



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:04 am GMT

PDB ID : 1LD4
Title : Placement of the Structural Proteins in Sindbis Virus
Authors : Zhang, W.; Mukhopadhyay, S.; Pletnev, S.V.; Baker, T.S.; Kuhn, R.J.; Rossmann, M.G.
Deposited on : 2002-04-08
Resolution : 11.40 Å (reported)
Based on PDB ID : 1SVB, 1YSA, 1I9W

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

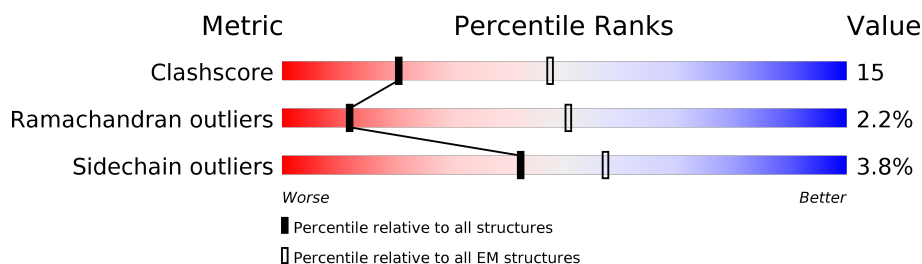
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.40 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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

Mol	Chain	Length	Quality of chain
1	A	264	
1	B	264	
1	C	264	
1	D	264	
2	E	57	
2	F	57	
2	G	57	
2	H	57	
2	I	57	

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Mol	Chain	Length	Quality of chain
2	J	57	<div><div></div><div>49%</div><div>51%</div></div>
2	K	57	<div><div></div><div>49%</div><div>51%</div></div>
2	L	57	<div><div></div><div>49%</div><div>51%</div></div>
3	M	439	<div><div></div><div>54%</div><div>28%</div><div>•</div><div>16%</div></div>
3	N	439	<div><div></div><div>55%</div><div>28%</div><div>•</div><div>16%</div></div>
3	O	439	<div><div></div><div>55%</div><div>28%</div><div>•</div><div>16%</div></div>
3	P	439	<div><div></div><div>55%</div><div>27%</div><div>•</div><div>16%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15680 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 Coat protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	151	Total	C	N	O	S	0	0
			1162	731	207	219	5		
1	B	151	Total	C	N	O	S	0	0
			1162	731	207	219	5		
1	C	151	Total	C	N	O	S	0	0
			1162	731	207	219	5		
1	D	151	Total	C	N	O	S	0	0
			1162	731	207	219	5		

- Molecule 2 is a protein called GENERAL CONTROL PROTEIN GCN4.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	E	28	Total	C	0	28
			28	28		
2	F	28	Total	C	0	28
			28	28		
2	G	28	Total	C	0	28
			28	28		
2	H	28	Total	C	0	28
			28	28		
2	I	28	Total	C	0	28
			28	28		
2	J	28	Total	C	0	28
			28	28		
2	K	28	Total	C	0	28
			28	28		
2	L	28	Total	C	0	28
			28	28		

- Molecule 3 is a protein called Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	369	Total	C	N	O	S	0	15
			2694	1709	446	519	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	369	Total	C	N	O	S	0	15
			2694	1709	446	519	20		
3	O	369	Total	C	N	O	S	0	15
			2694	1709	446	519	20		
3	P	369	Total	C	N	O	S	0	15
			2694	1709	446	519	20		

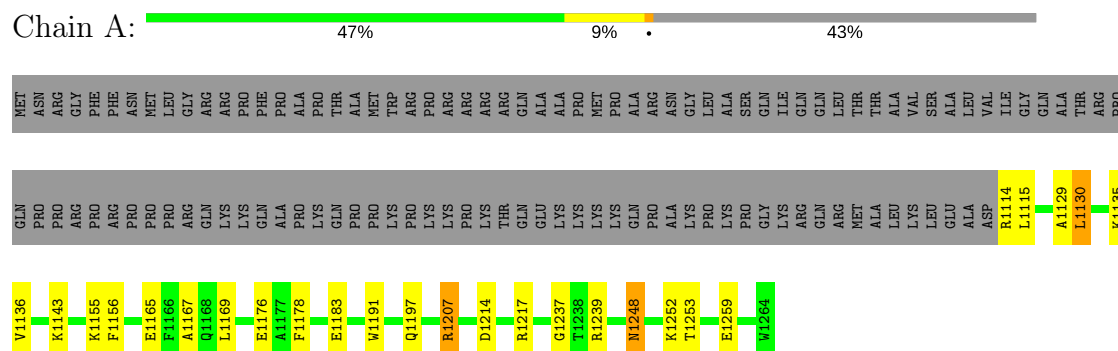
- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
4	P	6	Total	X	0
			6	6	
4	J	1	Total	X	0
			1	1	
4	H	1	Total	X	0
			1	1	
4	N	6	Total	X	0
			6	6	
4	O	8	Total	X	0
			8	8	
4	L	1	Total	X	0
			1	1	
4	F	2	Total	X	0
			2	2	
4	M	7	Total	X	0
			7	7	

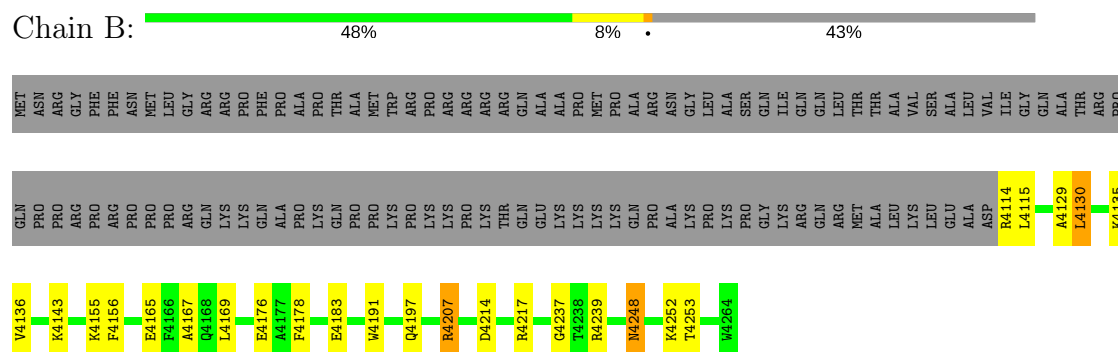
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

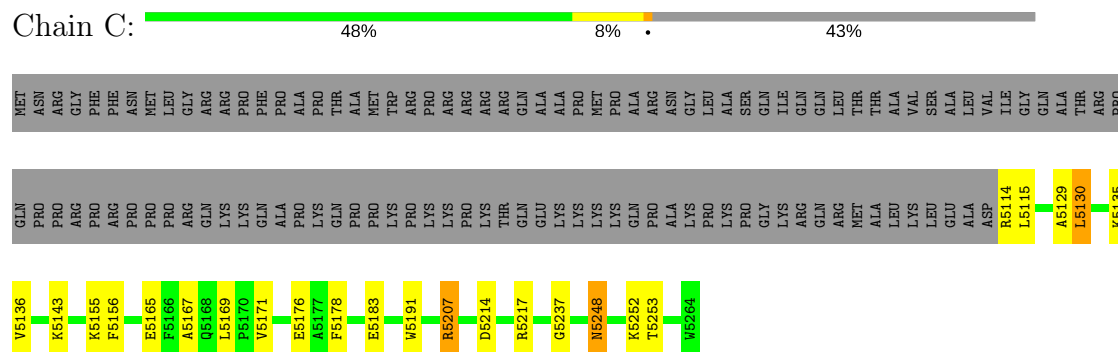
- Molecule 1: Coat protein C



- Molecule 1: Coat protein C



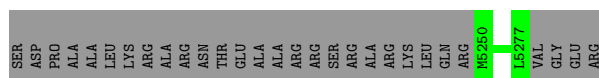
- Molecule 1: Coat protein C



- Molecule 1: Coat protein C

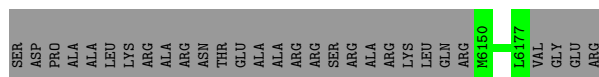
43%





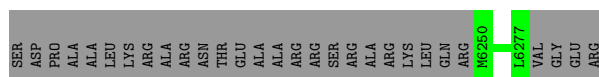
• Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain K: 49% 51%



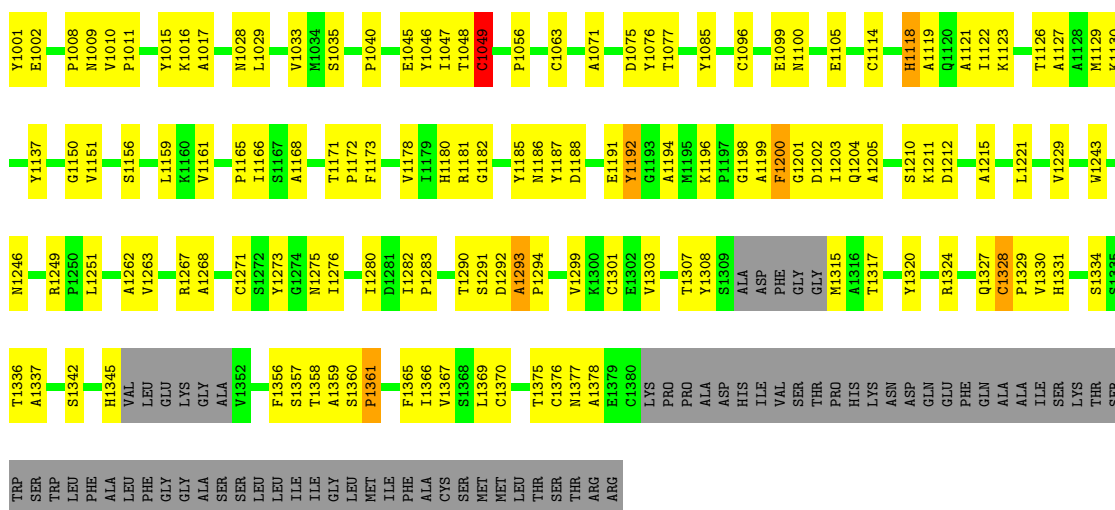
• Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain L: 49% 51%



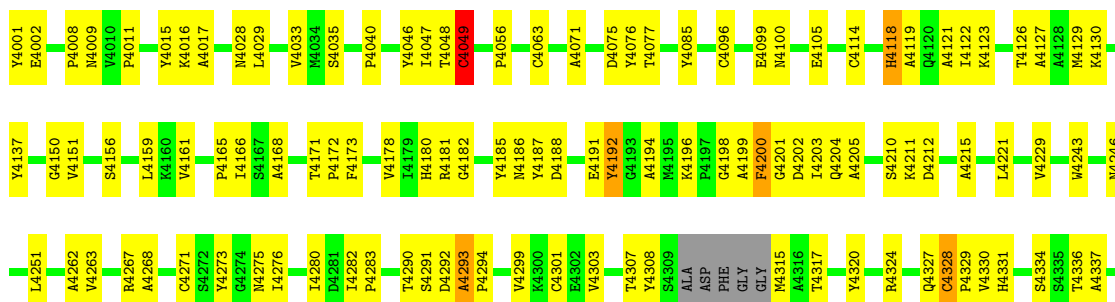
• Molecule 3: Spike glycoprotein E1

Chain M: 54% 28% 16%



• Molecule 3: Spike glycoprotein E1

Chain N: 55% 28% 16%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	each viral image was CTF corrected before reconstruction, based on the following equation: $F(\text{corr})=F(\text{obs})/[CTF +wiener]$	Depositor
Microscope	PHILLIPS CM200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1840	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2580	Depositor
Magnification	38000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 >2	RMSZ	# Z >2
1	A	0.52	0/1190	0.81	1/1607 (0.1%)
1	B	0.52	0/1190	0.81	1/1607 (0.1%)
1	C	0.52	0/1190	0.81	1/1607 (0.1%)
1	D	0.52	0/1190	0.81	1/1607 (0.1%)
3	M	0.34	0/2743	0.54	0/3740
3	N	0.34	0/2743	0.54	0/3740
3	O	0.34	0/2743	0.54	0/3740
3	P	0.34	0/2743	0.54	0/3740
All	All	0.41	0/15732	0.63	4/21388 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	6130	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	1130	LEU	CA-CB-CG	5.10	127.04	115.30
1	B	4130	LEU	CA-CB-CG	5.09	127.02	115.30
1	C	5130	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1162	0	1131	16	0
1	B	1162	0	1131	11	0
1	C	1162	0	1131	14	0
1	D	1162	0	1131	9	0
2	E	28	0	0	0	0
2	F	28	0	0	0	0
2	G	28	0	0	0	0
2	H	28	0	0	0	0
2	I	28	0	0	0	0
2	J	28	0	0	0	0
2	K	28	0	0	0	0
2	L	28	0	0	0	0
3	M	2694	0	2605	139	0
3	N	2694	0	2605	135	0
3	O	2694	0	2605	91	0
3	P	2694	0	2605	95	0
4	F	2	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
4	M	7	0	0	0	0
4	N	6	0	0	0	0
4	O	8	0	0	0	0
4	P	6	0	0	0	0
All	All	15680	0	14944	464	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 15.

All (464) 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:M:1194:ALA:CB	3:N:4151:VAL:HG12	1.36	1.54
3:M:1151:VAL:HG12	3:N:4194:ALA:CB	1.36	1.48
3:M:1151:VAL:CG1	3:N:4194:ALA:CB	2.05	1.34
3:M:1194:ALA:CB	3:N:4151:VAL:CG1	2.05	1.31
3:O:5330:VAL:HG22	3:O:5369:LEU:CA	1.62	1.29
3:P:6330:VAL:HG22	3:P:6369:LEU:CA	1.62	1.29
3:M:1330:VAL:HG22	3:M:1369:LEU:CA	1.62	1.29
3:N:4330:VAL:HG22	3:N:4369:LEU:CA	1.62	1.28
3:M:1151:VAL:CG1	3:N:4194:ALA:HB3	1.64	1.27
3:M:1151:VAL:HG21	3:N:4191:GLU:CD	1.55	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:1194:ALA:HB3	3:N:4151:VAL:CG1	1.64	1.25
3:M:1191:GLU:CD	3:N:4151:VAL:HG21	1.55	1.24
3:M:1191:GLU:CB	3:N:4151:VAL:HG11	1.75	1.15
3:M:1151:VAL:HG11	3:N:4191:GLU:CB	1.75	1.14
1:A:1259:GLU:OE1	1:C:5171:VAL:CG2	1.99	1.10
3:N:4001:TYR:CA	3:N:4282:ILE:O	2.02	1.08
3:O:5001:TYR:CA	3:O:5282:ILE:O	2.02	1.07
3:M:1001:TYR:CA	3:M:1282:ILE:O	2.02	1.07
3:P:6330:VAL:CG2	3:P:6369:LEU:CA	2.33	1.07
3:O:5330:VAL:CG2	3:O:5369:LEU:CA	2.33	1.06
3:N:4330:VAL:CG2	3:N:4369:LEU:CA	2.33	1.06
3:P:6001:TYR:CA	3:P:6282:ILE:O	2.02	1.05
3:M:1330:VAL:CG2	3:M:1369:LEU:CA	2.33	1.05
3:P:6303:VAL:HG23	3:P:6377:ASN:CA	1.88	1.04
3:M:1191:GLU:HB2	3:N:4151:VAL:CG1	1.87	1.04
3:M:1303:VAL:HG23	3:M:1377:ASN:CA	1.88	1.04
3:M:1151:VAL:HG12	3:N:4194:ALA:HB2	1.08	1.04
3:N:4303:VAL:HG23	3:N:4377:ASN:CA	1.88	1.03
3:M:1194:ALA:HB2	3:N:4151:VAL:HG12	1.08	1.03
3:M:1151:VAL:HG11	3:N:4191:GLU:HB2	1.03	1.03
3:O:5303:VAL:HG23	3:O:5377:ASN:CA	1.88	1.03
3:M:1151:VAL:CG1	3:N:4191:GLU:HB2	1.87	1.03
3:M:1191:GLU:HB2	3:N:4151:VAL:HG11	1.04	1.01
3:O:5301:CYS:CB	3:O:5376:CYS:CA	2.45	0.94
3:N:4301:CYS:CB	3:N:4376:CYS:CA	2.45	0.94
3:P:6301:CYS:CB	3:P:6376:CYS:CA	2.45	0.93
3:M:1301:CYS:CB	3:M:1376:CYS:CA	2.45	0.93
3:O:5301:CYS:HB3	3:O:5376:CYS:CA	2.00	0.92
3:N:4301:CYS:HB3	3:N:4376:CYS:CA	2.00	0.91
3:P:6301:CYS:HB3	3:P:6376:CYS:CA	2.00	0.91
3:M:1301:CYS:HB3	3:M:1376:CYS:CA	1.99	0.91
3:O:5366:ILE:HA	3:O:5375:THR:CA	2.01	0.91
3:N:4366:ILE:HA	3:N:4375:THR:CA	2.01	0.90
3:M:1366:ILE:HA	3:M:1375:THR:CA	2.01	0.90
1:A:1259:GLU:OE1	1:C:5171:VAL:HG21	1.68	0.90
3:M:1151:VAL:CG2	3:N:4191:GLU:CD	2.39	0.90
3:M:1191:GLU:CD	3:N:4151:VAL:CG2	2.39	0.90
3:P:6366:ILE:HA	3:P:6375:THR:CA	2.01	0.88
3:M:1151:VAL:HG21	3:N:4191:GLU:CG	2.06	0.86
3:M:1151:VAL:HG13	3:N:4194:ALA:CB	2.07	0.85
3:M:1194:ALA:CB	3:N:4151:VAL:HG13	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:6301:CYS:HB2	3:P:6376:CYS:CA	2.07	0.84
3:M:1191:GLU:CG	3:N:4151:VAL:HG21	2.06	0.84
3:O:5301:CYS:HB2	3:O:5376:CYS:CA	2.07	0.84
3:M:1301:CYS:HB2	3:M:1376:CYS:CA	2.07	0.83
3:N:4301:CYS:HB2	3:N:4376:CYS:CA	2.07	0.82
3:P:6002:GLU:CA	3:P:6002:GLU:CG	2.58	0.82
3:M:1002:GLU:CG	3:M:1002:GLU:CA	2.58	0.82
3:N:4002:GLU:CA	3:N:4002:GLU:CG	2.58	0.82
3:O:5002:GLU:CG	3:O:5002:GLU:CA	2.58	0.81
3:M:1049:CYS:SG	3:M:1118:HIS:HA	2.24	0.78
3:O:5049:CYS:SG	3:O:5118:HIS:HA	2.24	0.78
3:P:6049:CYS:SG	3:P:6118:HIS:HA	2.24	0.78
3:N:4049:CYS:SG	3:N:4118:HIS:HA	2.24	0.78
3:M:1191:GLU:OE2	3:N:4151:VAL:HG21	1.84	0.78
3:M:1151:VAL:HG12	3:N:4194:ALA:HB3	1.32	0.77
1:A:1259:GLU:OE1	1:C:5171:VAL:HG22	1.84	0.77
3:M:1151:VAL:HG21	3:N:4191:GLU:OE2	1.84	0.76
3:M:1194:ALA:HB3	3:N:4151:VAL:HG13	1.65	0.76
3:M:1151:VAL:HG13	3:N:4194:ALA:HB3	1.65	0.75
3:O:5358:THR:HG22	3:O:5359:ALA:H	1.55	0.72
3:M:1358:THR:HG22	3:M:1359:ALA:H	1.55	0.72
3:P:6049:CYS:HB3	3:P:6114:CYS:SG	2.30	0.71
3:N:4049:CYS:HB3	3:N:4114:CYS:SG	2.30	0.71
3:P:6009:ASN:HD21	3:P:6166:ILE:HD13	1.56	0.71
3:P:6358:THR:HG22	3:P:6359:ALA:H	1.55	0.71
3:O:5049:CYS:HB3	3:O:5114:CYS:SG	2.30	0.71
3:M:1049:CYS:HB3	3:M:1114:CYS:SG	2.30	0.71
3:O:5200:PHE:H	3:O:5243:TRP:HE1	1.39	0.71
3:M:1009:ASN:HD21	3:M:1166:ILE:HD13	1.56	0.70
3:P:6016:LYS:HD3	3:P:6331:HIS:HE1	1.55	0.70
3:O:5016:LYS:HD3	3:O:5331:HIS:HE1	1.55	0.70
3:N:4009:ASN:HD21	3:N:4166:ILE:HD13	1.55	0.70
3:N:4358:THR:HG22	3:N:4359:ALA:H	1.55	0.70
3:M:1016:LYS:HD3	3:M:1331:HIS:HE1	1.55	0.70
3:N:4016:LYS:HD3	3:N:4331:HIS:HE1	1.55	0.70
3:O:5009:ASN:HD21	3:O:5166:ILE:HD13	1.56	0.70
3:P:6180:HIS:HB2	3:P:6185:TYR:HE1	1.57	0.69
3:M:1290:THR:O	3:M:1294:PRO:HD2	1.92	0.69
3:N:4200:PHE:H	3:N:4243:TRP:HE1	1.39	0.69
3:M:1151:VAL:CG1	3:N:4194:ALA:HB1	2.21	0.69
3:P:6200:PHE:H	3:P:6243:TRP:HE1	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:4290:THR:O	3:N:4294:PRO:HD2	1.92	0.69
3:O:5290:THR:O	3:O:5294:PRO:HD2	1.92	0.69
3:P:6290:THR:O	3:P:6294:PRO:HD2	1.92	0.69
3:M:1180:HIS:HB2	3:M:1185:TYR:HE1	1.57	0.68
3:N:4040:PRO:HA	3:N:4127:ALA:HA	1.76	0.68
3:O:5040:PRO:HA	3:O:5127:ALA:HA	1.76	0.68
3:M:1200:PHE:H	3:M:1243:TRP:HE1	1.39	0.68
3:M:1366:ILE:O	3:M:1367:VAL:CA	2.42	0.68
3:M:1040:PRO:HA	3:M:1127:ALA:HA	1.76	0.68
3:O:5180:HIS:HB2	3:O:5185:TYR:HE1	1.57	0.68
3:O:5366:ILE:O	3:O:5367:VAL:CA	2.42	0.68
3:N:4366:ILE:O	3:N:4367:VAL:CA	2.42	0.68
3:N:4180:HIS:HB2	3:N:4185:TYR:HE1	1.57	0.67
1:B:4156:PHE:HB3	1:B:4165:GLU:HG2	1.76	0.67
1:A:1156:PHE:HB3	1:A:1165:GLU:HG2	1.76	0.67
1:D:6156:PHE:HB3	1:D:6165:GLU:HG2	1.76	0.67
3:P:6040:PRO:HA	3:P:6127:ALA:HA	1.76	0.67
1:C:5156:PHE:HB3	1:C:5165:GLU:HG2	1.76	0.66
3:M:1191:GLU:OE2	3:N:4151:VAL:CG2	2.43	0.66
3:P:6366:ILE:O	3:P:6367:VAL:CA	2.42	0.66
3:O:5017:ALA:HB3	3:O:5029:LEU:HD12	1.77	0.66
3:N:4017:ALA:HB3	3:N:4029:LEU:HD12	1.77	0.66
3:P:6017:ALA:HB3	3:P:6029:LEU:HD12	1.77	0.65
3:M:1017:ALA:HB3	3:M:1029:LEU:HD12	1.77	0.65
3:M:1194:ALA:HB1	3:N:4151:VAL:CG1	2.21	0.65
3:M:1151:VAL:CG2	3:N:4191:GLU:OE2	2.43	0.65
3:M:1194:ALA:HB3	3:N:4151:VAL:HG12	1.32	0.63
3:P:6129:MET:SD	3:P:6166:ILE:HD12	2.39	0.63
3:O:5129:MET:SD	3:O:5166:ILE:HD12	2.39	0.63
3:O:5330:VAL:HG21	3:O:5369:LEU:CA	2.29	0.63
3:M:1129:MET:SD	3:M:1166:ILE:HD12	2.39	0.62
3:P:6365:PHE:O	3:P:6375:THR:CA	2.48	0.62
3:O:5365:PHE:O	3:O:5375:THR:CA	2.48	0.62
3:M:1365:PHE:O	3:M:1375:THR:CA	2.48	0.62
3:N:4365:PHE:O	3:N:4375:THR:CA	2.48	0.62
3:N:4129:MET:SD	3:N:4166:ILE:HD12	2.39	0.61
3:N:4330:VAL:HG21	3:N:4369:LEU:CA	2.29	0.61
3:O:5171:THR:HG22	3:O:5173:PHE:H	1.66	0.60
3:O:5342:SER:O	3:O:5356:PHE:HZ	1.84	0.60
3:P:6342:SER:O	3:P:6356:PHE:HZ	1.84	0.60
3:M:1171:THR:HG22	3:M:1173:PHE:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:6330:VAL:HG21	3:P:6369:LEU:CA	2.29	0.60
3:N:4200:PHE:N	3:N:4243:TRP:HE1	2.00	0.60
3:M:1151:VAL:HG11	3:N:4191:GLU:HB3	1.81	0.60
3:N:4171:THR:HG22	3:N:4173:PHE:H	1.66	0.59
3:P:6171:THR:HG22	3:P:6173:PHE:H	1.66	0.59
3:O:5303:VAL:CG2	3:O:5377:ASN:CA	2.75	0.59
3:P:6200:PHE:N	3:P:6243:TRP:HE1	2.00	0.59
3:M:1342:SER:O	3:M:1356:PHE:HZ	1.84	0.59
3:O:5200:PHE:N	3:O:5243:TRP:HE1	2.00	0.59
3:N:4342:SER:O	3:N:4356:PHE:HZ	1.84	0.59
3:M:1180:HIS:NE2	3:M:1187:TYR:HE1	2.02	0.58
3:P:6180:HIS:NE2	3:P:6187:TYR:HE1	2.02	0.58
3:M:1200:PHE:N	3:M:1243:TRP:HE1	2.00	0.58
3:P:6159:LEU:CD2	3:P:6283:PRO:HD2	2.34	0.58
3:N:4159:LEU:CD2	3:N:4283:PRO:HD2	2.34	0.57
3:P:6360:SER:HB2	3:P:6361:PRO:HD2	1.86	0.57
3:M:1330:VAL:HG21	3:M:1369:LEU:CA	2.29	0.57
3:O:5159:LEU:CD2	3:O:5283:PRO:HD2	2.34	0.57
3:M:1159:LEU:CD2	3:M:1283:PRO:HD2	2.34	0.57
3:O:5121:ALA:HA	3:O:5178:VAL:HG22	1.87	0.57
3:O:5180:HIS:NE2	3:O:5187:TYR:HE1	2.02	0.57
3:N:4180:HIS:NE2	3:N:4187:TYR:HE1	2.02	0.57
3:M:1360:SER:HB2	3:M:1361:PRO:HD2	1.86	0.56
1:D:6207:ARG:HH21	1:D:6237:GLY:HA2	1.71	0.56
1:B:4207:ARG:HH21	1:B:4237:GLY:HA2	1.71	0.56
3:N:4121:ALA:HA	3:N:4178:VAL:HG22	1.86	0.56
3:N:4360:SER:HB2	3:N:4361:PRO:HD2	1.86	0.56
3:O:5360:SER:HB2	3:O:5361:PRO:HD2	1.86	0.56
3:O:5315:MET:HG2	3:O:5317:THR:H	1.71	0.56
3:P:6121:ALA:HA	3:P:6178:VAL:HG22	1.87	0.56
1:C:5207:ARG:HH21	1:C:5237:GLY:HA2	1.71	0.56
3:N:4192:TYR:HD1	3:N:4192:TYR:H	1.54	0.56
3:M:1121:ALA:HA	3:M:1178:VAL:HG22	1.87	0.56
1:A:1207:ARG:HH21	1:A:1237:GLY:HA2	1.71	0.55
3:P:6315:MET:HG2	3:P:6317:THR:H	1.71	0.55
3:P:6303:VAL:CG2	3:P:6377:ASN:CA	2.75	0.55
3:M:1192:TYR:HD1	3:M:1192:TYR:H	1.54	0.55
3:P:6161:VAL:HA	3:P:6280:ILE:HG12	1.89	0.55
3:O:5008:PRO:HA	3:O:5275:ASN:HA	1.88	0.55
3:P:6192:TYR:H	3:P:6192:TYR:HD1	1.54	0.55
3:M:1161:VAL:HA	3:M:1280:ILE:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:4315:MET:HG2	3:N:4317:THR:H	1.71	0.54
3:N:4016:LYS:HD3	3:N:4331:HIS:CE1	2.39	0.54
3:N:4008:PRO:HA	3:N:4275:ASN:HA	1.89	0.54
3:O:5016:LYS:HD3	3:O:5331:HIS:CE1	2.39	0.54
3:P:6008:PRO:HA	3:P:6275:ASN:HA	1.89	0.54
3:M:1315:MET:HG2	3:M:1317:THR:H	1.71	0.54
3:M:1290:THR:HG22	3:M:1291:SER:H	1.73	0.54
3:M:1191:GLU:HB3	3:N:4151:VAL:HG11	1.81	0.54
3:N:4161:VAL:HA	3:N:4280:ILE:HG12	1.89	0.54
3:N:4290:THR:HG22	3:N:4291:SER:H	1.73	0.54
3:M:1008:PRO:HA	3:M:1275:ASN:HA	1.89	0.54
3:O:5161:VAL:HA	3:O:5280:ILE:HG12	1.89	0.54
3:O:5192:TYR:HD1	3:O:5192:TYR:H	1.54	0.54
3:M:1016:LYS:HD3	3:M:1331:HIS:CE1	2.39	0.54
3:O:5290:THR:HG22	3:O:5291:SER:H	1.73	0.53
3:P:6016:LYS:HD3	3:P:6331:HIS:CE1	2.39	0.53
3:P:6290:THR:HG22	3:P:6291:SER:H	1.73	0.53
3:N:4303:VAL:CG2	3:N:4377:ASN:CA	2.75	0.53
1:A:1248:ASN:ND2	1:A:1252:LYS:H	2.07	0.53
3:M:1303:VAL:CG2	3:M:1377:ASN:CA	2.75	0.52
3:M:1011:PRO:HA	3:M:1033:VAL:HB	1.92	0.52
3:N:4063:CYS:HA	3:N:4099:GLU:O	2.10	0.52
1:D:6248:ASN:ND2	1:D:6252:LYS:H	2.07	0.52
3:N:4192:TYR:N	3:N:4192:TYR:CD1	2.78	0.52
3:O:5192:TYR:CD1	3:O:5192:TYR:N	2.78	0.52
3:P:6262:ALA:HB3	3:P:6267:ARG:H	1.75	0.52
1:B:4248:ASN:ND2	1:B:4252:LYS:H	2.07	0.52
3:M:1063:CYS:HA	3:M:1099:GLU:O	2.10	0.52
3:M:1151:VAL:O	3:N:4194:ALA:CB	2.58	0.52
3:N:4011:PRO:HA	3:N:4033:VAL:HB	1.91	0.52
3:N:4243:TRP:HA	3:N:4243:TRP:CE3	2.45	0.52
3:P:6336:THR:HG22	3:P:6337:ALA:N	2.25	0.52
1:C:5248:ASN:ND2	1:C:5252:LYS:H	2.07	0.51
3:M:1194:ALA:CB	3:N:4151:VAL:O	2.58	0.51
3:O:5063:CYS:HA	3:O:5099:GLU:O	2.10	0.51
3:O:5336:THR:HG22	3:O:5337:ALA:N	2.25	0.51
3:P:6011:PRO:HA	3:P:6033:VAL:HB	1.91	0.51
3:P:6063:CYS:HA	3:P:6099:GLU:O	2.10	0.51
3:O:5262:ALA:HB3	3:O:5267:ARG:H	1.75	0.51
3:N:4262:ALA:HB3	3:N:4267:ARG:H	1.75	0.51
3:O:5028:ASN:HD22	3:O:5342:SER:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:6243:TRP:CE3	3:P:6243:TRP:HA	2.45	0.51
3:M:1262:ALA:HB3	3:M:1267:ARG:H	1.75	0.51
3:O:5011:PRO:HA	3:O:5033:VAL:HB	1.91	0.51
3:M:1243:TRP:CE3	3:M:1243:TRP:HA	2.45	0.51
3:O:5243:TRP:CE3	3:O:5243:TRP:HA	2.45	0.51
3:M:1192:TYR:N	3:M:1192:TYR:CD1	2.78	0.50
3:N:4049:CYS:CB	3:N:4114:CYS:SG	2.99	0.50
3:N:4336:THR:HG22	3:N:4337:ALA:N	2.25	0.50
3:O:5049:CYS:CB	3:O:5114:CYS:SG	2.99	0.50
3:P:6192:TYR:CD1	3:P:6192:TYR:N	2.78	0.50
3:M:1336:THR:HG22	3:M:1337:ALA:N	2.25	0.50
3:M:1194:ALA:HB1	3:N:4151:VAL:O	2.12	0.50
3:M:1028:ASN:HD22	3:M:1342:SER:HB2	1.76	0.50
3:N:4028:ASN:HD22	3:N:4342:SER:HB2	1.76	0.50
3:P:6009:ASN:OD1	3:P:6276:ILE:HG13	2.11	0.50
3:N:4009:ASN:OD1	3:N:4276:ILE:HG13	2.11	0.49
3:O:5009:ASN:OD1	3:O:5276:ILE:HG13	2.11	0.49
3:M:1009:ASN:OD1	3:M:1276:ILE:HG13	2.11	0.49
3:M:1210:SER:O	3:M:1211:LYS:HG3	2.12	0.49
3:P:6028:ASN:HD22	3:P:6342:SER:HB2	1.76	0.49
3:P:6358:THR:HG22	3:P:6359:ALA:N	2.27	0.49
1:A:1214:ASP:O	1:A:1217:ARG:HG3	2.13	0.49
3:M:1049:CYS:CB	3:M:1114:CYS:SG	2.99	0.49
1:B:4214:ASP:O	1:B:4217:ARG:HG3	2.13	0.49
1:C:5214:ASP:O	1:C:5217:ARG:HG3	2.13	0.49
3:M:1151:VAL:O	3:N:4194:ALA:HB1	2.12	0.49
3:O:5210:SER:O	3:O:5211:LYS:HG3	2.12	0.49
3:P:6210:SER:O	3:P:6211:LYS:HG3	2.12	0.48
1:D:6214:ASP:O	1:D:6217:ARG:HG3	2.13	0.48
3:N:4210:SER:O	3:N:4211:LYS:HG3	2.12	0.48
1:A:1259:GLU:CD	1:C:5171:VAL:HG21	2.31	0.48
3:P:6049:CYS:CB	3:P:6114:CYS:SG	2.99	0.48
3:M:1186:ASN:ND2	3:M:1251:LEU:HD21	2.29	0.48
3:M:1194:ALA:HB1	3:N:4151:VAL:HG13	1.89	0.48
3:O:5172:PRO:HD3	3:O:5273:TYR:OH	2.14	0.48
3:M:1358:THR:HG22	3:M:1359:ALA:N	2.27	0.47
3:N:4172:PRO:HD3	3:N:4273:TYR:OH	2.14	0.47
3:M:1337:ALA:HB2	3:M:1360:SER:HB3	1.96	0.47
3:O:5186:ASN:ND2	3:O:5251:LEU:HD21	2.29	0.47
3:M:1172:PRO:HD3	3:M:1273:TYR:OH	2.14	0.47
3:N:4192:TYR:N	3:N:4192:TYR:HD1	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:5192:TYR:N	3:O:5192:TYR:HD1	2.12	0.47
3:M:1192:TYR:HD1	3:M:1192:TYR:N	2.12	0.47
3:N:4337:ALA:HB2	3:N:4360:SER:HB3	1.96	0.47
3:P:6186:ASN:ND2	3:P:6251:LEU:HD21	2.29	0.47
3:P:6172:PRO:HD3	3:P:6273:TYR:OH	2.14	0.47
3:N:4186:ASN:ND2	3:N:4251:LEU:HD21	2.29	0.47
3:O:5337:ALA:HB2	3:O:5360:SER:HB3	1.96	0.47
1:B:4136:VAL:HG22	1:B:4169:LEU:HD23	1.97	0.47
1:D:6136:VAL:HG22	1:D:6169:LEU:HD23	1.97	0.46
3:N:4290:THR:HG22	3:N:4291:SER:N	2.30	0.46
3:O:5122:ILE:HG22	3:O:5123:LYS:N	2.30	0.46
3:O:5166:ILE:HG22	3:O:5168:ALA:H	1.81	0.46
3:P:6182:GLY:HA2	3:P:6263:VAL:HG13	1.97	0.46
3:M:1001:TYR:CA	3:M:1282:ILE:C	2.82	0.46
3:P:6122:ILE:HG22	3:P:6123:LYS:N	2.30	0.46
3:M:1182:GLY:HA2	3:M:1263:VAL:HG13	1.96	0.46
3:N:4182:GLY:HA2	3:N:4263:VAL:HG13	1.96	0.46
3:O:5182:GLY:HA2	3:O:5263:VAL:HG13	1.96	0.46
3:P:6290:THR:HG22	3:P:6291:SER:N	2.30	0.46
3:O:5358:THR:HG22	3:O:5359:ALA:N	2.27	0.46
3:P:6337:ALA:HB2	3:P:6360:SER:HB3	1.96	0.46
3:P:6192:TYR:HD1	3:P:6192:TYR:N	2.12	0.46
3:M:1166:ILE:HG22	3:M:1168:ALA:H	1.81	0.46
1:A:1136:VAL:HG22	1:A:1169:LEU:HD23	1.97	0.46
3:N:4358:THR:HG22	3:N:4359:ALA:N	2.27	0.46
1:A:1135:LYS:HB2	1:A:1167:ALA:O	2.16	0.46
3:M:1290:THR:HG22	3:M:1291:SER:N	2.30	0.46
3:M:1327:GLN:H	3:M:1345:HIS:CE1	2.34	0.46
3:M:1356:PHE:HB3	3:M:1357:SER:H	1.63	0.46
3:P:6327:GLN:H	3:P:6345:HIS:CE1	2.34	0.46
1:C:5135:LYS:HB2	1:C:5167:ALA:O	2.16	0.46
3:N:4166:ILE:HG22	3:N:4168:ALA:H	1.81	0.46
3:O:5008:PRO:HG2	3:O:5015:TYR:CE2	2.51	0.46
1:C:5130:LEU:HD11	1:C:5178:PHE:CD2	2.52	0.45
3:N:4122:ILE:HG22	3:N:4123:LYS:N	2.30	0.45
1:B:4135:LYS:HB2	1:B:4167:ALA:O	2.16	0.45
1:C:5114:ARG:HH21	1:C:5176:GLU:HB2	1.82	0.45
3:M:1008:PRO:HG2	3:M:1015:TYR:CE2	2.51	0.45
3:N:4303:VAL:HG21	3:N:4378:ALA:CA	2.47	0.45
3:P:6356:PHE:HB3	3:P:6357:SER:H	1.63	0.45
1:B:4130:LEU:HD11	1:B:4178:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:1151:VAL:HG13	3:N:4194:ALA:HB1	1.89	0.45
3:O:5327:GLN:H	3:O:5345:HIS:CE1	2.34	0.45
3:P:6166:ILE:HG22	3:P:6168:ALA:H	1.81	0.45
1:A:1114:ARG:HH21	1:A:1176:GLU:HB2	1.82	0.45
1:D:6114:ARG:HH21	1:D:6176:GLU:HB2	1.82	0.45
1:D:6130:LEU:HD11	1:D:6178:PHE:CD2	2.52	0.45
3:M:1122:ILE:HG22	3:M:1123:LYS:N	2.30	0.45
3:M:1329:PRO:O	3:M:1370:CYS:CA	2.65	0.45
3:P:6303:VAL:HG21	3:P:6378:ALA:CA	2.47	0.45
1:B:4114:ARG:HH21	1:B:4176:GLU:HB2	1.82	0.45
3:O:5290:THR:HG22	3:O:5291:SER:N	2.30	0.45
1:A:1130:LEU:HD11	1:A:1178:PHE:CD2	2.51	0.45
3:M:1096:CYS:HB2	3:M:1100:ASN:HD21	1.82	0.45
1:C:5136:VAL:HG22	1:C:5169:LEU:HD23	1.97	0.45
1:D:6135:LYS:HB2	1:D:6167:ALA:O	2.16	0.45
3:M:1268:ALA:HB1	3:M:1271:CYS:SG	2.57	0.45
3:M:1303:VAL:HG21	3:M:1378:ALA:CA	2.47	0.45
3:N:4008:PRO:HG2	3:N:4015:TYR:CE2	2.51	0.45
3:N:4268:ALA:HB1	3:N:4271:CYS:SG	2.57	0.45
3:O:5329:PRO:O	3:O:5370:CYS:CA	2.65	0.45
3:P:6329:PRO:O	3:P:6370:CYS:CA	2.65	0.45
3:N:4047:ILE:HG23	3:N:4119:ALA:O	2.18	0.44
3:O:5303:VAL:HG21	3:O:5378:ALA:CA	2.47	0.44
3:N:4327:GLN:H	3:N:4345:HIS:CE1	2.34	0.44
3:O:5268:ALA:HB1	3:O:5271:CYS:SG	2.57	0.44
3:P:6268:ALA:HB1	3:P:6271:CYS:SG	2.57	0.44
3:N:4096:CYS:HB2	3:N:4100:ASN:HD21	1.82	0.44
3:N:4307:THR:HG22	3:N:4308:TYR:N	2.32	0.44
3:N:4329:PRO:O	3:N:4370:CYS:CA	2.65	0.44
3:O:5001:TYR:CA	3:O:5282:ILE:C	2.82	0.44
3:O:5307:THR:HG22	3:O:5308:TYR:N	2.32	0.44
3:P:6008:PRO:HG2	3:P:6015:TYR:CE2	2.51	0.44
3:M:1085:TYR:OH	3:M:1229:VAL:HA	2.18	0.44
3:P:6096:CYS:HB2	3:P:6100:ASN:HD21	1.82	0.44
3:P:6085:TYR:OH	3:P:6229:VAL:HA	2.18	0.44
3:P:6307:THR:HG22	3:P:6308:TYR:N	2.32	0.44
3:P:6327:GLN:H	3:P:6345:HIS:HE1	1.66	0.44
3:M:1200:PHE:HD2	3:M:1200:PHE:HA	1.61	0.43
3:O:5047:ILE:HG23	3:O:5119:ALA:O	2.18	0.43
3:O:5096:CYS:HB2	3:O:5100:ASN:HD21	1.82	0.43
3:P:6047:ILE:HG23	3:P:6119:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:1327:GLN:H	3:M:1345:HIS:HE1	1.66	0.43
3:N:4356:PHE:HB3	3:N:4357:SER:H	1.63	0.43
3:P:6203:ILE:HA	3:P:6215:ALA:HB2	2.00	0.43
3:M:1249:ARG:H	3:M:1249:ARG:HG3	1.67	0.43
3:P:6077:THR:HG22	3:P:6221:LEU:HG	2.01	0.43
3:M:1047:ILE:HG23	3:M:1119:ALA:O	2.18	0.43
3:M:1199:ALA:HB1	3:M:1243:TRP:NE1	2.33	0.43
3:M:1071:ALA:HB3	3:M:1076:TYR:OH	2.19	0.43
3:M:1077:THR:HG22	3:M:1221:LEU:HG	2.01	0.43
3:M:1307:THR:HG22	3:M:1308:TYR:N	2.32	0.43
3:N:4085:TYR:OH	3:N:4229:VAL:HA	2.18	0.43
3:O:5077:THR:HG22	3:O:5221:LEU:HG	2.01	0.43
1:C:5115:LEU:HD12	1:C:5129:ALA:O	2.19	0.43
3:O:5071:ALA:HB3	3:O:5076:TYR:OH	2.19	0.43
3:O:5249:ARG:H	3:O:5249:ARG:HG3	1.67	0.43
3:P:6056:PRO:HD2	3:P:6105:GLU:O	2.19	0.43
1:D:6115:LEU:HD12	1:D:6129:ALA:O	2.19	0.43
3:M:1320:TYR:CE1	3:M:1369:LEU:CA	3.02	0.43
3:N:4001:TYR:CA	3:N:4282:ILE:C	2.82	0.43
3:O:5056:PRO:HD2	3:O:5105:GLU:O	2.19	0.43
3:P:6199:ALA:HB1	3:P:6243:TRP:NE1	2.34	0.43
3:P:6320:TYR:CE1	3:P:6369:LEU:CA	3.02	0.43
3:M:1029:LEU:HD22	3:M:1137:TYR:CE2	2.54	0.43
3:N:4203:ILE:HA	3:N:4215:ALA:HB2	2.00	0.43
3:O:5085:TYR:OH	3:O:5229:VAL:HA	2.18	0.43
3:N:4029:LEU:HD22	3:N:4137:TYR:CE2	2.54	0.43
3:O:5327:GLN:H	3:O:5345:HIS:HE1	1.66	0.43
3:N:4056:PRO:HD2	3:N:4105:GLU:O	2.19	0.43
3:N:4327:GLN:H	3:N:4345:HIS:HE1	1.66	0.43
3:P:6071:ALA:HB3	3:P:6076:TYR:OH	2.19	0.43
3:N:4199:ALA:HB1	3:N:4243:TRP:NE1	2.33	0.42
3:O:5203:ILE:HA	3:O:5215:ALA:HB2	2.01	0.42
3:P:6001:TYR:CA	3:P:6282:ILE:C	2.82	0.42
3:M:1203:ILE:HA	3:M:1215:ALA:HB2	2.01	0.42
3:O:5130:LYS:HD2	3:O:5267:ARG:NH2	2.35	0.42
3:O:5199:ALA:HB1	3:O:5243:TRP:NE1	2.33	0.42
3:P:6029:LEU:HD22	3:P:6137:TYR:CE2	2.54	0.42
1:B:4115:LEU:HD12	1:B:4129:ALA:O	2.19	0.42
3:N:4077:THR:HG22	3:N:4221:LEU:HG	2.01	0.42
3:N:4320:TYR:CE1	3:N:4369:LEU:CA	3.02	0.42
1:A:1115:LEU:HD12	1:A:1129:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:4071:ALA:HB3	3:N:4076:TYR:OH	2.19	0.42
3:O:5320:TYR:CE1	3:O:5369:LEU:CA	3.02	0.42
3:P:6130:LYS:HD2	3:P:6267:ARG:NH2	2.35	0.42
3:M:1056:PRO:HD2	3:M:1105:GLU:O	2.19	0.42
3:O:5063:CYS:N	3:O:5096:CYS:SG	2.93	0.42
3:P:6048:THR:CG2	3:P:6204:GLN:HG2	2.50	0.42
3:N:4327:GLN:O	3:N:4328:CYS:HB3	2.20	0.42
3:O:5029:LEU:HD22	3:O:5137:TYR:CE2	2.54	0.42
3:O:5009:ASN:ND2	3:O:5166:ILE:HD13	2.31	0.42
3:P:6048:THR:HG23	3:P:6204:GLN:HG2	2.02	0.42
3:P:6299:VAL:HG13	3:P:6320:TYR:HE2	1.85	0.42
3:P:6327:GLN:O	3:P:6328:CYS:HB3	2.20	0.42
3:M:1320:TYR:OH	3:M:1369:LEU:CA	2.68	0.42
3:O:5046:TYR:HA	3:O:5205:ALA:O	2.20	0.42
3:P:6203:ILE:HG12	3:P:6215:ALA:CB	2.50	0.42
3:M:1299:VAL:HG13	3:M:1320:TYR:HE2	1.85	0.42
3:N:4203:ILE:HG12	3:N:4215:ALA:CB	2.50	0.42
3:N:4048:THR:CG2	3:N:4204:GLN:HG2	2.50	0.42
3:O:5150:GLY:N	3:O:5165:PRO:HD3	2.35	0.42
3:O:5048:THR:CG2	3:O:5204:GLN:HG2	2.50	0.42
3:M:1063:CYS:N	3:M:1096:CYS:SG	2.93	0.41
3:N:4063:CYS:N	3:N:4096:CYS:SG	2.93	0.41
3:M:1151:VAL:HG21	3:N:4191:GLU:CB	2.50	0.41
3:M:1150:GLY:N	3:M:1165:PRO:HD3	2.35	0.41
3:M:1327:GLN:O	3:M:1328:CYS:HB3	2.20	0.41
3:N:4200:PHE:HD2	3:N:4200:PHE:HA	1.61	0.41
3:N:4299:VAL:HG13	3:N:4320:TYR:HE2	1.85	0.41
3:O:5029:LEU:HD22	3:O:5137:TYR:HE2	1.85	0.41
3:M:1130:LYS:HD2	3:M:1267:ARG:NH2	2.35	0.41
3:N:4029:LEU:HD22	3:N:4137:TYR:HE2	1.85	0.41
3:O:5299:VAL:HG13	3:O:5320:TYR:HE2	1.85	0.41
3:O:5327:GLN:O	3:O:5328:CYS:HB3	2.20	0.41
3:P:6342:SER:O	3:P:6356:PHE:CZ	2.71	0.41
3:M:1048:THR:HG23	3:M:1204:GLN:HG2	2.02	0.41
3:N:4130:LYS:HD2	3:N:4267:ARG:NH2	2.35	0.41
3:P:6029:LEU:HD22	3:P:6137:TYR:HE2	1.85	0.41
3:P:6009:ASN:ND2	3:P:6166:ILE:HD13	2.31	0.41
3:P:6320:TYR:OH	3:P:6369:LEU:CA	2.68	0.41
3:M:1191:GLU:CB	3:N:4151:VAL:HG21	2.50	0.41
3:N:4196:LYS:C	3:N:4198:GLY:H	2.24	0.41
3:N:4317:THR:O	3:N:4317:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:6046:TYR:HA	3:P:6205:ALA:O	2.20	0.41
3:P:6063:CYS:N	3:P:6096:CYS:SG	2.93	0.41
1:A:1197:GLN:NE2	1:A:1239:ARG:HH12	2.19	0.41
1:B:4197:GLN:NE2	1:B:4239:ARG:HH12	2.19	0.41
1:B:4248:ASN:C	1:B:4248:ASN:HD22	2.24	0.41
3:M:1010:VAL:HA	3:M:1011:PRO:HD2	1.92	0.41
3:M:1293:ALA:HB3	3:M:1294:PRO:CD	2.51	0.41
3:M:1317:THR:HG22	3:M:1317:THR:O	2.20	0.41
3:N:4293:ALA:HB3	3:N:4294:PRO:CD	2.51	0.41
3:P:6150:GLY:N	3:P:6165:PRO:HD3	2.35	0.41
3:M:1203:ILE:HG12	3:M:1215:ALA:CB	2.50	0.41
3:M:1336:THR:O	3:M:1337:ALA:HB3	2.21	0.41
3:O:5243:TRP:HZ3	3:O:5246:ASN:HB3	1.86	0.41
3:O:5336:THR:O	3:O:5337:ALA:HB3	2.21	0.41
3:O:5320:TYR:OH	3:O:5369:LEU:CA	2.68	0.41
3:P:6336:THR:O	3:P:6337:ALA:HB3	2.21	0.41
1:A:1248:ASN:C	1:A:1248:ASN:HD22	2.24	0.41
3:M:1196:LYS:C	3:M:1198:GLY:H	2.24	0.41
3:M:1243:TRP:HZ3	3:M:1246:ASN:HB3	1.86	0.41
3:N:4243:TRP:HZ3	3:N:4246:ASN:HB3	1.86	0.41
3:N:4336:THR:O	3:N:4337:ALA:HB3	2.21	0.41
3:N:4320:TYR:OH	3:N:4369:LEU:CA	2.68	0.41
3:M:1046:TYR:HA	3:M:1205:ALA:O	2.20	0.41
3:O:5317:THR:HG22	3:O:5317:THR:O	2.20	0.41
3:M:1049:CYS:HG	3:M:1118:HIS:HA	1.86	0.41
3:N:4150:GLY:N	3:N:4165:PRO:HD3	2.35	0.41
3:O:5073:HIS:H	3:O:5076:TYR:HE1	1.69	0.41
3:P:6196:LYS:C	3:P:6198:GLY:H	2.24	0.41
3:P:6293:ALA:HB3	3:P:6294:PRO:CD	2.51	0.41
3:P:6317:THR:O	3:P:6317:THR:HG22	2.20	0.41
3:N:4048:THR:HG23	3:N:4204:GLN:HG2	2.02	0.41
3:P:6243:TRP:HZ3	3:P:6246:ASN:HB3	1.86	0.40
1:C:5248:ASN:C	1:C:5248:ASN:HD22	2.24	0.40
3:M:1048:THR:CG2	3:M:1204:GLN:HG2	2.50	0.40
1:A:1156:PHE:CB	1:A:1165:GLU:HG2	2.49	0.40
3:M:1029:LEU:HD22	3:M:1137:TYR:HE2	1.85	0.40
3:M:1045:GLU:O	3:M:1046:TYR:HD2	2.05	0.40
3:N:4009:ASN:ND2	3:N:4166:ILE:HD13	2.31	0.40
3:O:5203:ILE:HG12	3:O:5215:ALA:CB	2.50	0.40
3:P:6045:GLU:O	3:P:6046:TYR:HD2	2.05	0.40
3:M:1166:ILE:HG12	3:M:1276:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:4046:TYR:HA	3:N:4205:ALA:O	2.20	0.40
3:O:5196:LYS:C	3:O:5198:GLY:H	2.24	0.40
3:P:6180:HIS:O	3:P:6182:GLY:N	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	A	149/264 (56%)	144 (97%)	5 (3%)	0	100	100
1	B	149/264 (56%)	144 (97%)	5 (3%)	0	100	100
1	C	149/264 (56%)	144 (97%)	5 (3%)	0	100	100
1	D	149/264 (56%)	144 (97%)	5 (3%)	0	100	100
3	M	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	5	36
3	N	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	5	36
3	O	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	5	36
3	P	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	5	36
All	All	1988/2812 (71%)	1656 (83%)	288 (14%)	44 (2%)	12	44

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	1126	THR
3	M	1361	PRO
3	N	4126	THR
3	N	4361	PRO
3	O	5126	THR
3	O	5361	PRO
3	P	6126	THR

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Mol	Chain	Res	Type
3	P	6361	PRO
3	M	1156	SER
3	M	1201	GLY
3	M	1202	ASP
3	N	4156	SER
3	N	4201	GLY
3	N	4202	ASP
3	O	5156	SER
3	O	5201	GLY
3	O	5202	ASP
3	P	6156	SER
3	P	6201	GLY
3	P	6202	ASP
3	M	1075	ASP
3	M	1181	ARG
3	M	1324	ARG
3	N	4049	CYS
3	N	4075	ASP
3	N	4181	ARG
3	N	4324	ARG
3	O	5049	CYS
3	O	5075	ASP
3	O	5181	ARG
3	O	5324	ARG
3	P	6075	ASP
3	P	6181	ARG
3	P	6324	ARG
3	M	1049	CYS
3	P	6049	CYS
3	M	1293	ALA
3	M	1328	CYS
3	N	4293	ALA
3	N	4328	CYS
3	O	5293	ALA
3	O	5328	CYS
3	P	6293	ALA
3	P	6328	CYS

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	122/218 (56%)	115 (94%)	7 (6%)	24	56
1	B	122/218 (56%)	115 (94%)	7 (6%)	24	56
1	C	122/218 (56%)	115 (94%)	7 (6%)	24	56
1	D	122/218 (56%)	115 (94%)	7 (6%)	24	56
3	M	299/370 (81%)	290 (97%)	9 (3%)	46	72
3	N	299/370 (81%)	290 (97%)	9 (3%)	46	72
3	O	299/370 (81%)	290 (97%)	9 (3%)	46	72
3	P	299/370 (81%)	290 (97%)	9 (3%)	46	72
All	All	1684/2352 (72%)	1620 (96%)	64 (4%)	42	67

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1143	LYS
1	A	1155	LYS
1	A	1183	GLU
1	A	1191	TRP
1	A	1207	ARG
1	A	1248	ASN
1	A	1253	THR
1	B	4143	LYS
1	B	4155	LYS
1	B	4183	GLU
1	B	4191	TRP
1	B	4207	ARG
1	B	4248	ASN
1	B	4253	THR
1	C	5143	LYS
1	C	5155	LYS
1	C	5183	GLU
1	C	5191	TRP
1	C	5207	ARG
1	C	5248	ASN
1	C	5253	THR
1	D	6143	LYS
1	D	6155	LYS

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Mol	Chain	Res	Type
1	D	6183	GLU
1	D	6191	TRP
1	D	6207	ARG
1	D	6248	ASN
1	D	6253	THR
3	M	1035	SER
3	M	1049	CYS
3	M	1118	HIS
3	M	1188	ASP
3	M	1192	TYR
3	M	1200	PHE
3	M	1212	ASP
3	M	1292	ASP
3	M	1334	SER
3	N	4035	SER
3	N	4049	CYS
3	N	4118	HIS
3	N	4188	ASP
3	N	4192	TYR
3	N	4200	PHE
3	N	4212	ASP
3	N	4292	ASP
3	N	4334	SER
3	O	5035	SER
3	O	5049	CYS
3	O	5118	HIS
3	O	5188	ASP
3	O	5192	TYR
3	O	5200	PHE
3	O	5212	ASP
3	O	5292	ASP
3	O	5334	SER
3	P	6035	SER
3	P	6049	CYS
3	P	6118	HIS
3	P	6188	ASP
3	P	6192	TYR
3	P	6200	PHE
3	P	6212	ASP
3	P	6292	ASP
3	P	6334	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	1190	ASN
1	A	1197	GLN
1	A	1248	ASN
1	B	4128	HIS
1	B	4190	ASN
1	B	4197	GLN
1	B	4248	ASN
1	C	5128	HIS
1	C	5190	ASN
1	C	5197	GLN
1	C	5248	ASN
1	D	6128	HIS
1	D	6190	ASN
1	D	6197	GLN
1	D	6248	ASN
3	M	1073	HIS
3	M	1100	ASN
3	M	1331	HIS
3	M	1345	HIS
3	M	1355	HIS
3	N	4073	HIS
3	N	4100	ASN
3	N	4331	HIS
3	N	4345	HIS
3	N	4355	HIS
3	O	5073	HIS
3	O	5100	ASN
3	O	5331	HIS
3	O	5345	HIS
3	O	5355	HIS
3	P	6073	HIS
3	P	6100	ASN
3	P	6331	HIS
3	P	6345	HIS
3	P	6355	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 32 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.