



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Aug 9, 2017 – 12:46 PM EDT

PDB ID : 5XLR
EMDB ID: : EMD-6732
Title : Structure of SARS-CoV spike glycoprotein
Authors : Gui, M.; Song, W.; Xiang, Y.; Wang, X.
Deposited on : unknown
Resolution : 3.80 Å(reported)

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) : rb-20029824

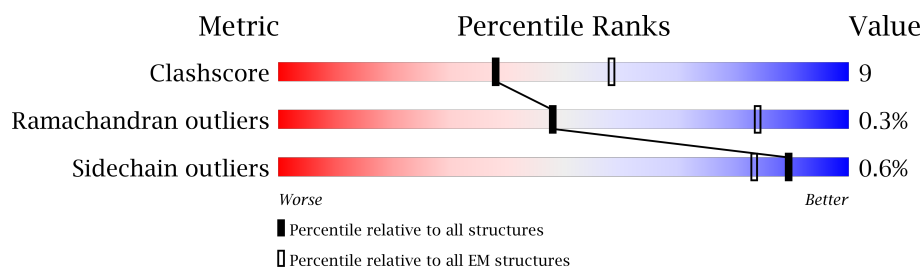
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	1203	
1	B	1203	
1	C	1203	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23901 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0
			7967	5093	1318	1512	44		
1	B	1022	Total	C	N	O	S	0	0
			7967	5093	1318	1512	44		
1	C	1022	Total	C	N	O	S	0	0
			7967	5093	1318	1512	44		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	667	ALA	ARG	engineered mutation	UNP P59594
A	1197	SER	-	expression tag	UNP P59594
A	1198	HIS	-	expression tag	UNP P59594
A	1199	PRO	-	expression tag	UNP P59594
A	1200	GLN	-	expression tag	UNP P59594
A	1201	PHE	-	expression tag	UNP P59594
A	1202	GLU	-	expression tag	UNP P59594
A	1203	LYS	-	expression tag	UNP P59594
B	667	ALA	ARG	engineered mutation	UNP P59594
B	1197	SER	-	expression tag	UNP P59594
B	1198	HIS	-	expression tag	UNP P59594
B	1199	PRO	-	expression tag	UNP P59594
B	1200	GLN	-	expression tag	UNP P59594
B	1201	PHE	-	expression tag	UNP P59594
B	1202	GLU	-	expression tag	UNP P59594
B	1203	LYS	-	expression tag	UNP P59594
C	667	ALA	ARG	engineered mutation	UNP P59594
C	1197	SER	-	expression tag	UNP P59594
C	1198	HIS	-	expression tag	UNP P59594
C	1199	PRO	-	expression tag	UNP P59594
C	1200	GLN	-	expression tag	UNP P59594
C	1201	PHE	-	expression tag	UNP P59594
C	1202	GLU	-	expression tag	UNP P59594
C	1203	LYS	-	expression tag	UNP P59594



I1097	I1098	F1103	V1110	V1111	Y1120	ASP	PRO	LEU	GLN	PRO	GLY	LEU	LYS	TYR	GLN	TYR	ILE	LYS	TRP	PRO	SER	HIS	PRO	PHE	GLU	LYS	I1078	P879	M882	M889	M896	Y899	Q904	Q917	T921	T922	T923	I927	L959	Q987	T988	Y989	V990	L1031	V1043	F1044	Y1049	Q1053	F1057	I1058	T1059	I1063	Y1070	G1075	V1076	F1077	V1078	F1079	N1080	S1083	I1086	T1087	Q1088	F1092
ALA	LYS	ASN	ASN	GLU	SER	LEU	ILE	ASP	LEU	GLN	GLU	LEU	LYS	TYR	GLN	TYR	ILE	LYS	TRP	PRO	SER	HIS	PRO	PHE	GLU	LYS	I1078	P879	M882	M889	M896	Y899	Q904	Q917	T921	T922	T923	I927	L959	Q987	T988	Y989	V990	L1031	V1043	F1044	Y1049	Q1053	F1057	I1058	T1059	I1063	Y1070	G1075	V1076	F1077	V1078	F1079	N1080	S1083	I1086	T1087	Q1088	F1092
ALA	LYS	ASN	ASN	GLU	SER	LEU	ILE	ASP	LEU	GLN	GLU	LEU	LYS	TYR	GLN	TYR	ILE	LYS	TRP	PRO	SER	HIS	PRO	PHE	GLU	LYS	I1078	P879	M882	M889	M896	Y899	Q904	Q917	T921	T922	T923	I927	L959	Q987	T988	Y989	V990	L1031	V1043	F1044	Y1049	Q1053	F1057	I1058	T1059	I1063	Y1070	G1075	V1076	F1077	V1078	F1079	N1080	S1083	I1086	T1087	Q1088	F1092

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	42135	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/8151	0.64	1/11085 (0.0%)
1	B	0.43	0/8151	0.64	1/11085 (0.0%)
1	C	0.43	0/8151	0.64	1/11085 (0.0%)
All	All	0.43	0/24453	0.64	3/33255 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	8
1	C	0	8
All	All	0	24

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1031	LEU	CA-CB-CG	5.73	128.48	115.30
1	C	1031	LEU	CA-CB-CG	5.69	128.39	115.30
1	A	1031	LEU	CA-CB-CG	5.68	128.36	115.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1075	GLY	Peptide
1	A	261	THR	Peptide
1	A	502	GLU	Mainchain,Peptide
1	A	548	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	A	573	ILE	Peptide
1	A	574	SER	Peptide
1	A	633	ALA	Peptide
1	B	1075	GLY	Peptide
1	B	261	THR	Peptide
1	B	502	GLU	Mainchain,Peptide
1	B	548	PHE	Peptide
1	B	573	ILE	Peptide
1	B	574	SER	Peptide
1	B	633	ALA	Peptide
1	C	1075	GLY	Peptide
1	C	261	THR	Peptide
1	C	502	GLU	Mainchain,Peptide
1	C	548	PHE	Peptide
1	C	573	ILE	Peptide
1	C	574	SER	Peptide
1	C	633	ALA	Peptide

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	7967	0	7762	185	0
1	B	7967	0	7762	166	0
1	C	7967	0	7762	170	0
All	All	23901	0	23286	432	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 9.

All (432) 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)
1:A:194:LEU:O	1:A:223:PRO:HA	1.72	0.88
1:B:194:LEU:O	1:B:223:PRO:HA	1.72	0.88
1:C:194:LEU:O	1:C:223:PRO:HA	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:HA	1:A:166:ASP:O	1.74	0.87
1:B:34:THR:O	1:B:66:VAL:HB	1.75	0.87
1:B:122:ASN:HA	1:B:166:ASP:O	1.74	0.87
1:A:34:THR:O	1:A:66:VAL:HB	1.75	0.86
1:C:34:THR:O	1:C:66:VAL:HB	1.75	0.86
1:C:122:ASN:HA	1:C:166:ASP:O	1.74	0.85
1:A:899:TYR:CE1	1:B:1111:VAL:HB	2.16	0.81
1:A:549:GLN:NE2	1:C:45:GLU:OE1	2.14	0.80
1:A:304:ASN:ND2	1:C:719:ASP:OD1	2.15	0.80
1:A:844:PRO:HG3	1:B:632:GLN:HG3	1.68	0.76
1:A:719:ASP:OD1	1:B:304:ASN:ND2	2.20	0.74
1:B:123:VAL:O	1:B:165:SER:HA	1.87	0.73
1:C:123:VAL:O	1:C:165:SER:HA	1.88	0.73
1:A:123:VAL:O	1:A:165:SER:HA	1.88	0.73
1:A:685:SER:HB3	1:C:771:TYR:HD1	1.54	0.72
1:C:37:MET:HA	1:C:63:TYR:H	1.55	0.72
1:A:37:MET:HA	1:A:63:TYR:H	1.55	0.71
1:B:37:MET:HA	1:B:63:TYR:H	1.55	0.71
1:A:769:GLN:HE22	1:B:683:ALA:C	1.95	0.70
1:B:405:ILE:HG23	1:B:409:ASN:HD22	1.57	0.70
1:A:36:SER:O	1:A:63:TYR:HA	1.92	0.70
1:A:1111:VAL:HB	1:C:899:TYR:CE1	2.27	0.70
1:B:36:SER:O	1:B:63:TYR:HA	1.92	0.70
1:A:549:GLN:HE21	1:C:45:GLU:CD	1.94	0.69
1:C:36:SER:O	1:C:63:TYR:HA	1.92	0.69
1:A:554:ASP:HB2	1:A:558:PHE:H	1.57	0.69
1:C:184:GLU:HB3	1:C:199:GLY:O	1.92	0.69
1:A:184:GLU:HB3	1:A:199:GLY:O	1.92	0.69
1:C:405:ILE:HG23	1:C:409:ASN:HD22	1.57	0.69
1:C:554:ASP:HB2	1:C:558:PHE:H	1.57	0.69
1:A:405:ILE:HG23	1:A:409:ASN:HD22	1.57	0.68
1:B:184:GLU:HB3	1:B:199:GLY:O	1.92	0.68
1:B:554:ASP:HB2	1:B:558:PHE:H	1.57	0.68
1:C:597:LEU:HD11	1:C:633:ALA:HB1	1.76	0.67
1:B:707:GLU:O	1:B:1043:VAL:HA	1.94	0.67
1:B:597:LEU:HD11	1:B:633:ALA:HB1	1.76	0.67
1:B:719:ASP:OD1	1:C:304:ASN:ND2	2.26	0.67
1:A:707:GLU:O	1:A:1043:VAL:HA	1.94	0.66
1:A:100:GLY:HA3	1:A:235:LEU:HB2	1.78	0.66
1:A:597:LEU:HD11	1:A:633:ALA:HB1	1.76	0.66
1:B:100:GLY:HA3	1:B:235:LEU:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:GLY:HA2	1:C:46:ILE:HG23	1.79	0.65
1:C:707:GLU:O	1:C:1043:VAL:HA	1.94	0.65
1:C:59:PHE:HB3	1:C:257:LEU:HB2	1.78	0.65
1:A:578:PHE:CE2	1:C:839:GLY:HA2	2.31	0.65
1:A:59:PHE:HB3	1:A:257:LEU:HB2	1.78	0.64
1:A:771:TYR:HD1	1:B:685:SER:HB3	1.61	0.64
1:C:100:GLY:HA3	1:C:235:LEU:HB2	1.78	0.64
1:B:59:PHE:HB3	1:B:257:LEU:HB2	1.78	0.64
1:A:768:LYS:HD2	1:A:874:ALA:HB2	1.80	0.64
1:C:91:ALA:HB3	1:C:183:ARG:HB2	1.80	0.64
1:C:768:LYS:HD2	1:C:874:ALA:HB2	1.80	0.63
1:A:899:TYR:CZ	1:B:1110:VAL:HG22	2.33	0.63
1:B:35:SER:HA	1:B:64:SER:O	1.99	0.63
1:C:35:SER:HA	1:C:64:SER:O	1.98	0.63
1:A:844:PRO:CG	1:B:632:GLN:HG3	2.29	0.63
1:A:582:SER:HB2	1:A:597:LEU:HB3	1.81	0.63
1:B:561:SER:HB3	1:B:571:LEU:HD23	1.80	0.63
1:B:768:LYS:HD2	1:B:874:ALA:HB2	1.80	0.63
1:A:899:TYR:HE1	1:B:1111:VAL:HB	1.64	0.63
1:C:582:SER:HB2	1:C:597:LEU:HB3	1.81	0.62
1:B:582:SER:HB2	1:B:597:LEU:HB3	1.81	0.62
1:A:35:SER:HA	1:A:64:SER:O	1.98	0.62
1:C:561:SER:HB3	1:C:571:LEU:HD23	1.80	0.62
1:B:91:ALA:HB3	1:B:183:ARG:HB2	1.80	0.62
1:A:561:SER:HB3	1:A:571:LEU:HD23	1.80	0.62
1:C:80:VAL:HG22	1:C:81:ILE:HG13	1.82	0.61
1:A:769:GLN:NE2	1:B:683:ALA:O	2.34	0.61
1:A:91:ALA:HB3	1:A:183:ARG:HB2	1.80	0.61
1:B:844:PRO:HG3	1:C:632:GLN:HG3	1.83	0.61
1:B:80:VAL:HG22	1:B:81:ILE:HG13	1.82	0.61
1:A:899:TYR:CE2	1:B:1110:VAL:HG22	2.35	0.60
1:A:347:ASN:H	1:A:509:THR:HB	1.67	0.60
1:A:80:VAL:HG22	1:A:81:ILE:HG13	1.82	0.60
1:A:422:ALA:HA	1:A:495:ARG:O	2.02	0.60
1:C:422:ALA:HA	1:C:495:ARG:O	2.02	0.60
1:B:347:ASN:H	1:B:509:THR:HB	1.67	0.59
1:A:698:THR:H	1:A:1053:GLN:HB2	1.68	0.59
1:A:550:GLN:HA	1:A:563:ARG:HB3	1.85	0.59
1:B:422:ALA:HA	1:B:495:ARG:O	2.02	0.59
1:C:698:THR:H	1:C:1053:GLN:HB2	1.68	0.59
1:B:899:TYR:CE1	1:C:1111:VAL:HB	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:870:PHE:HA	1:B:874:ALA:HA	1.84	0.59
1:C:347:ASN:H	1:C:509:THR:HB	1.67	0.59
1:B:341:GLU:O	1:B:385:ASP:HA	2.03	0.59
1:B:550:GLN:HA	1:B:563:ARG:HB3	1.85	0.59
1:C:870:PHE:HA	1:C:874:ALA:HA	1.84	0.59
1:A:341:GLU:O	1:A:385:ASP:HA	2.03	0.59
1:B:698:THR:H	1:B:1053:GLN:HB2	1.68	0.59
1:C:341:GLU:O	1:C:385:ASP:HA	2.03	0.59
1:A:745:LEU:HD22	1:A:990:VAL:HG21	1.85	0.58
1:A:771:TYR:CD1	1:B:685:SER:HB3	2.38	0.58
1:A:201:GLN:NE2	1:A:215:THR:OG1	2.37	0.58
1:A:870:PHE:HA	1:A:874:ALA:HA	1.84	0.58
1:C:550:GLN:HA	1:C:563:ARG:HB3	1.85	0.58
1:B:771:TYR:HD1	1:C:685:SER:HB3	1.69	0.58
1:B:745:LEU:HD22	1:B:990:VAL:HG21	1.85	0.58
1:C:745:LEU:HD22	1:C:990:VAL:HG21	1.85	0.58
1:A:632:GLN:HG3	1:C:844:PRO:HG3	1.85	0.57
1:B:201:GLN:NE2	1:B:215:THR:OG1	2.37	0.57
1:C:201:GLN:NE2	1:C:215:THR:OG1	2.37	0.56
1:A:45:GLU:HB2	1:B:549:GLN:NE2	2.21	0.56
1:A:807:LYS:NZ	1:A:923:THR:O	2.38	0.56
1:B:807:LYS:NZ	1:B:923:THR:O	2.38	0.56
1:C:807:LYS:NZ	1:C:923:THR:O	2.38	0.55
1:B:314:VAL:HG22	1:B:528:ASN:HB2	1.89	0.55
1:B:128:CYS:HB3	1:B:161:PHE:HB3	1.89	0.55
1:A:128:CYS:HB3	1:A:161:PHE:HB3	1.89	0.55
1:C:314:VAL:HG22	1:C:528:ASN:HB2	1.89	0.55
1:B:769:GLN:HE22	1:C:683:ALA:C	2.09	0.55
1:A:770:MET:SD	1:B:681:LEU:HB3	2.47	0.55
1:A:314:VAL:HG22	1:A:528:ASN:HB2	1.89	0.55
1:B:424:ASN:ND2	1:B:492:GLN:OE1	2.40	0.55
1:A:1098:THR:HA	1:A:1120:TYR:HB2	1.90	0.54
1:A:551:PHE:O	1:C:46:ILE:HG12	2.08	0.54
1:C:1070:TYR:HA	1:C:1103:PHE:O	2.08	0.54
1:C:128:CYS:HB3	1:C:161:PHE:HB3	1.89	0.54
1:B:127:ALA:HB3	1:B:161:PHE:HB2	1.89	0.54
1:C:1098:THR:HA	1:C:1120:TYR:HB2	1.90	0.54
1:A:228:ILE:HD11	1:B:452:GLU:CD	2.27	0.54
1:C:424:ASN:ND2	1:C:492:GLN:OE1	2.40	0.54
1:B:1070:TYR:HA	1:B:1103:PHE:O	2.07	0.54
1:C:767:VAL:HG12	1:C:769:GLN:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:THR:HB	1:A:422:ALA:HB3	1.90	0.54
1:A:424:ASN:ND2	1:A:492:GLN:OE1	2.40	0.54
1:A:685:SER:HB3	1:C:771:TYR:CD1	2.40	0.54
1:B:1098:THR:HA	1:B:1120:TYR:HB2	1.90	0.54
1:C:363:THR:HB	1:C:422:ALA:HB3	1.90	0.54
1:A:127:ALA:HB3	1:A:161:PHE:HB2	1.89	0.53
1:A:484:TYR:HB2	1:A:487:THR:HG23	1.91	0.53
1:C:127:ALA:HB3	1:C:161:PHE:HB2	1.89	0.53
1:A:1070:TYR:HA	1:A:1103:PHE:O	2.08	0.53
1:B:190:LYS:NZ	1:B:191:ASP:OD2	2.40	0.53
1:B:767:VAL:HG12	1:B:769:GLN:H	1.72	0.53
1:A:692:ASN:HA	1:A:1059:THR:HG22	1.91	0.53
1:B:363:THR:HB	1:B:422:ALA:HB3	1.90	0.53
1:B:692:ASN:HA	1:B:1059:THR:HG22	1.91	0.53
1:A:767:VAL:HG12	1:A:769:GLN:H	1.72	0.53
1:B:540:PRO:HA	1:B:570:ILE:HG22	1.90	0.53
1:C:540:PRO:HA	1:C:570:ILE:HG22	1.90	0.53
1:A:719:ASP:OD2	1:B:306:ARG:NH2	2.42	0.53
1:B:484:TYR:HB2	1:B:487:THR:HG23	1.91	0.53
1:A:1051:PRO:HD2	1:C:872:ALA:HB1	1.90	0.53
1:A:540:PRO:HA	1:A:570:ILE:HG22	1.90	0.53
1:A:879:PRO:HB2	1:A:882:MET:HG2	1.91	0.53
1:C:598:TYR:HB2	1:C:635:CYS:HB2	1.91	0.53
1:C:626:ASN:ND2	1:C:639:ALA:O	2.42	0.53
1:A:1089:ARG:NH1	1:C:868:TRP:HE1	2.07	0.53
1:B:101:TRP:HB2	1:B:116:ILE:HB	1.92	0.52
1:C:484:TYR:HB2	1:C:487:THR:HG23	1.91	0.52
1:C:879:PRO:HB2	1:C:882:MET:HG2	1.91	0.52
1:A:101:TRP:HB2	1:A:116:ILE:HB	1.92	0.52
1:A:190:LYS:NZ	1:A:191:ASP:OD2	2.40	0.52
1:C:921:THR:HG22	1:C:922:THR:HG23	1.91	0.52
1:A:921:THR:HG22	1:A:922:THR:HG23	1.91	0.52
1:B:899:TYR:CZ	1:C:1110:VAL:HG22	2.44	0.52
1:A:549:GLN:HG3	1:C:45:GLU:HB3	1.92	0.52
1:A:626:ASN:ND2	1:A:639:ALA:O	2.42	0.52
1:B:626:ASN:ND2	1:B:639:ALA:O	2.42	0.52
1:C:707:GLU:HB3	1:C:1044:PHE:HB2	1.92	0.52
1:C:692:ASN:HA	1:C:1059:THR:HG22	1.91	0.52
1:A:598:TYR:HB2	1:A:635:CYS:HB2	1.91	0.52
1:A:46:ILE:HG23	1:B:551:PHE:O	2.09	0.52
1:B:598:TYR:HB2	1:B:635:CYS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:921:THR:HG22	1:B:922:THR:HG23	1.91	0.52
1:A:1111:VAL:CG1	1:C:899:TYR:HE1	2.23	0.52
1:B:228:ILE:HD11	1:C:452:GLU:CD	2.29	0.52
1:A:1089:ARG:NH1	1:C:868:TRP:NE1	2.57	0.51
1:B:879:PRO:HB2	1:B:882:MET:HG2	1.91	0.51
1:C:101:TRP:HB2	1:C:116:ILE:HB	1.92	0.51
1:A:707:GLU:HB3	1:A:1044:PHE:HB2	1.92	0.51
1:C:190:LYS:NZ	1:C:191:ASP:OD2	2.40	0.51
1:A:551:PHE:O	1:C:46:ILE:HG23	2.11	0.51
1:C:49:SER:OG	1:C:50:ASP:N	2.45	0.51
1:A:965:ARG:HG3	1:B:369:VAL:HG12	1.94	0.50
1:C:917:GLN:O	1:C:921:THR:OG1	2.26	0.50
1:A:93:GLU:O	1:A:181:HIS:ND1	2.44	0.50
1:A:917:GLN:O	1:A:921:THR:OG1	2.26	0.50
1:A:839:GLY:HA2	1:B:578:PHE:CE2	2.47	0.50
1:A:1059:THR:O	1:A:1080:ASN:ND2	2.39	0.50
1:A:228:ILE:HD11	1:B:452:GLU:OE2	2.11	0.50
1:B:93:GLU:O	1:B:181:HIS:ND1	2.44	0.50
1:C:93:GLU:O	1:C:181:HIS:ND1	2.44	0.50
1:C:564:ASP:HB2	1:C:568:SER:H	1.77	0.50
1:A:879:PRO:HG3	1:B:689:TYR:CE1	2.47	0.50
1:A:306:ARG:NH2	1:C:722:MET:HG3	2.27	0.50
1:A:564:ASP:HB2	1:A:568:SER:H	1.77	0.49
1:A:49:SER:OG	1:A:50:ASP:N	2.45	0.49
1:A:805:PHE:O	1:A:809:THR:OG1	2.22	0.49
1:B:707:GLU:HB3	1:B:1044:PHE:HB2	1.92	0.49
1:C:394:VAL:HG21	1:C:494:TYR:HD2	1.77	0.49
1:B:564:ASP:HB2	1:B:568:SER:H	1.77	0.49
1:A:201:GLN:HB3	1:A:203:ILE:HG12	1.94	0.49
1:B:201:GLN:HB3	1:B:203:ILE:HG12	1.94	0.49
1:B:49:SER:OG	1:B:50:ASP:N	2.44	0.49
1:B:839:GLY:HA2	1:C:578:PHE:CE2	2.47	0.49
1:B:260:THR:OG1	1:B:261:THR:N	2.42	0.49
1:B:394:VAL:HG21	1:B:494:TYR:HD2	1.77	0.49
1:A:38:ARG:HE	1:A:214:ASN:HB2	1.78	0.49
1:A:879:PRO:HG3	1:B:689:TYR:OH	2.12	0.49
1:A:394:VAL:HG21	1:A:494:TYR:HD2	1.77	0.49
1:B:1086:ILE:HG13	1:B:1097:ILE:HD12	1.95	0.49
1:A:1111:VAL:HB	1:C:899:TYR:CD1	2.48	0.48
1:C:1059:THR:O	1:C:1080:ASN:ND2	2.39	0.48
1:B:228:ILE:HD11	1:C:452:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLU:CD	1:B:549:GLN:HE21	2.14	0.48
1:C:805:PHE:O	1:C:809:THR:OG1	2.21	0.48
1:A:695:ALA:HB3	1:C:876:LEU:HA	1.95	0.48
1:C:38:ARG:HE	1:C:214:ASN:HB2	1.78	0.48
1:B:987:GLN:NE2	1:C:988:THR:OG1	2.46	0.48
1:A:844:PRO:CD	1:B:632:GLN:HG3	2.42	0.48
1:C:201:GLN:HB3	1:C:203:ILE:HG12	1.94	0.48
1:A:545:PHE:CE1	1:C:47:PHE:CD1	3.02	0.48
1:B:108:ASN:HA	1:B:131:GLU:HB2	1.96	0.48
1:A:549:GLN:CD	1:C:45:GLU:HB2	2.34	0.48
1:B:917:GLN:O	1:B:921:THR:OG1	2.26	0.48
1:A:310:SER:OG	1:A:523:GLN:NE2	2.47	0.48
1:B:36:SER:O	1:B:63:TYR:CA	2.61	0.48
1:B:310:SER:OG	1:B:523:GLN:NE2	2.47	0.47
1:C:1086:ILE:HG13	1:C:1097:ILE:HD12	1.95	0.47
1:A:385:ASP:O	1:A:497:VAL:HA	2.14	0.47
1:A:646:TYR:HB2	1:A:677:TYR:CZ	2.49	0.47
1:C:108:ASN:HA	1:C:131:GLU:HB2	1.96	0.47
1:A:988:THR:OG1	1:C:987:GLN:NE2	2.46	0.47
1:B:1059:THR:O	1:B:1080:ASN:ND2	2.39	0.47
1:B:38:ARG:HE	1:B:214:ASN:HB2	1.78	0.47
1:A:846:LEU:HA	1:B:653:GLY:O	2.14	0.47
1:A:108:ASN:HA	1:A:131:GLU:HB2	1.96	0.47
1:A:1110:VAL:HG22	1:C:899:TYR:CE2	2.49	0.47
1:B:1031:LEU:HD22	1:B:1049:TYR:HB2	1.97	0.47
1:B:769:GLN:NE2	1:C:683:ALA:O	2.47	0.47
1:A:1031:LEU:HD22	1:A:1049:TYR:HB2	1.96	0.47
1:C:310:SER:OG	1:C:523:GLN:NE2	2.47	0.47
1:C:385:ASP:O	1:C:497:VAL:HA	2.14	0.47
1:C:866:ALA:HA	1:C:877:GLN:H	1.80	0.47
1:A:304:ASN:HA	1:A:580:GLY:HA2	1.97	0.47
1:A:866:ALA:HA	1:A:877:GLN:H	1.80	0.47
1:B:304:ASN:HA	1:B:580:GLY:HA2	1.97	0.47
1:C:304:ASN:HA	1:C:580:GLY:HA2	1.97	0.47
1:C:36:SER:O	1:C:63:TYR:CA	2.61	0.47
1:A:1086:ILE:HG13	1:A:1097:ILE:HD12	1.95	0.47
1:C:646:TYR:HB2	1:C:677:TYR:CZ	2.49	0.47
1:A:36:SER:O	1:A:63:TYR:CA	2.61	0.47
1:B:844:PRO:CG	1:C:632:GLN:HG3	2.44	0.47
1:A:545:PHE:CZ	1:C:47:PHE:CD2	3.03	0.46
1:B:646:TYR:HB2	1:B:677:TYR:CZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:LEU:HD11	1:A:921:THR:HA	1.97	0.46
1:B:118:ASN:HA	1:B:123:VAL:HA	1.98	0.46
1:B:771:TYR:CD1	1:C:685:SER:HB3	2.49	0.46
1:A:899:TYR:HE1	1:B:1111:VAL:CG1	2.29	0.46
1:A:549:GLN:NE2	1:C:45:GLU:CD	2.65	0.46
1:A:118:ASN:HA	1:A:123:VAL:HA	1.98	0.46
1:A:260:THR:OG1	1:A:261:THR:N	2.42	0.46
1:B:385:ASP:O	1:B:497:VAL:HA	2.14	0.46
1:C:118:ASN:HA	1:C:123:VAL:HA	1.98	0.46
1:C:260:THR:OG1	1:C:261:THR:N	2.42	0.46
1:B:397:ILE:HG23	1:B:412:LEU:HD21	1.98	0.46
1:C:1031:LEU:HD22	1:C:1049:TYR:HB2	1.96	0.46
1:A:397:ILE:HG23	1:A:412:LEU:HD21	1.98	0.46
1:C:397:ILE:HG23	1:C:412:LEU:HD21	1.98	0.46
1:B:37:MET:O	1:B:38:ARG:NH1	2.42	0.46
1:B:441:ARG:NH2	1:B:456:SER:O	2.48	0.46
1:B:866:ALA:HA	1:B:877:GLN:H	1.80	0.46
1:C:116:ILE:HG12	1:C:125:ILE:HG12	1.98	0.46
1:B:803:LEU:HD11	1:B:921:THR:HA	1.97	0.46
1:A:552:GLY:O	1:A:560:ASP:N	2.49	0.45
1:A:36:SER:OG	1:A:37:MET:N	2.49	0.45
1:A:945:VAL:HG13	1:B:556:SER:HB3	1.96	0.45
1:C:552:GLY:O	1:C:560:ASP:N	2.49	0.45
1:A:1080:ASN:HA	1:A:1083:SER:H	1.81	0.45
1:B:116:ILE:HG12	1:B:125:ILE:HG12	1.98	0.45
1:B:38:ARG:HG3	1:B:214:ASN:H	1.82	0.45
1:C:37:MET:O	1:C:38:ARG:NH1	2.42	0.45
1:C:36:SER:OG	1:C:37:MET:N	2.49	0.45
1:C:803:LEU:HD11	1:C:921:THR:HA	1.97	0.45
1:A:681:LEU:HB3	1:C:770:MET:SD	2.57	0.45
1:A:116:ILE:HG12	1:A:125:ILE:HG12	1.98	0.45
1:B:388:VAL:HG22	1:B:495:ARG:HG2	1.98	0.45
1:B:552:GLY:O	1:B:560:ASP:N	2.49	0.45
1:C:441:ARG:NH2	1:C:456:SER:O	2.48	0.45
1:A:388:VAL:HG22	1:A:495:ARG:HG2	1.98	0.44
1:C:38:ARG:HG3	1:C:214:ASN:H	1.82	0.44
1:A:345:ILE:HB	1:A:382:VAL:HG23	1.99	0.44
1:A:444:ARG:NH2	1:A:452:GLU:OE2	2.51	0.44
1:B:1080:ASN:HA	1:B:1083:SER:H	1.81	0.44
1:A:899:TYR:CD1	1:B:1111:VAL:HB	2.50	0.44
1:C:38:ARG:HG3	1:C:214:ASN:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:VAL:HG22	1:C:495:ARG:HG2	1.98	0.44
1:C:693:THR:HA	1:C:1057:PHE:O	2.18	0.44
1:A:877:GLN:HG2	1:B:687:ILE:CG2	2.47	0.44
1:C:440:TYR:HB3	1:C:481:TYR:HE1	1.83	0.44
1:A:38:ARG:HG3	1:A:214:ASN:N	2.32	0.44
1:B:693:THR:HA	1:B:1057:PHE:O	2.18	0.44
1:B:804:LEU:HD22	1:B:927:LEU:HD21	1.99	0.44
1:A:987:GLN:NE2	1:B:988:THR:OG1	2.51	0.44
1:B:345:ILE:HB	1:B:382:VAL:HG23	1.99	0.44
1:B:444:ARG:NH2	1:B:452:GLU:OE2	2.51	0.44
1:C:1080:ASN:HA	1:C:1083:SER:H	1.81	0.44
1:C:345:ILE:HB	1:C:382:VAL:HG23	1.99	0.44
1:A:452:GLU:CD	1:C:228:ILE:HD11	2.37	0.44
1:C:1063:ILE:HD11	1:C:1078:VAL:HG21	2.00	0.44
1:C:149:HIS:HD2	1:C:150:THR:HG23	1.83	0.44
1:C:615:LEU:HG	1:C:617:PRO:HD2	2.00	0.44
1:A:45:GLU:HB2	1:B:549:GLN:CD	2.38	0.43
1:A:1071:PHE:HE2	1:C:896:ASN:HA	1.82	0.43
1:A:693:THR:HA	1:A:1057:PHE:O	2.18	0.43
1:B:198:LYS:HE2	1:B:221:LYS:HD3	2.00	0.43
1:A:198:LYS:HE2	1:A:221:LYS:HD3	2.00	0.43
1:A:615:LEU:HG	1:A:617:PRO:HD2	2.00	0.43
1:A:868:TRP:HE1	1:B:1089:ARG:NH1	2.16	0.43
1:A:104:GLY:O	1:A:230:ASN:N	2.42	0.43
1:B:38:ARG:HG3	1:B:214:ASN:N	2.32	0.43
1:B:440:TYR:HB3	1:B:481:TYR:HE1	1.83	0.43
1:C:198:LYS:HE2	1:C:221:LYS:HD3	2.01	0.43
1:C:804:LEU:HD22	1:C:927:LEU:HD21	1.99	0.43
1:B:149:HIS:HD2	1:B:150:THR:HG23	1.83	0.43
1:A:1063:ILE:HD11	1:A:1078:VAL:HG21	2.00	0.43
1:A:38:ARG:HG3	1:A:214:ASN:H	1.82	0.43
1:A:943:THR:CG2	1:C:744:GLN:HE21	2.31	0.43
1:B:615:LEU:HG	1:B:617:PRO:HD2	2.00	0.43
1:B:36:SER:OG	1:B:37:MET:N	2.49	0.43
1:B:45:GLU:OE1	1:C:549:GLN:NE2	2.32	0.43
1:B:527:PHE:O	1:B:533:THR:HA	2.19	0.43
1:B:529:PHE:HE2	1:B:562:VAL:HG21	1.83	0.43
1:A:440:TYR:HB3	1:A:481:TYR:HE1	1.83	0.43
1:A:545:PHE:CE1	1:C:47:PHE:CG	3.07	0.43
1:A:337:VAL:HG12	1:A:409:ASN:HB3	2.01	0.43
1:B:770:MET:SD	1:C:681:LEU:HB3	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:HIS:HD2	1:A:150:THR:HG23	1.83	0.43
1:A:348:CYS:SG	1:A:349:VAL:N	2.92	0.43
1:B:182:LEU:HD23	1:B:201:GLN:HB2	2.01	0.43
1:C:444:ARG:NH2	1:C:452:GLU:OE2	2.51	0.43
1:A:1110:VAL:HG22	1:C:899:TYR:CZ	2.54	0.42
1:A:632:GLN:HG3	1:C:844:PRO:CG	2.48	0.42
1:A:804:LEU:HD22	1:A:927:LEU:HD21	2.00	0.42
1:C:527:PHE:O	1:C:533:THR:HA	2.19	0.42
1:A:529:PHE:HE2	1:A:562:VAL:HG21	1.83	0.42
1:C:348:CYS:SG	1:C:349:VAL:N	2.92	0.42
1:C:529:PHE:HE2	1:C:562:VAL:HG21	1.84	0.42
1:A:182:LEU:HD23	1:A:201:GLN:HB2	2.01	0.42
1:A:90:ALA:HB3	1:A:253:PHE:HB2	2.02	0.42
1:B:348:CYS:SG	1:B:349:VAL:N	2.92	0.42
1:B:899:TYR:CE2	1:C:1110:VAL:HG22	2.54	0.42
1:C:90:ALA:HB3	1:C:253:PHE:HB2	2.02	0.42
1:A:859:LEU:HD23	1:A:859:LEU:HA	1.90	0.42
1:A:959:LEU:HA	1:A:959:LEU:HD23	1.86	0.42
1:A:899:TYR:HE1	1:B:1111:VAL:CB	2.29	0.42
1:A:527:PHE:O	1:A:533:THR:HA	2.19	0.42
1:A:529:PHE:HB2	1:A:532:LEU:HB3	2.02	0.42
1:B:1063:ILE:HD11	1:B:1078:VAL:HG21	2.00	0.42
1:C:182:LEU:HD23	1:C:201:GLN:HB2	2.01	0.42
1:C:529:PHE:HB2	1:C:532:LEU:HB3	2.02	0.42
1:A:265:LYS:HD3	1:A:293:PHE:HE2	1.85	0.42
1:B:325:PHE:HE1	1:B:345:ILE:HD13	1.85	0.42
1:C:124:VAL:HG13	1:C:163:TYR:HE1	1.85	0.42
1:C:337:VAL:HG12	1:C:409:ASN:HB3	2.01	0.42
1:B:529:PHE:HB2	1:B:532:LEU:HB3	2.02	0.42
1:C:325:PHE:HE1	1:C:345:ILE:HD13	1.85	0.42
1:C:182:LEU:HB3	1:C:201:GLN:O	2.20	0.42
1:C:265:LYS:HD3	1:C:293:PHE:HE2	1.85	0.42
1:A:101:TRP:O	1:A:115:ILE:HA	2.20	0.41
1:A:182:LEU:HB3	1:A:201:GLN:O	2.20	0.41
1:A:549:GLN:HG3	1:C:45:GLU:CB	2.50	0.41
1:B:101:TRP:O	1:B:115:ILE:HA	2.20	0.41
1:B:118:ASN:HD21	1:B:121:THR:HA	1.85	0.41
1:A:118:ASN:HD21	1:A:121:THR:HA	1.85	0.41
1:B:182:LEU:HB3	1:B:201:GLN:O	2.20	0.41
1:B:90:ALA:HB3	1:B:253:PHE:HB2	2.02	0.41
1:B:265:LYS:HD3	1:B:293:PHE:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASP:OD1	1:A:268:GLU:N	2.53	0.41
1:B:124:VAL:HG13	1:B:163:TYR:HE1	1.85	0.41
1:B:335:PRO:HG3	1:B:341:GLU:HG2	2.03	0.41
1:A:286:LEU:HG	1:A:295:ILE:HD13	2.02	0.41
1:B:337:VAL:HG12	1:B:409:ASN:HB3	2.01	0.41
1:B:45:GLU:HB2	1:C:549:GLN:NE2	2.35	0.41
1:C:805:PHE:O	1:C:809:THR:CB	2.69	0.41
1:A:325:PHE:HE1	1:A:345:ILE:HD13	1.85	0.41
1:B:1076:VAL:HB	1:B:1088:GLN:HA	2.02	0.41
1:B:267:ASP:OD1	1:B:268:GLU:N	2.53	0.41
1:C:267:ASP:OD1	1:C:268:GLU:N	2.53	0.41
1:C:286:LEU:HG	1:C:295:ILE:HD13	2.02	0.41
1:A:1076:VAL:HB	1:A:1088:GLN:HA	2.02	0.41
1:A:335:PRO:HG3	1:A:341:GLU:HG2	2.03	0.41
1:B:286:LEU:HG	1:B:295:ILE:HD13	2.02	0.41
1:C:101:TRP:O	1:C:115:ILE:HA	2.20	0.41
1:C:292:SER:OG	1:C:293:PHE:N	2.53	0.41
1:A:124:VAL:HG13	1:A:163:TYR:HE1	1.85	0.41
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.90	0.41
1:A:632:GLN:HG3	1:C:844:PRO:CD	2.50	0.41
1:A:943:THR:HG22	1:C:744:GLN:HE21	1.85	0.41
1:B:292:SER:OG	1:B:293:PHE:N	2.54	0.41
1:B:805:PHE:O	1:B:809:THR:OG1	2.22	0.41
1:A:945:VAL:CG1	1:B:556:SER:HB3	2.51	0.41
1:B:650:ILE:O	1:B:657:CYS:HA	2.21	0.41
1:A:805:PHE:O	1:A:809:THR:CB	2.69	0.41
1:B:805:PHE:O	1:B:809:THR:CB	2.69	0.41
1:C:335:PRO:HG3	1:C:341:GLU:HG2	2.03	0.41
1:C:650:ILE:O	1:C:657:CYS:HA	2.21	0.41
1:A:1080:ASN:OD1	1:A:1083:SER:N	2.54	0.41
1:A:604:THR:O	1:A:608:THR:OG1	2.30	0.41
1:B:859:LEU:HD23	1:B:859:LEU:HA	1.90	0.41
1:C:1080:ASN:OD1	1:C:1083:SER:N	2.54	0.41
1:A:545:PHE:CD1	1:C:47:PHE:CD1	3.09	0.41
1:C:959:LEU:HD23	1:C:959:LEU:HA	1.86	0.41
1:B:104:GLY:O	1:B:230:ASN:N	2.42	0.41
1:C:1076:VAL:HB	1:C:1088:GLN:HA	2.02	0.41
1:C:98:VAL:HG13	1:C:236:THR:HA	2.03	0.41
1:B:1080:ASN:OD1	1:B:1083:SER:N	2.54	0.40
1:B:537:VAL:O	1:B:572:ASP:HA	2.22	0.40
1:B:98:VAL:HG13	1:B:236:THR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:PHE:CE1	1:C:47:PHE:CE1	3.09	0.40
1:A:37:MET:O	1:A:38:ARG:NH1	2.42	0.40
1:A:411:LYS:HB2	1:A:448:LEU:HB2	2.03	0.40
1:B:337:VAL:HG22	1:B:387:PHE:HB2	2.04	0.40
1:C:118:ASN:HD21	1:C:121:THR:HA	1.85	0.40
1:C:411:LYS:HB2	1:C:448:LEU:HB2	2.03	0.40
1:B:299:ILE:HD13	1:B:584:ILE:HG12	2.04	0.40
1:B:411:LYS:HB2	1:B:448:LEU:HB2	2.03	0.40
1:C:350:ALA:N	1:C:511:CYS:O	2.51	0.40
1:C:299:ILE:HD13	1:C:584:ILE:HG12	2.04	0.40
1:A:337:VAL:HG22	1:A:387:PHE:HB2	2.04	0.40
1:A:537:VAL:O	1:A:572:ASP:HA	2.22	0.40
1:A:887:ARG:HB2	1:A:1031:LEU:HD12	2.04	0.40
1:C:181:HIS:CE1	1:C:183:ARG:HG2	2.56	0.40
1:A:628:VAL:HB	1:A:636:LEU:HB3	2.04	0.40
1:B:597:LEU:HD12	1:B:597:LEU:HA	1.85	0.40
1:B:879:PRO:HG3	1:C:689:TYR:OH	2.22	0.40
1:C:699:ASN:HD21	1:C:904:GLN:HE22	1.68	0.40
1:A:1111:VAL:HG12	1:C:899:TYR:HE1	1.86	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	1008/1203 (84%)	859 (85%)	146 (14%)	3 (0%)	44	81
1	B	1008/1203 (84%)	858 (85%)	147 (15%)	3 (0%)	44	81
1	C	1008/1203 (84%)	858 (85%)	147 (15%)	3 (0%)	44	81
All	All	3024/3609 (84%)	2575 (85%)	440 (15%)	9 (0%)	48	81

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	549	GLN
1	B	549	GLN
1	C	549	GLN
1	A	1092	PHE
1	B	1092	PHE
1	C	1092	PHE
1	A	574	SER
1	B	574	SER
1	C	574	SER

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	881/1047 (84%)	876 (99%)	5 (1%)	89	95
1	B	881/1047 (84%)	876 (99%)	5 (1%)	89	95
1	C	881/1047 (84%)	876 (99%)	5 (1%)	89	95
All	All	2643/3141 (84%)	2628 (99%)	15 (1%)	89	95

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	323	CYS
1	A	333	LYS
1	A	563	ARG
1	A	889	ASN
1	B	214	ASN
1	B	323	CYS
1	B	333	LYS
1	B	563	ARG
1	B	889	ASN
1	C	214	ASN
1	C	323	CYS
1	C	333	LYS
1	C	563	ARG

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Mol	Chain	Res	Type
1	C	889	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	149	HIS
1	A	201	GLN
1	A	214	ASN
1	A	409	ASN
1	A	435	ASN
1	A	437	ASN
1	A	523	GLN
1	A	744	GLN
1	A	759	ASN
1	A	769	GLN
1	A	818	GLN
1	A	889	ASN
1	A	904	GLN
1	A	987	GLN
1	A	1046	HIS
1	B	129	ASN
1	B	149	HIS
1	B	201	GLN
1	B	214	ASN
1	B	409	ASN
1	B	435	ASN
1	B	437	ASN
1	B	523	GLN
1	B	744	GLN
1	B	759	ASN
1	B	769	GLN
1	B	889	ASN
1	B	904	GLN
1	B	987	GLN
1	B	1046	HIS
1	C	129	ASN
1	C	149	HIS
1	C	201	GLN
1	C	214	ASN
1	C	409	ASN
1	C	435	ASN

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Mol	Chain	Res	Type
1	C	437	ASN
1	C	523	GLN
1	C	744	GLN
1	C	769	GLN
1	C	889	ASN
1	C	904	GLN
1	C	987	GLN
1	C	1046	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.