



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 09:04 PM UTC

PDB ID : 1LD4 / pdb_00001ld4
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 initial models : 1I9W, 1SVB, 1YSA

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB 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:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

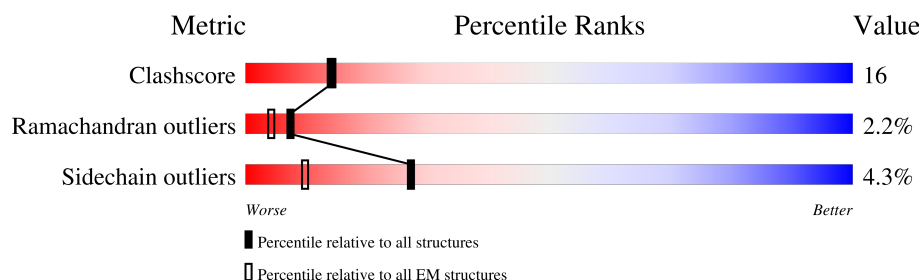
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	A	264	45% 11% . 43%
1	B	264	45% 11% . 43%
1	C	264	45% 10% . 43%
1	D	264	46% 10% . 43%
2	E	57	49% 51%
2	F	57	49% 51%
2	G	57	49% 51%
2	H	57	49% 51%
2	I	57	49% 51%

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Mol	Chain	Length	Quality of chain
2	J	57	 49% 51%
2	K	57	 49% 51%
2	L	57	 49% 51%
3	M	439	 53% 29% • 16%
3	N	439	 54% 28% • 16%
3	O	439	 54% 28% • 16%
3	P	439	 54% 28% • 16%

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		

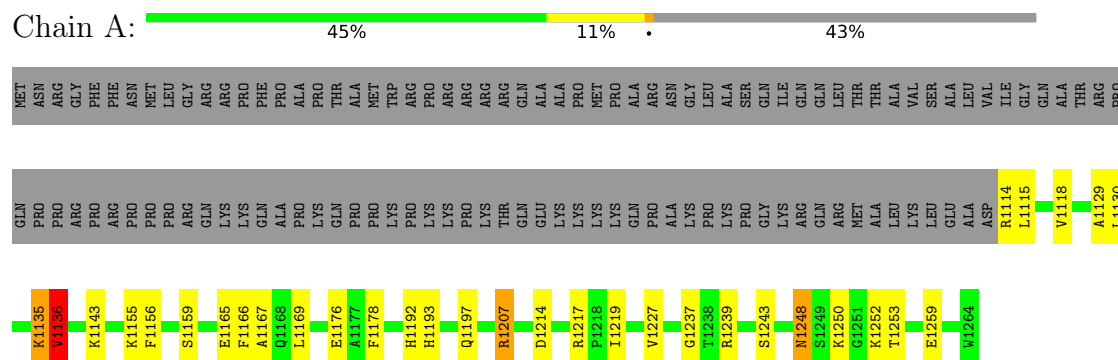
- Molecule 4 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

3 Residue-property plots

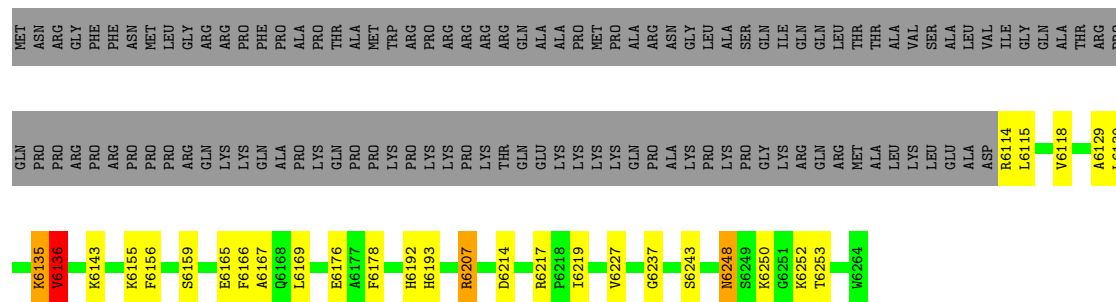
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Coat protein C



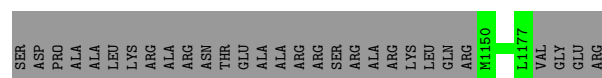
- Molecule 1: Coat protein C

Chain D: 46% 10% • 43%

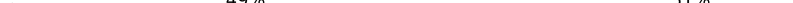


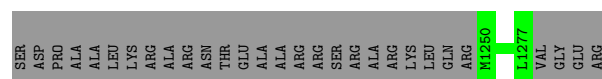
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain E: 49% 51%

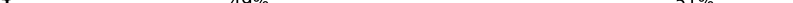


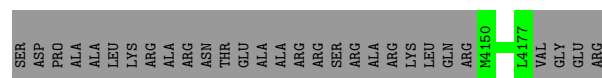
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain F:  49% 51%

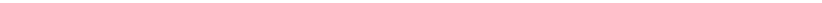


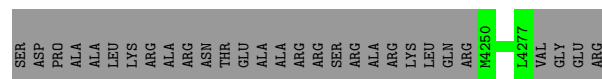
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain G:  49% 51%

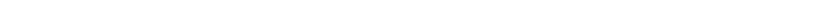


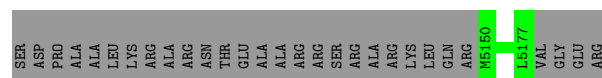
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain H:  49% 51%



- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain I:  49% 51%



- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain J:  49% 51%

SER	ASP	PRO	ALA	ALA	LEU	LYS	ARG	ALA	ALA	ASN	THR	GLU	ALA	ALA	ARG	ARG	ARG	ALA	LYS	LEU	GLN	ARG	H6250	L6277	VAL	GLY	GLU	ARG
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- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain K:  49% 51%

SER	ASP	PRO	ALA	ALA	LEU	LYS	ARG	ALA	ALA	ASN	THR	GLU	ALA	ALA	ARG	ARG	ARG	ALA	LYS	LEU	GLN	ARG	H6150	L6177	VAL	GLY	GLU	ARG
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- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain L:  49% 51%

SER	ASP	PRO	ALA	ALA	LEU	LYS	ARG	ALA	ALA	ASN	THR	GLU	ALA	ALA	ARG	ARG	ARG	ALA	LYS	LEU	GLN	ARG	H6250	L6277	VAL	GLY	GLU	ARG
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- Molecule 3: Spike glycoprotein E1

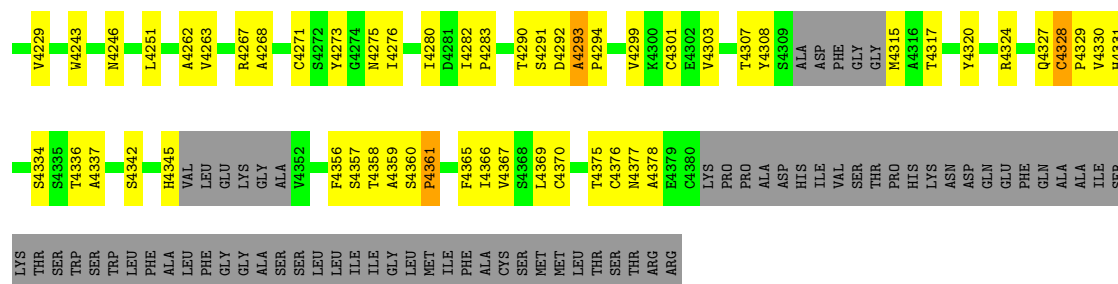
Chain M:  53% 29% 16%

Y1001	E1002	P1008	N1009	V1010	P1011	Y1015	K1016	A1017	N1028	L1029	V1033	M1034	S1035	P1040	E1045	Y1046	I1047	T1048	C1049	P1056	C1063	A1071	D1075	Y1076	T1077	Y1085	C1096	E1099	N1100	E1105	C1114	H1118	A1119	Q1120	A1121	I1122	K1123	T1126	A1127	A1128	M1129	K1130									
Y1137	T1141	G1150	V1151	S1156	L1159	K1160	P1165	I1166	S1167	A1168	T1171	P1172	F1173	D1174	H1175	V1178	I1179	H1180	R1181	G1182	Y1185	N1186	Y1187	D1188	E1191	Y1192	G1193	A1194	M1195	K1196	P1197	A1198	F1200	G1201	D1202	T1203	Q1204	A1205	T1206	S1207	S1210	K1211	D1212	A1215							
L1221	V1229	W1243	N1246	R1249	L1251	A1262	V1263	R1267	A1268	C1271	S1272	Y1273	G1274	N1275	I1276	I1280	D1281	I1282	P1283	T1290	S1291	A1293	P1294	V1299	K1300	C1301	E1302	V1303	T1307	Y1308	S1309	ALA	ASP	PHE	GLY	M1315	A1316	T1317	Y1320	R1324	Q1327	C1328									
P1329	V1330	H1331	S1334	S1335	T1336	A1337	S1342	H1345	VAL	LEU	GLY	LYS	ALA	V1352	F1356	S1357	T1358	A1359	S1360	P1361	F1365	T1366	V1367	L1369	C1370	T1375	C1376	N1377	A1378	E1379	C1380	LYS	PRO	PRO	ALA	ASP	HIS	ILE	VAL	SER	THR	PRO	HIS	LYS	ASN	ASP	GLN	GLU	PHE	GLN	ALA
ALA	ILE	LYS	THR	SER	TRP	SER	TRP	PHE	LEU	ALA	LEU	PHE	GLY	GLY	SER	SER	LEU	ILE	ILE	ALA	CYS	SER	MET	MET	LEU	THR	SER	THR	ARG	ARG	ALA	ILE	LYS	THR	ASP	HIS	ILE	VAL	SER	THR	PRO	HIS	LYS	ASN	ASP	GLN	GLU	PHE	GLN	ALA	

- Molecule 3: Spike glycoprotein E1

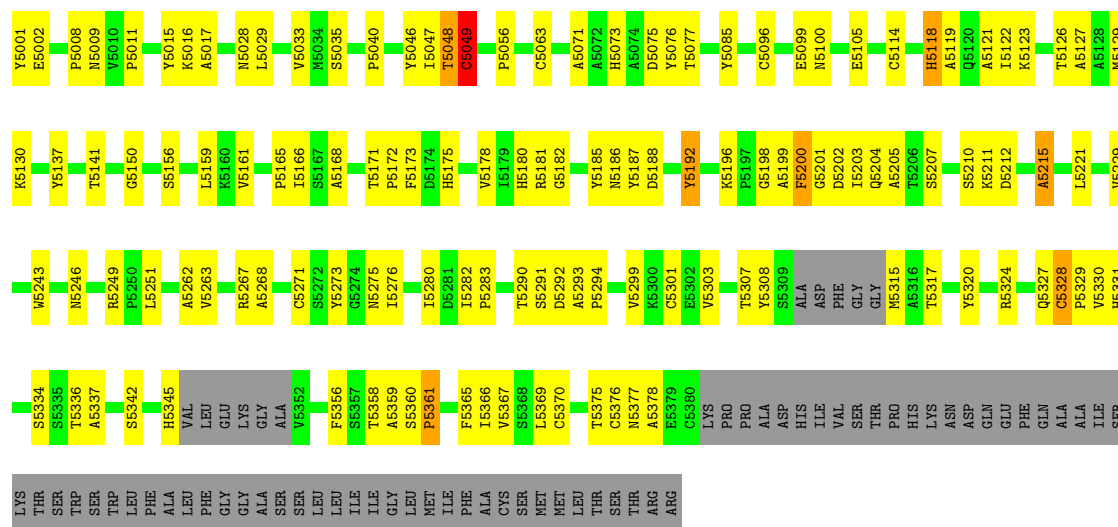
Chain N:  54% 28% 16%

Y4001	E4002	P4008	N4009	V4010	P4011	Y4015	K4016	A4017	N4028	L4029	V4033	M4034	S4035	P4040	Y4046	I4047	T4048	C4049	P4056	C4063	A4071	D4075	Y4076	T4077	Y4085	C4096	E4099	N4100	E4105	C4114	H4118	A4119	Q4120	A4121	I4122	K4123	T4126	A4127	A4128	M4129	K4130							
Y4137	T4141	G4150	V4151	S4156	L4159	K4160	V4161	P4165	T4166	S4167	A4168	T4171	P4172	F4173	D4174	H4175	Y4178	T4179	H4180	A4181	C4182	Y4185	N4186	Y4187	D4188	E4191	Y4192	G4193	A4194	M4195	K4196	P4197	Q4198	A4199	F4200	G4201	D4202	I4203	Q4204	A4205	T4206	S4207	S4210	K4211	D4212	A4215	M4219	K4221



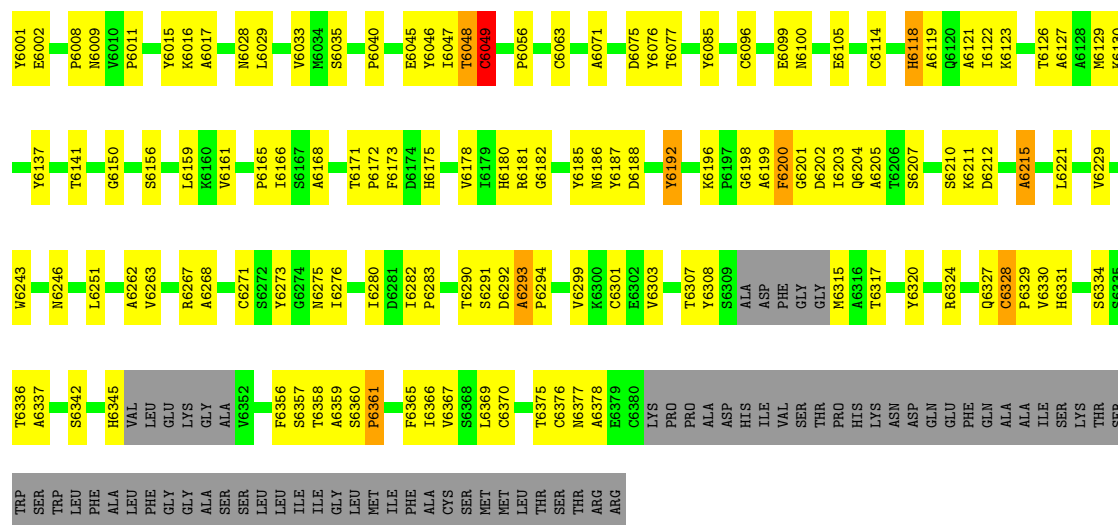
• Molecule 3: Spike glycoprotein E1

Chain O: 54% 28% 16%



• Molecule 3: Spike glycoprotein E1

Chain P: 54% 28% 16%



4 Data and refinement statistics

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 11.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-11.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15680	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

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 > 5$	RMSZ	# $ Z > 5$
1	A	0.65	0/1190	1.04	9/1607 (0.6%)
1	B	0.65	0/1190	1.04	9/1607 (0.6%)
1	C	0.65	0/1190	1.04	9/1607 (0.6%)
1	D	0.65	0/1190	1.04	9/1607 (0.6%)
3	M	0.44	0/2743	0.85	4/3740 (0.1%)
3	N	0.44	0/2743	0.85	4/3740 (0.1%)
3	O	0.44	0/2743	0.85	4/3740 (0.1%)
3	P	0.44	0/2743	0.85	4/3740 (0.1%)
All	All	0.51	0/15732	0.91	52/21388 (0.2%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	4215	ALA	N-CA-C	6.61	117.20	107.88
3	P	6215	ALA	N-CA-C	6.61	117.20	107.88
3	M	1215	ALA	N-CA-C	6.59	117.18	107.88
3	O	5215	ALA	N-CA-C	6.59	117.18	107.88
1	B	4219	ILE	N-CA-C	-6.58	98.95	108.17
1	D	6219	ILE	N-CA-C	-6.58	98.96	108.17
1	C	5219	ILE	N-CA-C	-6.57	98.98	108.17
1	A	1219	ILE	N-CA-C	-6.56	98.98	108.17
1	A	1159	SER	N-CA-C	-6.07	101.22	109.54
1	B	4159	SER	N-CA-C	-6.07	101.23	109.54
1	D	6159	SER	N-CA-C	-6.05	101.26	109.54
1	C	5159	SER	N-CA-C	-6.04	101.26	109.54
1	A	1136	VAL	CB-CA-C	-6.02	102.96	111.21
1	B	4136	VAL	CB-CA-C	-6.01	102.97	111.21
1	D	6136	VAL	CB-CA-C	-6.01	102.98	111.21
1	C	5136	VAL	CB-CA-C	-5.99	103.00	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1048	THR	N-CA-C	5.79	117.59	108.96
3	O	5048	THR	N-CA-C	5.78	117.57	108.96
3	N	4048	THR	N-CA-C	5.75	117.52	108.96
3	P	6048	THR	N-CA-C	5.75	117.52	108.96
1	D	6243	SER	N-CA-C	-5.45	99.84	108.73
1	A	1243	SER	N-CA-C	-5.44	99.86	108.73
1	C	5243	SER	N-CA-C	-5.44	99.86	108.73
1	B	4243	SER	N-CA-C	-5.43	99.87	108.73
3	O	5207	SER	N-CA-C	5.34	115.08	108.19
3	M	1207	SER	N-CA-C	5.33	115.07	108.19
1	C	5135	LYS	N-CA-C	5.32	117.27	109.24
3	P	6207	SER	N-CA-C	5.32	115.05	108.19
3	N	4207	SER	N-CA-C	5.31	115.05	108.19
1	B	4135	LYS	N-CA-C	5.30	117.25	109.24
1	D	6135	LYS	N-CA-C	5.29	117.23	109.24
1	A	1135	LYS	N-CA-C	5.29	117.22	109.24
1	C	5166	PHE	N-CA-C	5.28	117.21	109.24
1	A	1166	PHE	N-CA-C	5.26	117.19	109.24
1	D	6166	PHE	N-CA-C	5.23	117.14	109.24
1	B	4166	PHE	N-CA-C	5.23	117.14	109.24
1	A	1192	HIS	N-CA-C	5.20	117.62	111.33
3	P	6175	HIS	N-CA-C	5.19	117.84	111.82
1	B	4192	HIS	N-CA-C	5.19	117.61	111.33
1	C	5192	HIS	N-CA-C	5.18	117.60	111.33
1	D	6192	HIS	N-CA-C	5.17	117.59	111.33
3	M	1175	HIS	N-CA-C	5.16	117.81	111.82
3	N	4175	HIS	N-CA-C	5.14	117.78	111.82
3	O	5175	HIS	N-CA-C	5.13	117.77	111.82
1	A	1118	VAL	N-CA-C	-5.11	100.40	107.80
1	B	4118	VAL	N-CA-C	-5.11	100.40	107.80
1	B	4193	HIS	N-CA-C	5.09	119.18	112.92
1	C	5118	VAL	N-CA-C	-5.09	100.42	107.80
1	D	6118	VAL	N-CA-C	-5.09	100.42	107.80
1	D	6193	HIS	N-CA-C	5.05	119.14	112.92
1	C	5193	HIS	N-CA-C	5.04	119.12	112.92
1	A	1193	HIS	N-CA-C	5.03	119.11	112.92

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	10	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	142	0
3	N	2694	0	2605	137	0
3	O	2694	0	2605	94	0
3	P	2694	0	2605	97	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	475	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 16.

All (475) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:1194:ALA:CB	3:N:4151:VAL:CG1	2.05	1.31
3:M:1151:VAL:HG21	3:N:4191:GLU:CD	1.55	1.30
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:1191:GLU:CD	3:N:4151:VAL:HG21	1.55	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:1194:ALA:HB3	3:N:4151:VAL:CG1	1.64	1.25
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:M:1330:VAL:CG2	3:M:1369:LEU:CA	2.33	1.05
3:P:6001:TYR:CA	3:P:6282:ILE:O	2.02	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:1151:VAL:HG12	3:N:4194:ALA:HB2	1.08	1.04
3:M:1303:VAL:HG23	3:M:1377:ASN:CA	1.88	1.04
3:N:4303:VAL:HG23	3:N:4377:ASN:CA	1.88	1.03
3:M:1151:VAL:HG11	3:N:4191:GLU:HB2	1.03	1.03
3:M:1194:ALA:HB2	3:N:4151:VAL:HG12	1.08	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:M:1151:VAL:CG2	3:N:4191:GLU:CD	2.39	0.95
3:M:1191:GLU:CD	3:N:4151:VAL:CG2	2.39	0.95
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:CG	3:P:6002:GLU:CA	2.58	0.82
3:M:1002:GLU:CA	3:M:1002:GLU:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:M:1191:GLU:OE2	3:N:4151:VAL:CG2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:4207:ARG:HH21	1:B:4237:GLY:HA2	1.71	0.56
1:D:6207:ARG:HH21	1:D:6237: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:GLU:CD	1:C:5171:VAL:HG21	2.31	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:HD1	3:P:6192:TYR:H	1.54	0.55
3:M:1161:VAL:HA	3:M:1280:ILE:HG12	1.89	0.55
3:N:4016:LYS:HD3	3:N:4331:HIS:CE1	2.39	0.54
3:N:4315:MET:HG2	3:N:4317:THR:H	1.71	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:1191:GLU:HB3	3:N:4151:VAL:HG11	1.81	0.54
3:M:1290:THR:HG22	3:M:1291:SER:H	1.73	0.54
3:N:4161:VAL:HA	3:N:4280:ILE:HG12	1.89	0.54
3:O:5049:CYS:HG	3:O:5118:HIS:HA	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:P:6243:TRP:CE3	3:P:6243:TRP:HA	2.45	0.51
3:M:1001:TYR:CA	3:M:1282:ILE:C	2.82	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:HA	3:M:1243:TRP:CE3	2.45	0.51
3:O:5243:TRP:HA	3:O:5243:TRP:CE3	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:1194:ALA:HB1	3:N:4151:VAL:O	2.12	0.50
3:M:1336:THR:HG22	3:M:1337:ALA:N	2.25	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:O:5001:TYR:CA	3:O:5282:ILE:C	2.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:4001:TYR:CA	3:N:4282:ILE:C	2.82	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:P:6001:TYR:CA	3:P:6282:ILE:C	2.82	0.47
3:M:1192:TYR:HD1	3:M:1192:TYR:N	2.12	0.47
3:N:4192:TYR:HD1	3:N:4192:TYR:N	2.12	0.47
3:N:4337:ALA:HB2	3:N:4360:SER:HB3	1.96	0.47
3:O:5192:TYR:HD1	3:O:5192:TYR:N	2.12	0.47
3:P:6172:PRO:HD3	3:P:6273:TYR:OH	2.14	0.47
3:P:6186:ASN:ND2	3:P:6251:LEU:HD21	2.29	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: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:N:4196:LYS:C	3:N:4198:GLY:H	2.24	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
1:B:4248:ASN:C	1:B:4248:ASN:HD22	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1248:ASN:C	1:A:1248:ASN:HD22	2.24	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
3:P:6196:LYS:C	3:P:6198:GLY:H	2.24	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
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:C:5248:ASN:C	1:C:5248:ASN:HD22	2.24	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
1:D:6248:ASN:C	1:D:6248:ASN:HD22	2.24	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:5196:LYS:C	3:O:5198:GLY:H	2.24	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:M:1196:LYS:C	3:M:1198:GLY:H	2.24	0.45
3:N:4047:ILE:HG23	3:N:4119:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N:4315:MET:HE3	3:N:4317:THR:HA	2.00	0.44
3:N:4049:CYS:HG	3:N:4118:HIS:HA	1.81	0.44
3:P:6085:TYR:OH	3:P:6229:VAL:HA	2.18	0.44
3:P:6096:CYS:HB2	3:P:6100:ASN:HD21	1.82	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
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
3:P:6315:MET:HE3	3:P:6317:THR:HA	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:5315:MET:HE3	3:O:5317:THR:HA	2.00	0.42
3:M:1315:MET:HE3	3:M:1317:THR:HA	2.00	0.42
3:O:5203:ILE:HA	3:O:5215:ALA:HB2	2.01	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
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:5009:ASN:ND2	3:O:5166:ILE:HD13	2.31	0.42
3:O:5029:LEU:HD22	3:O:5137:TYR:CE2	2.54	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:4048:THR:CG2	3:N:4204:GLN:HG2	2.50	0.42
3:N:4203:ILE:HG12	3:N:4215:ALA:CB	2.50	0.42
3:O:5048:THR:CG2	3:O:5204:GLN:HG2	2.50	0.42
3:O:5150:GLY:N	3:O:5165:PRO:HD3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1150:GLY:N	3:M:1165:PRO:HD3	2.35	0.41
3:M:1151:VAL:HG21	3:N:4191:GLU:CB	2.50	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:6009:ASN:ND2	3:P:6166:ILE:HD13	2.31	0.41
3:P:6029:LEU:HD22	3:P:6137:TYR:HE2	1.85	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:4317:THR:O	3:N:4317:THR:HG22	2.20	0.41
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
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:O	3:M:1317:THR:HG22	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:1071:ALA:HB3	3:M:1076:TYR:HH	1.84	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:5320:TYR:OH	3:O:5369:LEU:CA	2.68	0.41
3:O:5336:THR:O	3:O:5337:ALA:HB3	2.21	0.41
3:P:6186:ASN:CG	3:P:6251:LEU:HD11	2.46	0.41
3:P:6336:THR:O	3:P:6337:ALA:HB3	2.21	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:4320:TYR:OH	3:N:4369:LEU:CA	2.68	0.41
3:N:4336:THR:O	3:N:4337:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:1046:TYR:HA	3:M:1205:ALA: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:O:5186:ASN:CG	3:O:5251:LEU:HD11	2.46	0.41
3:O:5317:THR:O	3:O:5317:THR:HG22	2.20	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:M:1186:ASN:CG	3:M:1251:LEU:HD11	2.46	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
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
3:N:4046:TYR:HA	3:N:4205:ALA:O	2.20	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	3	21
3	N	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	3	21
3	O	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	3	21
3	P	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	3	21
All	All	1988/2812 (71%)	1656 (83%)	288 (14%)	44 (2%)	7	29

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
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

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Mol	Chain	Res	Type
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%)	114 (93%)	8 (7%)	15	37
1	B	122/218 (56%)	114 (93%)	8 (7%)	15	37
1	C	122/218 (56%)	114 (93%)	8 (7%)	15	37
1	D	122/218 (56%)	114 (93%)	8 (7%)	15	37
3	M	299/370 (81%)	289 (97%)	10 (3%)	33	55
3	N	299/370 (81%)	289 (97%)	10 (3%)	33	55
3	O	299/370 (81%)	289 (97%)	10 (3%)	33	55
3	P	299/370 (81%)	289 (97%)	10 (3%)	33	55
All	All	1684/2352 (72%)	1612 (96%)	72 (4%)	27	47

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1136	VAL
1	A	1143	LYS
1	A	1155	LYS

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Mol	Chain	Res	Type
1	A	1207	ARG
1	A	1227	VAL
1	A	1248	ASN
1	A	1250	LYS
1	A	1253	THR
1	B	4136	VAL
1	B	4143	LYS
1	B	4155	LYS
1	B	4207	ARG
1	B	4227	VAL
1	B	4248	ASN
1	B	4250	LYS
1	B	4253	THR
1	C	5136	VAL
1	C	5143	LYS
1	C	5155	LYS
1	C	5207	ARG
1	C	5227	VAL
1	C	5248	ASN
1	C	5250	LYS
1	C	5253	THR
1	D	6136	VAL
1	D	6143	LYS
1	D	6155	LYS
1	D	6207	ARG
1	D	6227	VAL
1	D	6248	ASN
1	D	6250	LYS
1	D	6253	THR
3	M	1035	SER
3	M	1049	CYS
3	M	1118	HIS
3	M	1141	THR
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

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Mol	Chain	Res	Type
3	N	4141	THR
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	5141	THR
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	6141	THR
3	P	6188	ASP
3	P	6192	TYR
3	P	6200	PHE
3	P	6212	ASP
3	P	6292	ASP
3	P	6334	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1128	HIS
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

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Mol	Chain	Res	Type
1	D	6128	HIS
1	D	6190	ASN
1	D	6197	GLN
1	D	6248	ASN
3	M	1100	ASN
3	M	1102	GLN
3	M	1125	HIS
3	M	1275	ASN
3	M	1331	HIS
3	M	1345	HIS
3	N	4073	HIS
3	N	4100	ASN
3	N	4102	GLN
3	N	4275	ASN
3	N	4331	HIS
3	N	4345	HIS
3	O	5073	HIS
3	O	5100	ASN
3	O	5102	GLN
3	O	5125	HIS
3	O	5275	ASN
3	O	5331	HIS
3	O	5345	HIS
3	P	6100	ASN
3	P	6102	GLN
3	P	6125	HIS
3	P	6204	GLN
3	P	6275	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.