



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:01 AM UTC

PDB ID : 8GA8 / pdb_00008ga8
EMDB ID : EMD-29892
Title : Structure of the yeast (HDAC) Rpd3L complex
Authors : Patel, A.B.; Radhakrishnan, I.; He, Y.
Deposited on : 2023-02-22
Resolution : 3.50 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

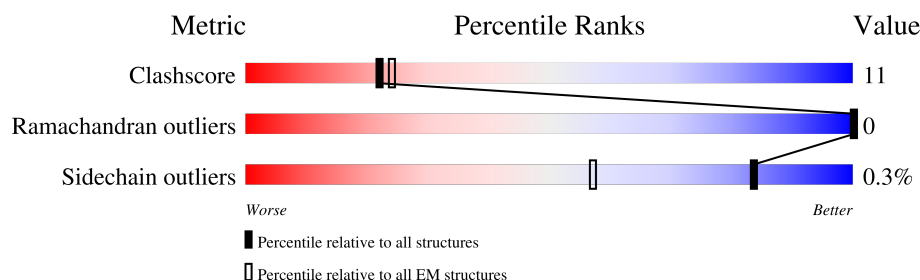
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	H	327	34% 10% 56%
2	A	1536	25% 10% 66%
2	D	1536	23% 10% 67%
3	J	201	32% 13% 55%
4	L	330	28% 11% 61%
5	M	430	37% 15% 48%
6	G	405	20% . 76%
7	B	433	65% 23% 12%
7	E	433	63% 25% 12%

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Mol	Chain	Length	Quality of chain
8	K	294	 A horizontal bar chart showing the quality of chain K. The bar is divided into three segments: a green segment on the left representing 52%, a yellow segment in the middle representing 16%, and a grey segment on the right representing 32%. The percentages are labeled below each segment.

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 22011 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 SDS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	144	Total	C	N	O	S	0	0
			1206	749	222	234	1		

- Molecule 2 is a protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	525	Total	C	N	O	S	0	0
			4417	2838	749	815	15		
2	D	503	Total	C	N	O	S	0	0
			4240	2731	724	772	13		

- Molecule 3 is a protein called Transcriptional regulatory protein SAP30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	90	Total	C	N	O	S	0	0
			767	486	142	138	1		

- Molecule 4 is a protein called Transcriptional regulatory protein PHO23.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	129	Total	C	N	O	S	0	0
			1052	659	182	204	7		

- Molecule 5 is a protein called Transcriptional regulatory protein RXT2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	223	Total	C	N	O	S	1	0
			1832	1156	334	339	3		

- Molecule 6 is a protein called Transcriptional regulatory protein DEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	97	Total	C	N	O	S	0	0
			838	527	155	154	2		

- Molecule 7 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	383	Total	C	N	O	S	0	0
			3039	1935	510	568	26		
7	E	382	Total	C	N	O	S	0	0
			3031	1930	509	567	25		

- Molecule 8 is a protein called Transcriptional regulatory protein RXT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	199	Total	C	N	O	S	0	0
			1587	1012	268	305	2		

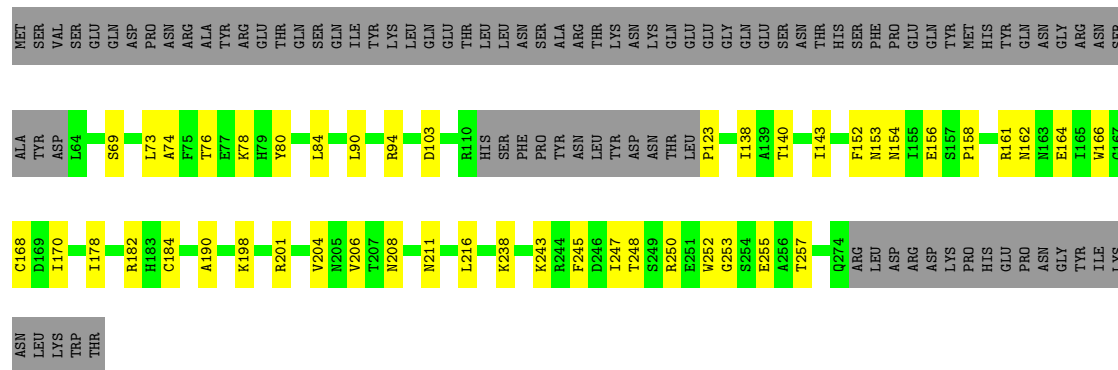
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	B	1	Total	Zn	0
			1	1	
9	E	1	Total	Zn	0
			1	1	

- Molecule 2: Transcriptional regulatory protein SIN3



- Molecule 8: Transcriptional regulatory protein RXT3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	210993	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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

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	H	0.11	0/1222	0.30	0/1637
2	A	0.11	0/4509	0.28	0/6072
2	D	0.10	0/4333	0.26	0/5836
3	J	0.10	0/784	0.26	0/1050
4	L	0.16	0/1067	0.36	0/1434
5	M	0.13	0/1856	0.33	0/2493
6	G	0.12	0/855	0.26	0/1153
7	B	0.13	0/3118	0.32	1/4220 (0.0%)
7	E	0.12	0/3110	0.31	0/4210
8	K	0.10	0/1626	0.26	0/2209
All	All	0.12	0/22480	0.29	1/30314 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	111	PRO	CA-N-CD	-6.09	103.47	112.00

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	H	1206	0	1210	35	0
2	A	4417	0	4398	113	0
2	D	4240	0	4237	104	0
3	J	767	0	759	24	0
4	L	1052	0	1060	29	0
5	M	1832	0	1888	55	0
6	G	838	0	820	16	0
7	B	3039	0	2919	82	0
7	E	3031	0	2907	84	0
8	K	1587	0	1556	29	0
9	B	1	0	0	0	0
9	E	1	0	0	0	0
All	All	22011	0	21754	501	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 11.

All (501) 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)
7:E:200:THR:HG21	2:D:777:VAL:HA	1.63	0.79
2:D:1219:LEU:HD11	2:D:1223:TRP:HB2	1.70	0.73
2:A:1228:LEU:HD11	2:A:1240:TYR:HE2	1.51	0.72
8:K:143:ILE:HG21	8:K:178:ILE:HD11	1.71	0.72
2:D:814:ARG:HH21	2:D:916:TRP:HB3	1.56	0.69
2:D:1253:ALA:HA	2:D:1256:LEU:HD12	1.75	0.69
7:E:184:ASP:HB3	7:E:207:SER:HA	1.76	0.68
7:E:221:LEU:HD21	7:E:372:VAL:HG13	1.77	0.67
2:D:1291:ARG:HA	2:D:1294:MET:HB3	1.75	0.67
5:M:63:ASN:H	5:M:66:ASN:HD21	1.42	0.67
2:A:1234:ASN:HB3	7:B:359:ASN:HD21	1.58	0.67
2:D:952:ILE:HD12	2:D:1316:TYR:HB2	1.76	0.66
5:M:56:GLU:N	5:M:56:GLU:OE2	2.29	0.66
5:M:227:TYR:H	5:M:230:ASN:HB2	1.61	0.66
2:A:951:GLU:OE2	2:A:1149:ARG:NH1	2.29	0.65
5:M:169[A]:ILE:HG13	5:M:171:SER:H	1.61	0.65
5:M:187:SER:O	5:M:373:ARG:NH1	2.30	0.65
7:E:327:GLY:HA3	7:E:334:LEU:HD21	1.78	0.65
2:A:773:MET:HE1	5:M:360:GLN:HE22	1.61	0.65
7:B:43:HIS:CE1	7:B:46:ARG:HD2	2.32	0.65
2:D:1300:MET:SD	2:D:1300:MET:N	2.70	0.65
5:M:169[B]:ILE:HG13	5:M:171:SER:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:74:ALA:O	8:K:78:LYS:HG2	1.97	0.64
2:D:851:LEU:HB3	2:D:884:HIS:HA	1.78	0.64
7:B:50:SER:O	7:B:54:ASN:ND2	2.31	0.64
7:E:210:LYS:NZ	7:E:211:TYR:O	2.31	0.64
7:E:181:LEU:HD22	7:E:267:VAL:HG22	1.79	0.63
4:L:84:GLU:HA	4:L:87:MET:HG3	1.79	0.63
2:A:814:ARG:NH2	7:B:345:GLU:O	2.30	0.63
7:B:197:PHE:HB3	7:B:203:VAL:HG21	1.79	0.63
2:D:1228:LEU:HD12	2:D:1232:TYR:HE2	1.63	0.63
3:J:126:ASN:HB3	3:J:162:LEU:HD23	1.79	0.63
2:D:865:LYS:O	2:D:865:LYS:NZ	2.32	0.63
1:H:304:VAL:HG23	2:A:871:TYR:HD2	1.62	0.63
7:B:48:ALA:O	7:B:52:ILE:HG13	1.98	0.62
2:A:975:LEU:HD12	2:A:1314:ILE:HD11	1.81	0.62
2:D:1212:ARG:O	2:D:1216:ASN:ND2	2.32	0.62
1:H:311:ILE:HD12	1:H:314:LEU:HD21	1.82	0.62
3:J:176:LYS:HD2	3:J:178:THR:HG23	1.81	0.62
4:L:80:MET:HA	4:L:83:LEU:HD12	1.82	0.62
8:K:94:ARG:NH2	8:K:156:GLU:O	2.33	0.62
2:D:1261:LYS:HE3	2:D:1265:ILE:HD11	1.82	0.62
7:E:359:ASN:ND2	2:D:1234:ASN:OD1	2.33	0.61
7:B:150:HIS:HB3	7:B:166:ILE:HD12	1.83	0.61
7:E:345:GLU:O	2:D:814:ARG:NH1	2.33	0.61
7:B:30:GLY:O	7:B:46:ARG:NH1	2.31	0.61
3:J:161:ASP:OD2	3:J:162:LEU:N	2.34	0.61
8:K:103:ASP:O	2:D:965:HIS:NE2	2.33	0.61
5:M:226:ILE:O	6:G:265:GLN:NE2	2.32	0.60
2:D:897:ARG:NH2	2:D:900:GLN:OE1	2.34	0.60
8:K:73:LEU:HD22	8:K:206:VAL:HG13	1.84	0.60
7:B:177:HIS:O	7:B:202:ARG:NH2	2.34	0.60
7:E:191:ASP:OD1	7:E:191:ASP:N	2.35	0.60
7:E:47:MET:HE2	7:E:315:MET:HB3	1.84	0.59
2:D:999:THR:HG21	2:D:1002:TYR:HD2	1.66	0.59
4:L:31:LEU:O	4:L:35:ILE:HG13	2.02	0.59
5:M:207:SER:OG	5:M:210:ARG:NH2	2.36	0.59
7:E:17:ASP:O	7:E:331:ASN:ND2	2.36	0.58
7:E:204:MET:HG3	7:E:258:ILE:HD11	1.84	0.58
5:M:348:ALA:O	5:M:352:ASN:ND2	2.33	0.58
7:E:289:GLU:OE2	7:E:336:LYS:NZ	2.36	0.58
3:J:109:ASP:OD1	3:J:126:ASN:ND2	2.30	0.58
1:H:17:ARG:HH12	3:J:178:THR:HG22	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:195:GLU:OE2	2:D:779:ASN:ND2	2.36	0.58
1:H:23:SER:OG	1:H:27:LYS:NZ	2.37	0.58
7:B:43:HIS:O	7:B:47:MET:HG3	2.03	0.58
2:D:1140:ALA:HB1	2:D:1144:ILE:HD13	1.84	0.58
5:M:35:LYS:NZ	5:M:40:ASN:OD1	2.37	0.58
2:D:932:GLY:O	2:D:936:LYS:NZ	2.33	0.58
5:M:83:SER:HB2	7:E:280:ARG:HD3	1.86	0.58
2:A:779:ASN:ND2	2:A:782:TRP:O	2.34	0.57
7:E:204:MET:HE2	7:E:258:ILE:HD13	1.86	0.57
2:D:940:LYS:O	2:D:940:LYS:NZ	2.33	0.57
7:B:242:ILE:HB	7:B:364:ASN:HD22	1.69	0.57
2:A:714:LYS:O	2:A:718:THR:OG1	2.21	0.57
5:M:174:ASP:O	5:M:177:ASN:ND2	2.32	0.57
2:A:1220:GLU:HG3	2:A:1222:GLN:H	1.69	0.57
7:B:43:HIS:HE1	7:B:46:ARG:HD2	1.69	0.57
7:B:152:ALA:HB3	7:B:164:ASN:HB2	1.86	0.57
1:H:35:GLU:HB2	1:H:38:ASN:HD21	1.70	0.57
7:B:224:ILE:HB	7:B:231:ASN:HA	1.86	0.57
7:E:53:MET:HE3	7:E:53:MET:HA	1.87	0.57
2:D:832:GLU:HG2	2:D:895:LEU:HD21	1.87	0.57
2:D:1214:LEU:HD21	2:D:1224:PHE:HB2	1.86	0.57
2:A:976:ASP:OD1	2:A:1311:HIS:NE2	2.37	0.56
2:D:678:ASN:HB3	2:D:681:LEU:HB2	1.86	0.56
5:M:177:ASN:HD21	5:M:182:SER:HB2	1.70	0.56
2:A:917:ARG:NH1	2:A:1184:LEU:O	2.38	0.56
2:A:1286:TYR:O	2:A:1290:VAL:HG13	2.06	0.56
4:L:59:ASN:OD1	4:L:65:GLN:NE2	2.38	0.56
2:D:960:THR:HB	2:D:970:LYS:HB2	1.87	0.56
2:D:943:LEU:HB2	2:D:1150:HIS:HE1	1.68	0.56
2:D:1152:THR:O	2:D:1156:GLU:HG2	2.06	0.56
7:E:350:ASP:OD1	7:E:350:ASP:N	2.36	0.56
7:E:199:THR:HG22	2:D:779:ASN:HB3	1.87	0.56
1:H:40:TYR:HB3	6:G:293:ARG:HH21	1.71	0.56
1:H:67:ARG:NH2	3:J:154:ASP:O	2.38	0.56
7:E:179:ARG:NH1	7:E:263:GLN:O	2.39	0.56
2:A:1189:SER:O	2:A:1193:GLU:N	2.36	0.56
1:H:11:LEU:HB3	1:H:14:LYS:HB3	1.88	0.55
2:A:1142:THR:HG22	2:A:1301:PHE:HE2	1.71	0.55
7:B:285:ASN:ND2	7:B:358:SER:O	2.39	0.55
8:K:69:SER:O	8:K:69:SER:OG	2.23	0.55
2:D:810:ILE:HD11	2:D:919:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:927:SER:O	2:D:927:SER:OG	2.21	0.55
7:E:258:ILE:O	7:E:262:TYR:N	2.33	0.55
2:A:1004:ASN:HA	2:A:1007:LYS:HD2	1.87	0.55
2:A:1228:LEU:HD11	2:A:1240:TYR:CE2	2.39	0.55
4:L:102:SER:O	4:L:106:LEU:HG	2.07	0.55
7:B:82:TYR:OH	7:B:162:TYR:O	2.19	0.55
7:B:250:VAL:HA	7:B:373:MET:HE2	1.88	0.55
7:E:165:ASP:HA	7:E:168:LEU:HD12	1.87	0.55
7:E:181:LEU:HG	7:E:204:MET:HE3	1.87	0.55
2:D:1137:ASN:OD1	2:D:1302:ARG:NH2	2.34	0.55
2:A:985:PHE:HA	2:A:988:ILE:HD12	1.89	0.55
7:E:26:ASP:OD2	7:E:65:ARG:NH1	2.39	0.55
1:H:80:LEU:HD21	6:G:256:THR:HG23	1.89	0.54
4:L:101:THR:O	4:L:105:GLU:HG3	2.07	0.54
5:M:371:ARG:HH12	5:M:375:ARG:HH21	1.55	0.54
2:A:851:LEU:HD13	2:A:855:LEU:HD22	1.89	0.54
7:E:221:LEU:HD11	7:E:372:VAL:HG22	1.90	0.54
1:H:75:LEU:HD13	3:J:130:GLN:HB2	1.89	0.54
2:A:858:THR:OG1	7:B:28:ASP:OD2	2.23	0.54
2:A:1213:ARG:NE	2:A:1218:ASP:OD2	2.35	0.54
4:L:80:MET:HE3	5:M:344:LEU:HB2	1.90	0.54
2:D:940:LYS:HD2	2:D:1244:LYS:HZ3	1.72	0.54
1:H:49:THR:HA	1:H:52:THR:HG22	1.90	0.54
2:D:947:GLN:O	2:D:951:GLU:HG2	2.07	0.54
1:H:41:LYS:NZ	1:H:45:THR:OG1	2.39	0.53
2:A:1140:ALA:HB1	2:A:1144:ILE:HG23	1.90	0.53
7:B:60:LYS:O	7:B:330:ASN:ND2	2.41	0.53
1:H:18:ARG:HG2	2:A:666:VAL:HG11	1.90	0.53
2:A:1180:PHE:HZ	7:B:338:LEU:O	1.92	0.53
7:B:19:ARG:NH2	7:B:303:ILE:O	2.41	0.53
2:D:1291:ARG:NH2	2:D:1296:ASN:OD1	2.41	0.53
6:G:403:TRP:HE1	2:D:893:VAL:HG11	1.73	0.53
7:E:54:ASN:ND2	7:E:340:TYR:O	2.41	0.53
2:A:842:THR:HG22	2:A:844:ASN:H	1.74	0.53
5:M:179:LYS:O	5:M:183:ARG:NH2	2.42	0.53
3:J:123:VAL:HG21	3:J:165:VAL:HG11	1.90	0.53
5:M:56:GLU:HA	5:M:70:GLN:HB2	1.90	0.53
2:A:886:HIS:O	2:A:890:THR:OG1	2.21	0.53
6:G:229:LYS:O	6:G:233:ILE:HG23	2.08	0.53
1:H:301:PRO:HA	1:H:304:VAL:HG12	1.91	0.53
2:A:1204:TYR:HA	2:A:1207:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:76:TYR:O	4:L:80:MET:HE2	2.08	0.53
4:L:81:PRO:O	4:L:84:GLU:HG2	2.09	0.53
2:D:1208:LEU:O	2:D:1212:ARG:HG2	2.09	0.52
2:D:1227:SER:O	2:D:1230:GLN:NE2	2.43	0.52
2:D:960:THR:HG22	2:D:971:PRO:HD2	1.92	0.52
7:E:202:ARG:O	7:E:262:TYR:OH	2.28	0.52
2:D:1018:ILE:HG13	2:D:1019:SER:N	2.25	0.52
2:D:1304:GLU:HG3	2:D:1313:SER:HB3	1.90	0.52
7:B:44:ARG:NH2	7:B:310:GLY:O	2.42	0.52
7:B:273:GLY:HA3	7:B:318:VAL:HG22	1.91	0.52
7:B:281:LEU:HD12	7:B:313:TYR:HE2	1.74	0.52
8:K:182:ARG:NH1	8:K:245:PHE:O	2.43	0.52
7:B:40:MET:HE1	7:B:44:ARG:HH22	1.74	0.52
7:E:295:VAL:HG11	7:E:325:GLU:HG2	1.92	0.52
8:K:208:ASN:HB3	8:K:211:ASN:HB2	1.92	0.51
8:K:255:GLU:N	8:K:255:GLU:OE1	2.42	0.51
2:D:685:PHE:HE1	2:D:706:VAL:HG23	1.75	0.51
2:A:777:VAL:HG23	2:A:778:LEU:HD12	1.93	0.51
8:K:162:ASN:O	8:K:250:ARG:NH1	2.43	0.51
5:M:71:ARG:NH1	5:M:85:PRO:O	2.41	0.51
5:M:233:LEU:HD13	6:G:260:ARG:HH11	1.75	0.51
7:B:81:GLU:HG2	7:B:104:PHE:HZ	1.76	0.51
7:B:224:ILE:HG21	7:B:379:ASN:HD22	1.74	0.51
2:D:659:ASN:HA	2:D:662:LEU:HD12	1.93	0.51
2:A:913:ASN:ND2	7:B:345:GLU:OE1	2.44	0.51
2:A:1196:LEU:HD13	2:A:1227:SER:HB3	1.92	0.51
7:B:210:LYS:HG2	7:B:214:PHE:HE2	1.76	0.51
2:A:1264:GLU:O	2:A:1268:LEU:HG	2.10	0.51
7:E:170:ILE:HD11	7:E:268:VAL:HG11	1.93	0.51
2:A:1145:TYR:OH	2:A:1149:ARG:NH1	2.42	0.50
2:D:989:LEU:HD13	2:D:1015:LYS:HD3	1.93	0.50
7:E:320:ARG:HG2	7:E:353:LEU:HD12	1.93	0.50
2:D:934:THR:O	2:D:937:GLN:HG3	2.12	0.50
2:D:998:HIS:ND1	2:D:1215:ILE:O	2.44	0.50
7:E:204:MET:SD	7:E:205:THR:N	2.85	0.50
8:K:184:CYS:HB3	8:K:201:ARG:HA	1.92	0.50
2:A:1239:LEU:HD23	2:A:1239:LEU:H	1.77	0.50
7:E:9:ASP:OD1	7:E:9:ASP:N	2.44	0.50
7:E:277:SER:O	7:E:317:ASN:ND2	2.45	0.50
2:A:1309:THR:HG23	2:A:1311:HIS:HB3	1.93	0.50
7:B:270:GLN:OE1	7:B:272:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:766:PRO:HB2	7:B:80:ASP:HB2	1.93	0.50
7:B:238:LEU:HB3	7:B:364:ASN:HD21	1.77	0.50
7:B:255:ILE:O	7:B:259:MET:HG2	2.11	0.50
1:H:106:HIS:CE1	6:G:230:ILE:HG22	2.46	0.50
2:A:686:LEU:HG	3:J:175:ILE:HD13	1.94	0.50
7:E:254:VAL:O	7:E:258:ILE:HG22	2.11	0.50
8:K:182:ARG:HD3	8:K:247:ILE:HD11	1.94	0.50
2:A:755:TYR:CD1	2:A:784:GLY:HA2	2.47	0.50
7:B:167:VAL:HG22	7:B:197:PHE:HE2	1.76	0.50
7:E:376:ILE:HA	7:E:379:ASN:HD21	1.77	0.50
3:J:138:LEU:HA	3:J:141:LYS:HZ3	1.77	0.49
7:E:184:ASP:OD1	7:E:186:ASP:N	2.45	0.49
3:J:116:LYS:HG2	3:J:121:LEU:HB2	1.92	0.49
7:B:261:TRP:HE3	7:B:380:LEU:HG	1.77	0.49
7:B:114:ASP:N	7:B:114:ASP:OD1	2.45	0.49
7:E:273:GLY:HA2	7:E:291:HIS:HE1	1.77	0.49
2:D:665:GLU:N	2:D:665:GLU:OE1	2.43	0.49
5:M:224:GLU:OE1	5:M:297:SER:OG	2.29	0.49
7:E:51:LEU:O	7:E:55:TYR:HB2	2.12	0.49
7:E:94:LEU:HD23	7:E:94:LEU:H	1.76	0.49
7:E:370:ASP:O	7:E:374:THR:OG1	2.25	0.49
1:H:302:ASP:O	1:H:306:GLU:HG2	2.13	0.49
5:M:86:MET:HB2	2:D:805:GLU:HG3	1.95	0.49
4:L:94:LEU:HD21	5:M:361:LYS:HE3	1.95	0.49
5:M:32:ARG:NH2	2:D:695:ASP:OD1	2.42	0.48
5:M:66:ASN:HB2	5:M:69:LEU:HD12	1.93	0.48
7:E:41:LYS:NZ	2:D:812:GLU:OE2	2.46	0.48
2:A:686:LEU:HD11	3:J:180:CYS:SG	2.52	0.48
2:A:706:VAL:HG21	2:A:720:PHE:CE2	2.48	0.48
8:K:153:ASN:OD1	8:K:153:ASN:N	2.44	0.48
2:D:1009:ARG:O	2:D:1013:LEU:HG	2.14	0.48
5:M:57:ALA:HB3	5:M:72:SER:HB3	1.94	0.48
5:M:359:LEU:HA	5:M:362:ILE:HD12	1.94	0.48
2:D:992:ALA:O	2:D:996:ILE:HD13	2.14	0.48
7:B:55:TYR:CE1	7:B:339:PRO:HD2	2.49	0.48
7:B:180:VAL:HG12	7:B:266:ALA:HB3	1.95	0.48
7:E:375:ASN:O	7:E:379:ASN:ND2	2.46	0.48
2:A:1204:TYR:O	2:A:1208:LEU:HG	2.14	0.48
4:L:80:MET:HB3	5:M:351:ARG:NH1	2.28	0.48
7:B:51:LEU:HD21	7:B:347:TYR:HE2	1.78	0.48
2:D:703:VAL:HA	2:D:706:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:83:SER:HA	5:M:86:MET:HE2	1.94	0.48
2:A:1009:ARG:HH12	2:A:1077:LEU:HD22	1.79	0.48
8:K:73:LEU:HD21	8:K:204:VAL:HA	1.96	0.48
2:A:1180:PHE:HE1	7:B:344:TYR:CZ	2.32	0.48
5:M:339:GLU:OE1	5:M:342:ARG:NH2	2.47	0.48
2:D:822:GLU:OE2	2:D:826:ARG:NH1	2.47	0.48
1:H:79:ARG:HH12	2:A:857:HIS:CE1	2.32	0.48
7:B:78:HIS:HB3	7:B:82:TYR:HD2	1.78	0.48
7:B:194:GLU:OE2	7:B:205:THR:OG1	2.26	0.48
1:H:67:ARG:HB3	3:J:156:ARG:HH12	1.80	0.47
5:M:340:SER:O	5:M:344:LEU:HG	2.14	0.47
5:M:368:LYS:O	5:M:372:ILE:HG12	2.14	0.47
7:E:174:LEU:HD21	7:E:202:ARG:HB3	1.94	0.47
2:D:1152:THR:OG1	2:D:1156:GLU:OE2	2.26	0.47
2:A:1065:LEU:N	2:A:1257:MET:SD	2.88	0.47
5:M:184:THR:O	5:M:187:SER:OG	2.28	0.47
7:E:259:MET:HE1	7:E:301:PHE:CD2	2.49	0.47
7:E:184:ASP:OD2	7:E:207:SER:OG	2.23	0.47
5:M:202:GLU:OE2	7:B:177:HIS:ND1	2.47	0.47
2:D:1138:LEU:HD13	2:D:1269:PHE:CD1	2.49	0.47
1:H:311:ILE:HD11	2:A:889:VAL:HG23	1.97	0.47
2:A:820:TYR:HE2	2:A:869:LYS:HG2	1.80	0.47
2:A:901:LYS:HD2	2:A:901:LYS:HA	1.74	0.47
2:A:1019:SER:HA	2:A:1024:ILE:HG13	1.96	0.47
5:M:222:HIS:NE2	5:M:296:GLN:OE1	2.48	0.47
6:G:403:TRP:CZ2	2:D:890:THR:HG23	2.50	0.47
7:B:46:ARG:HD3	7:B:343:TYR:OH	2.14	0.47
2:D:1014:LEU:HA	2:D:1017:PHE:CD1	2.50	0.47
7:B:109:ASP:OD2	7:B:110:CYS:N	2.48	0.47
8:K:238:LYS:HA	8:K:253:GLY:HA3	1.96	0.47
1:H:83:PHE:HB2	2:A:829:GLN:HG3	1.97	0.47
7:B:211:TYR:CE2	7:B:220:GLU:HG3	2.49	0.47
7:E:19:ARG:HB2	7:E:140:ASP:HB2	1.96	0.47
7:E:55:TYR:CE2	7:E:334:LEU:HD12	2.50	0.47
1:H:16:LYS:HA	1:H:19:PHE:CD1	2.50	0.47
3:J:111:PHE:HD2	3:J:112:LEU:HD23	1.81	0.47
2:A:1256:LEU:HG	2:A:1262:THR:HB	1.97	0.46
7:B:317:ASN:O	7:B:321:THR:HG22	2.16	0.46
7:E:75:CYS:HB3	2:D:769:GLY:H	1.80	0.46
7:E:209:HIS:HE1	7:E:235:ASN:HB3	1.80	0.46
2:D:673:LYS:HE2	2:D:674:ARG:HH12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1015:LYS:HA	2:D:1018:ILE:HG12	1.97	0.46
2:A:691:LEU:HD13	3:J:111:PHE:HZ	1.79	0.46
2:A:979:PHE:HZ	2:A:1152:THR:HG22	1.79	0.46
5:M:209:VAL:O	5:M:213:GLN:HG2	2.15	0.46
5:M:231:LEU:HD12	6:G:261:THR:HG23	1.98	0.46
7:E:41:LYS:HG3	7:E:315:MET:HE1	1.97	0.46
8:K:90:LEU:N	8:K:140:THR:O	2.47	0.46
2:A:1226:GLU:H	2:A:1226:GLU:CD	2.24	0.46
4:L:35:ILE:HG23	4:L:38:LYS:HE3	1.96	0.46
6:G:262:PHE:HE2	7:B:58:TYR:HB2	1.80	0.46
1:H:40:TYR:CD2	6:G:289:ILE:HG23	2.51	0.46
4:L:75:ILE:O	4:L:79:LEU:HD23	2.15	0.46
7:E:259:MET:HE1	7:E:301:PHE:CG	2.50	0.46
2:D:1203:ALA:O	2:D:1207:VAL:HG12	2.16	0.46
2:A:670:GLU:OE2	2:A:674:ARG:NH1	2.46	0.46
2:A:1234:ASN:HB3	7:B:359:ASN:ND2	2.30	0.46
4:L:93:MET:HE2	5:M:362:ILE:HD13	1.98	0.46
8:K:161:ARG:HD2	8:K:161:ARG:HA	1.73	0.46
8:K:164:GLU:HG3	8:K:166:TRP:HZ3	1.80	0.46
2:D:1247:GLN:HA	2:D:1250:VAL:HG22	1.98	0.46
4:L:108:TYR:CD2	5:M:372:ILE:HD12	2.51	0.46
5:M:344:LEU:HD12	5:M:345:SER:N	2.31	0.46
7:B:204:MET:HB2	7:B:262:TYR:CZ	2.51	0.46
7:E:128:MET:HE1	7:E:172:GLU:HG3	1.98	0.46
7:E:269:LEU:HD23	7:E:307:VAL:HG22	1.97	0.46
2:D:675:TYR:HE2	2:D:712:SER:HB2	1.81	0.46
2:A:713:ASN:HB3	2:A:716:LEU:HB3	1.98	0.45
8:K:73:LEU:HD12	8:K:73:LEU:H	1.81	0.45
2:D:1161:ILE:HA	2:D:1164:MET:HG2	1.98	0.45
1:H:31:ASN:O	1:H:35:GLU:HG2	2.15	0.45
1:H:83:PHE:HE1	2:A:825:LEU:HD21	1.82	0.45
7:E:179:ARG:O	7:E:265:SER:OG	2.31	0.45
2:D:945:THR:HG23	2:D:1146:ILE:HD11	1.98	0.45
2:D:987:ASP:O	2:D:991:LEU:HD23	2.16	0.45
1:H:35:GLU:HB2	1:H:38:ASN:ND2	2.30	0.45
2:A:827:THR:HG21	2:A:866:VAL:HG21	1.98	0.45
2:A:897:ARG:HD2	2:A:897:ARG:HA	1.71	0.45
7:E:189:HIS:H	7:E:216:PRO:HG3	1.82	0.45
2:D:824:ASN:ND2	2:D:902:ASP:OD1	2.50	0.45
2:D:1228:LEU:HD12	2:D:1232:TYR:CE2	2.49	0.45
2:A:706:VAL:HG21	2:A:720:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1262:THR:O	2:A:1265:ILE:HG22	2.17	0.45
4:L:15:THR:O	4:L:19:GLU:HG2	2.16	0.45
7:B:127:SER:OG	7:B:165:ASP:OD2	2.34	0.45
7:E:189:HIS:HD2	7:E:209:HIS:CE1	2.35	0.45
4:L:55:LYS:HG3	4:L:57:ASP:H	1.82	0.45
7:B:111:PRO:O	7:B:111:PRO:HD2	2.17	0.45
2:A:1194:MET:HB2	2:A:1196:LEU:HG	1.99	0.45
4:L:80:MET:HB3	5:M:351:ARG:HH12	1.82	0.45
5:M:63:ASN:HA	5:M:66:ASN:OD1	2.17	0.45
2:A:860:MET:SD	2:A:860:MET:N	2.89	0.45
5:M:206:MET:HG2	5:M:210:ARG:HH12	1.80	0.45
7:B:153:LYS:HE3	7:B:156:GLU:HB2	1.99	0.45
2:D:1171:GLU:O	2:D:1174:THR:OG1	2.33	0.45
2:A:1268:LEU:HD12	2:A:1290:VAL:HG12	1.98	0.44
2:A:1302:ARG:NH1	2:A:1304:GLU:HB2	2.33	0.44
8:K:168:CYS:C	8:K:170:ILE:H	2.25	0.44
2:A:907:ARG:HA	2:A:910:ARG:HH21	1.82	0.44
7:E:314:THR:O	7:E:318:VAL:HG12	2.17	0.44
2:D:774:CYS:O	2:D:778:LEU:HB2	2.18	0.44
2:D:823:SER:HB3	2:D:866:VAL:HG22	1.98	0.44
2:A:837:LYS:HE3	3:J:133:LEU:HA	1.99	0.44
7:E:258:ILE:HB	7:E:380:LEU:HD21	2.00	0.44
2:D:851:LEU:HD21	2:D:855:LEU:HG	2.00	0.44
1:H:82:LEU:HB3	2:A:832:GLU:CD	2.42	0.44
2:A:841:MET:HE1	2:A:846:LYS:HG2	1.99	0.44
5:M:73:GLU:HB3	8:K:257:THR:HG22	1.99	0.44
7:E:194:GLU:HG2	7:E:198:TYR:HE1	1.83	0.44
8:K:84:LEU:HD12	8:K:138:ILE:HG12	1.99	0.44
7:E:270:GLN:OE1	7:E:272:GLY:N	2.51	0.44
2:D:1168:VAL:HG11	2:D:1232:TYR:CD1	2.53	0.44
1:H:67:ARG:NH1	3:J:154:ASP:HB3	2.33	0.44
5:M:353:LYS:NZ	6:G:280:ASN:HD21	2.15	0.44
2:D:996:ILE:HG23	2:D:1007:LYS:HG2	2.00	0.44
2:D:1251:LYS:HD2	2:D:1251:LYS:HA	1.69	0.44
2:A:803:TYR:CD1	2:A:926:LYS:HD3	2.53	0.43
7:B:59:LYS:HB2	7:B:59:LYS:HE3	1.77	0.43
7:E:322:TRP:O	7:E:326:THR:OG1	2.32	0.43
2:D:1225:GLU:HG3	2:D:1240:TYR:HD2	1.83	0.43
2:D:1302:ARG:HH11	2:D:1315:GLN:HB3	1.83	0.43
2:A:1212:ARG:O	2:A:1215:ILE:HG22	2.18	0.43
7:B:47:MET:SD	7:B:315:MET:HB3	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:81:GLU:HG2	7:B:104:PHE:CZ	2.53	0.43
7:E:293:ASN:OD1	7:E:293:ASN:C	2.61	0.43
1:H:67:ARG:HH21	3:J:148:ASN:ND2	2.16	0.43
7:E:185:ILE:HD13	7:E:291:HIS:CD2	2.54	0.43
7:E:305:MET:HE3	7:E:305:MET:HB2	1.86	0.43
2:D:901:LYS:HA	2:D:901:LYS:HD3	1.69	0.43
2:D:939:ASP:OD1	2:D:1157:ARG:NH2	2.51	0.43
2:A:836:ASN:OD1	3:J:136:SER:OG	2.30	0.43
5:M:347:ILE:O	5:M:351:ARG:HG3	2.18	0.43
8:K:198:LYS:HA	8:K:198:LYS:HD2	1.77	0.43
1:H:79:ARG:HG2	2:A:829:GLN:HE21	1.84	0.43
2:A:673:LYS:HG3	2:A:682:TYR:CE1	2.53	0.43
3:J:149:THR:N	3:J:152:GLN:OE1	2.51	0.43
7:E:53:MET:HE1	7:E:58:TYR:HB3	2.00	0.43
2:A:917:ARG:HG3	2:A:1186:LEU:HD13	2.00	0.43
1:H:67:ARG:HH12	3:J:154:ASP:HB3	1.84	0.43
1:H:111:LYS:HA	1:H:111:LYS:HD3	1.83	0.43
2:A:820:TYR:CE2	2:A:869:LYS:HG2	2.54	0.43
4:L:71:ASN:HD22	4:L:71:ASN:HA	1.66	0.43
2:D:855:LEU:HD13	2:D:863:TYR:CZ	2.54	0.43
2:A:701:ASP:O	2:A:704:GLU:HG2	2.19	0.43
2:A:990:CYS:O	2:A:994:THR:HG22	2.19	0.43
7:B:276:LEU:HD11	7:B:321:THR:HG21	1.99	0.43
7:E:175:ARG:HD2	2:D:773:MET:CE	2.48	0.43
2:D:1305:PHE:HD1	2:D:1312:VAL:HG22	1.83	0.43
4:L:28:TYR:HB3	4:L:93:MET:HG3	2.01	0.43
7:E:272:GLY:HA2	7:E:310:GLY:O	2.19	0.43
7:E:288:MET:SD	7:E:354:SER:HA	2.59	0.43
2:D:1229:ARG:HG2	2:D:1229:ARG:HH11	1.83	0.43
2:A:851:LEU:HD23	2:A:852:PRO:HD2	2.00	0.43
2:A:1186:LEU:HD12	2:A:1186:LEU:O	2.19	0.43
8:K:243:LYS:HG3	8:K:248:THR:HG22	2.00	0.43
2:D:1210:LEU:HD23	2:D:1210:LEU:HA	1.84	0.43
3:J:127:LEU:HD12	3:J:127:LEU:HA	1.86	0.42
4:L:106:LEU:O	4:L:110:VAL:HG23	2.19	0.42
5:M:81:ASN:HB3	5:M:84:LYS:HE3	2.00	0.42
5:M:225:PRO:HG3	7:B:20:ARG:NE	2.33	0.42
7:E:3:TYR:N	7:E:370:ASP:OD2	2.40	0.42
2:D:826:ARG:HH21	2:D:862:ILE:HG23	1.84	0.42
5:M:376:ILE:HD12	5:M:376:ILE:HA	1.87	0.42
7:B:205:THR:OG1	7:B:205:THR:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:250:VAL:HA	7:B:373:MET:CE	2.49	0.42
7:E:151:HIS:HB2	7:E:161:CYS:HB2	2.01	0.42
7:E:248:ARG:HB2	7:E:293:ASN:ND2	2.34	0.42
2:D:999:THR:HG21	2:D:1002:TYR:CD2	2.52	0.42
5:M:80:LEU:N	7:E:109:ASP:OD2	2.30	0.42
2:D:814:ARG:HG2	2:D:916:TRP:CZ3	2.55	0.42
2:A:755:TYR:HD1	2:A:784:GLY:HA2	1.83	0.42
2:A:1180:PHE:CE1	7:B:344:TYR:CZ	3.07	0.42
4:L:35:ILE:HD11	4:L:89:VAL:HG11	2.01	0.42
7:B:82:TYR:OH	7:B:157:ALA:HB2	2.19	0.42
2:D:1168:VAL:HG21	2:D:1232:TYR:HE1	1.85	0.42
2:A:1180:PHE:HE1	7:B:344:TYR:CE2	2.38	0.42
6:G:294:ARG:HA	6:G:294:ARG:HD3	1.63	0.42
2:A:778:LEU:HD11	7:B:171:ILE:HD11	2.01	0.42
7:E:267:VAL:O	7:E:305:MET:HA	2.20	0.42
2:D:1166:GLU:HG2	2:D:1167:ARG:N	2.35	0.42
1:H:36:ARG:H	1:H:36:ARG:HG3	1.68	0.42
2:A:826:ARG:HD2	2:A:826:ARG:HA	1.88	0.42
2:A:1228:LEU:HD12	2:A:1229:ARG:N	2.35	0.42
2:A:1255:THR:HA	2:A:1258:THR:HG22	2.02	0.42
4:L:58:PHE:CZ	4:L:65:GLN:HA	2.55	0.42
5:M:78:ARG:H	5:M:78:ARG:HG2	1.69	0.42
7:E:181:LEU:HD21	7:E:183:ILE:HD11	2.02	0.42
2:D:828:ILE:HD13	2:D:899:LYS:HD3	2.01	0.42
2:D:859:SER:HB2	2:D:862:ILE:HG13	2.00	0.42
2:A:692:TYR:HB2	2:A:702:LEU:HD13	2.00	0.42
7:B:3:TYR:HB3	7:B:370:ASP:OD1	2.20	0.42
7:E:141:VAL:HG11	7:E:329:LEU:HD22	2.00	0.42
1:H:40:TYR:HD2	6:G:289:ILE:HG23	1.84	0.42
2:A:667:THR:O	2:A:670:GLU:HG3	2.20	0.42
2:A:863:TYR:CE2	2:A:880:ILE:HD11	2.55	0.42
2:A:1244:LYS:HE2	2:A:1244:LYS:HB2	1.80	0.42
4:L:95:ASP:OD2	4:L:96:ASN:N	2.52	0.42
7:B:54:ASN:ND2	7:B:341:ASN:HB3	2.35	0.42
2:D:835:VAL:HA	2:D:838:ILE:HG22	2.02	0.42
2:A:1302:ARG:HH12	2:A:1304:GLU:HB2	1.85	0.42
4:L:64:THR:HA	4:L:67:ARG:HG2	2.02	0.42
7:E:134:LEU:HG	7:E:306:MET:HG2	2.02	0.42
8:K:76:THR:HA	8:K:80:TYR:HD2	1.83	0.42
7:B:151:HIS:HB2	7:B:161:CYS:SG	2.60	0.41
7:B:313:TYR:N	7:B:313:TYR:CD1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:830:CYS:O	2:D:833:THR:HG22	2.21	0.41
8:K:123:PRO:HG3	8:K:158:PRO:HB2	2.01	0.41
8:K:190:ALA:HA	8:K:216:LEU:HD11	2.02	0.41
2:A:686:LEU:HD12	2:A:686:LEU:O	2.20	0.41
2:A:800:LYS:HD3	2:A:800:LYS:HA	1.78	0.41
2:A:868:ARG:O	2:A:873:LYS:N	2.54	0.41
4:L:45:ASN:O	4:L:49:ARG:HG2	2.20	0.41
4:L:76:TYR:C	4:L:80:MET:HE2	2.45	0.41
7:E:127:SER:OG	7:E:165:ASP:OD2	2.39	0.41
2:D:757:ARG:HB2	2:D:782:TRP:CZ3	2.55	0.41
7:E:173:LEU:HD11	7:E:306:MET:SD	2.59	0.41
2:A:803:TYR:HB3	2:A:923:VAL:HG13	2.02	0.41
2:A:1157:ARG:NH1	2:A:1245:VAL:HG21	2.35	0.41
7:B:239:ARG:HB3	7:B:363:VAL:HB	2.03	0.41
7:E:316:ARG:H	7:E:316:ARG:HG3	1.51	0.41
2:D:1206:GLN:O	2:D:1209:ARG:HG3	2.21	0.41
2:A:768:SER:OG	7:B:80:ASP:OD1	2.26	0.41
2:A:932:GLY:HA2	2:A:935:PHE:HB2	2.03	0.41
5:M:63:ASN:N	5:M:66:ASN:HD21	2.16	0.41
7:B:149:LEU:HB3	7:B:161:CYS:SG	2.61	0.41
7:B:214:PHE:HB3	7:B:216:PRO:HD2	2.03	0.41
7:B:328:LEU:HD12	7:B:328:LEU:HA	1.89	0.41
8:K:178:ILE:HD13	8:K:178:ILE:HA	1.80	0.41
2:D:770:ARG:HE	2:D:775:TRP:HD1	1.69	0.41
2:A:1151:TRP:HE3	2:A:1249:LEU:HD11	1.85	0.41
2:D:1305:PHE:HB2	2:D:1312:VAL:HG13	2.03	0.41
2:A:933:LEU:HD23	2:A:933:LEU:HA	1.90	0.41
3:J:137:LYS:H	3:J:137:LYS:HG2	1.58	0.41
5:M:164:GLU:H	5:M:164:GLU:HG3	1.70	0.41
2:A:803:TYR:CE2	2:A:933:LEU:HD11	2.56	0.41
2:A:816:GLU:O	2:A:820:TYR:HD1	2.04	0.41
2:A:1153:THR:O	2:A:1156:GLU:HG3	2.21	0.41
2:A:1180:PHE:HD1	2:A:1180:PHE:O	2.04	0.41
2:A:1210:LEU:HA	2:A:1210:LEU:HD12	1.79	0.41
2:A:1273:ARG:HH21	2:A:1305:PHE:HE2	1.68	0.41
3:J:138:LEU:O	3:J:141:LYS:HG3	2.21	0.41
7:B:210:LYS:HG2	7:B:214:PHE:CE2	2.55	0.41
7:B:270:GLN:NE2	7:B:310:GLY:HA3	2.35	0.41
2:D:851:LEU:HD12	2:D:852:PRO:HD2	2.03	0.41
2:D:952:ILE:HA	2:D:955:ILE:HG22	2.02	0.41
2:D:962:LYS:HE3	2:D:964:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:989:LEU:HD11	2:D:1018:ILE:HD13	2.03	0.41
2:A:678:ASN:HB3	2:A:681:LEU:HB2	2.03	0.41
2:A:757:ARG:NH1	2:A:781:GLU:OE1	2.54	0.41
2:A:929:ASP:OD2	2:A:932:GLY:HA3	2.21	0.41
1:H:296:LEU:HD23	1:H:296:LEU:HA	1.88	0.40
5:M:63:ASN:HD21	8:K:252:TRP:HZ2	1.68	0.40
7:B:343:TYR:CD1	7:B:343:TYR:N	2.89	0.40
2:D:1149:ARG:HA	2:D:1152:THR:HG22	2.03	0.40
2:A:808:PHE:CZ	7:B:280:ARG:HA	2.56	0.40
4:L:19:GLU:OE2	5:M:184:THR:HG21	2.21	0.40
6:G:248:GLU:O	6:G:252:ILE:HG12	2.21	0.40
7:B:179:ARG:HB3	7:B:262:TYR:CE2	2.57	0.40
7:B:181:LEU:HA	7:B:204:MET:HB3	2.03	0.40
7:B:189:HIS:ND1	7:B:218:THR:OG1	2.54	0.40
7:E:3:TYR:HB2	7:E:373:MET:HE2	2.02	0.40
7:E:247:TYR:CD2	7:E:286:LEU:HD11	2.57	0.40
1:H:16:LYS:HA	1:H:19:PHE:HD1	1.85	0.40
2:A:1307:LYS:HA	2:A:1307:LYS:HD3	1.89	0.40
4:L:89:VAL:HA	4:L:92:ILE:HD12	2.04	0.40
7:B:379:ASN:OD1	7:B:379:ASN:N	2.54	0.40
7:E:305:MET:HE2	7:E:307:VAL:HG23	2.02	0.40
7:E:314:THR:HG23	7:E:317:ASN:HB2	2.03	0.40
2:D:1226:GLU:HA	2:D:1229:ARG:HG3	2.02	0.40
2:A:673:LYS:HG3	2:A:682:TYR:CZ	2.57	0.40
6:G:398:ASP:HA	6:G:401:HIS:HB3	2.03	0.40
7:B:242:ILE:HB	7:B:364:ASN:ND2	2.35	0.40
7:E:181:LEU:HD13	7:E:264:PRO:HG3	2.03	0.40
2:D:1305:PHE:CD1	2:D:1312:VAL:HG22	2.55	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	H	140/327 (43%)	139 (99%)	1 (1%)	0	100	100
2	A	513/1536 (33%)	507 (99%)	6 (1%)	0	100	100
2	D	491/1536 (32%)	478 (97%)	13 (3%)	0	100	100
3	J	88/201 (44%)	86 (98%)	2 (2%)	0	100	100
4	L	125/330 (38%)	123 (98%)	2 (2%)	0	100	100
5	M	214/430 (50%)	206 (96%)	8 (4%)	0	100	100
6	G	93/405 (23%)	90 (97%)	3 (3%)	0	100	100
7	B	381/433 (88%)	369 (97%)	12 (3%)	0	100	100
7	E	380/433 (88%)	366 (96%)	14 (4%)	0	100	100
8	K	195/294 (66%)	187 (96%)	8 (4%)	0	100	100
All	All	2620/5925 (44%)	2551 (97%)	69 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	134/290 (46%)	134 (100%)	0	100	100
2	A	492/1391 (35%)	491 (100%)	1 (0%)	87	85
2	D	471/1391 (34%)	467 (99%)	4 (1%)	73	77
3	J	83/179 (46%)	83 (100%)	0	100	100
4	L	123/290 (42%)	123 (100%)	0	100	100
5	M	209/393 (53%)	209 (100%)	0	100	100
6	G	91/371 (24%)	91 (100%)	0	100	100
7	B	325/367 (89%)	325 (100%)	0	100	100
7	E	324/367 (88%)	323 (100%)	1 (0%)	86	83
8	K	180/269 (67%)	178 (99%)	2 (1%)	65	74
All	All	2432/5308 (46%)	2424 (100%)	8 (0%)	84	83

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

Mol	Chain	Res	Type
2	A	765	MET
7	E	224	ILE
8	K	152	PHE
8	K	154	ASN
2	D	807	LEU
2	D	825	LEU
2	D	928	LEU
2	D	948	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	690	ASN
2	A	694	GLN
2	A	829	GLN
2	A	844	ASN
2	A	921	GLN
2	A	998	HIS
4	L	65	GLN
5	M	63	ASN
5	M	230	ASN
5	M	360	GLN
6	G	253	ASN
6	G	280	ASN
6	G	401	HIS
6	G	405	GLN
7	B	54	ASN
7	B	151	HIS
7	E	38	HIS
7	E	189	HIS
7	E	293	ASN
7	E	296	ASN
7	E	379	ASN
8	K	211	ASN
2	D	694	GLN
2	D	913	ASN
2	D	1230	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29892. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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.