6:N:41:DA:C8	3.08	0.41
2:C:181:GLY:HA3	2:C:395:TYR:CD1	2.56	0.41
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.56	0.41
3:D:132:LEU:HD12	3:D:132:LEU:HA	1.92	0.41
3:D:225:GLU:OE1	3:D:229:GLN:HB2	2.21	0.41
3:D:1256:ILE:HD13	3:D:1256:ILE:HA	1.82	0.41
5:F:54:LEU:HD22	5:F:99:THR:HG23	2.03	0.41
1:A:74:VAL:HA	1:A:132:HIS:O	2.20	0.41
2:C:49:LEU:HD22	2:C:464:PHE:CE2	2.55	0.41
2:C:870:ILE:HG21	2:C:931:VAL:HG11	2.03	0.41
3:D:44:ILE:HD13	3:D:44:ILE:HA	1.90	0.41
3:D:195:GLU:H	3:D:195:GLU:CD	2.29	0.41
3:D:857:LEU:HD23	3:D:872:LEU:HD23	2.02	0.41
3:D:974:VAL:HG23	3:D:1001:ALA:C	2.46	0.41
4:T:12:DT:H2'	4:T:13:DA:H8	1.83	0.41
5:F:20:ILE:HD12	5:F:20:ILE:HA	1.88	0.41
5:F:61:SER:HA	5:F:68:LYS:HZ2	1.86	0.41
5:F:68:LYS:HB2	5:F:68:LYS:HE2	1.70	0.41
5:F:75:GLY:HA2	5:F:105:ALA:HB3	2.02	0.41
1:B:59:VAL:HG23	1:B:144:ILE:HG22	2.03	0.41
2:C:560:PRO:O	3:D:780:ARG:NH2	2.45	0.41
2:C:672:GLU:HB3	2:C:1187:PHE:CD1	2.56	0.41
2:C:712:SER:OG	2:C:713:GLY:N	2.54	0.41
2:C:801:ARG:HD3	2:C:1094:VAL:HA	2.03	0.41
2:C:921:PRO:HG2	2:C:924:VAL:HG11	2.02	0.41
2:C:1098:LEU:HA	2:C:1098:LEU:HD23	1.80	0.41
2:C:1246:ARG:HD2	2:C:1265:PHE:O	2.20	0.41
2:C:1303:LYS:HD3	2:C:1303:LYS:HA	1.71	0.41
2:C:1333:LEU:HG	3:D:327:LEU:HD22	2.02	0.41
3:D:127:LEU:HD12	3:D:127:LEU:HA	1.75	0.41
3:D:390:LEU:O	3:D:400:MET:HE1	2.21	0.41
3:D:718:SER:OG	3:D:719:PHE:N	2.53	0.41
3:D:930:LEU:HD11	3:D:1241:TYR:CE1	2.56	0.41
3:D:1051:ASP:OD2	3:D:1053:LEU:HG	2.21	0.41
3:D:1096:PRO:HB2	3:D:1098:GLN:HE22	1.86	0.41
1:B:66:HIS:HD2	1:B:68:TYR:HB2	1.86	0.41
2:C:339:ASN:OD1	2:C:340:ASP:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:755:LYS:HD2	2:C:755:LYS:HA	1.80	0.41
2:C:985:GLU:OE2	2:C:1000:LEU:HD21	2.21	0.41
2:C:1043:ALA:O	2:C:1046:VAL:HG22	2.21	0.41
3:D:35:PHE:CE2	3:D:101:ARG:HG2	2.56	0.41
3:D:275:ARG:NH1	3:D:302:ALA:HB2	2.32	0.41
3:D:518:VAL:HG13	3:D:519:ASN:N	2.35	0.41
3:D:712:GLN:HG2	3:D:713:GLU:N	2.35	0.41
4:T:9:DC:H2"	4:T:10:DA:C8	2.56	0.41
1:A:176:CYS:O	1:A:178:SER:N	2.53	0.40
2:C:59:ILE:HG12	2:C:472:GLU:OE2	2.20	0.40
2:C:81:ASP:OD2	2:C:82:VAL:N	2.54	0.40
2:C:396:ASP:OD1	2:C:397:LEU:N	2.54	0.40
2:C:452:ARG:HB3	2:C:586:PHE:CE1	2.55	0.40
3:D:1104:LYS:HD3	3:D:1104:LYS:HA	1.86	0.40
4:T:27:DA:C6	4:T:28:DC:N4	2.88	0.40
1:A:40:GLY:HA3	1:A:185:TYR:CE2	2.56	0.40
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	2.02	0.40
3:D:783:LEU:O	3:D:786:THR:OG1	2.27	0.40
3:D:974:VAL:HA	3:D:1002:VAL:HA	2.02	0.40
3:D:1174:ARG:C	3:D:1175:LEU:HD12	2.46	0.40
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.81	0.40
1:B:86:LYS:HD3	1:B:173:VAL:HG12	2.02	0.40
2:C:611:GLU:C	2:C:613:ASN:H	2.29	0.40
2:C:811:ASN:OD1	2:C:811:ASN:N	2.51	0.40
3:D:212:THR:OG1	3:D:213:LYS:N	2.54	0.40
3:D:259:ARG:HG3	5:F:139:LEU:HD13	2.03	0.40
3:D:801:VAL:O	3:D:805:GLN:HB2	2.22	0.40
2:C:39:ILE:O	2:C:40:GLU:HG3	2.22	0.40
2:C:490:GLN:O	2:C:493:ILE:HG22	2.21	0.40
2:C:624:ASP:C	2:C:626:GLU:N	2.80	0.40
2:C:799:ASN:OD1	2:C:799:ASN:N	2.50	0.40
2:C:865:LEU:HD23	2:C:865:LEU:HA	1.87	0.40
2:C:1023:HIS:HA	2:C:1026:GLU:OE2	2.21	0.40
2:C:1295:SER:OG	3:D:346:ARG:O	2.37	0.40
3:D:661:VAL:HG23	3:D:682:VAL:HG22	2.03	0.40
3:D:670:SER:OG	3:D:672:LEU:HD23	2.21	0.40
3:D:783:LEU:HD23	3:D:783:LEU:HA	1.93	0.40
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.33	0.40
3:D:962:ASN:HB2	3:D:979:ASN:O	2.22	0.40
2:C:153:PRO:O	2:C:401:GLY:HA2	2.21	0.40
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:518:VAL:HG11	3:D:707:ILE:HG23	2.04	0.40
3:D:527:LEU:HD23	3:D:532:GLU:HB3	2.04	0.40
3:D:797:THR:O	3:D:801:VAL:HG12	2.22	0.40
3:D:1002:VAL:O	3:D:1018:ALA:HA	2.22	0.40
3:D:1194:ARG:HD3	3:D:1194:ARG:HA	1.91	0.40
3:D:1306:LEU:HD12	3:D:1306:LEU:HA	1.80	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	215/329 (65%)	193 (90%)	22 (10%)	0	100	100
1	B	214/329 (65%)	193 (90%)	21 (10%)	0	100	100
2	C	1312/1342 (98%)	1140 (87%)	170 (13%)	2 (0%)	43	72
3	D	1329/1407 (94%)	1181 (89%)	147 (11%)	1 (0%)	48	79
5	F	133/185 (72%)	118 (89%)	15 (11%)	0	100	100
All	All	3203/3592 (89%)	2825 (88%)	375 (12%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	45	GLY
2	C	50	GLU
3	D	805	GLN

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	186/286 (65%)	185 (100%)	1 (0%)	81	80
1	B	186/286 (65%)	186 (100%)	0	100	100
2	C	1135/1157 (98%)	1133 (100%)	2 (0%)	87	85
3	D	1120/1168 (96%)	1118 (100%)	2 (0%)	87	85
5	F	121/166 (73%)	118 (98%)	3 (2%)	42	63
All	All	2748/3063 (90%)	2740 (100%)	8 (0%)	84	83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	VAL
2	C	528	ARG
2	C	1225	VAL
3	D	434	ILE
3	D	1345	ARG
5	F	128	VAL
5	F	129	TYR
5	F	133	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	93	GLN
1	A	117	HIS
1	B	23	HIS
1	B	37	HIS
1	B	41	ASN
1	B	66	HIS
1	B	93	GLN
1	B	117	HIS
2	C	41	GLN

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Mol	Chain	Res	Type
2	C	65	ASN
2	C	150	HIS
2	C	343	HIS
2	C	618	GLN
2	C	856	ASN
2	C	1038	GLN
2	C	1116	HIS
2	C	1136	GLN
2	C	1157	GLN
2	C	1268	GLN
3	D	94	GLN
3	D	465	GLN
3	D	504	GLN
3	D	651	HIS
3	D	805	GLN
3	D	929	GLN
3	D	1366	HIS
5	F	126	HIS
5	F	127	ASN

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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30604. 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.