



Full wwPDB EM Validation Report ⓘ

Jun 25, 2023 – 12:08 AM JST

PDB ID : 8HPO
EMDB ID : EMD-34935
Title : Cryo-EM structure of a SIN3/HDAC complex from budding yeast
Authors : Guo, Z.; Zhan, X.; Wang, C.
Deposited on : 2022-12-12
Resolution : 2.60 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:

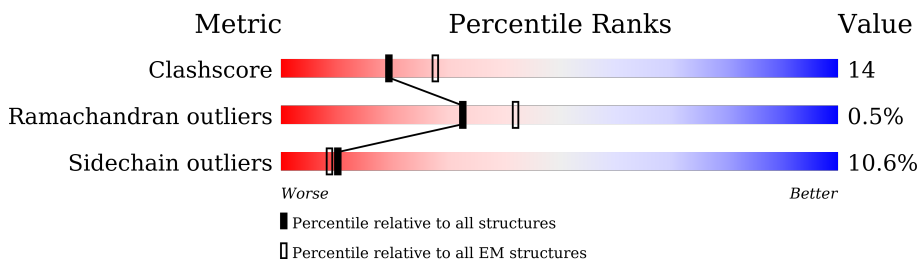
EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	K	460	86% (Green), 10% (Grey), 4% (Yellow), 0% (Orange), 0% (Red)
2	D	327	28% (Green), 16% (Yellow), 6% (Orange), 50% (Grey)
3	F	433	66% (Green), 21% (Yellow), 9% (Orange), 4% (Red), 0% (Grey)
4	G	433	63% (Green), 22% (Yellow), 11% (Orange), 0% (Red), 0% (Grey)
5	I	201	38% (Green), 23% (Yellow), 35% (Grey), 4% (Orange), 0% (Red)
6	A	1536	26% (Green), 14% (Yellow), 59% (Grey), 1% (Orange), 0% (Red)
6	B	1536	22% (Green), 16% (Yellow), 60% (Grey), 2% (Orange), 0% (Red)
7	H	405	36% (Green), 18% (Yellow), 42% (Grey), 4% (Orange), 0% (Red)
8	C	330	27% (Green), 13% (Yellow), 58% (Grey), 2% (Orange), 0% (Red)

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Mol	Chain	Length	Quality of chain
9	E	430	
10	J	294	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SEP	F	265	-	-	X	-
3	TPO	F	365	-	-	X	-
9	TPO	E	167	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 27951 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 Transcriptional regulatory protein UME1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	K	413	2038	1212	413	413	0	0

- Molecule 2 is a protein called Transcriptional regulatory protein SDS3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
2	D	165	1385	863	248	271	1	2	0	0

- Molecule 3 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
3	F	392	3132	1982	524	596	5	25	0	0

- Molecule 4 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	385	3057	1948	513	571	25	0	0

- Molecule 5 is a protein called Transcriptional regulatory protein SAP30.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
5	I	130	1104	696	203	201	1	3	0	0

- Molecule 6 is a protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	637	5283	3392	887	987	17	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	613	5129	3295	862	955	17	0	0

- Molecule 7 is a protein called Transcriptional regulatory protein DEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	233	1936	1218	340	368	10	0	0

- Molecule 8 is a protein called Transcriptional regulatory protein PHO23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	C	138	1116	703	195	211	7	0	0

- Molecule 9 is a protein called Transcriptional regulatory protein RXT2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
9	E	255	2077	1306	375	391	2	3	0	0

- Molecule 10 is a protein called Transcriptional regulatory protein RXT3.


Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	209	1676	1069	284	321	2	0	0

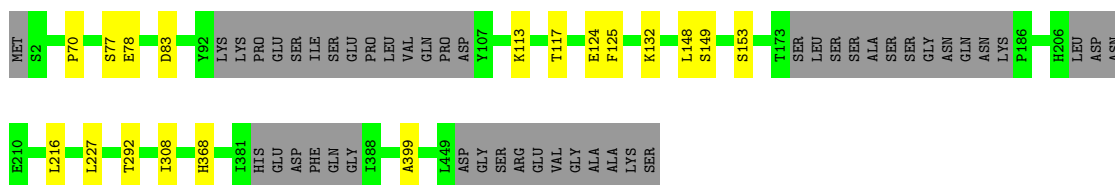
- Molecule 11 is PHOSPHOTHREONINE (three-letter code: TPO) (formula: C₄H₁₀NO₆P).

3 Residue-property plots [i](#)

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.

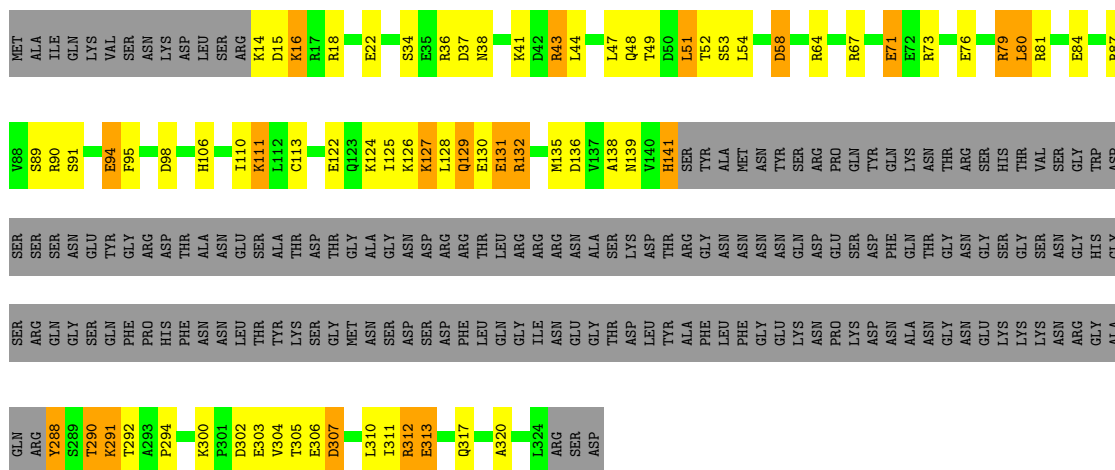
- Molecule 1: Transcriptional regulatory protein UME1

Chain K:  86% 10%



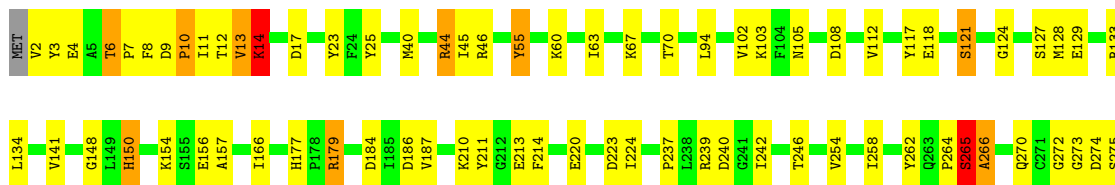
- Molecule 2: Transcriptional regulatory protein SDS3

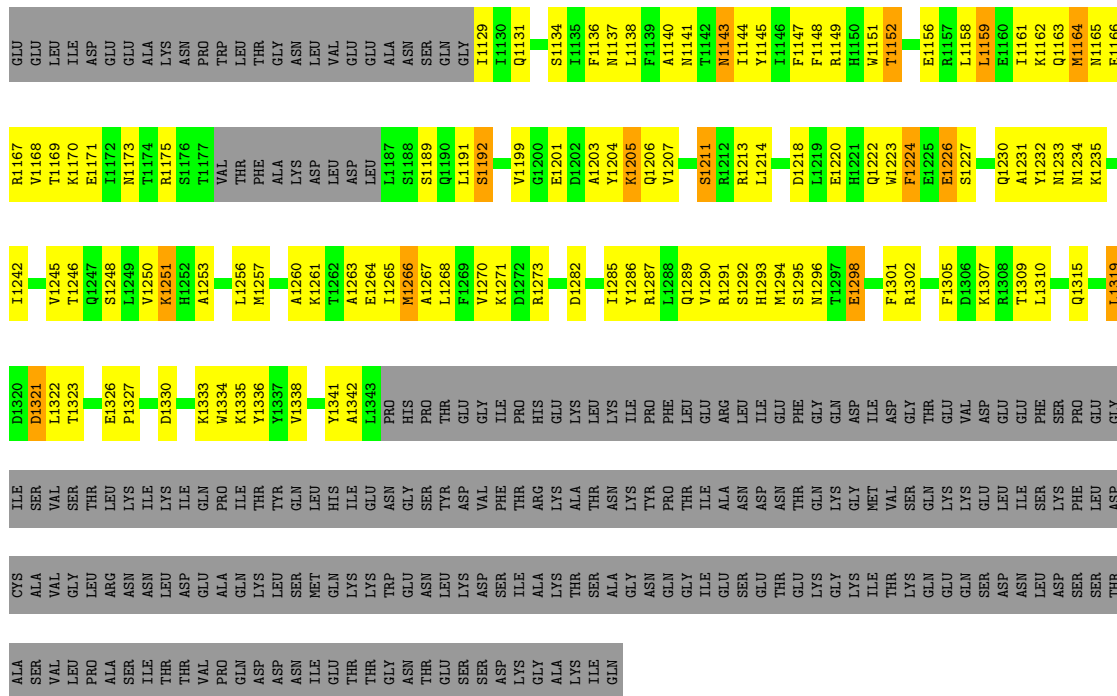
Chain D:  28% 16% 6% 50%



- Molecule 3: Histone deacetylase RPD3

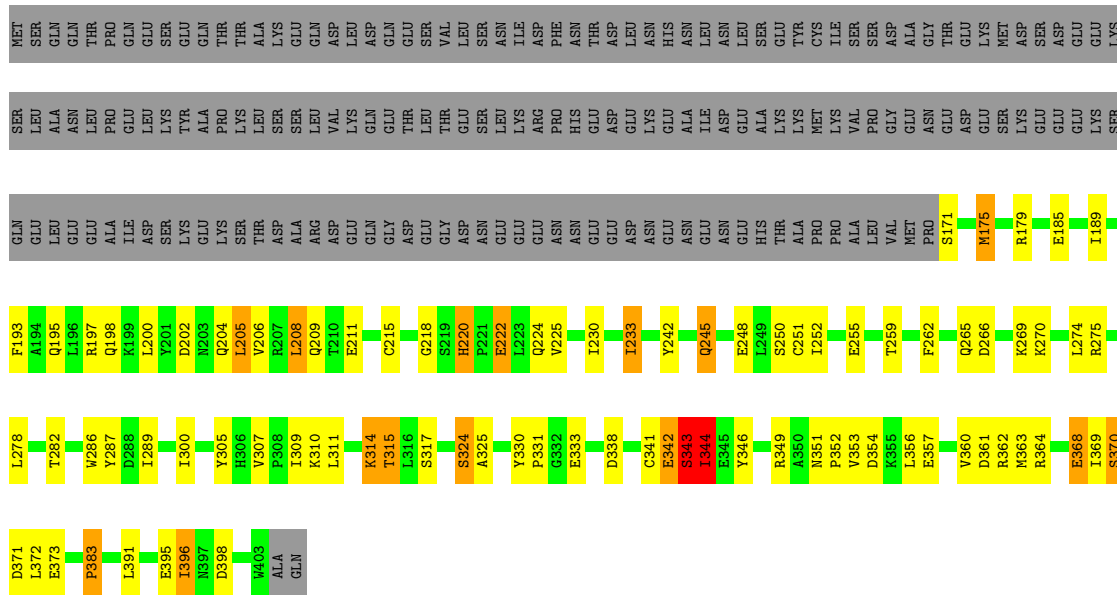
Chain F:  66% 21% 9%





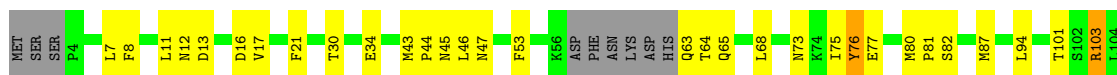
• Molecule 7: Transcriptional regulatory protein DEP1

Chain H:



• Molecule 8: Transcriptional regulatory protein PHO23

Chain C:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	665105	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)	1800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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: SEP, K, ZN, TPO

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	K	0.24	0/2033	0.44	0/2822
2	D	0.50	1/1393 (0.1%)	0.69	1/1866 (0.1%)
3	F	0.55	3/3156 (0.1%)	0.63	6/4262 (0.1%)
4	G	0.35	0/3137	0.48	0/4246
5	I	0.38	0/1119	0.61	1/1500 (0.1%)
6	A	0.32	0/5400	0.48	0/7289
6	B	0.30	0/5245	0.51	1/7077 (0.0%)
7	H	0.34	0/1976	0.50	0/2674
8	C	0.30	0/1134	0.50	0/1529
9	E	0.42	0/2082	0.58	1/2799 (0.0%)
10	J	0.38	1/1718 (0.1%)	0.54	0/2335
All	All	0.37	5/28393 (0.0%)	0.53	10/38399 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1
5	I	0	1
6	A	0	1
6	B	0	2
7	H	0	4
9	E	0	2
All	All	0	11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	10	PRO	N-CA	13.06	1.69	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	294	PRO	C-N	8.63	1.50	1.34
3	F	14	LYS	C-N	8.37	1.50	1.34
10	J	123	PRO	C-N	7.87	1.49	1.34
3	F	9	ASP	C-N	6.27	1.46	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	307	ASP	CB-CA-C	-11.25	87.91	110.40
3	F	9	ASP	CB-CA-C	-7.49	95.42	110.40
3	F	266	ALA	N-CA-CB	7.36	120.40	110.10
3	F	10	PRO	CA-N-CD	-6.63	102.21	111.50
6	B	1033	LEU	CA-CB-CG	6.06	129.25	115.30
9	E	168	PRO	N-CA-CB	-5.91	96.10	102.60
5	I	109	ASP	CB-CG-OD1	5.54	123.29	118.30
3	F	14	LYS	CB-CA-C	-5.28	99.83	110.40
3	F	393	HIS	CB-CA-C	5.16	120.71	110.40
3	F	10	PRO	N-CA-C	-5.08	98.88	112.10

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	891	ALA	Peptide
6	B	741	HIS	Peptide
6	B	891	ALA	Peptide
9	E	41	TYR	Peptide
9	E	42	GLN	Peptide
3	F	265	SEP	Mainchain
7	H	314	LYS	Peptide
7	H	342	GLU	Peptide
7	H	343	SER	Peptide
7	H	344	ILE	Peptide
5	I	174	SEP	Mainchain

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	K	2038	0	890	9	0
2	D	1385	0	1388	84	0
3	F	3132	0	2978	85	0
4	G	3057	0	2932	69	0
5	I	1104	0	1087	46	0
6	A	5283	0	5216	166	0
6	B	5129	0	5096	193	0
7	H	1936	0	1896	65	0
8	C	1116	0	1133	38	0
9	E	2077	0	2136	75	0
10	J	1676	0	1637	44	0
11	F	12	0	5	3	0
12	F	1	0	0	0	0
12	G	1	0	0	0	0
13	F	2	0	0	0	0
13	G	2	0	0	0	0
All	All	27951	0	26394	767	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 14.

All (767) 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:F:10:PRO:N	3:F:10:PRO:CA	1.69	1.36
3:F:6:TPO:CG2	3:F:7:PRO:HD2	1.68	1.23
9:E:176:ILE:CD1	9:E:374:LEU:HD12	1.77	1.15
9:E:167:TPO:CG2	9:E:168:PRO:HD2	1.81	1.10
5:I:177:GLU:O	5:I:179:ASP:N	1.82	1.09
2:D:304:VAL:CG1	6:A:875:ARG:HH21	1.66	1.07
3:F:6:TPO:HG23	3:F:7:PRO:CD	1.84	1.06
2:D:312:ARG:HD2	2:D:317:GLN:OE1	1.55	1.05
3:F:365:TPO:HG23	3:F:366:PRO:HD2	1.39	1.01
9:E:167:TPO:HG23	9:E:168:PRO:HD2	1.03	1.01
9:E:167:TPO:HG23	9:E:168:PRO:CD	1.90	1.00
6:B:987:ASP:O	6:B:990:CYS:HB2	1.60	1.00
9:E:176:ILE:HD11	9:E:374:LEU:HD12	1.40	0.99
6:A:923:VAL:O	6:A:927:SER:HB2	1.63	0.96
9:E:176:ILE:HD11	9:E:374:LEU:CD1	1.96	0.96
2:D:291:LYS:HE3	2:D:291:LYS:HA	1.48	0.95
2:D:304:VAL:HG12	6:A:875:ARG:HH21	1.29	0.95
3:F:6:TPO:HG23	3:F:7:PRO:HD2	0.94	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:311:ILE:CD1	6:A:890:THR:HG23	2.00	0.91
9:E:176:ILE:CD1	9:E:374:LEU:CD1	2.49	0.90
6:A:837:LYS:NZ	6:A:841:MET:SD	2.46	0.88
3:F:265:SEP:O1P	3:F:265:SEP:N	2.06	0.88
9:E:176:ILE:HD12	9:E:374:LEU:HD12	1.56	0.88
4:G:90:THR:HG22	4:G:92:ASP:H	1.38	0.87
3:F:365:TPO:HG23	3:F:366:PRO:CD	2.07	0.83
2:D:132:ARG:HH12	7:H:198:GLN:HA	1.42	0.83
3:F:156:GLU:OE2	6:A:742:ARG:NH2	2.12	0.83
6:B:972:LYS:O	6:B:1315:GLN:NE2	2.12	0.82
6:B:1287:ARG:NH2	6:B:1321:ASP:O	2.12	0.81
2:D:291:LYS:HA	2:D:291:LYS:CE	2.06	0.81
6:B:1013:LEU:HD11	6:B:1257:MET:HG3	1.63	0.81
6:A:1330:ASP:HA	6:A:1333:LYS:HE2	1.62	0.81
10:J:227:GLU:HB2	10:J:271:VAL:HG22	1.64	0.80
2:D:304:VAL:HG12	6:A:875:ARG:NH2	1.96	0.79
6:A:770:ARG:HG2	6:A:774:CYS:HB3	1.64	0.79
6:B:1169:THR:O	6:B:1173:ASN:ND2	2.16	0.78
6:A:939:ASP:OD2	6:A:1157:ARG:NH2	2.15	0.77
5:I:177:GLU:C	5:I:179:ASP:H	1.88	0.77
2:D:302:ASP:HA	2:D:305:THR:HG22	1.67	0.77
5:I:177:GLU:O	5:I:180:CYS:N	2.15	0.76
2:D:312:ARG:HH12	2:D:320:ALA:HB2	1.51	0.76
3:F:4:GLU:N	3:F:4:GLU:OE1	2.18	0.76
10:J:162:ASN:O	10:J:250:ARG:NH1	2.19	0.76
6:B:1004:ASN:HA	6:B:1007:LYS:HD3	1.68	0.75
2:D:311:ILE:HD13	6:A:890:THR:HG23	1.68	0.75
4:G:50:SER:O	4:G:54:ASN:ND2	2.20	0.75
4:G:350:ASP:OD2	4:G:356:ARG:NH2	2.19	0.74
2:D:313:GLU:HA	2:D:313:GLU:OE2	1.85	0.74
9:E:103:THR:HG23	9:E:104:ASN:H	1.53	0.74
3:F:337:ASP:HB3	6:A:1178:VAL:HG22	1.69	0.74
9:E:164:GLU:HA	9:E:167:TPO:O2P	1.88	0.74
6:B:1033:LEU:HD22	6:B:1037:LYS:HZ1	1.53	0.74
6:B:1327:PRO:HB3	6:B:1333:LYS:HD3	1.69	0.73
3:F:365:TPO:CG2	3:F:366:PRO:HD2	2.15	0.73
4:G:148:GLY:HA2	4:G:166:ILE:HD11	1.70	0.73
5:I:79:TYR:OH	6:A:878:GLU:OE1	2.07	0.73
7:H:220:HIS:NE2	7:H:222:GLU:HB3	2.05	0.72
3:F:179:ARG:O	3:F:265:SEP:O1P	2.07	0.72
7:H:242:TYR:OH	9:E:243:PRO:O	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:2:VAL:N	4:G:370:ASP:OD1	2.23	0.72
6:B:1067:ASP:HA	6:B:1070:HIS:HB2	1.71	0.71
6:A:956:LYS:HE2	6:A:959:GLN:HE21	1.56	0.71
3:F:10:PRO:N	3:F:10:PRO:C	2.45	0.69
2:D:18:ARG:HG2	6:A:666:VAL:HG21	1.73	0.69
7:H:218:GLY:O	7:H:224:GLN:NE2	2.25	0.69
2:D:64:ARG:HD3	5:I:113:ARG:HD3	1.74	0.69
9:E:25:ILE:HD13	6:B:690:ASN:HB2	1.75	0.69
9:E:67:LYS:NZ	10:J:174:ASP:OD2	2.26	0.69
6:B:902:ASP:OD1	6:B:906:ARG:NH2	2.26	0.69
6:B:1287:ARG:NH2	6:B:1319:LEU:O	2.25	0.69
7:H:342:GLU:HG3	8:C:122:ARG:HH21	1.57	0.68
6:A:1140:ALA:HB1	6:A:1144:ILE:HB	1.75	0.68
3:F:154:LYS:NZ	6:A:780:ASP:OD1	2.27	0.68
9:E:30:THR:HB	6:B:662:LEU:HD11	1.74	0.68
3:F:265:SEP:HB2	11:F:501:TPO:HB	1.76	0.68
6:B:1291:ARG:HG3	6:B:1319:LEU:HD21	1.75	0.68
2:D:43:ARG:NH2	5:I:196:LYS:O	2.27	0.68
6:B:981:ASP:OD2	6:B:1162:LYS:NZ	2.24	0.68
2:D:95:PHE:HB2	7:H:245:GLN:HG3	1.75	0.67
2:D:15:ASP:OD2	2:D:18:ARG:NH1	2.22	0.67
4:G:19:ARG:HH22	4:G:302:GLY:HA2	1.59	0.67
8:C:128:HIS:O	8:C:130:ALA:N	2.27	0.67
6:A:1006:ASP:OD1	6:A:1006:ASP:N	2.22	0.67
4:G:280:ARG:NH1	6:B:812:GLU:OE2	2.25	0.67
10:J:239:TYR:OH	10:J:264:SER:OG	2.10	0.67
2:D:310:LEU:C	2:D:310:LEU:HD23	2.15	0.66
4:G:15:PRO:O	4:G:18:LYS:NZ	2.28	0.66
5:I:186:TYR:O	5:I:190:ASN:ND2	2.28	0.66
6:B:1191:LEU:HD12	6:B:1191:LEU:H	1.60	0.66
6:A:1295:SER:OG	6:A:1296:ASN:N	2.28	0.66
8:C:135:HIS:O	8:C:139:GLU:HB2	1.96	0.66
2:D:291:LYS:HE3	2:D:291:LYS:CA	2.24	0.66
7:H:204:GLN:HE22	7:H:205:LEU:HD13	1.61	0.66
6:A:1265:ILE:HG12	6:A:1290:VAL:HG23	1.78	0.65
8:C:8:PHE:O	8:C:12:ASN:ND2	2.24	0.65
6:B:1175:ARG:NH1	6:B:1231:ALA:O	2.29	0.65
6:B:1009:ARG:NH2	6:B:1069:LEU:O	2.28	0.65
6:B:1213:ARG:HE	6:B:1218:ASP:HB3	1.62	0.65
6:B:860:MET:SD	6:B:860:MET:N	2.65	0.65
2:D:80:LEU:HD11	7:H:259:THR:HG23	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:95:GLU:HA	4:G:98:LYS:HD2	1.78	0.65
2:D:304:VAL:HG22	6:A:871:TYR:HD1	1.62	0.65
6:A:1268:LEU:HD23	6:A:1286:TYR:HD2	1.61	0.65
10:J:85:LYS:HZ3	10:J:86:ASN:H	1.45	0.65
6:A:951:GLU:HG2	6:A:969:PRO:HG2	1.79	0.64
6:A:1042:GLU:OE1	6:A:1209:ARG:NH1	2.30	0.64
9:E:70:GLN:O	9:E:72:SER:N	2.30	0.64
6:A:976:ASP:OD1	6:A:1311:HIS:NE2	2.20	0.64
7:H:317:SER:OG	7:H:354:ASP:OD1	2.09	0.64
2:D:90:ARG:NH1	6:A:902:ASP:OD2	2.30	0.64
6:A:1233:ASN:OD1	6:A:1233:ASN:N	2.28	0.64
3:F:4:GLU:O	3:F:4:GLU:HG2	1.95	0.64
8:C:94:LEU:HD23	9:E:352:ILE:HG13	1.79	0.64
6:A:1343:LEU:HD12	6:A:1344:PRO:HD2	1.78	0.64
9:E:169:ILE:HG13	9:E:181:ILE:HD13	1.80	0.64
6:B:790:SER:HA	10:J:129:ALA:HB3	1.80	0.64
6:B:996:ILE:HD13	6:B:1010:LEU:HD21	1.78	0.64
9:E:41:TYR:O	9:E:42:GLN:HB2	1.96	0.64
6:B:990:CYS:O	6:B:994:THR:OG1	2.15	0.63
2:D:311:ILE:HD11	6:A:890:THR:HG23	1.79	0.63
5:I:177:GLU:C	5:I:179:ASP:N	2.49	0.63
3:F:129:GLU:OE1	7:H:269:LYS:NZ	2.31	0.63
6:B:1037:LYS:O	6:B:1041:SER:OG	2.14	0.63
4:G:258:ILE:HG22	4:G:380:LEU:HD21	1.80	0.63
6:A:767:CYS:SG	6:A:770:ARG:NH1	2.71	0.63
6:A:1181:ALA:HA	6:A:1186:LEU:HD12	1.80	0.63
6:A:1019:SER:HA	6:A:1024:ILE:HB	1.80	0.63
2:D:58:ASP:N	2:D:58:ASP:OD1	2.31	0.63
6:A:1161:ILE:HG12	6:A:1239:LEU:HD11	1.81	0.63
7:H:324:SER:OG	7:H:325:ALA:N	2.31	0.63
6:A:1325:LYS:H	6:A:1325:LYS:HD2	1.64	0.62
6:B:1233:ASN:HD22	6:B:1235:LYS:HG3	1.64	0.62
6:B:1166:GLU:O	6:B:1169:THR:OG1	2.16	0.62
9:E:176:ILE:HG13	9:E:374:LEU:HD11	1.81	0.62
6:B:959:GLN:OE1	6:B:974:GLN:NE2	2.28	0.62
6:B:652:PRO:O	6:B:653:THR:OG1	2.17	0.62
9:E:197:ILE:HG21	9:E:353:ARG:HB2	1.79	0.62
2:D:18:ARG:NH2	2:D:22:GLU:OE2	2.32	0.61
4:G:368:TYR:HD2	4:G:371:LYS:HZ3	1.46	0.61
10:J:180:VAL:HG22	10:J:267:ILE:HD11	1.82	0.61
3:F:359:ASN:HB3	6:A:1234:ASN:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:684:GLU:OE2	6:B:709:TYR:OH	2.16	0.61
2:D:304:VAL:HG11	6:A:875:ARG:HH21	1.62	0.61
5:I:121:LEU:HD21	5:I:169:HIS:CD2	2.35	0.61
6:A:1262:THR:HA	6:A:1265:ILE:HD12	1.83	0.61
9:E:84:LYS:O	9:E:87:ILE:HG13	2.01	0.61
5:I:105:GLU:O	5:I:159:LYS:NZ	2.26	0.61
5:I:100:HIS:HD2	5:I:102:MET:H	1.48	0.61
5:I:169:HIS:O	5:I:169:HIS:ND1	2.33	0.61
1:K:216:LEU:O	1:K:227:LEU:N	2.32	0.60
3:F:2:VAL:HG13	3:F:2:VAL:O	2.01	0.60
6:A:678:ASN:OD1	6:A:679:LYS:N	2.33	0.60
8:C:16:ASP:OD1	6:B:910:ARG:NH1	2.34	0.60
6:B:1189:SER:O	6:B:1192:SER:HB2	2.02	0.60
8:C:45:ASN:OD1	8:C:45:ASN:N	2.35	0.60
6:B:1065:LEU:HA	6:B:1068:ILE:HB	1.82	0.60
6:A:639:ILE:HG22	7:H:368:GLU:HA	1.83	0.60
6:A:945:THR:HG23	6:A:1146:ILE:HG13	1.84	0.60
7:H:175:MET:O	7:H:179:ARG:HG2	2.02	0.60
2:D:48:GLN:O	2:D:48:GLN:NE2	2.35	0.60
2:D:312:ARG:HB2	2:D:312:ARG:HH11	1.66	0.60
9:E:81:ASN:OD1	9:E:83:SER:OG	2.18	0.60
10:J:93:ASN:OD1	10:J:94:ARG:N	2.35	0.59
4:G:141:VAL:HG22	4:G:305:MET:HG2	1.83	0.59
6:B:993:ASP:HA	6:B:996:ILE:HG13	1.83	0.59
10:J:120:ASN:HD22	10:J:121:THR:H	1.49	0.59
2:D:125:ILE:HD12	7:H:208:LEU:HD11	1.85	0.59
4:G:99:ARG:HH21	4:G:103:LYS:HB2	1.68	0.59
6:A:1133:ARG:NH1	6:A:1272:ASP:O	2.34	0.59
6:A:1303:ILE:HG12	6:A:1314:ILE:HG12	1.83	0.59
9:E:70:GLN:C	9:E:72:SER:H	2.04	0.59
9:E:372:GLU:HG3	9:E:372:GLU:O	2.03	0.59
6:A:986:TYR:HB3	6:A:1033:LEU:HD23	1.84	0.59
9:E:167:TPO:O1P	9:E:167:TPO:HG21	2.01	0.59
6:B:1167:ARG:HA	6:B:1170:LYS:HG2	1.84	0.59
6:B:1305:PHE:HE2	6:B:1310:LEU:HA	1.68	0.59
6:A:1288:LEU:HD22	6:A:1345:HIS:HD2	1.68	0.59
5:I:74:ALA:O	5:I:78:GLN:NE2	2.33	0.59
6:A:978:ASP:OD1	6:A:979:PHE:N	2.36	0.59
6:B:732:CYS:HA	10:J:65:PRO:HB3	1.83	0.59
6:B:929:ASP:OD1	6:B:929:ASP:N	2.35	0.58
10:J:104:SER:HB2	10:J:107:TYR:CE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:ARG:HB3	7:H:252:ILE:HD13	1.84	0.58
6:A:838:ILE:HD13	6:A:888:ALA:HA	1.86	0.58
4:G:371:LYS:HA	4:G:374:THR:HG22	1.85	0.58
6:A:1288:LEU:O	6:A:1292:SER:OG	2.21	0.58
7:H:311:LEU:HB2	7:H:314:LYS:HB2	1.84	0.58
6:B:1140:ALA:HB1	6:B:1144:ILE:HB	1.84	0.58
3:F:6:TPO:CG2	3:F:7:PRO:CD	2.61	0.58
7:H:265:GLN:NE2	9:E:226:ILE:O	2.33	0.58
8:C:122:ARG:HG3	9:E:369:TRP:CZ2	2.39	0.58
3:F:343:TYR:OH	6:A:822:GLU:OE1	2.11	0.58
6:B:1203:ALA:O	6:B:1207:VAL:HG23	2.04	0.58
2:D:87:ARG:NH2	7:H:255:GLU:OE1	2.34	0.58
2:D:306:GLU:OE2	2:D:306:GLU:HA	2.02	0.58
3:F:365:TPO:N	3:F:365:TPO:O1P	2.36	0.58
4:G:246:THR:O	4:G:250:VAL:HG23	2.04	0.58
9:E:361:ARG:O	9:E:365:ARG:HG2	2.04	0.58
2:D:288:TYR:N	2:D:288:TYR:CD2	2.72	0.57
6:A:1331:GLU:O	6:A:1335:LYS:HG3	2.04	0.57
6:B:890:THR:O	6:B:890:THR:OG1	2.20	0.57
6:B:985:PHE:HD1	6:B:1151:TRP:HZ2	1.50	0.57
7:H:341:CYS:O	9:E:361:ARG:NH1	2.37	0.57
6:A:1134:SER:OG	6:A:1308:ARG:NE	2.38	0.57
4:G:20:ARG:HG3	4:G:139:CYS:HA	1.87	0.57
6:B:1261:LYS:O	6:B:1265:ILE:HG12	2.04	0.57
4:G:238:LEU:HD13	4:G:242:ILE:HD13	1.87	0.57
4:G:294:CYS:O	4:G:298:VAL:HG23	2.04	0.57
2:D:291:LYS:HE3	2:D:292:THR:H	1.69	0.57
5:I:148:ASN:O	5:I:148:ASN:ND2	2.38	0.57
3:F:14:LYS:HG3	3:F:14:LYS:O	2.05	0.57
9:E:323:GLN:O	9:E:326:GLU:HG2	2.04	0.57
6:A:1009:ARG:HA	6:A:1068:ILE:HD11	1.86	0.56
7:H:208:LEU:O	7:H:211:GLU:HG3	2.05	0.56
9:E:160:VAL:HG21	6:B:919:LEU:HD12	1.86	0.56
6:A:929:ASP:HB3	6:A:933:LEU:HD13	1.85	0.56
6:A:932:GLY:HA2	6:A:935:PHE:HB3	1.86	0.56
7:H:215:CYS:HB2	7:H:220:HIS:ND1	2.19	0.56
6:B:951:GLU:O	6:B:954:SER:OG	2.22	0.56
7:H:342:GLU:OE1	9:E:365:ARG:NH2	2.39	0.56
7:H:343:SER:OG	7:H:344:ILE:N	2.39	0.56
6:B:691:LEU:HD12	6:B:697:LEU:HD22	1.88	0.56
4:G:44:ARG:NH1	4:G:311:GLY:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:280:ARG:HH21	9:E:83:SER:HB2	1.71	0.56
6:A:1331:GLU:HA	6:A:1334:TRP:HB3	1.88	0.55
6:B:738:HIS:ND1	6:B:739:GLU:O	2.36	0.55
6:B:1162:LYS:HE2	6:B:1204:TYR:CZ	2.41	0.55
6:A:1261:LYS:H	6:A:1261:LYS:HZ3	1.53	0.55
7:H:398:ASP:OD2	6:B:871:TYR:OH	2.17	0.55
6:B:700:ASP:N	6:B:700:ASP:OD1	2.39	0.55
1:K:78:GLU:HA	1:K:124:GLU:HA	1.88	0.55
6:A:678:ASN:HD21	6:A:680:HIS:HB3	1.71	0.55
6:A:1268:LEU:HD21	6:A:1289:GLN:HB3	1.88	0.55
8:C:53:PHE:HB2	8:C:68:LEU:HD22	1.88	0.55
3:F:390:GLN:O	9:E:199:LEU:HD13	2.06	0.55
9:E:24:ASN:O	9:E:28:THR:HG23	2.06	0.55
4:G:245:ALA:O	4:G:249:SER:OG	2.25	0.55
8:C:13:ASP:OD2	8:C:103:ARG:NH2	2.38	0.55
7:H:369:ILE:HD11	9:E:166:LEU:O	2.06	0.55
3:F:258:ILE:HG12	3:F:380:LEU:HD11	1.88	0.55
4:G:368:TYR:O	4:G:371:LYS:HD3	2.07	0.55
6:B:1214:LEU:HD13	6:B:1224:PHE:HD2	1.70	0.55
1:K:292:THR:O	1:K:308:ILE:N	2.36	0.55
6:A:1173:ASN:HD21	6:A:1200:GLY:HA2	1.72	0.54
7:H:363:MET:HG2	6:B:648:VAL:HG11	1.88	0.54
2:D:122:GLU:O	2:D:125:ILE:HG22	2.06	0.54
3:F:6:TPO:O1P	3:F:6:TPO:HG21	2.07	0.54
3:F:211:TYR:HB2	3:F:237:PRO:HB3	1.88	0.54
6:A:738:HIS:ND1	6:A:764:PHE:HB2	2.23	0.54
10:J:175:SER:O	10:J:265:TYR:OH	2.21	0.54
6:A:732:CYS:SG	6:A:733:ILE:N	2.81	0.54
1:K:70:PRO:HA	1:K:83:ASP:HA	1.89	0.54
7:H:195:GLN:HA	7:H:198:GLN:HG2	1.88	0.54
7:H:200:LEU:O	7:H:204:GLN:HG3	2.08	0.54
2:D:304:VAL:CG1	6:A:875:ARG:NH2	2.50	0.54
3:F:211:TYR:OH	3:F:220:GLU:OE2	2.23	0.54
6:B:1167:ARG:O	6:B:1171:GLU:HG2	2.07	0.54
11:F:501:TPO:O2P	11:F:501:TPO:HG22	2.08	0.54
6:B:1152:THR:HG22	6:B:1156:GLU:OE1	2.08	0.54
2:D:312:ARG:CD	2:D:317:GLN:OE1	2.43	0.54
3:F:365:TPO:N	3:F:365:TPO:P	2.80	0.54
3:F:389:VAL:HG12	3:F:389:VAL:O	2.08	0.54
8:C:73:ASN:O	8:C:77:GLU:HG3	2.08	0.54
6:B:1168:VAL:HG21	6:B:1232:TYR:CZ	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:312:ARG:HG3	2:D:317:GLN:HB2	1.89	0.53
2:D:71:GLU:HG2	5:I:131:GLY:HA3	1.90	0.53
9:E:226:ILE:HD12	9:E:231:LEU:HD21	1.90	0.53
2:D:290:THR:HG23	2:D:290:THR:O	2.07	0.53
8:C:101:THR:O	8:C:105:GLU:HG3	2.08	0.53
3:F:134:LEU:HD22	3:F:304:PRO:HB3	1.90	0.53
4:G:24:PHE:CE1	4:G:129:GLU:HG2	2.43	0.53
4:G:209:HIS:HE1	4:G:235:ASN:HB3	1.73	0.53
5:I:173:HIS:C	5:I:173:HIS:CD2	2.82	0.53
6:B:1012:ASP:HA	6:B:1015:LYS:HE2	1.90	0.53
6:A:1268:LEU:HD23	6:A:1286:TYR:CD2	2.43	0.53
6:B:838:ILE:HD11	6:B:849:PHE:CE1	2.44	0.53
2:D:126:LYS:O	2:D:130:GLU:HG2	2.09	0.52
2:D:135:MET:HA	2:D:138:ALA:HB3	1.91	0.52
4:G:62:GLU:OE1	4:G:64:TYR:OH	2.16	0.52
4:G:292:ALA:HB1	4:G:328:LEU:HD21	1.90	0.52
6:B:987:ASP:OD1	6:B:1204:TYR:OH	2.23	0.52
3:F:346:TYR:OH	6:A:818:ASP:OD1	2.17	0.52
5:I:127:LEU:N	5:I:157:ILE:O	2.40	0.52
6:A:692:TYR:CG	6:A:702:LEU:HD22	2.44	0.52
6:A:1165:ASN:O	6:A:1169:THR:HG22	2.10	0.52
8:C:47:ASN:HD22	9:E:210:ARG:HD2	1.73	0.52
5:I:157:ILE:HD12	5:I:161:ASP:HB2	1.91	0.52
7:H:193:PHE:O	7:H:197:ARG:HG3	2.10	0.52
6:B:678:ASN:OD1	6:B:680:HIS:N	2.42	0.52
6:B:993:ASP:O	6:B:997:THR:HG23	2.09	0.52
2:D:138:ALA:HA	2:D:141:HIS:CD2	2.45	0.52
3:F:277:SER:OG	3:F:286:LEU:O	2.27	0.52
6:B:1156:GLU:HA	6:B:1159:LEU:HD23	1.91	0.52
6:A:864:LYS:O	6:A:868:ARG:HG2	2.10	0.52
6:B:1065:LEU:HA	6:B:1068:ILE:HD12	1.92	0.52
2:D:136:ASP:HA	2:D:139:ASN:ND2	2.25	0.52
6:A:944:THR:HB	6:A:946:LYS:HD2	1.92	0.52
2:D:84:GLU:OE1	9:E:238:HIS:ND1	2.39	0.51
9:E:167:TPO:CB	9:E:168:PRO:HD2	2.33	0.51
6:B:1213:ARG:O	6:B:1218:ASP:N	2.43	0.51
6:B:1263:ALA:O	6:B:1266:MET:HG3	2.10	0.51
3:F:223:ASP:OD2	6:A:754:SER:OG	2.22	0.51
6:B:721:LYS:HG2	6:B:726:TYR:HD2	1.76	0.51
5:I:128:THR:OG1	5:I:129:LEU:N	2.39	0.51
6:B:987:ASP:HA	6:B:990:CYS:SG	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:177:HIS:ND1	3:F:265:SEP:O2P	2.40	0.51
4:G:366:PRO:O	4:G:370:ASP:HB2	2.11	0.51
6:A:727:GLN:O	6:A:727:GLN:NE2	2.44	0.51
10:J:69:SER:O	10:J:69:SER:OG	2.25	0.51
7:H:266:ASP:O	7:H:270:LYS:HG3	2.11	0.51
4:G:191:ASP:OD1	4:G:191:ASP:N	2.36	0.51
6:A:1280:ALA:O	6:A:1284:ILE:HG12	2.10	0.51
2:D:18:ARG:HB3	2:D:18:ARG:CZ	2.41	0.51
3:F:370:ASP:O	3:F:374:THR:OG1	2.26	0.51
6:A:841:MET:HE3	6:A:846:LYS:HA	1.93	0.51
6:A:948:LEU:HA	6:A:951:GLU:OE1	2.11	0.51
6:B:1338:VAL:O	6:B:1342:ALA:HB2	2.11	0.51
9:E:167:TPO:CG2	9:E:168:PRO:CD	2.70	0.51
4:G:261:TRP:HB3	4:G:383:THR:O	2.11	0.51
6:B:1223:TRP:O	6:B:1227:SER:OG	2.17	0.51
3:F:210:LYS:HD2	3:F:283:CYS:SG	2.51	0.50
6:A:1012:ASP:O	6:A:1016:TYR:HD2	1.93	0.50
6:A:1322:LEU:HA	6:A:1348:GLU:HG3	1.92	0.50
2:D:91:SER:OG	7:H:248:GLU:HG2	2.11	0.50
4:G:109:ASP:OD1	4:G:109:ASP:N	2.43	0.50
6:A:1321:ASP:OD2	6:A:1321:ASP:N	2.39	0.50
10:J:169:ASP:OD1	10:J:244:ARG:NH2	2.44	0.50
2:D:307:ASP:OD2	6:A:871:TYR:HE1	1.95	0.50
4:G:346:TYR:OH	6:B:818:ASP:OD2	2.16	0.50
6:A:1013:LEU:HD13	6:A:1257:MET:HE3	1.93	0.50
6:A:1295:SER:HB3	6:A:1298:GLU:HG3	1.94	0.50
9:E:286:ASP:OD1	9:E:286:ASP:N	2.44	0.50
2:D:110:ILE:HG13	2:D:111:LYS:N	2.27	0.50
4:G:105:ASN:HB2	4:G:156:GLU:HG2	1.93	0.50
6:A:760:LYS:O	6:A:763:THR:OG1	2.27	0.50
6:B:1004:ASN:OD1	6:B:1004:ASN:N	2.43	0.50
6:B:1162:LYS:HG3	6:B:1204:TYR:CG	2.46	0.50
7:H:300:ILE:HD13	6:B:895:LEU:HD23	1.94	0.50
4:G:77:PHE:HA	6:B:770:ARG:HH21	1.77	0.50
2:D:300:LYS:HB2	2:D:303:GLU:HG3	1.93	0.50
6:A:1214:LEU:HD11	6:A:1221:HIS:ND1	2.27	0.50
7:H:330:TYR:HD1	7:H:331:PRO:HD2	1.76	0.50
10:J:85:LYS:NZ	10:J:86:ASN:H	2.10	0.50
2:D:106:HIS:HE1	7:H:230:ILE:HG23	1.76	0.49
3:F:118:GLU:OE2	3:F:118:GLU:N	2.41	0.49
3:F:336:LYS:O	3:F:353:LEU:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:76:TYR:O	8:C:80:MET:HG2	2.12	0.49
6:B:942:LEU:HG	6:B:947:GLN:HG2	1.94	0.49
6:B:1158:LEU:O	6:B:1161:ILE:HG22	2.13	0.49
2:D:124:LYS:O	2:D:127:LYS:HB3	2.12	0.49
7:H:310:LYS:HG2	7:H:354:ASP:HB2	1.95	0.49
9:E:172:LEU:HD12	9:E:175:ILE:HD12	1.93	0.49
6:B:986:TYR:HE1	6:B:1029:ILE:HG22	1.76	0.49
6:B:1207:VAL:O	6:B:1211:SER:OG	2.29	0.49
2:D:64:ARG:HH11	5:I:113:ARG:HB3	1.77	0.49
3:F:210:LYS:HE3	3:F:240:ASP:OD1	2.12	0.49
4:G:209:HIS:CE1	4:G:235:ASN:HB3	2.47	0.49
6:B:924:PHE:O	6:B:927:SER:OG	2.29	0.49
4:G:244:ASP:OD1	4:G:244:ASP:N	2.45	0.49
6:B:954:SER:HA	6:B:957:VAL:HG12	1.95	0.49
9:E:73:GLU:HB3	10:J:257:THR:HG22	1.94	0.49
6:B:857:HIS:HB3	6:B:860:MET:HA	1.94	0.49
2:D:307:ASP:OD2	6:A:871:TYR:CE1	2.66	0.49
2:D:312:ARG:HH11	2:D:312:ARG:CB	2.25	0.49
6:A:672:ALA:O	6:A:676:ILE:HG13	2.11	0.49
6:A:1288:LEU:HD22	6:A:1345:HIS:CD2	2.46	0.49
6:A:1286:TYR:O	6:A:1290:VAL:HG12	2.13	0.49
7:H:275:ARG:NH1	9:E:219:LEU:HB3	2.27	0.49
6:B:1065:LEU:HD11	6:B:1270:VAL:HG11	1.95	0.49
3:F:148:GLY:HA2	3:F:166:ILE:HD11	1.93	0.49
8:C:77:GLU:HA	8:C:80:MET:HG2	1.95	0.49
6:B:1285:ILE:O	6:B:1289:GLN:NE2	2.46	0.49
1:K:132:LYS:O	1:K:148:LEU:N	2.34	0.49
2:D:138:ALA:O	2:D:141:HIS:HB2	2.13	0.49
6:B:739:GLU:HG3	6:B:740:LYS:N	2.27	0.49
6:B:830:CYS:SG	6:B:831:LEU:N	2.85	0.49
4:G:86:LEU:HD22	4:G:116:LEU:HD11	1.95	0.48
6:A:1030:GLU:O	6:A:1034:TYR:HB2	2.13	0.48
6:B:1138:LEU:HD22	6:B:1140:ALA:HB2	1.95	0.48
3:F:102:VAL:HG21	8:C:141:ILE:HD11	1.94	0.48
6:A:667:THR:O	6:A:671:LYS:HG2	2.13	0.48
6:A:1322:LEU:HD23	6:A:1322:LEU:H	1.78	0.48
6:B:960:THR:HA	6:B:963:LYS:HE3	1.95	0.48
3:F:105:ASN:ND2	3:F:157:ALA:O	2.46	0.48
10:J:89:THR:HA	10:J:140:THR:HB	1.96	0.48
6:A:1229:ARG:O	6:A:1233:ASN:HA	2.13	0.48
6:B:1014:LEU:O	6:B:1018:ILE:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:LEU:HD21	7:H:259:THR:HG21	1.96	0.48
6:B:1129:ILE:HG12	6:B:1131:GLN:HG3	1.96	0.48
6:B:1148:PHE:O	6:B:1152:THR:OG1	2.29	0.48
4:G:359:ASN:HB3	6:B:1234:ASN:HD22	1.78	0.48
6:B:963:LYS:HE2	6:B:971:PRO:HD3	1.95	0.48
8:C:16:ASP:OD2	8:C:103:ARG:NH1	2.39	0.48
6:B:951:GLU:O	6:B:955:ILE:HG13	2.14	0.48
2:D:312:ARG:NH1	2:D:312:ARG:CG	2.72	0.48
6:A:1335:LYS:O	6:A:1339:THR:HG22	2.13	0.48
10:J:120:ASN:N	10:J:120:ASN:ND2	2.60	0.48
10:J:223:PRO:O	10:J:275:ARG:HB2	2.14	0.48
3:F:117:TYR:O	3:F:121:SER:OG	2.28	0.48
8:C:17:VAL:HG22	8:C:103:ARG:HG2	1.96	0.48
6:B:1164:MET:O	6:B:1168:VAL:HG23	2.14	0.48
4:G:368:TYR:HA	4:G:371:LYS:NZ	2.29	0.47
6:A:663:ASN:O	6:A:667:THR:OG1	2.22	0.47
6:B:1295:SER:OG	6:B:1296:ASN:N	2.46	0.47
7:H:342:GLU:OE2	9:E:365:ARG:NH1	2.48	0.47
6:B:729:LYS:O	6:B:731:LYS:N	2.46	0.47
2:D:291:LYS:HE3	2:D:292:THR:N	2.28	0.47
6:A:1261:LYS:H	6:A:1261:LYS:NZ	2.11	0.47
10:J:123:PRO:HG3	10:J:158:PRO:HG2	1.96	0.47
4:G:99:ARG:O	4:G:102:VAL:HG22	2.15	0.47
7:H:346:TYR:CZ	8:C:113:LYS:HE2	2.49	0.47
9:E:176:ILE:CG1	9:E:374:LEU:HD11	2.43	0.47
6:B:851:LEU:HD12	6:B:851:LEU:HA	1.79	0.47
3:F:103:LYS:HD2	6:A:740:LYS:O	2.14	0.47
5:I:126:ASN:HD22	5:I:159:LYS:HG2	1.80	0.47
6:A:699:LEU:O	6:A:703:VAL:HG23	2.13	0.47
6:A:1004:ASN:O	6:A:1008:GLU:HG2	2.15	0.47
6:A:1283:GLN:HB2	6:A:1324:LEU:HD21	1.95	0.47
6:B:1282:ASP:HA	6:B:1285:ILE:HB	1.97	0.47
2:D:94:GLU:HG2	6:A:910:ARG:NH1	2.30	0.47
2:D:312:ARG:HH22	2:D:320:ALA:HA	1.79	0.47
3:F:326:THR:O	3:F:330:ASN:ND2	2.47	0.47
6:A:965:HIS:CE1	6:A:967:LEU:HD12	2.49	0.47
2:D:122:GLU:HA	2:D:125:ILE:HG22	1.95	0.47
2:D:312:ARG:HD2	2:D:317:GLN:HB2	1.97	0.47
2:D:312:ARG:HH11	2:D:312:ARG:CG	2.26	0.47
3:F:213:GLU:HG2	6:A:789:ALA:O	2.15	0.47
5:I:113:ARG:NH2	5:I:126:ASN:OD1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:807:LEU:O	6:A:811:GLU:HG3	2.14	0.47
6:B:820:TYR:CE2	6:B:869:LYS:HD2	2.50	0.47
6:B:993:ASP:N	6:B:993:ASP:OD1	2.46	0.47
6:B:1004:ASN:O	6:B:1008:GLU:HG2	2.14	0.47
6:B:1222:GLN:OE1	6:B:1222:GLN:N	2.47	0.47
10:J:216:LEU:HD23	10:J:217:PRO:HD2	1.97	0.47
6:B:851:LEU:HD23	6:B:855:LEU:HD22	1.96	0.47
3:F:265:SEP:P	3:F:265:SEP:O	2.73	0.47
4:G:199:THR:O	4:G:199:THR:OG1	2.27	0.47
7:H:356:LEU:O	7:H:360:VAL:HG23	2.14	0.47
6:B:739:GLU:HG3	6:B:741:HIS:H	1.80	0.47
2:D:18:ARG:CD	6:A:663:ASN:ND2	2.78	0.47
7:H:233:ILE:HD12	7:H:233:ILE:HA	1.69	0.47
2:D:81:ARG:HB2	9:E:288:PHE:CE1	2.50	0.46
6:B:803:TYR:CD1	6:B:923:VAL:HG13	2.50	0.46
6:B:1026:PHE:O	6:B:1029:ILE:HG12	2.15	0.46
6:B:1035:SER:O	6:B:1039:ASN:ND2	2.48	0.46
10:J:90:LEU:N	10:J:140:THR:O	2.43	0.46
3:F:186:ASP:OD2	3:F:272:GLY:HA3	2.14	0.46
5:I:92:HIS:CD2	5:I:93:PRO:HD2	2.50	0.46
7:H:185:GLU:O	7:H:189:ILE:HG13	2.14	0.46
9:E:56:GLU:HG3	9:E:70:GLN:HG3	1.97	0.46
9:E:64:ARG:NH1	10:J:127:LEU:O	2.41	0.46
10:J:123:PRO:O	10:J:123:PRO:HG2	2.15	0.46
3:F:94:LEU:HD13	3:F:112:VAL:HG21	1.97	0.46
8:C:46:LEU:HB2	8:C:75:ILE:HG21	1.97	0.46
9:E:167:TPO:CB	9:E:168:PRO:CD	2.90	0.46
4:G:73:GLU:O	4:G:76:GLN:HG3	2.15	0.46
5:I:173:HIS:CD2	5:I:173:HIS:O	2.69	0.46
8:C:43:MET:N	8:C:44:PRO:HD2	2.31	0.46
6:B:1036:HIS:O	6:B:1040:VAL:HG23	2.14	0.46
6:B:1147:PHE:CE2	6:B:1253:ALA:HB2	2.51	0.46
2:D:94:GLU:HG2	6:A:910:ARG:HH11	1.80	0.46
6:A:792:ASP:OD1	6:A:792:ASP:N	2.48	0.46
6:A:1197:ASP:OD1	6:A:1198:PHE:N	2.49	0.46
7:H:307:VAL:HG12	7:H:353:VAL:HG23	1.98	0.46
9:E:71:ARG:O	9:E:74:VAL:HG22	2.15	0.46
6:B:868:ARG:HD2	6:B:873:LYS:HG2	1.97	0.46
10:J:136:ASN:ND2	10:J:136:ASN:O	2.49	0.46
7:H:305:TYR:O	8:C:103:ARG:HD2	2.15	0.46
6:B:958:ASP:HA	6:B:961:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1006:ASP:HA	6:B:1009:ARG:HD3	1.96	0.46
6:B:1033:LEU:O	6:B:1037:LYS:NZ	2.49	0.46
2:D:126:LYS:HA	2:D:129:GLN:HB2	1.98	0.46
5:I:194:LYS:HB3	7:H:289:ILE:HD13	1.97	0.46
6:A:1237:PHE:H	6:A:1237:PHE:HD1	1.64	0.46
6:B:894:VAL:O	6:B:898:LEU:HG	2.16	0.46
6:B:901:LYS:HA	6:B:901:LYS:HD2	1.58	0.46
6:B:1168:VAL:HA	6:B:1171:GLU:HG2	1.96	0.46
10:J:92:TYR:HB2	10:J:141:LEU:HD11	1.98	0.46
3:F:3:TYR:O	3:F:3:TYR:CD1	2.68	0.46
3:F:55:TYR:OH	3:F:335:ASP:O	2.22	0.46
4:G:151:HIS:ND1	4:G:191:ASP:OD1	2.42	0.46
5:I:180:CYS:SG	6:A:686:LEU:HD22	2.56	0.46
6:B:702:LEU:O	6:B:706:VAL:HG23	2.16	0.46
4:G:71:LYS:NZ	4:G:84:ASP:OD1	2.36	0.45
4:G:78:HIS:CD2	4:G:163:LEU:HD12	2.51	0.45
5:I:90:ASP:OD1	5:I:90:ASP:N	2.40	0.45
6:A:802:GLN:H	6:A:802:GLN:HG3	1.46	0.45
7:H:346:TYR:CE2	8:C:113:LYS:HE2	2.51	0.45
9:E:56:GLU:HA	9:E:70:GLN:HB2	1.97	0.45
9:E:87:ILE:HG22	9:E:87:ILE:O	2.16	0.45
8:C:65:GLN:HB3	9:E:303:LEU:HD23	1.97	0.45
5:I:100:HIS:CD2	5:I:102:MET:H	2.31	0.45
5:I:181:ILE:HB	5:I:182:PRO:HD3	1.97	0.45
6:A:1139:PHE:HD2	6:A:1286:TYR:CE1	2.34	0.45
6:A:1256:LEU:HD13	6:A:1266:MET:SD	2.56	0.45
8:C:121:LEU:HD21	9:E:372:GLU:HG2	1.99	0.45
6:B:1020:LEU:HD12	6:B:1021:PHE:N	2.31	0.45
3:F:179:ARG:HG2	3:F:262:TYR:CZ	2.51	0.45
3:F:341:ASN:ND2	3:F:343:TYR:H	2.14	0.45
5:I:92:HIS:HD2	5:I:93:PRO:HD2	1.82	0.45
7:H:343:SER:O	7:H:344:ILE:HB	2.15	0.45
6:B:842:THR:OG1	6:B:845:GLU:HG2	2.17	0.45
6:B:1289:GLN:O	6:B:1293:HIS:NE2	2.48	0.45
4:G:171:ILE:HA	4:G:174:LEU:HD12	1.98	0.45
8:C:47:ASN:ND2	9:E:210:ARG:HD2	2.32	0.45
9:E:70:GLN:C	9:E:72:SER:N	2.69	0.45
6:B:849:PHE:O	6:B:850:LYS:HD2	2.16	0.45
4:G:24:PHE:HE1	4:G:129:GLU:HG2	1.81	0.45
5:I:193:LYS:HA	5:I:193:LYS:HD3	1.74	0.45
6:A:802:GLN:O	6:A:806:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:345:GLU:O	3:F:346:TYR:HB2	2.16	0.45
6:A:940:LYS:HE3	6:A:940:LYS:HB3	1.74	0.45
6:A:1164:MET:SD	6:A:1235:LYS:HD2	2.57	0.45
7:H:396:ILE:HG13	6:B:875:ARG:HH22	1.81	0.45
6:B:863:TYR:O	6:B:867:ILE:HD12	2.16	0.45
6:B:1143:ASN:N	6:B:1143:ASN:OD1	2.47	0.45
6:B:1199:VAL:C	6:B:1201:GLU:H	2.19	0.45
10:J:86:ASN:HA	10:J:138:ILE:HD12	1.99	0.45
1:K:77:SER:O	1:K:125:PHE:N	2.40	0.45
2:D:67:ARG:HH11	5:I:156:ARG:HD2	1.81	0.45
2:D:304:VAL:HG22	6:A:871:TYR:CD1	2.48	0.45
5:I:136:SER:HB3	6:A:837:LYS:HA	1.98	0.45
10:J:188:ILE:HA	10:J:216:LEU:HD11	1.99	0.45
2:D:79:ARG:NH2	6:A:830:CYS:SG	2.85	0.45
6:A:1022:PHE:HA	6:A:1305:PHE:CZ	2.51	0.45
6:B:770:ARG:HB2	6:B:775:TRP:NE1	2.32	0.45
6:B:1201:GLU:HB3	6:B:1206:GLN:NE2	2.32	0.45
2:D:73:ARG:O	2:D:76:GLU:HB2	2.17	0.45
3:F:46:ARG:HD3	3:F:343:TYR:OH	2.16	0.44
4:G:218:THR:HG22	4:G:219:GLY:H	1.82	0.44
5:I:98:LYS:HB2	5:I:98:LYS:HE2	1.73	0.44
6:B:1260:ALA:O	6:B:1264:GLU:HG3	2.18	0.44
6:B:1286:TYR:HA	6:B:1289:GLN:NE2	2.32	0.44
3:F:365:TPO:CB	3:F:366:PRO:HD2	2.47	0.44
6:B:946:LYS:O	6:B:950:SER:OG	2.29	0.44
4:G:45:ILE:HD13	4:G:146:ALA:HA	1.99	0.44
7:H:370:SER:HA	7:H:373:GLU:HG2	1.98	0.44
8:C:8:PHE:HD1	8:C:11:LEU:HD12	1.83	0.44
6:B:949:ILE:O	6:B:953:SER:OG	2.32	0.44
2:D:18:ARG:O	2:D:22:GLU:HG3	2.16	0.44
4:G:241:GLY:HA2	4:G:360:MET:SD	2.58	0.44
9:E:70:GLN:HB3	9:E:71:ARG:H	1.61	0.44
6:B:653:THR:HG22	6:B:654:GLU:N	2.32	0.44
6:B:1010:LEU:O	6:B:1013:LEU:HB2	2.17	0.44
3:F:141:VAL:HG11	3:F:329:LEU:HD22	1.98	0.44
3:F:150:HIS:ND1	3:F:184:ASP:OD2	2.47	0.44
8:C:30:THR:O	8:C:34:GLU:HG3	2.17	0.44
10:J:181:LEU:HD23	10:J:181:LEU:HA	1.86	0.44
2:D:14:LYS:HD2	2:D:16:LYS:HZ3	1.82	0.44
6:A:844:ASN:O	6:A:848:ASN:HB2	2.17	0.44
6:A:1327:PRO:HD2	6:A:1333:LYS:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:691:LEU:HD13	6:B:696:ILE:HB	1.99	0.44
3:F:274:ASP:O	3:F:282:GLY:HA3	2.16	0.44
6:A:864:LYS:HE3	6:A:864:LYS:HB3	1.83	0.44
6:A:1276:SER:OG	6:A:1277:THR:N	2.50	0.44
6:A:1343:LEU:HG	6:A:1345:HIS:H	1.83	0.44
9:E:166:LEU:HD23	9:E:166:LEU:HA	1.81	0.44
6:B:1020:LEU:O	6:B:1273:ARG:NH2	2.47	0.44
6:B:1333:LYS:HA	6:B:1336:TYR:HB3	2.00	0.44
5:I:72:LEU:HD12	5:I:73:THR:HG23	2.00	0.44
6:A:982:LYS:HB2	6:A:982:LYS:HE2	1.78	0.44
9:E:66:ASN:HB3	9:E:69:LEU:HD12	2.00	0.44
6:B:957:VAL:HA	6:B:960:THR:HG22	2.00	0.44
10:J:223:PRO:HB2	10:J:275:ARG:HD2	1.99	0.44
4:G:257:LYS:HG3	4:G:380:LEU:HD23	2.00	0.43
5:I:107:TYR:O	5:I:109:ASP:N	2.50	0.43
6:A:1173:ASN:ND2	6:A:1200:GLY:HA2	2.33	0.43
9:E:176:ILE:CG1	9:E:374:LEU:CD1	2.96	0.43
6:B:684:GLU:O	6:B:687:LYS:HB3	2.18	0.43
6:B:984:ILE:O	6:B:988:ILE:HG13	2.18	0.43
6:B:1305:PHE:CE2	6:B:1310:LEU:HA	2.50	0.43
10:J:126:PHE:HB2	10:J:159:ARG:NH2	2.33	0.43
10:J:155:ILE:HD12	10:J:155:ILE:O	2.18	0.43
4:G:86:LEU:HD23	4:G:86:LEU:HA	1.90	0.43
4:G:186:ASP:OD2	4:G:272:GLY:HA3	2.17	0.43
9:E:317:THR:N	9:E:320:GLU:OE1	2.51	0.43
10:J:274:GLN:HE21	10:J:274:GLN:HB3	1.59	0.43
6:A:851:LEU:HD12	6:A:887:PRO:HB3	2.00	0.43
6:A:1003:SER:OG	6:A:1004:ASN:N	2.50	0.43
6:A:1199:VAL:O	6:A:1201:GLU:N	2.50	0.43
6:A:1334:TRP:O	6:A:1338:VAL:HG23	2.18	0.43
7:H:372:LEU:HD22	7:H:383:PRO:HB3	2.00	0.43
6:B:889:VAL:HG13	6:B:890:THR:HG22	1.99	0.43
6:B:1013:LEU:HD13	6:B:1256:LEU:HD23	2.01	0.43
6:B:1152:THR:H	6:B:1152:THR:HG1	1.41	0.43
6:B:1242:ILE:O	6:B:1245:VAL:HG12	2.18	0.43
10:J:73:LEU:HA	10:J:76:THR:HG22	1.99	0.43
7:H:278:LEU:O	7:H:282:THR:HG23	2.18	0.43
8:C:63:GLN:HG2	8:C:64:THR:HG23	2.01	0.43
6:B:1327:PRO:CB	6:B:1333:LYS:HD3	2.43	0.43
2:D:131:GLU:O	2:D:135:MET:HG3	2.18	0.43
3:F:390:GLN:H	3:F:390:GLN:HG2	1.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:114:ASP:HB3	6:B:859:SER:HB3	2.00	0.43
6:A:1157:ARG:O	6:A:1160:GLU:HG2	2.19	0.43
6:A:1168:VAL:HG21	6:A:1232:TYR:CE1	2.54	0.43
6:B:936:LYS:HB2	6:B:936:LYS:HE2	1.62	0.43
6:B:1145:TYR:CE2	6:B:1149:ARG:HD2	2.53	0.43
6:B:1253:ALA:O	6:B:1256:LEU:HB3	2.18	0.43
6:B:1268:LEU:HB3	6:B:1286:TYR:HE2	1.84	0.43
2:D:64:ARG:NH1	5:I:113:ARG:HB3	2.34	0.43
4:G:150:HIS:CD2	4:G:150:HIS:H	2.35	0.43
6:A:983:ASN:HA	6:A:986:TYR:CE2	2.54	0.43
6:A:1214:LEU:HD11	6:A:1221:HIS:CE1	2.54	0.43
7:H:309:ILE:HG23	7:H:352:PRO:HB2	2.00	0.43
8:C:13:ASP:O	8:C:17:VAL:HG23	2.19	0.43
6:B:979:PHE:HB2	6:B:1310:LEU:HD23	2.01	0.43
6:B:1235:LYS:HB2	6:B:1235:LYS:HE2	1.74	0.43
6:B:1069:LEU:HG	6:B:1257:MET:HG2	2.00	0.43
6:B:1136:PHE:CE2	6:B:1307:LYS:HD2	2.54	0.43
10:J:85:LYS:HZ2	10:J:85:LYS:HG3	1.71	0.43
6:A:943:LEU:HD12	6:A:943:LEU:HA	1.82	0.43
6:A:1268:LEU:HD21	6:A:1289:GLN:CB	2.48	0.43
7:H:205:LEU:HA	7:H:208:LEU:HD22	2.00	0.43
8:C:80:MET:N	8:C:81:PRO:HD2	2.33	0.43
6:B:986:TYR:CE1	6:B:1029:ILE:HG22	2.53	0.43
2:D:37:ASP:O	2:D:41:LYS:NZ	2.38	0.43
6:A:1237:PHE:HA	6:A:1240:TYR:CE1	2.53	0.43
6:A:1258:THR:HG22	6:A:1258:THR:O	2.19	0.43
6:A:1331:GLU:HG3	6:A:1334:TRP:HD1	1.84	0.43
4:G:79:THR:HB	6:B:765:MET:SD	2.59	0.43
5:I:118:HIS:NE2	6:A:694:GLN:OE1	2.52	0.43
7:H:222:GLU:O	7:H:225:VAL:HG12	2.18	0.43
9:E:226:ILE:O	9:E:226:ILE:HG13	2.18	0.43
2:D:51:LEU:HD21	9:E:336:GLN:NE2	2.34	0.42
3:F:211:TYR:CB	3:F:237:PRO:HB3	2.49	0.42
3:F:341:ASN:HD22	3:F:343:TYR:H	1.67	0.42
3:F:360:MET:HB3	6:A:930:HIS:CD2	2.54	0.42
5:I:121:LEU:HD21	5:I:169:HIS:HD2	1.81	0.42
6:A:986:TYR:O	6:A:989:LEU:HB2	2.19	0.42
6:A:1327:PRO:HG2	6:A:1333:LYS:HG2	2.00	0.42
6:B:736:ILE:HB	10:J:236:LEU:HD13	2.01	0.42
6:B:943:LEU:HD12	6:B:943:LEU:HA	1.76	0.42
6:B:1031:GLU:O	6:B:1035:SER:OG	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1205:LYS:HE2	6:B:1205:LYS:HB2	1.68	0.42
2:D:312:ARG:NH1	2:D:312:ARG:HG2	2.33	0.42
4:G:88:ARG:HH21	4:G:97:PHE:HE1	1.67	0.42
5:I:133:LEU:HD23	6:A:837:LYS:HD2	2.01	0.42
5:I:133:LEU:HA	6:A:837:LYS:HG3	2.01	0.42
6:A:983:ASN:HA	6:A:986:TYR:CD2	2.54	0.42
6:B:787:VAL:O	6:B:787:VAL:HG13	2.19	0.42
6:B:1007:LYS:O	6:B:1010:LEU:HD23	2.19	0.42
6:B:1159:LEU:O	6:B:1163:GLN:HG3	2.19	0.42
2:D:49:THR:HA	2:D:52:THR:HG22	2.01	0.42
4:G:269:LEU:HD21	4:G:295:VAL:HG22	2.01	0.42
6:B:685:PHE:HE2	6:B:706:VAL:HG13	1.84	0.42
6:B:787:VAL:O	6:B:789:ALA:N	2.52	0.42
2:D:16:LYS:HD2	2:D:16:LYS:H	1.85	0.42
6:A:714:LYS:HE3	6:A:714:LYS:HB3	1.64	0.42
6:A:1004:ASN:N	6:A:1004:ASN:OD1	2.53	0.42
7:H:391:LEU:HD11	6:B:897:ARG:HD3	2.01	0.42
9:E:296:GLN:HB3	9:E:301:LEU:HD23	2.02	0.42
2:D:111:LYS:HB3	2:D:111:LYS:HE3	1.66	0.42
4:G:185:ILE:HG12	4:G:270:GLN:O	2.19	0.42
5:I:113:ARG:NH2	5:I:156:ARG:HH21	2.17	0.42
6:A:673:LYS:HG3	6:A:682:TYR:CE1	2.54	0.42
6:A:1162:LYS:HE2	6:A:1162:LYS:HB3	1.88	0.42
10:J:91:TYR:CD2	10:J:102:GLU:HG2	2.54	0.42
6:B:1016:TYR:O	6:B:1020:LEU:HG	2.20	0.42
6:B:1242:ILE:O	6:B:1246:THR:HG23	2.19	0.42
10:J:217:PRO:HG3	10:J:274:GLN:CD	2.40	0.42
3:F:23:TYR:CE1	3:F:25:TYR:HB2	2.55	0.42
6:A:690:ASN:HA	6:A:693:SER:OG	2.19	0.42
6:A:745:LEU:O	6:A:756:LYS:HD2	2.19	0.42
6:B:1302:ARG:O	6:B:1302:ARG:HG3	2.20	0.42
3:F:13:VAL:O	3:F:13:VAL:CG2	2.68	0.42
4:G:341:ASN:H	4:G:341:ASN:ND2	2.18	0.42
9:E:48:LEU:HA	9:E:48:LEU:HD23	1.74	0.42
6:B:684:GLU:HB3	6:B:709:TYR:OH	2.20	0.42
10:J:140:THR:HG23	10:J:229:GLU:OE2	2.20	0.42
3:F:44:ARG:HG2	3:F:45:ILE:N	2.35	0.42
3:F:63:ILE:HD12	7:H:262:PHE:CZ	2.55	0.42
7:H:362:ARG:CZ	9:E:168:PRO:HG3	2.50	0.42
9:E:165:ILE:HG23	9:E:180:THR:HG21	2.02	0.42
6:B:995:PHE:CD1	6:B:1250:VAL:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:714:LYS:O	6:A:718:THR:HG22	2.19	0.41
6:A:1333:LYS:H	6:A:1333:LYS:HG3	1.69	0.41
9:E:26:ILE:HD13	6:B:669:PHE:CG	2.55	0.41
9:E:73:GLU:HA	10:J:252:TRP:CH2	2.55	0.41
3:F:239:ARG:HB2	3:F:364:ASN:OD1	2.20	0.41
3:F:365:TPO:CB	3:F:366:PRO:CD	2.97	0.41
9:E:231:LEU:O	9:E:233:LEU:N	2.45	0.41
6:B:1141:ASN:HB2	6:B:1298:GLU:OE2	2.21	0.41
2:D:310:LEU:HD23	2:D:310:LEU:O	2.20	0.41
3:F:3:TYR:O	3:F:3:TYR:CG	2.70	0.41
3:F:274:ASP:HA	3:F:279:ASP:OD1	2.20	0.41
7:H:344:ILE:HD12	7:H:344:ILE:HA	1.83	0.41
6:B:735:ASN:ND2	10:J:68:SER:O	2.54	0.41
6:B:1267:ALA:O	6:B:1271:LYS:HG3	2.20	0.41
4:G:257:LYS:HD2	4:G:261:TRP:CE3	2.56	0.41
5:I:118:HIS:HD2	5:I:119:PHE:CD2	2.37	0.41
6:A:1228:LEU:HD23	6:A:1228:LEU:HA	1.93	0.41
7:H:315:THR:HB	7:H:357:GLU:OE2	2.20	0.41
6:B:701:ASP:O	6:B:705:LYS:HG2	2.20	0.41
6:B:1226:GLU:O	6:B:1230:GLN:HG2	2.20	0.41
6:B:1289:GLN:O	6:B:1292:SER:OG	2.38	0.41
10:J:261:ASP:OD1	10:J:261:ASP:N	2.54	0.41
1:K:113:LYS:O	1:K:117:THR:N	2.53	0.41
6:A:831:LEU:HD22	6:A:891:ALA:HB1	2.01	0.41
6:A:960:THR:HG22	6:A:962:LYS:HG2	2.03	0.41
6:A:1203:ALA:O	6:A:1207:VAL:HG12	2.21	0.41
6:A:1304:GLU:OE2	6:A:1325:LYS:HE2	2.19	0.41
7:H:353:VAL:HB	8:C:110:VAL:HG21	2.03	0.41
6:B:938:ALA:O	6:B:942:LEU:HB2	2.20	0.41
6:B:1165:ASN:OD1	6:B:1204:TYR:N	2.47	0.41
6:B:1287:ARG:HD2	6:B:1323:THR:HB	2.01	0.41
3:F:14:LYS:HB2	3:F:14:LYS:HE2	1.75	0.41
3:F:265:SEP:O1P	3:F:265:SEP:CA	2.67	0.41
11:F:501:TPO:O2P	11:F:501:TPO:CG2	2.69	0.41
6:A:679:LYS:O	6:A:683:THR:OG1	2.24	0.41
3:F:254:VAL:O	3:F:258:ILE:HG13	2.21	0.41
3:F:365:TPO:CG2	3:F:366:PRO:CD	2.85	0.41
5:I:108:THR:C	5:I:110:ALA:H	2.24	0.41
8:C:143:SER:OG	8:C:144:LYS:N	2.54	0.41
6:B:729:LYS:O	6:B:729:LYS:HD2	2.20	0.41
6:B:1330:ASP:O	6:B:1334:TRP:HD1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:124:GLY:O	3:F:128:MET:HG3	2.20	0.41
4:G:19:ARG:NH2	4:G:302:GLY:HA2	2.32	0.41
6:A:744:ASP:HB2	8:C:133:LEU:HB2	2.02	0.41
6:A:993:ASP:HA	6:A:996:ILE:HD12	2.03	0.41
7:H:361:ASP:OD1	7:H:364:ARG:NH1	2.54	0.41
8:C:47:ASN:ND2	9:E:210:ARG:HH11	2.18	0.41
6:B:864:LYS:HG2	6:B:880:ILE:HD13	2.02	0.41
6:B:885:GLU:O	6:B:886:HIS:ND1	2.54	0.41
6:B:1322:LEU:HD21	6:B:1326:GLU:OE1	2.20	0.41
3:F:8:PHE:O	3:F:8:PHE:CD1	2.74	0.41
3:F:239:ARG:N	3:F:364:ASN:OD1	2.41	0.41
3:F:273:GLY:H	3:F:311:GLY:C	2.23	0.41
4:G:124:GLY:O	4:G:128:MET:HG3	2.21	0.41
5:I:90:ASP:O	5:I:92:HIS:N	2.46	0.41
6:A:1162:LYS:HD2	6:A:1204:TYR:CE1	2.56	0.41
6:A:1168:VAL:O	6:A:1172:ILE:HG13	2.21	0.41
7:H:202:ASP:O	7:H:206:VAL:HG23	2.21	0.41
7:H:287:TYR:CE1	8:C:87:MET:HE1	2.56	0.41
7:H:362:ARG:NH2	8:C:7:LEU:HD12	2.36	0.41
6:B:1004:ASN:N	6:B:1005:PRO:HD2	2.36	0.41
6:B:1201:GLU:HB3	6:B:1206:GLN:CD	2.41	0.41
1:K:149:SER:N	1:K:153:SER:O	2.35	0.41
3:F:242:ILE:HG13	3:F:246:THR:HB	2.02	0.41
6:A:770:ARG:HH21	6:A:778:LEU:HD13	1.86	0.41
9:E:103:THR:HG23	9:E:104:ASN:N	2.30	0.41
9:E:324:LEU:O	9:E:328:ILE:HG13	2.20	0.41
6:B:651:GLU:H	6:B:651:GLU:CD	2.24	0.41
6:B:1220:GLU:HG3	6:B:1223:TRP:HD1	1.86	0.41
6:B:1251:LYS:HB3	6:B:1251:LYS:HE3	1.72	0.41
5:I:113:ARG:O	5:I:117:ASP:HB2	2.21	0.40
6:A:1274:ASN:N	6:A:1274:ASN:OD1	2.54	0.40
10:J:182:ARG:HE	10:J:182:ARG:HB3	1.77	0.40
4:G:14:LYS:HE3	4:G:14:LYS:HB3	1.94	0.40
4:G:257:LYS:HD2	4:G:261:TRP:CD2	2.56	0.40
6:A:1281:LYS:HD3	6:A:1281:LYS:H	1.86	0.40
6:B:913:ASN:HA	6:B:916:TRP:HB2	2.03	0.40
10:J:176:ASP:O	10:J:180:VAL:HG12	2.22	0.40
3:F:67:LYS:HE2	3:F:67:LYS:HB2	1.71	0.40
3:F:224:ILE:HD13	3:F:379:ASN:OD1	2.21	0.40
4:G:153:LYS:HE2	4:G:158:SER:OG	2.21	0.40
6:A:809:LYS:HB3	6:A:809:LYS:HE2	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:125:VAL:HG12	8:C:126:ASP:N	2.36	0.40
1:K:368:HIS:O	1:K:399:ALA:N	2.50	0.40
3:F:388:SEP:O3P	4:G:54:ASN:O	2.40	0.40
3:F:389:VAL:O	3:F:389:VAL:CG1	2.69	0.40
4:G:221:LEU:O	4:G:221:LEU:HD13	2.22	0.40
4:G:359:ASN:HD22	6:B:1234:ASN:HD22	1.69	0.40
6:A:906:ARG:O	6:A:910:ARG:HG2	2.21	0.40
2:D:44:LEU:HG	7:H:286:TRP:HE1	1.86	0.40
4:G:341:ASN:H	4:G:341:ASN:HD22	1.68	0.40
6:A:636:ARG:HA	6:A:636:ARG:HD2	1.76	0.40
6:B:1287:ARG:O	6:B:1290:VAL:HG12	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	K	403/460 (88%)	396 (98%)	7 (2%)	0	100	100
2	D	160/327 (49%)	157 (98%)	3 (2%)	0	100	100
3	F	385/433 (89%)	356 (92%)	26 (7%)	3 (1%)	19	39
4	G	383/433 (88%)	360 (94%)	23 (6%)	0	100	100
5	I	127/201 (63%)	110 (87%)	14 (11%)	3 (2%)	6	10
6	A	627/1536 (41%)	593 (95%)	32 (5%)	2 (0%)	41	64
6	B	605/1536 (39%)	551 (91%)	54 (9%)	0	100	100
7	H	231/405 (57%)	208 (90%)	20 (9%)	3 (1%)	12	24
8	C	134/330 (41%)	128 (96%)	3 (2%)	3 (2%)	6	12
9	E	245/430 (57%)	217 (89%)	24 (10%)	4 (2%)	9	19
10	J	205/294 (70%)	188 (92%)	17 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3505/6385 (55%)	3264 (93%)	223 (6%)	18 (0%)	32	52

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	177	GLU
5	I	178	THR
7	H	344	ILE
9	E	42	GLN
9	E	71	ARG
3	F	266	ALA
3	F	389	VAL
7	H	343	SER
5	I	128	THR
8	C	129	PRO
9	E	72	SER
9	E	103	THR
3	F	366	PRO
6	A	1233	ASN
7	H	315	THR
8	C	128	HIS
8	C	130	ALA
6	A	1200	GLY

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	
2	D	153/289 (53%)	124 (81%)	29 (19%)	1	2
3	F	328/362 (91%)	301 (92%)	27 (8%)	11	22
4	G	326/367 (89%)	292 (90%)	34 (10%)	7	13
5	I	119/178 (67%)	105 (88%)	14 (12%)	5	9
6	A	585/1391 (42%)	524 (90%)	61 (10%)	7	13
6	B	574/1391 (41%)	513 (89%)	61 (11%)	6	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	213/371 (57%)	190 (89%)	23 (11%)	6	12
8	C	129/290 (44%)	123 (95%)	6 (5%)	26	50
9	E	234/391 (60%)	210 (90%)	24 (10%)	7	13
10	J	190/269 (71%)	167 (88%)	23 (12%)	5	9
All	All	2851/5299 (54%)	2549 (89%)	302 (11%)	10	12

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	16	LYS
2	D	34	SER
2	D	36	ARG
2	D	38	ASN
2	D	43	ARG
2	D	47	LEU
2	D	51	LEU
2	D	53	SER
2	D	54	LEU
2	D	58	ASP
2	D	71	GLU
2	D	79	ARG
2	D	80	LEU
2	D	89	SER
2	D	94	GLU
2	D	98	ASP
2	D	111	LYS
2	D	113	CYS
2	D	127	LYS
2	D	128	LEU
2	D	129	GLN
2	D	131	GLU
2	D	132	ARG
2	D	141	HIS
2	D	288	TYR
2	D	290	THR
2	D	291	LYS
2	D	312	ARG
2	D	313	GLU
3	F	11	ILE
3	F	13	VAL
3	F	14	LYS

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Mol	Chain	Res	Type
3	F	17	ASP
3	F	40	MET
3	F	44	ARG
3	F	55	TYR
3	F	60	LYS
3	F	70	THR
3	F	108	ASP
3	F	121	SER
3	F	127	SER
3	F	133	ARG
3	F	150	HIS
3	F	179	ARG
3	F	187	VAL
3	F	214	PHE
3	F	264	PRO
3	F	270	GLN
3	F	275	SER
3	F	277	SER
3	F	287	SER
3	F	316	ARG
3	F	318	VAL
3	F	337	ASP
3	F	374	THR
3	F	389	VAL
4	G	17	ASP
4	G	20	ARG
4	G	28	ASP
4	G	29	VAL
4	G	41	LYS
4	G	44	ARG
4	G	50	SER
4	G	67	LYS
4	G	75	CYS
4	G	99	ARG
4	G	109	ASP
4	G	112	VAL
4	G	116	LEU
4	G	123	SER
4	G	150	HIS
4	G	154	LYS
4	G	160	PHE
4	G	199	THR

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Mol	Chain	Res	Type
4	G	205	THR
4	G	213	GLU
4	G	221	LEU
4	G	222	ARG
4	G	231	ASN
4	G	244	ASP
4	G	246	THR
4	G	249	SER
4	G	277	SER
4	G	280	ARG
4	G	314	THR
4	G	328	LEU
4	G	341	ASN
4	G	371	LYS
4	G	375	ASN
4	G	383	THR
5	I	72	LEU
5	I	109	ASP
5	I	117	ASP
5	I	123	VAL
5	I	149	THR
5	I	171	ASP
5	I	172	GLU
5	I	173	HIS
5	I	175	ILE
5	I	176	LYS
5	I	177	GLU
5	I	180	CYS
5	I	192	LYS
5	I	196	LYS
6	A	646	VAL
6	A	674	ARG
6	A	691	LEU
6	A	698	ASP
6	A	700	ASP
6	A	704	GLU
6	A	717	PHE
6	A	727	GLN
6	A	742	ARG
6	A	747	LEU
6	A	761	SER
6	A	780	ASP

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Mol	Chain	Res	Type
6	A	792	ASP
6	A	799	ARG
6	A	801	ASN
6	A	802	GLN
6	A	823	SER
6	A	825	LEU
6	A	826	ARG
6	A	827	THR
6	A	833	THR
6	A	848	ASN
6	A	859	SER
6	A	860	MET
6	A	861	THR
6	A	864	LYS
6	A	868	ARG
6	A	872	ASP
6	A	920	GLU
6	A	927	SER
6	A	929	ASP
6	A	946	LYS
6	A	950	SER
6	A	954	SER
6	A	981	ASP
6	A	982	LYS
6	A	999	THR
6	A	1004	ASN
6	A	1006	ASP
6	A	1013	LEU
6	A	1033	LEU
6	A	1036	HIS
6	A	1062	GLU
6	A	1067	ASP
6	A	1069	LEU
6	A	1149	ARG
6	A	1156	GLU
6	A	1161	ILE
6	A	1170	LYS
6	A	1199	VAL
6	A	1202	ASP
6	A	1248	SER
6	A	1274	ASN
6	A	1277	THR

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Mol	Chain	Res	Type
6	A	1281	LYS
6	A	1288	LEU
6	A	1295	SER
6	A	1319	LEU
6	A	1325	LYS
6	A	1337	TYR
6	A	1345	HIS
7	H	171	SER
7	H	175	MET
7	H	205	LEU
7	H	208	LEU
7	H	209	GLN
7	H	220	HIS
7	H	222	GLU
7	H	233	ILE
7	H	245	GLN
7	H	250	SER
7	H	251	CYS
7	H	274	LEU
7	H	324	SER
7	H	333	GLU
7	H	338	ASP
7	H	349	ARG
7	H	351	ASN
7	H	368	GLU
7	H	370	SER
7	H	371	ASP
7	H	383	PRO
7	H	395	GLU
7	H	396	ILE
8	C	21	PHE
8	C	76	TYR
8	C	82	SER
8	C	103	ARG
8	C	137	LEU
8	C	139	GLU
9	E	32	ARG
9	E	49	ASP
9	E	61	SER
9	E	76	THR
9	E	99	ARG
9	E	101	LEU

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Mol	Chain	Res	Type
9	E	102	GLN
9	E	159	LEU
9	E	162	VAL
9	E	187	SER
9	E	231	LEU
9	E	245	ASP
9	E	286	ASP
9	E	317	THR
9	E	320	GLU
9	E	322	GLN
9	E	324	LEU
9	E	329	GLU
9	E	340	GLN
9	E	361	ARG
9	E	367	LEU
9	E	371	ARG
9	E	372	GLU
9	E	376	ILE
6	B	657	GLU
6	B	664	GLU
6	B	671	LYS
6	B	687	LYS
6	B	695	ASP
6	B	697	LEU
6	B	714	LYS
6	B	729	LYS
6	B	734	GLU
6	B	742	ARG
6	B	744	ASP
6	B	748	CYS
6	B	760	LYS
6	B	765	MET
6	B	768	SER
6	B	826	ARG
6	B	830	CYS
6	B	844	ASN
6	B	850	LYS
6	B	860	MET
6	B	881	ASP
6	B	883	LEU
6	B	890	THR
6	B	901	LYS

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Mol	Chain	Res	Type
6	B	918	GLU
6	B	920	GLU
6	B	929	ASP
6	B	948	LEU
6	B	978	ASP
6	B	991	LEU
6	B	999	THR
6	B	1004	ASN
6	B	1006	ASP
6	B	1010	LEU
6	B	1016	TYR
6	B	1025	SER
6	B	1029	ILE
6	B	1036	HIS
6	B	1067	ASP
6	B	1134	SER
6	B	1137	ASN
6	B	1143	ASN
6	B	1152	THR
6	B	1159	LEU
6	B	1164	MET
6	B	1192	SER
6	B	1205	LYS
6	B	1211	SER
6	B	1224	PHE
6	B	1226	GLU
6	B	1248	SER
6	B	1251	LYS
6	B	1266	MET
6	B	1294	MET
6	B	1298	GLU
6	B	1301	PHE
6	B	1309	THR
6	B	1319	LEU
6	B	1321	ASP
6	B	1335	LYS
6	B	1341	TYR
10	J	63	ASP
10	J	64	LEU
10	J	68	SER
10	J	69	SER
10	J	71	SER

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Mol	Chain	Res	Type
10	J	106	SER
10	J	107	TYR
10	J	109	ASP
10	J	120	ASN
10	J	157	SER
10	J	161	ARG
10	J	169	ASP
10	J	172	SER
10	J	173	ASP
10	J	183	HIS
10	J	224	PHE
10	J	225	ASP
10	J	259	ILE
10	J	261	ASP
10	J	265	TYR
10	J	269	SER
10	J	273	LYS
10	J	276	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	20	ASN
2	D	38	ASN
2	D	106	HIS
2	D	141	HIS
3	F	231	ASN
3	F	341	ASN
3	F	382	ASN
3	F	392	ASN
4	G	38	HIS
4	G	177	HIS
4	G	231	ASN
4	G	235	ASN
4	G	341	ASN
5	I	82	ASN
5	I	92	HIS
5	I	100	HIS
5	I	173	HIS
6	A	663	ASN
6	A	690	ASN
6	A	741	HIS

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Mol	Chain	Res	Type
6	A	798	HIS
6	A	802	GLN
6	A	829	GLN
6	A	836	ASN
6	A	848	ASN
6	A	930	HIS
6	A	947	GLN
6	A	959	GLN
6	A	983	ASN
6	A	1036	HIS
6	A	1173	ASN
6	A	1252	HIS
6	A	1293	HIS
6	A	1299	ASN
6	A	1345	HIS
7	H	264	HIS
7	H	327	GLN
7	H	351	ASN
8	C	47	ASN
8	C	128	HIS
8	C	135	HIS
9	E	24	ASN
9	E	94	ASN
9	E	322	GLN
9	E	340	GLN
9	E	360	ASN
6	B	694	GLN
6	B	735	ASN
6	B	801	ASN
6	B	815	HIS
6	B	840	ASN
6	B	900	GLN
6	B	965	HIS
6	B	1070	HIS
6	B	1163	GLN
6	B	1206	GLN
6	B	1216	ASN
6	B	1233	ASN
6	B	1234	ASN
6	B	1296	ASN
10	J	120	ASN
10	J	237	GLN

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Mol	Chain	Res	Type
10	J	260	HIS
10	J	274	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SEP	E	171	9	8,9,10	0.69	0	8,12,14	1.52	1 (12%)
5	SEP	I	174	5	8,9,10	0.96	0	8,12,14	0.82	0
3	SEP	F	388	3	8,9,10	0.73	0	8,12,14	1.08	1 (12%)
3	TPO	F	365	3	8,10,11	0.86	0	10,14,16	1.19	2 (20%)
2	SEP	D	309	2	8,9,10	0.94	0	8,12,14	0.94	0
9	TPO	E	167	9	8,10,11	2.98	1 (12%)	10,14,16	1.56	2 (20%)
3	SEP	F	265	3	8,9,10	1.97	1 (12%)	8,12,14	2.22	3 (37%)
3	TPO	F	6	3	8,10,11	0.99	0	10,14,16	1.33	1 (10%)
3	TPO	F	12	3	8,10,11	0.81	0	10,14,16	1.12	1 (10%)

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
9	SEP	E	171	9	-	2/5/8/10	-
5	SEP	I	174	5	-	1/5/8/10	-
3	SEP	F	388	3	-	3/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPO	F	365	3	-	7/9/11/13	-
2	SEP	D	309	2	-	2/5/8/10	-
9	TPO	E	167	9	-	6/9/11/13	-
3	SEP	F	265	3	-	4/5/8/10	-
3	TPO	F	6	3	-	0/9/11/13	-
3	TPO	F	12	3	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	167	TPO	P-OG1	-7.95	1.44	1.59
3	F	265	SEP	O-C	-4.57	1.01	1.19

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	265	SEP	O2P-P-OG	-4.51	94.74	106.73
9	E	167	TPO	P-OG1-CB	-3.55	112.48	123.21
9	E	171	SEP	O3P-P-OG	-2.75	99.41	106.73
3	F	265	SEP	OG-P-O1P	2.72	114.11	106.47
3	F	388	SEP	OG-CB-CA	2.70	110.78	108.14
3	F	6	TPO	O-C-CA	-2.54	118.13	124.78
3	F	365	TPO	P-OG1-CB	-2.50	115.66	123.21
3	F	265	SEP	O3P-P-O2P	2.44	116.97	107.64
3	F	12	TPO	O-C-CA	-2.41	118.47	124.78
9	E	167	TPO	O2P-P-OG1	-2.25	95.91	105.99
3	F	365	TPO	O-C-CA	-2.24	118.91	124.78

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	12	TPO	O-C-CA-CB
3	F	265	SEP	N-CA-CB-OG
3	F	265	SEP	CB-OG-P-O2P
3	F	265	SEP	CB-OG-P-O3P
3	F	365	TPO	N-CA-CB-CG2
3	F	365	TPO	N-CA-CB-OG1
3	F	365	TPO	C-CA-CB-CG2
3	F	365	TPO	CA-CB-OG1-P

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Mol	Chain	Res	Type	Atoms
3	F	388	SEP	N-CA-CB-OG
9	E	167	TPO	N-CA-CB-CG2
9	E	167	TPO	N-CA-CB-OG1
9	E	167	TPO	C-CA-CB-CG2
9	E	167	TPO	O-C-CA-CB
9	E	167	TPO	CG2-CB-OG1-P
9	E	171	SEP	N-CA-CB-OG
3	F	365	TPO	CB-OG1-P-O1P
3	F	265	SEP	CA-CB-OG-P
3	F	388	SEP	CA-CB-OG-P
9	E	171	SEP	CA-CB-OG-P
5	I	174	SEP	N-CA-CB-OG
2	D	309	SEP	CB-OG-P-O1P
2	D	309	SEP	CB-OG-P-O2P
3	F	388	SEP	CB-OG-P-O2P
3	F	365	TPO	CB-OG1-P-O3P
9	E	167	TPO	CB-OG1-P-O2P
3	F	365	TPO	O-C-CA-CB

There are no ring outliers.

5 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	388	SEP	1	0
3	F	365	TPO	8	0
9	E	167	TPO	8	0
3	F	265	SEP	6	0
3	F	6	TPO	5	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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
11	TPO	F	501	3	9,11,11	0.83	0	13,16,16	1.79	1 (7%)

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
11	TPO	F	501	3	-	5/13/13/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	501	TPO	CB-CA-C	5.25	122.46	110.32

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	501	TPO	O-C-CA-N
11	F	501	TPO	OXT-C-CA-N
11	F	501	TPO	O-C-CA-CB
11	F	501	TPO	OXT-C-CA-CB
11	F	501	TPO	CG2-CB-OG1-P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	501	TPO	3	0

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.