Full wwPDB EM Model Validation Report

Feb 22, 2020 – 05:07 AM EST

PDB ID	:	6VSB
EMDB ID	:	EMD-21375
Title	:	Prefusion 2019-nCoV spike glycoprotein with a single receptor-binding domain up
Authors	:	Wrapp, D.; Wang, N.; Corbett, K.S.; Goldsmith, J.A.; Hsieh, C.; Abiona, O.; Graham, B.S.; McLellan, J.S.
Deposited on	:	2020-02-10
Resolution	:	3.46 Å(reported)

This is a Full wwPDB EM 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
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

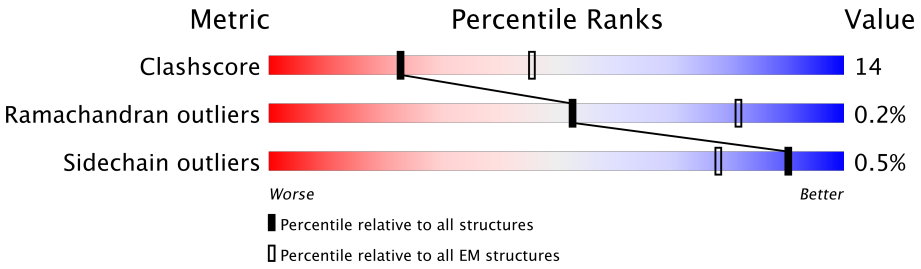
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.8

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 3.46 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1288	54% 20% 26%
1	B	1288	53% 22% 24%
1	C	1288	54% 21% 24%

2 Entry composition

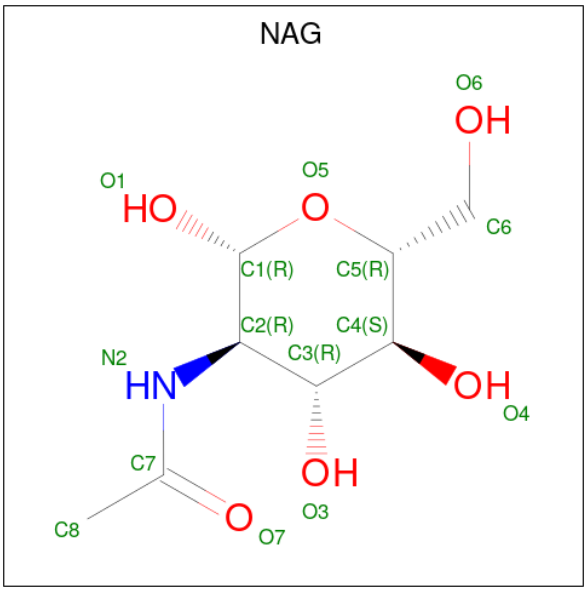
There are 2 unique types of molecules in this entry. The entry contains 22854 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	959	Total	C	N	O	S	0	0
			7311	4675	1215	1388	33		
1	B	973	Total	C	N	O	S	0	0
			7362	4704	1223	1401	34		
1	C	973	Total	C	N	O	S	0	0
			7327	4684	1213	1396	34		

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			266	152	19	95	
2	A	1	Total	C	N	O	0
			266	152	19	95	
2	A	1	Total	C	N	O	0
			266	152	19	95	
2	A	1	Total	C	N	O	0
			266	152	19	95	

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Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	A	1	Total C N O 266 152 19 95	0
2	B	1	Total C N O 294 168 21 105	0
2	B	1	Total C N O 294 168 21 105	0
2	B	1	Total C N O 294 168 21 105	0
2	B	1	Total C N O 294 168 21 105	0
2	B	1	Total C N O 294 168 21 105	0
2	B	1	Total C N O 294 168 21 105	0

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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	B	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0

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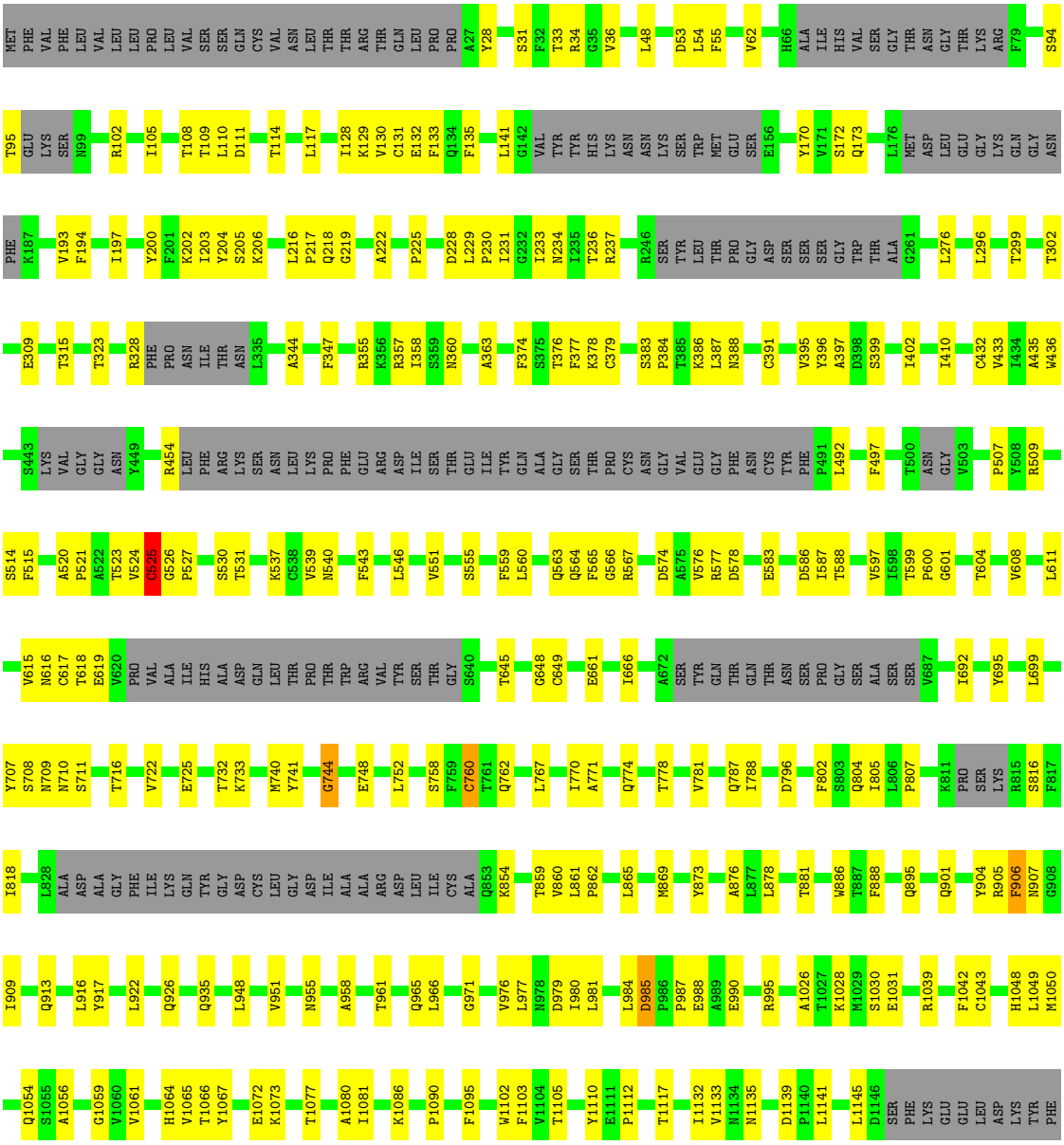
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0
2	C	1	Total 294	C 168	N 21	O 105	0

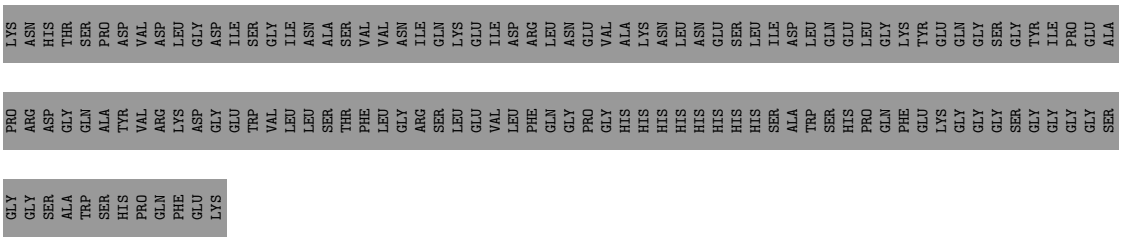
3 Residue-property plots (i)

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: Spike glycoprotein

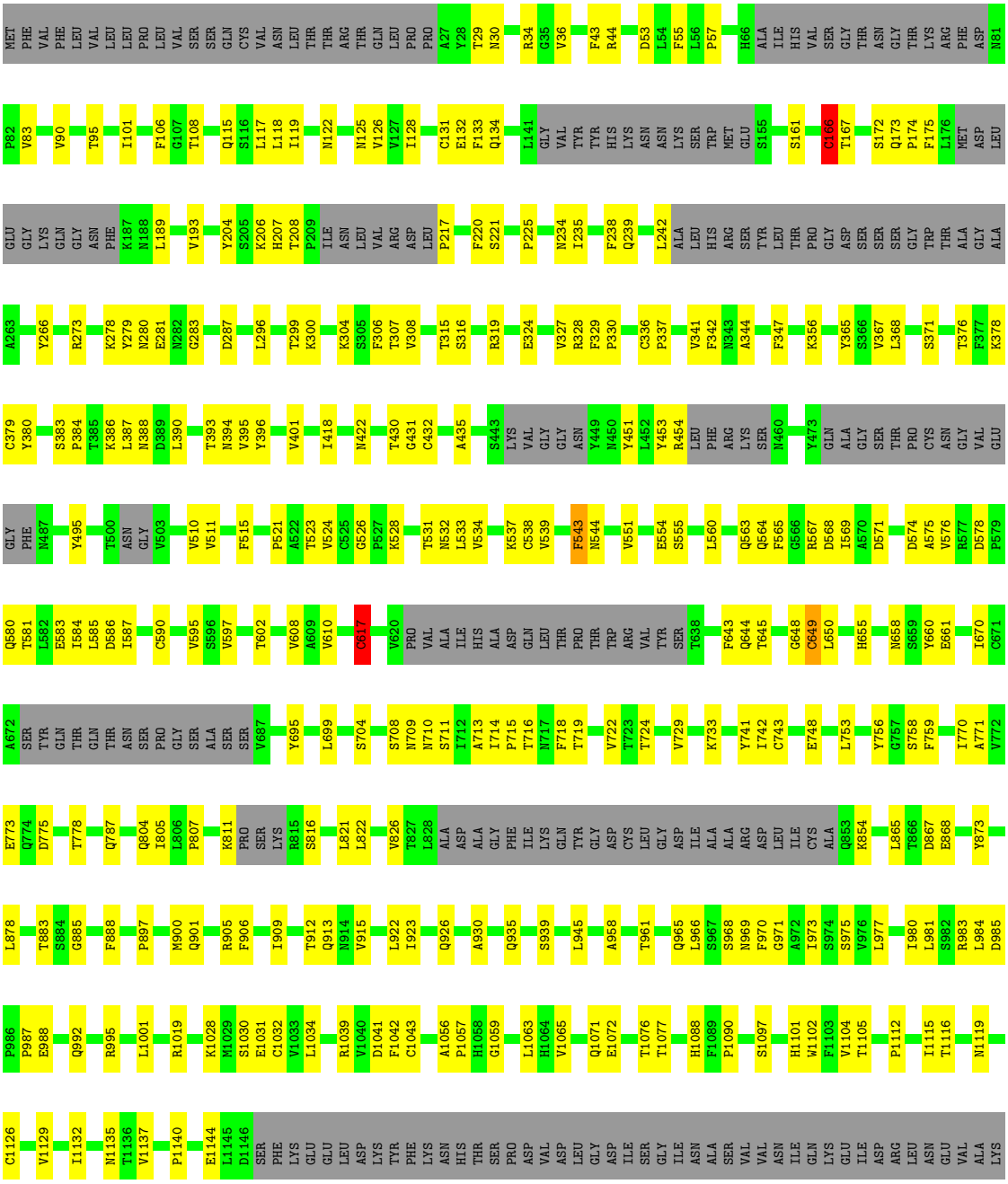
Chain A:

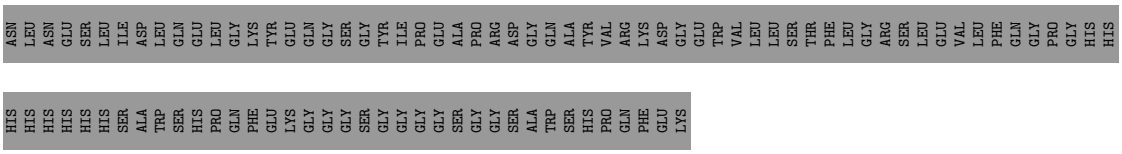




• Molecule 1: Spike glycoprotein

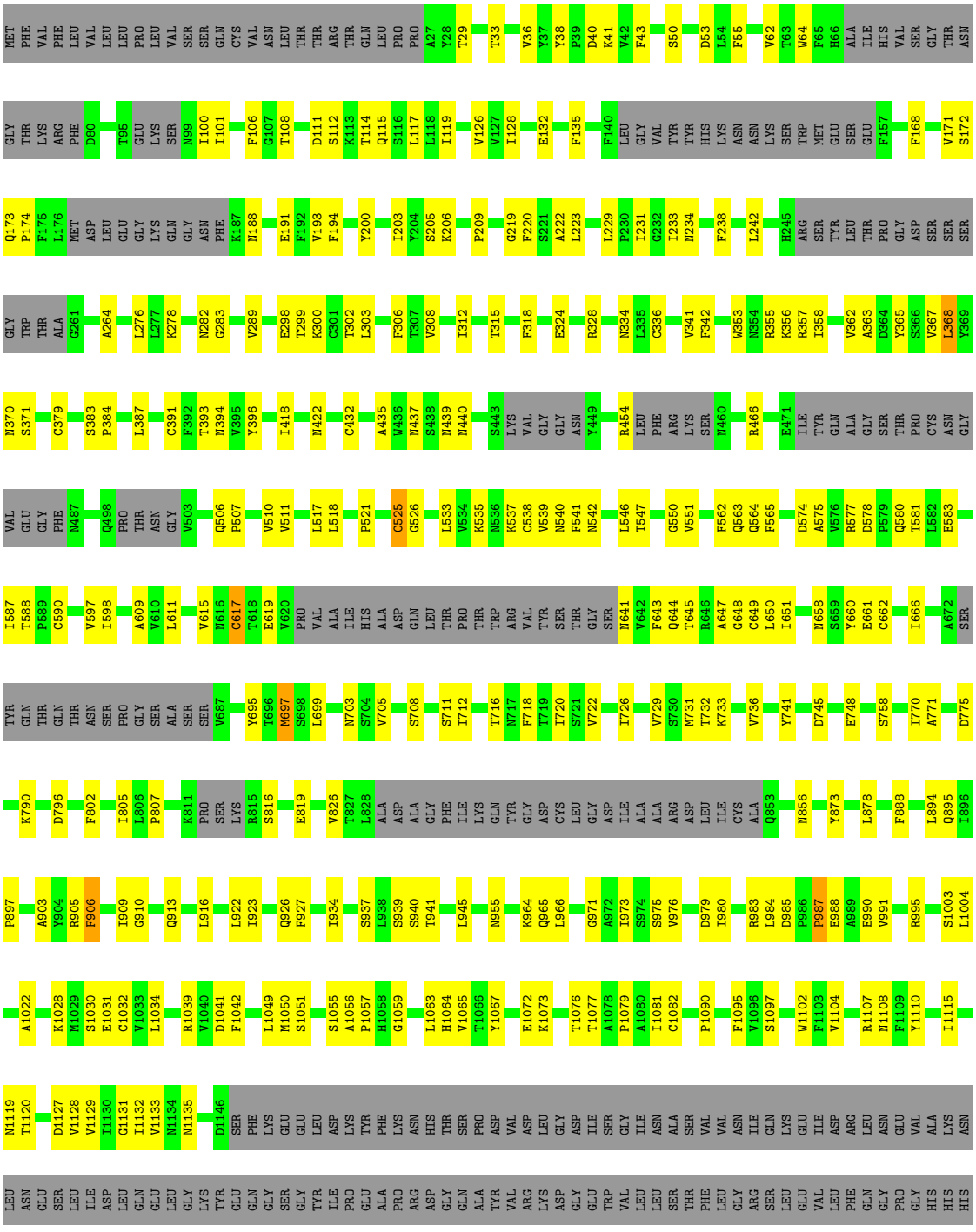
Chain B:





• Molecule 1: Spike glycoprotein

Chain C:



HIS HIS HIS HIS HIS SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	120001	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 ($e^-/Å^2$)	37.8	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	1/7467 (0.0%)	0.54	1/10174 (0.0%)
1	B	0.31	3/7519 (0.0%)	0.54	3/10249 (0.0%)
1	C	0.29	0/7482	0.55	4/10207 (0.0%)
All	All	0.31	4/22468 (0.0%)	0.55	8/30630 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	CYS	CB-SG	-5.99	1.72	1.81
1	B	617	CYS	CB-SG	-5.70	1.72	1.81
1	A	760	CYS	CB-SG	-5.49	1.72	1.81
1	B	649	CYS	CB-SG	-5.37	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	525	CYS	CA-CB-SG	7.48	127.47	114.00
1	B	166	CYS	CA-CB-SG	6.60	125.88	114.00
1	C	1032	CYS	CA-CB-SG	-5.87	103.43	114.00
1	B	1032	CYS	CA-CB-SG	-5.57	103.98	114.00
1	C	697	MET	CA-CB-CG	5.28	122.27	113.30
1	C	697	MET	CB-CG-SD	-5.12	97.03	112.40
1	B	1043	CYS	CA-CB-SG	-5.06	104.89	114.00
1	C	368	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	7311	0	7003	207	0
1	B	7362	0	6991	210	0
1	C	7327	0	6943	205	0
2	A	266	0	242	13	0
2	B	294	0	267	13	0
2	C	294	0	267	13	0
All	All	22854	0	21713	603	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (603) 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)
2:C:1311:NAG:H82	2:C:1311:NAG:H3	1.46	0.96
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.55	0.89
1:B:342:PHE:HB3	2:B:1315:NAG:H83	1.56	0.86
1:A:1103:PHE:HZ	2:A:1311:NAG:H61	1.40	0.86
1:B:1072:GLU:N	1:B:1072:GLU:OE1	2.10	0.84
1:A:895:GLN:HE22	2:C:1305:NAG:HN2	1.25	0.84
1:C:895:GLN:N	1:C:895:GLN:OE1	2.15	0.79
1:A:599:THR:HG22	1:A:601:GLY:H	1.48	0.78
1:B:965:GLN:HE22	1:C:758:SER:H	1.31	0.78
1:A:971:GLY:HA3	1:A:995:ARG:HH21	1.49	0.78
1:A:128:ILE:HD13	1:A:229:LEU:HD21	1.66	0.77
1:A:725:GLU:OE2	1:A:1028:LYS:NZ	2.16	0.77
2:A:1310:NAG:H3	2:A:1310:NAG:H83	1.66	0.76
1:B:126:VAL:HG13	1:B:174:PRO:HA	1.66	0.76
1:A:560:LEU:HB2	1:A:563:GLN:HE22	1.49	0.76
1:B:342:PHE:HB3	2:B:1315:NAG:C8	2.15	0.76
1:A:1103:PHE:CZ	2:A:1311:NAG:H61	2.20	0.75
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.67	0.74
1:A:1090:PRO:O	1:B:913:GLN:NE2	2.21	0.74
2:B:1306:NAG:O7	2:B:1306:NAG:O3	2.05	0.72
2:A:1310:NAG:C1	2:A:1310:NAG:H82	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:THR:HA	1:A:302:THR:HG22	1.70	0.72
1:B:57:PRO:HG3	1:B:273:ARG:HD2	1.71	0.72
2:C:1311:NAG:C8	2:C:1311:NAG:H3	2.20	0.71
1:A:604:THR:HA	2:A:1301:NAG:H82	1.73	0.71
1:A:363:ALA:O	1:A:526:GLY:HA2	1.90	0.71
1:B:328:ARG:HH12	1:B:533:LEU:HD22	1.55	0.71
1:A:965:GLN:HE22	1:B:758:SER:H	1.39	0.71
1:A:197:ILE:HD11	1:A:202:LYS:HD2	1.71	0.71
1:A:578:ASP:OD1	1:A:583:GLU:N	2.14	0.71
1:C:303:LEU:HD23	1:C:308:VAL:HG12	1.71	0.70
2:C:1304:NAG:H82	2:C:1304:NAG:H3	1.74	0.70
1:C:367:VAL:HG23	1:C:368:LEU:HD12	1.74	0.70
1:A:722:VAL:HG12	1:A:1065:VAL:HG22	1.73	0.69
1:A:391:CYS:CA	1:A:525:CYS:HB3	2.21	0.69
2:B:1305:NAG:H62	2:B:1306:NAG:HN2	1.57	0.69
1:B:341:VAL:HG22	1:B:356:LYS:HD2	1.73	0.69
1:B:708:SER:OG	1:B:710:ASN:OD1	2.09	0.69
1:C:805:ILE:HD12	1:C:878:LEU:HD11	1.75	0.69
1:B:1105:THR:HG22	1:B:1112:PRO:HA	1.74	0.69
1:C:906:PHE:HD2	1:C:916:LEU:HB2	1.58	0.69
1:A:708:SER:OG	1:A:710:ASN:OD1	2.09	0.69
1:B:319:ARG:NH2	1:C:745:ASP:OD2	2.26	0.69
2:B:1315:NAG:H3	2:B:1315:NAG:O7	1.92	0.68
1:C:365:TYR:HD2	1:C:387:LEU:HB3	1.58	0.68
1:B:578:ASP:OD1	1:B:583:GLU:N	2.27	0.68
1:B:821:LEU:HD11	1:B:939:SER:HB3	1.75	0.68
1:A:732:THR:OG1	1:A:955:ASN:ND2	2.27	0.68
1:B:1116:THR:H	1:B:1119:ASN:HD21	1.41	0.68
1:B:376:THR:OG1	1:B:378:LYS:NZ	2.24	0.68
1:A:395:VAL:HG23	1:A:524:VAL:HG21	1.76	0.67
1:B:299:THR:HG22	1:B:315:THR:HG21	1.76	0.67
1:C:191:GLU:HG3	1:C:223:LEU:HD11	1.76	0.67
2:A:1310:NAG:C8	2:A:1310:NAG:H3	2.24	0.67
1:A:388:ASN:HB2	1:A:527:PRO:HD2	1.75	0.66
1:C:1082:CYS:HB2	1:C:1132:ILE:HD12	1.75	0.66
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	1.76	0.66
1:A:645:THR:OG1	1:A:648:GLY:O	2.11	0.66
1:A:105:ILE:HG22	1:A:110:LEU:HD22	1.76	0.66
1:C:126:VAL:HG13	1:C:174:PRO:HA	1.78	0.66
1:B:742:ILE:HD11	1:B:753:LEU:HD22	1.76	0.66
1:A:33:THR:OG1	1:A:219:GLY:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:TYR:HD2	1:B:883:THR:HG23	1.62	0.65
1:A:1043:CYS:HB2	1:A:1048:HIS:HD2	1.62	0.65
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.30	0.65
1:A:906:PHE:O	1:A:909:ILE:HG12	1.97	0.65
1:C:1050:MET:HG2	1:C:1065:VAL:HB	1.79	0.65
1:A:878:LEU:HA	1:A:881:THR:HG22	1.80	0.64
1:C:318:PHE:HZ	1:C:615:VAL:HG21	1.62	0.64
1:B:804:GLN:OE1	1:B:935:GLN:NE2	2.30	0.64
1:C:106:PHE:HD1	1:C:238:PHE:HB2	1.63	0.64
1:A:1050:MET:HG2	1:A:1065:VAL:HB	1.78	0.64
1:C:658:ASN:ND2	1:C:660:TYR:OH	2.31	0.64
1:A:1039:ARG:HB2	1:B:1031:GLU:HG2	1.80	0.64
1:B:575:ALA:HB1	1:B:584:ILE:HD11	1.80	0.64
1:C:363:ALA:O	1:C:526:GLY:HA2	1.98	0.64
1:B:716:THR:OG1	1:B:1071:GLN:O	2.14	0.64
1:C:334:ASN:O	1:C:362:VAL:N	2.24	0.64
1:A:108:THR:O	1:A:237:ARG:NH1	2.32	0.63
1:B:722:VAL:HG12	1:B:1065:VAL:HG22	1.81	0.63
1:C:328:ARG:HH21	1:C:580:GLN:HB2	1.63	0.63
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.80	0.63
1:B:1039:ARG:HB2	1:C:1031:GLU:HG2	1.80	0.63
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.63	0.63
1:B:565:PHE:HB3	1:B:576:VAL:HG13	1.80	0.62
1:C:732:THR:OG1	1:C:955:ASN:ND2	2.32	0.62
1:C:299:THR:HG22	1:C:315:THR:HG21	1.80	0.62
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.81	0.62
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.63	0.62
1:B:826:VAL:HG21	1:B:1057:PRO:HG2	1.82	0.62
1:A:328:ARG:NH2	1:A:531:THR:O	2.32	0.62
1:C:521:PRO:HB3	1:C:564:GLN:HG3	1.80	0.62
1:A:564:GLN:OE1	1:A:577:ARG:NH2	2.33	0.61
1:A:216:LEU:HD12	1:A:217:PRO:HD2	1.80	0.61
1:B:1072:GLU:HG3	1:C:894:LEU:HD22	1.83	0.61
1:B:324:GLU:OE1	1:B:537:LYS:NZ	2.30	0.61
1:C:108:THR:OG1	1:C:234:ASN:O	2.19	0.61
1:A:977:LEU:HD12	1:A:980:ILE:HD11	1.83	0.61
1:A:543:PHE:HZ	1:A:577:ARG:O	1.83	0.61
1:B:393:THR:O	1:B:523:THR:OG1	2.19	0.61
1:B:586:ASP:OD1	1:B:587:ILE:N	2.34	0.61
1:A:984:LEU:HD22	1:A:988:GLU:HG3	1.83	0.60
1:B:977:LEU:HD12	1:B:980:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:PRO:HD3	1:A:1095:PHE:HE1	1.66	0.60
1:A:1105:THR:HG22	1:A:1112:PRO:HA	1.81	0.60
1:A:565:PHE:HB2	1:A:576:VAL:HG12	1.82	0.60
1:A:1043:CYS:HB2	1:A:1048:HIS:CD2	2.37	0.60
1:B:119:ILE:HG12	1:B:128:ILE:HG23	1.83	0.60
1:B:543:PHE:CZ	1:B:578:ASP:HA	2.37	0.60
1:B:645:THR:HG22	1:B:648:GLY:O	2.00	0.60
1:C:966:LEU:O	1:C:975:SER:OG	2.19	0.60
1:B:574:ASP:O	1:B:587:ILE:N	2.28	0.60
1:C:903:ALA:HB1	1:C:913:GLN:HB2	1.84	0.60
1:C:542:ASN:HA	1:C:546:LEU:O	2.02	0.60
1:C:988:GLU:O	1:C:991:VAL:HG12	2.01	0.60
1:A:802:PHE:CD1	1:A:805:ILE:HD11	2.37	0.59
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.50	0.59
1:B:578:ASP:OD2	1:B:581:THR:HB	2.03	0.59
1:C:117:LEU:HD11	1:C:231:ILE:HG21	1.84	0.59
1:C:299:THR:HG21	1:C:597:VAL:HG21	1.85	0.58
1:C:564:GLN:HA	1:C:577:ARG:HG2	1.85	0.58
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.26	0.58
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.36	0.58
1:B:521:PRO:HB3	1:B:564:GLN:HE21	1.68	0.58
1:C:888:PHE:CZ	1:C:1034:LEU:HG	2.38	0.58
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.38	0.58
1:B:906:PHE:O	1:B:909:ILE:HG12	2.04	0.58
1:B:1116:THR:H	1:B:1119:ASN:ND2	2.01	0.58
1:C:748:GLU:OE2	1:C:748:GLU:N	2.35	0.57
1:A:985:ASP:N	1:C:383:SER:OG	2.36	0.57
1:A:699:LEU:HD12	1:B:873:TYR:CZ	2.40	0.57
1:A:907:ASN:HD22	1:A:913:GLN:HG3	1.69	0.57
1:A:328:ARG:HB2	1:A:543:PHE:HA	1.85	0.57
1:B:722:VAL:HG22	1:B:930:ALA:HB1	1.86	0.57
1:A:1056:ALA:HB3	1:A:1059:GLY:O	2.05	0.57
1:A:560:LEU:HB2	1:A:563:GLN:NE2	2.20	0.57
1:B:29:THR:HG22	1:B:30:ASN:H	1.70	0.57
2:C:1306:NAG:H83	2:C:1306:NAG:H3	1.86	0.57
1:B:1056:ALA:HB3	1:B:1059:GLY:O	2.05	0.57
1:B:569:ILE:HD11	1:C:964:LYS:HD3	1.86	0.57
1:B:867:ASP:OD1	1:B:868:GLU:N	2.38	0.57
1:B:83:VAL:HA	1:B:239:GLN:HB2	1.85	0.56
1:C:720:ILE:HD11	1:C:927:PHE:HB2	1.87	0.56
1:B:418:ILE:HA	1:B:422:ASN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:CYS:HA	1:C:432:CYS:HA	1.87	0.56
1:B:1140:PRO:O	1:B:1144:GLU:HG2	2.05	0.56
1:A:53:ASP:OD1	1:A:54:LEU:N	2.35	0.56
1:A:586:ASP:OD1	1:A:587:ILE:N	2.38	0.56
1:A:987:PRO:O	1:A:990:GLU:HG3	2.06	0.56
2:C:1307:NAG:H61	2:C:1308:NAG:HN2	1.69	0.56
1:A:193:VAL:HB	1:A:204:TYR:HB2	1.86	0.56
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.86	0.56
1:A:296:LEU:HB2	1:A:608:VAL:HG21	1.88	0.56
1:A:31:SER:HA	1:A:216:LEU:HD23	1.87	0.56
1:A:34:ARG:NH2	1:A:218:GLN:O	2.38	0.55
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.41	0.55
1:A:1103:PHE:HZ	2:A:1311:NAG:C6	2.15	0.55
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.71	0.55
1:A:117:LEU:HG	1:A:130:VAL:HG22	1.88	0.55
1:C:643:PHE:O	1:C:650:LEU:N	2.38	0.55
1:B:280:ASN:OD1	1:B:281:GLU:N	2.38	0.55
1:B:709:ASN:HA	1:C:897:PRO:HB3	1.88	0.55
2:C:1315:NAG:H83	2:C:1315:NAG:H3	1.87	0.55
1:C:50:SER:HA	1:C:276:LEU:HA	1.88	0.55
1:C:905:ARG:HD3	1:C:1049:LEU:O	2.07	0.55
1:A:108:THR:HA	1:A:236:THR:HG22	1.89	0.55
1:A:299:THR:HG21	1:A:597:VAL:HG21	1.89	0.55
1:B:756:TYR:HB3	1:B:759:PHE:CD2	2.41	0.55
1:C:33:THR:OG1	1:C:219:GLY:O	2.23	0.55
1:A:904:TYR:HB2	1:C:1107:ARG:NH1	2.22	0.55
2:C:1311:NAG:C8	2:C:1311:NAG:C3	2.86	0.54
2:A:1318:NAG:H83	2:A:1318:NAG:H3	1.89	0.54
1:A:218:GLN:HG2	1:A:219:GLY:H	1.72	0.54
1:C:188:ASN:HA	1:C:209:PRO:HA	1.87	0.54
1:B:394:ASN:ND2	1:B:396:TYR:OH	2.40	0.54
1:B:521:PRO:HB3	1:B:564:GLN:NE2	2.23	0.54
1:A:172:SER:OG	1:A:173:GLN:N	2.41	0.54
1:B:704:SER:HB2	1:C:790:LYS:HB3	1.88	0.54
1:C:708:SER:HB2	1:C:711:SER:HB3	1.88	0.54
1:A:358:ILE:N	1:A:395:VAL:O	2.37	0.54
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.40	0.54
1:B:431:GLY:HA3	1:B:515:PHE:CD1	2.43	0.54
1:C:353:TRP:O	1:C:466:ARG:NH1	2.40	0.54
1:C:619:GLU:OE1	1:C:619:GLU:N	2.40	0.54
1:A:574:ASP:O	1:A:587:ILE:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ASN:H	1:C:362:VAL:HG23	1.73	0.53
1:A:53:ASP:HB3	1:A:55:PHE:CE1	2.43	0.53
1:A:922:LEU:HD11	1:A:926:GLN:HE21	1.73	0.53
1:A:948:LEU:O	1:A:951:VAL:HG12	2.07	0.53
1:C:517:LEU:HG	1:C:518:LEU:HD23	1.90	0.53
1:B:342:PHE:HE1	1:B:511:VAL:HG11	1.74	0.53
1:A:299:THR:HG22	1:A:315:THR:HB	1.91	0.53
1:A:616:ASN:OD1	1:A:618:THR:HG23	2.08	0.53
1:A:854:LYS:HD3	1:A:860:VAL:HG23	1.91	0.53
1:C:819:GLU:HG2	1:C:1055:SER:HB3	1.91	0.53
1:C:598:ILE:HB	1:C:609:ALA:HB3	1.91	0.53
1:B:172:SER:OG	1:B:173:GLN:N	2.42	0.53
1:B:532:ASN:OD1	1:B:533:LEU:N	2.42	0.53
1:B:36:VAL:HG21	1:B:220:PHE:HE1	1.74	0.53
1:A:543:PHE:HB3	1:A:546:LEU:HB2	1.91	0.53
2:B:1306:NAG:C7	2:B:1306:NAG:HO3	2.15	0.53
1:C:341:VAL:HG22	1:C:356:LYS:HD3	1.90	0.53
1:B:965:GLN:NE2	1:C:758:SER:H	2.01	0.53
1:A:230:PRO:HG3	1:C:357:ARG:HH12	1.73	0.52
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.38	0.52
1:A:229:LEU:HB3	1:A:231:ILE:HD11	1.90	0.52
1:A:383:SER:OG	1:A:386:LYS:NZ	2.41	0.52
1:B:971:GLY:HA3	1:B:995:ARG:HH21	1.73	0.52
1:C:342:PHE:CE2	1:C:511:VAL:HG11	2.45	0.52
1:A:905:ARG:HD3	1:A:1049:LEU:O	2.10	0.52
1:B:108:THR:OG1	1:B:234:ASN:O	2.22	0.52
1:B:336:CYS:SG	1:B:337:PRO:HD2	2.49	0.52
1:B:365:TYR:HD1	1:B:368:LEU:HD21	1.73	0.52
1:B:742:ILE:HG13	1:B:743:CYS:N	2.24	0.52
1:B:748:GLU:H	1:B:748:GLU:CD	2.12	0.52
2:A:1308:NAG:O7	2:A:1308:NAG:H3	2.08	0.52
1:A:611:LEU:HD22	1:A:666:ILE:HG23	1.90	0.52
1:C:1056:ALA:HB3	1:C:1059:GLY:O	2.09	0.52
1:C:172:SER:OG	1:C:173:GLN:N	2.43	0.52
1:A:873:TYR:CZ	1:C:699:LEU:HD12	2.45	0.52
1:A:709:ASN:OD1	1:A:709:ASN:N	2.35	0.52
1:C:644:GLN:NE2	1:C:649:CYS:HB2	2.25	0.52
1:C:36:VAL:HG11	1:C:220:PHE:CZ	2.44	0.52
1:B:922:LEU:HD11	1:B:926:GLN:HE21	1.75	0.52
1:C:299:THR:CG2	1:C:597:VAL:HG21	2.39	0.52
1:C:987:PRO:O	1:C:990:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:973:ILE:N	1:B:992:GLN:OE1	2.34	0.51
1:A:895:GLN:NE2	2:C:1305:NAG:HN2	2.03	0.51
1:C:976:VAL:HG13	1:C:979:ASP:HB2	1.92	0.51
1:B:299:THR:CG2	1:B:597:VAL:HG21	2.40	0.51
1:B:741:TYR:CE1	1:B:966:LEU:HD11	2.46	0.51
1:C:355:ARG:HD3	1:C:396:TYR:HD2	1.75	0.51
1:C:802:PHE:CD1	1:C:805:ILE:HD11	2.45	0.51
1:B:367:VAL:O	1:B:371:SER:HB2	2.11	0.51
1:C:971:GLY:HA3	1:C:995:ARG:HH21	1.74	0.51
1:B:329:PHE:O	1:B:580:GLN:NE2	2.37	0.51
1:C:191:GLU:OE1	1:C:191:GLU:N	2.44	0.51
1:B:885:GLY:O	1:B:888:PHE:HD1	1.93	0.51
2:B:1319:NAG:H3	2:B:1319:NAG:H83	1.92	0.51
1:A:1117:THR:OG1	1:A:1139:ASP:HB3	2.10	0.51
1:A:225:PRO:HD2	1:C:562:PHE:CE2	2.45	0.51
1:B:379:CYS:HA	1:B:432:CYS:HA	1.93	0.51
1:C:506:GLN:HG3	1:C:507:PRO:HD2	1.92	0.51
1:A:752:LEU:HD21	1:A:990:GLU:HB2	1.92	0.51
1:B:115:GLN:HA	1:B:132:GLU:HG2	1.93	0.51
2:B:1305:NAG:HO3	2:B:1305:NAG:C7	2.24	0.51
1:C:922:LEU:HD11	1:C:926:GLN:HE21	1.76	0.51
1:A:48:LEU:HB3	1:A:276:LEU:HD21	1.93	0.50
1:C:965:GLN:HG3	1:C:1003:SER:OG	2.10	0.50
1:B:193:VAL:HB	1:B:204:TYR:HB2	1.92	0.50
1:B:807:PRO:HA	1:B:816:SER:HA	1.92	0.50
1:C:101:ILE:HD12	1:C:101:ILE:H	1.75	0.50
2:B:1315:NAG:C3	2:B:1315:NAG:O7	2.56	0.50
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.46	0.50
1:C:578:ASP:OD1	1:C:583:GLU:N	2.39	0.50
1:A:796:ASP:N	1:A:796:ASP:OD1	2.45	0.50
1:B:1041:ASP:HB2	1:C:1030:SER:HB3	1.93	0.50
1:C:718:PHE:HZ	1:C:923:ILE:HD11	1.77	0.50
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.46	0.50
1:C:106:PHE:CD1	1:C:238:PHE:HB2	2.45	0.50
1:C:910:GLY:C	1:C:1108:ASN:HD22	2.15	0.50
1:B:189:LEU:N	1:B:208:THR:O	2.40	0.50
1:C:641:ASN:O	1:C:651:ILE:HG13	2.12	0.50
1:B:1090:PRO:O	1:C:913:GLN:NE2	2.45	0.50
1:B:287:ASP:HB3	1:B:306:PHE:CE2	2.47	0.50
1:A:619:GLU:OE1	1:A:619:GLU:N	2.45	0.50
1:B:568:ASP:HB2	1:B:574:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:736:VAL:HG11	1:C:1004:LEU:HD11	1.93	0.50
1:B:711:SER:HA	1:B:1076:THR:HA	1.94	0.49
1:B:610:VAL:O	1:B:650:LEU:HD12	2.11	0.49
1:C:439:ASN:OD1	1:C:440:ASN:N	2.45	0.49
1:C:1127:ASP:OD1	1:C:1128:VAL:N	2.45	0.49
1:C:100:ILE:O	1:C:242:LEU:HD21	2.12	0.49
1:C:563:GLN:O	1:C:577:ARG:NE	2.45	0.49
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.47	0.49
1:C:1076:THR:HB	1:C:1097:SER:HB3	1.94	0.49
1:B:708:SER:HB3	1:B:711:SER:OG	2.11	0.49
1:A:396:TYR:HB2	1:A:514:SER:OG	2.12	0.49
1:B:308:VAL:HG22	1:B:602:THR:OG1	2.12	0.49
1:B:729:VAL:HG22	1:B:1059:GLY:HA2	1.95	0.49
2:C:1312:NAG:O3	2:C:1312:NAG:O7	2.30	0.49
1:C:916:LEU:HD12	1:C:923:ILE:HD12	1.95	0.49
1:A:854:LYS:HD2	1:A:859:THR:HA	1.93	0.49
1:A:758:SER:O	1:A:762:GLN:HG3	2.12	0.49
1:B:805:ILE:HG22	1:B:878:LEU:HD21	1.95	0.49
1:A:895:GLN:HB3	1:C:705:VAL:HG12	1.95	0.49
1:B:390:LEU:HD21	1:C:983:ARG:HB3	1.95	0.48
1:B:583:GLU:OE1	1:B:584:ILE:N	2.45	0.48
1:B:973:ILE:HG23	1:B:980:ILE:HG22	1.94	0.48
1:A:395:VAL:HG22	1:A:515:PHE:CD1	2.47	0.48
1:B:316:SER:O	1:B:595:VAL:HG12	2.13	0.48
1:C:437:ASN:HD21	1:C:506:GLN:HG2	1.78	0.48
1:A:551:VAL:HG12	1:A:588:THR:O	2.13	0.48
1:A:1043:CYS:HB3	1:A:1064:HIS:CE1	2.48	0.48
1:A:299:THR:HG21	1:A:597:VAL:CG2	2.43	0.48
1:B:644:GLN:HA	1:B:649:CYS:CB	2.44	0.48
1:C:1090:PRO:HD3	1:C:1095:PHE:HE2	1.79	0.48
1:A:965:GLN:NE2	1:B:758:SER:OG	2.46	0.48
1:B:122:ASN:HB3	1:B:125:ASN:OD1	2.14	0.48
1:A:1090:PRO:HG2	1:B:913:GLN:HE22	1.79	0.48
2:C:1301:NAG:H61	2:C:1302:NAG:C7	2.43	0.48
1:B:330:PRO:HD3	1:B:544:ASN:ND2	2.29	0.48
1:C:1102:TRP:CZ2	1:C:1133:VAL:HG21	2.49	0.48
1:A:788:ILE:HG23	1:A:876:ALA:HB2	1.96	0.48
1:B:431:GLY:HA3	1:B:515:PHE:HD1	1.79	0.48
1:B:554:GLU:HA	1:B:585:LEU:HD23	1.94	0.48
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.49	0.48
1:A:599:THR:HG22	1:A:601:GLY:N	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:ILE:HG13	1:A:981:LEU:N	2.29	0.48
1:A:454:ARG:HA	1:A:492:LEU:HA	1.96	0.47
1:B:555:SER:HB3	1:B:586:ASP:N	2.29	0.47
1:C:278:LYS:HB2	1:C:306:PHE:CE1	2.49	0.47
1:B:578:ASP:OD2	1:B:583:GLU:HB3	2.14	0.47
1:C:379:CYS:SG	1:C:384:PRO:HG3	2.53	0.47
1:A:1049:LEU:HD11	1:A:1067:TYR:HB2	1.96	0.47
1:A:230:PRO:HG3	1:C:357:ARG:NH1	2.29	0.47
1:A:402:ILE:HD13	1:A:410:ILE:HD11	1.96	0.47
1:B:1129:VAL:O	1:B:1132:ILE:HG12	2.14	0.47
1:B:538:CYS:HB2	1:B:590:CYS:HB3	1.51	0.47
1:A:904:TYR:HB2	1:C:1107:ARG:HH12	1.78	0.47
1:B:658:ASN:ND2	1:B:660:TYR:OH	2.48	0.47
1:B:897:PRO:HG2	1:B:900:MET:SD	2.55	0.47
1:B:980:ILE:HG13	1:B:981:LEU:N	2.30	0.47
1:C:741:TYR:CE1	1:C:966:LEU:HD11	2.49	0.47
1:A:1077:THR:HG22	1:A:1095:PHE:O	2.14	0.47
1:A:741:TYR:CE1	1:A:966:LEU:HD11	2.50	0.47
1:B:435:ALA:HB2	1:B:510:VAL:HG13	1.96	0.47
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.62	0.47
1:C:276:LEU:HB3	1:C:289:VAL:HG22	1.97	0.47
1:B:1088:HIS:ND1	1:B:1137:VAL:HG21	2.29	0.47
1:B:644:GLN:CD	1:B:649:CYS:HB3	2.36	0.47
1:C:888:PHE:CE1	1:C:1034:LEU:HA	2.50	0.47
1:B:748:GLU:OE1	1:B:748:GLU:N	2.32	0.46
1:C:38:TYR:HE1	1:C:222:ALA:HB1	1.79	0.46
1:A:228:ASP:OD1	1:A:229:LEU:N	2.47	0.46
1:C:1079:PRO:HD2	1:C:1131:GLY:O	2.15	0.46
1:B:396:TYR:HH	1:C:200:TYR:HE1	1.63	0.46
1:C:551:VAL:HG22	1:C:588:THR:O	2.15	0.46
1:B:537:LYS:HB3	1:B:537:LYS:HE2	1.71	0.46
1:C:565:PHE:HB2	1:C:575:ALA:O	2.15	0.46
1:C:807:PRO:HA	1:C:816:SER:HA	1.96	0.46
1:C:906:PHE:O	1:C:909:ILE:HG12	2.15	0.46
1:A:906:PHE:HD2	1:A:916:LEU:HB2	1.79	0.46
2:B:1304:NAG:H83	2:B:1304:NAG:H3	1.97	0.46
1:A:309:GLU:N	1:A:309:GLU:OE1	2.48	0.46
1:B:217:PRO:HG3	1:B:266:TYR:HE2	1.80	0.46
1:C:645:THR:OG1	1:C:648:GLY:O	2.15	0.46
1:C:370:ASN:OD1	1:C:371:SER:N	2.48	0.46
1:A:205:SER:OG	1:A:206:LYS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:LYS:N	1:B:551:VAL:HG23	2.30	0.46
1:A:1031:GLU:HG2	1:C:1039:ARG:HB3	1.97	0.46
1:A:716:THR:HG22	1:A:1110:TYR:CB	2.46	0.46
1:A:233:ILE:HG12	1:A:234:ASN:N	2.31	0.46
2:C:1308:NAG:O7	2:C:1308:NAG:O3	2.34	0.46
1:C:391:CYS:CA	1:C:525:CYS:HB3	2.41	0.46
1:A:206:LYS:HD2	1:A:222:ALA:O	2.16	0.46
1:B:1030:SER:O	1:B:1034:LEU:HB2	2.16	0.46
1:C:111:ASP:OD1	1:C:135:PHE:N	2.49	0.46
1:C:726:ILE:HD13	1:C:945:LEU:HD23	1.98	0.46
1:B:134:GLN:HB2	1:B:161:SER:OG	2.16	0.45
1:C:661:GLU:OE1	1:C:662:CYS:N	2.49	0.45
1:A:384:PRO:HA	1:A:387:LEU:HD23	1.98	0.45
1:B:106:PHE:CD2	1:B:235:ILE:HG21	2.51	0.45
1:C:578:ASP:OD2	1:C:581:THR:HB	2.16	0.45
1:A:781:VAL:HG22	1:A:1026:ALA:HB2	1.96	0.45
1:A:323:THR:O	1:A:539:VAL:HG23	2.15	0.45
1:A:770:ILE:O	1:A:774:GLN:HG2	2.17	0.45
1:C:119:ILE:HG12	1:C:128:ILE:HG23	1.99	0.45
2:A:1310:NAG:C8	2:A:1310:NAG:C1	2.86	0.45
1:A:1141:LEU:O	1:A:1145:LEU:HG	2.17	0.45
1:A:376:THR:HB	1:A:435:ALA:HB3	1.98	0.45
1:A:28:TYR:HA	1:A:62:VAL:O	2.16	0.45
1:C:298:GLU:O	1:C:302:THR:HG23	2.15	0.45
1:C:644:GLN:HE22	1:C:649:CYS:HB2	1.82	0.45
1:C:939:SER:OG	1:C:940:SER:N	2.50	0.45
1:A:36:VAL:HG23	1:A:222:ALA:HA	1.97	0.45
1:A:497:PHE:CD2	1:A:507:PRO:HB3	2.52	0.45
1:A:976:VAL:HG13	1:A:979:ASP:HB2	1.98	0.45
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.99	0.45
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.46	0.45
1:C:1073:LYS:HE2	1:C:1073:LYS:HB3	1.70	0.45
1:C:112:SER:HA	1:C:132:GLU:HB3	1.97	0.45
1:A:344:ALA:O	1:A:509:ARG:NH2	2.41	0.45
1:B:661:GLU:O	1:B:695:TYR:OH	2.24	0.45
1:B:699:LEU:HD12	1:C:873:TYR:CZ	2.51	0.45
1:B:1039:ARG:NE	1:C:1031:GLU:OE2	2.37	0.45
1:A:787:GLN:HG3	1:C:703:ASN:OD1	2.17	0.45
1:A:114:THR:N	1:A:132:GLU:OE2	2.50	0.45
1:A:194:PHE:CE1	1:A:203:ILE:HG23	2.52	0.45
1:A:34:ARG:NE	1:A:217:PRO:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ASN:HD22	1:A:523:THR:HB	1.82	0.45
1:B:395:VAL:HG23	1:B:524:VAL:HG11	1.98	0.45
1:C:1119:ASN:OD1	1:C:1120:THR:HG23	2.17	0.45
1:A:537:LYS:HE2	1:A:537:LYS:HB3	1.80	0.44
1:B:44:ARG:O	1:B:283:GLY:HA2	2.16	0.44
1:B:534:VAL:HG21	1:B:539:VAL:HG11	1.99	0.44
1:B:715:PRO:HA	1:B:1072:GLU:CB	2.47	0.44
1:B:822:LEU:HD22	1:B:945:LEU:HD11	1.99	0.44
1:A:560:LEU:H	1:A:563:GLN:HE21	1.65	0.44
1:A:984:LEU:HB3	1:A:988:GLU:HG2	1.99	0.44
1:A:1073:LYS:HE2	1:A:1073:LYS:HB3	1.72	0.44
1:A:117:LEU:HD21	1:A:231:ILE:HG13	1.98	0.44
1:A:566:GLY:HA3	1:B:43:PHE:HB3	2.00	0.44
1:A:708:SER:HB3	1:A:711:SER:OG	2.17	0.44
1:A:94:SER:OG	1:A:95:THR:N	2.50	0.44
1:B:1039:ARG:HB2	1:C:1031:GLU:CG	2.45	0.44
1:C:538:CYS:HB2	1:C:590:CYS:HB3	1.68	0.44
1:C:888:PHE:CZ	1:C:1034:LEU:HA	2.53	0.44
1:B:401:VAL:HG21	1:B:451:TYR:CE2	2.53	0.44
1:B:565:PHE:HB2	1:B:576:VAL:HG22	1.99	0.44
1:A:965:GLN:NE2	1:B:758:SER:H	2.12	0.44
1:B:299:THR:HG21	1:B:597:VAL:HG21	1.98	0.44
1:B:327:VAL:HB	1:B:531:THR:HG22	1.98	0.44
1:B:90:VAL:HG11	1:B:238:PHE:CE2	2.52	0.44
1:C:984:LEU:HD23	1:C:984:LEU:HA	1.72	0.44
1:A:565:PHE:CB	1:A:576:VAL:HG12	2.48	0.44
1:A:617:CYS:HB2	1:A:649:CYS:HB3	1.80	0.44
1:A:566:GLY:HA2	1:B:43:PHE:H	1.82	0.44
1:A:130:VAL:O	1:A:130:VAL:HG12	2.18	0.44
1:C:233:ILE:HG12	1:C:234:ASN:N	2.33	0.44
1:C:367:VAL:O	1:C:371:SER:HB3	2.18	0.44
1:C:205:SER:OG	1:C:206:LYS:N	2.51	0.44
1:B:131:CYS:HA	1:B:166:CYS:HB2	1.99	0.43
1:C:336:CYS:SG	1:C:358:ILE:HG23	2.58	0.43
1:A:615:VAL:HG12	1:A:616:ASN:N	2.33	0.43
1:A:988:GLU:OE2	1:C:383:SER:OG	2.36	0.43
1:B:365:TYR:CD1	1:B:368:LEU:HD21	2.51	0.43
1:B:379:CYS:SG	1:B:384:PRO:HG3	2.58	0.43
1:B:1101:HIS:CD2	2:B:1311:NAG:H5	2.53	0.43
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.33	0.43
1:A:917:TYR:HB3	1:C:1129:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:TYR:CD2	1:C:387:LEU:HB3	2.45	0.43
1:C:796:ASP:N	1:C:796:ASP:OD1	2.49	0.43
1:A:1090:PRO:HD3	1:A:1095:PHE:CE1	2.51	0.43
1:A:886:TRP:H	1:A:886:TRP:HE3	1.62	0.43
1:C:574:ASP:O	1:C:587:ILE:N	2.36	0.43
1:C:644:GLN:HA	1:C:649:CYS:HA	1.99	0.43
1:C:964:LYS:HA	1:C:964:LYS:HD2	1.83	0.43
1:B:1126:CYS:SG	1:B:1132:ILE:HD12	2.58	0.43
1:C:36:VAL:O	1:C:223:LEU:HB2	2.18	0.43
1:C:895:GLN:O	1:C:895:GLN:HG2	2.17	0.43
1:B:307:THR:HA	1:B:602:THR:HB	1.99	0.43
1:B:296:LEU:HB2	1:B:608:VAL:HG21	2.00	0.43
1:C:418:ILE:HG23	1:C:422:ASN:HB2	2.00	0.43
1:C:856:ASN:N	1:C:856:ASN:OD1	2.52	0.43
1:A:377:PHE:HE1	1:A:384:PRO:HB3	1.84	0.43
1:A:565:PHE:HE1	1:A:567:ARG:HH21	1.67	0.43
1:A:733:LYS:HB2	1:A:861:LEU:HB2	1.99	0.43
1:B:773:GLU:OE2	1:B:1019:ARG:HD3	2.19	0.43
1:B:770:ILE:HG13	1:B:771:ALA:N	2.33	0.43
1:B:778:THR:HG22	1:B:865:LEU:HD12	2.01	0.43
1:C:40:ASP:OD1	1:C:41:LYS:N	2.52	0.43
1:A:543:PHE:CZ	1:A:578:ASP:HA	2.54	0.43
1:A:543:PHE:CE1	1:A:578:ASP:HA	2.53	0.43
1:B:95:THR:HB	1:B:189:LEU:HD13	2.01	0.43
1:A:379:CYS:HA	1:A:432:CYS:HA	2.00	0.43
1:C:324:GLU:OE2	1:C:537:LYS:NZ	2.51	0.43
1:C:357:ARG:HD2	1:C:358:ILE:N	2.34	0.43
1:B:330:PRO:HD3	1:B:544:ASN:HD22	1.84	0.42
1:B:811:LYS:NZ	1:B:868:GLU:OE2	2.47	0.42
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.54	0.42
1:A:200:TYR:HB3	1:A:228:ASP:OD1	2.18	0.42
1:A:980:ILE:HG13	1:A:981:LEU:H	1.84	0.42
1:B:643:PHE:CZ	1:B:655:HIS:CD2	3.07	0.42
2:C:1311:NAG:H61	2:C:1312:NAG:HN2	1.84	0.42
1:C:422:ASN:OD1	1:C:454:ARG:N	2.38	0.42
1:A:111:ASP:HA	1:A:135:PHE:N	2.34	0.42
1:A:895:GLN:HB3	1:C:705:VAL:CG1	2.50	0.42
1:B:1097:SER:HB3	1:B:1102:TRP:CE3	2.55	0.42
1:B:300:LYS:O	1:B:304:LYS:N	2.50	0.42
1:B:969:ASN:OD1	1:B:975:SER:HB3	2.19	0.42
1:C:539:VAL:HG12	1:C:540:ASN:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:MET:CG	1:C:699:LEU:HD11	2.50	0.42
1:A:895:GLN:O	1:C:712:ILE:HA	2.19	0.42
1:B:106:PHE:HD2	1:B:235:ILE:HG21	1.84	0.42
1:B:787:GLN:OE1	1:B:787:GLN:N	2.53	0.42
1:C:53:ASP:HB2	1:C:55:PHE:CE2	2.54	0.42
1:A:1080:ALA:O	1:A:1132:ILE:HG22	2.19	0.42
1:A:129:LYS:HB3	1:A:131:CYS:SG	2.58	0.42
1:A:328:ARG:HH21	1:A:530:SER:HB3	1.84	0.42
1:B:543:PHE:HZ	1:B:578:ASP:HA	1.83	0.42
1:C:729:VAL:HG12	1:C:1022:ALA:HA	2.01	0.42
1:C:934:ILE:HD13	1:C:1063:LEU:HD23	2.00	0.42
1:C:661:GLU:O	1:C:695:TYR:OH	2.36	0.42
1:C:973:ILE:HG22	1:C:980:ILE:HD13	2.00	0.42
1:A:520:ALA:HB1	1:A:521:PRO:HD2	2.00	0.42
1:A:804:GLN:O	1:A:818:ILE:HD12	2.20	0.42
1:C:1051:SER:OG	1:C:1064:HIS:ND1	2.39	0.42
1:C:435:ALA:HB2	1:C:510:VAL:HG22	2.02	0.42
1:C:985:ASP:OD2	1:C:987:PRO:HD2	2.19	0.42
1:A:1043:CYS:HB3	1:A:1064:HIS:ND1	2.35	0.42
1:A:778:THR:HG22	1:A:865:LEU:HD12	2.02	0.42
1:B:1030:SER:HA	1:B:1034:LEU:HD12	2.01	0.42
1:B:645:THR:OG1	1:B:670:ILE:HG13	2.20	0.42
1:B:714:ILE:O	1:B:1072:GLU:HB2	2.20	0.42
1:C:1081:ILE:HG21	1:C:1135:ASN:HB3	2.02	0.42
1:C:973:ILE:CG2	1:C:980:ILE:HD13	2.50	0.42
1:A:117:LEU:HD11	1:A:231:ILE:HG21	2.02	0.42
1:A:388:ASN:HA	1:A:526:GLY:HA3	2.01	0.42
1:B:1102:TRP:HB2	1:B:1135:ASN:HD21	1.85	0.42
1:B:383:SER:OG	1:B:386:LYS:HB2	2.20	0.42
1:B:718:PHE:HZ	1:B:923:ILE:HD11	1.85	0.42
1:B:724:THR:HG22	1:B:1063:LEU:HD23	2.00	0.42
1:C:126:VAL:O	1:C:171:VAL:HA	2.19	0.42
1:C:662:CYS:HB2	1:C:697:MET:HG2	2.02	0.42
1:A:1030:SER:HB3	1:C:1041:ASP:HB3	2.01	0.42
1:A:555:SER:HB3	1:A:586:ASP:N	2.34	0.42
1:B:101:ILE:HD13	1:B:242:LEU:HD21	2.02	0.42
1:B:342:PHE:HB3	2:B:1315:NAG:H82	2.00	0.42
1:B:560:LEU:HB2	1:B:563:GLN:OE1	2.20	0.42
1:B:984:LEU:HD13	1:B:988:GLU:OE1	2.19	0.42
1:C:168:PHE:CE2	1:C:229:LEU:HD23	2.55	0.42
1:C:206:LYS:HD2	1:C:206:LYS:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:MET:HE2	1:C:731:MET:HB3	1.87	0.42
1:A:374:PHE:HA	1:A:436:TRP:HB3	2.02	0.42
1:A:560:LEU:H	1:A:563:GLN:NE2	2.17	0.42
1:B:567:ARG:HD3	1:B:571:ASP:HA	2.01	0.42
1:C:716:THR:HG22	1:C:1110:TYR:CB	2.50	0.42
1:A:1090:PRO:CD	1:A:1095:PHE:HE1	2.30	0.41
1:A:661:GLU:O	1:A:695:TYR:OH	2.23	0.41
1:A:965:GLN:HE22	1:B:758:SER:N	2.12	0.41
1:B:748:GLU:HG3	1:B:981:LEU:HD22	2.01	0.41
1:A:355:ARG:HA	1:A:397:ALA:O	2.20	0.41
1:B:106:PHE:HB2	1:B:117:LEU:HB2	2.02	0.41
1:B:204:TYR:HD1	1:B:225:PRO:HA	1.86	0.41
1:B:206:LYS:HG2	1:B:207:HIS:H	1.85	0.41
1:C:393:THR:OG1	1:C:394:ASN:N	2.53	0.41
1:C:312:ILE:HD12	1:C:598:ILE:HD11	2.01	0.41
1:A:378:LYS:HG3	1:A:433:VAL:HB	2.01	0.41
1:A:559:PHE:O	1:A:560:LEU:HD23	2.21	0.41
1:A:807:PRO:HA	1:A:816:SER:HA	2.02	0.41
1:B:453:TYR:HB3	1:B:495:TYR:CE2	2.55	0.41
1:C:106:PHE:CE2	1:C:119:ILE:HD12	2.54	0.41
1:A:1028:LYS:HG2	1:A:1042:PHE:CE2	2.55	0.41
1:A:1081:ILE:HG21	1:A:1135:ASN:HB3	2.02	0.41
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.81	0.41
1:B:388:ASN:O	1:B:526:GLY:HA3	2.20	0.41
1:B:710:ASN:O	1:B:1077:THR:N	2.38	0.41
1:C:1077:THR:HG22	1:C:1095:PHE:O	2.20	0.41
1:C:276:LEU:HB3	1:C:289:VAL:CG2	2.50	0.41
1:C:541:PHE:O	1:C:547:THR:HA	2.20	0.41
2:A:1310:NAG:C3	2:A:1310:NAG:C8	2.90	0.41
1:C:1049:LEU:HD11	1:C:1067:TYR:HB2	2.03	0.41
1:A:600:PRO:HD3	1:A:692:ILE:HD11	2.03	0.41
1:B:126:VAL:HG11	1:B:175:PHE:CE1	2.55	0.41
1:B:380:TYR:HB2	1:B:430:THR:O	2.21	0.41
1:B:617:CYS:SG	1:B:644:GLN:NE2	2.94	0.41
1:A:917:TYR:HB3	1:C:1129:VAL:HG21	2.03	0.41
1:B:206:LYS:HE3	1:B:221:SER:HB3	2.01	0.41
1:B:422:ASN:OD1	1:B:454:ARG:N	2.39	0.41
1:B:973:ILE:HD11	1:B:983:ARG:HH12	1.86	0.41
1:C:114:THR:HG22	1:C:115:GLN:H	1.86	0.41
1:C:660:TYR:HB2	1:C:695:TYR:CE2	2.56	0.41
1:A:102:ARG:HG3	1:A:141:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:826:VAL:HG21	1:C:1057:PRO:HG3	2.03	0.41
1:C:538:CYS:HA	1:C:550:GLY:O	2.21	0.41
1:A:357:ARG:NH2	1:B:167:THR:HG22	2.35	0.41
1:A:862:PRO:HG3	1:C:647:ALA:HA	2.02	0.41
1:A:958:ALA:O	1:A:961:THR:HG22	2.21	0.41
1:B:34:ARG:NH2	1:B:217:PRO:O	2.54	0.41
1:B:733:LYS:HE3	1:B:771:ALA:O	2.21	0.41
1:B:968:SER:HB3	1:B:970:PHE:CE2	2.56	0.41
1:C:611:LEU:HD22	1:C:666:ILE:HG23	2.03	0.41
1:A:1054:GLN:N	1:A:1061:VAL:O	2.46	0.41
1:A:1086:LYS:HE3	1:A:1086:LYS:HB2	1.75	0.41
1:B:888:PHE:CZ	1:B:1034:LEU:HD23	2.56	0.41
1:B:528:LYS:HA	1:B:528:LYS:HD2	1.85	0.41
1:B:985:ASP:HB2	1:B:987:PRO:HD2	2.02	0.41
1:A:740:MET:HA	1:A:744:GLY:HA2	2.03	0.41
1:B:118:LEU:HD13	1:B:133:PHE:CD2	2.55	0.41
1:B:278:LYS:HD3	1:B:287:ASP:HB2	2.03	0.41
1:B:299:THR:HG22	1:B:597:VAL:HG21	2.02	0.41
1:C:29:THR:O	1:C:62:VAL:HG22	2.20	0.41
1:B:699:LEU:HB3	1:C:873:TYR:CE1	2.55	0.41
1:A:360:ASN:ND2	1:A:523:THR:HB	2.37	0.40
1:A:770:ILE:HG13	1:A:771:ALA:N	2.34	0.40
1:B:344:ALA:HB3	1:B:347:PHE:CE1	2.56	0.40
2:A:1307:NAG:H62	2:A:1308:NAG:H83	2.03	0.40
1:A:132:GLU:HG2	2:A:1316:NAG:H82	2.03	0.40
1:B:365:TYR:CD2	1:B:387:LEU:HB3	2.56	0.40
1:C:119:ILE:HG23	1:C:128:ILE:HG13	2.03	0.40
1:C:194:PHE:CE1	1:C:203:ILE:HG23	2.56	0.40
1:C:299:THR:OG1	1:C:300:LYS:N	2.55	0.40
1:A:1072:GLU:N	1:A:1072:GLU:OE1	2.54	0.40
1:A:748:GLU:O	1:A:752:LEU:HD12	2.22	0.40
1:B:759:PHE:HD2	1:B:1001:LEU:HD11	1.86	0.40
1:B:44:ARG:HD2	1:B:279:TYR:CE2	2.56	0.40
1:B:719:THR:HA	1:B:926:GLN:OE1	2.21	0.40
1:B:912:THR:HG23	1:B:915:VAL:HG23	2.04	0.40
1:C:770:ILE:HG13	1:C:771:ALA:N	2.37	0.40
1:A:128:ILE:HD12	1:A:170:TYR:HD2	1.87	0.40
1:B:34:ARG:HD3	1:B:34:ARG:HA	1.93	0.40
1:C:289:VAL:HG13	1:C:306:PHE:CE2	2.57	0.40
1:C:533:LEU:HD11	1:C:535:LYS:HZ3	1.87	0.40
1:C:937:SER:O	1:C:941:THR:HB	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:HIS:HA	1:A:1066:THR:HG22	2.04	0.40
1:A:1102:TRP:CZ2	1:A:1133:VAL:HG11	2.57	0.40
1:A:109:THR:HA	1:A:237:ARG:NH1	2.37	0.40
1:A:539:VAL:HG22	1:A:540:ASN:N	2.37	0.40
2:B:1305:NAG:O3	2:B:1305:NAG:C7	2.70	0.40
1:B:805:ILE:HG22	1:B:878:LEU:HD11	2.04	0.40
1:B:958:ALA:O	1:B:961:THR:HG22	2.22	0.40
1:C:193:VAL:HG23	1:C:223:LEU:HD23	2.03	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	931/1288 (72%)	878 (94%)	51 (6%)	2 (0%)	49	83
1	B	945/1288 (73%)	899 (95%)	45 (5%)	1 (0%)	53	86
1	C	945/1288 (73%)	893 (94%)	50 (5%)	2 (0%)	49	83
All	All	2821/3864 (73%)	2670 (95%)	146 (5%)	5 (0%)	53	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	543	PHE
1	A	744	GLY
1	A	888	PHE
1	C	617	CYS
1	C	987	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	790/1113 (71%)	786 (100%)	4 (0%)	90 96
1	B	789/1113 (71%)	786 (100%)	3 (0%)	92 96
1	C	781/1113 (70%)	777 (100%)	4 (0%)	90 96
All	All	2360/3339 (71%)	2349 (100%)	11 (0%)	90 96

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	525	CYS
1	A	760	CYS
1	A	906	PHE
1	A	985	ASP
1	B	166	CYS
1	B	617	CYS
1	B	854	LYS
1	C	282	ASN
1	C	525	CYS
1	C	617	CYS
1	C	906	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	ASN
1	A	360	ASN
1	A	542	ASN
1	A	563	GLN
1	A	644	GLN
1	A	755	GLN
1	A	901	GLN
1	A	907	ASN
1	A	955	ASN
1	A	965	GLN

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Mol	Chain	Res	Type
1	B	66	HIS
1	B	207	HIS
1	B	394	ASN
1	B	564	GLN
1	B	644	GLN
1	B	655	HIS
1	B	658	ASN
1	B	755	GLN
1	B	762	GLN
1	B	804	GLN
1	B	913	GLN
1	B	935	GLN
1	B	954	GLN
1	B	955	ASN
1	B	965	GLN
1	B	1101	HIS
1	B	1119	ASN
1	C	536	ASN
1	C	606	ASN
1	C	644	GLN
1	C	655	HIS
1	C	658	ASN
1	C	751	ASN
1	C	755	GLN
1	C	955	ASN
1	C	965	GLN
1	C	1108	ASN
1	C	1113	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

61 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	1301	1	14,14,15	0.25	0	17,19,21	0.69	1 (5%)
2	NAG	A	1302	1	14,14,15	0.46	0	17,19,21	0.68	1 (5%)
2	NAG	A	1303	1	14,14,15	0.30	0	17,19,21	0.66	1 (5%)
2	NAG	A	1304	1	14,14,15	0.62	1 (7%)	17,19,21	0.63	1 (5%)
2	NAG	A	1305	1,2	14,14,15	0.23	0	17,19,21	0.39	0
2	NAG	A	1306	2	14,14,15	0.20	0	17,19,21	0.41	0
2	NAG	A	1307	1,2	14,14,15	0.34	0	17,19,21	0.60	0
2	NAG	A	1308	2	14,14,15	0.30	0	17,19,21	0.78	0
2	NAG	A	1309	1,2	14,14,15	0.34	0	17,19,21	0.75	0
2	NAG	A	1310	2	14,14,15	0.27	0	17,19,21	0.72	0
2	NAG	A	1311	1,2	14,14,15	0.36	0	17,19,21	0.78	0
2	NAG	A	1312	2	14,14,15	0.31	0	17,19,21	0.82	0
2	NAG	A	1313	1,2	14,14,15	0.17	0	17,19,21	0.43	0
2	NAG	A	1314	2	14,14,15	0.18	0	17,19,21	0.42	0
2	NAG	A	1315	1	14,14,15	0.22	0	17,19,21	0.54	0
2	NAG	A	1316	1	14,14,15	0.56	0	17,19,21	0.74	1 (5%)
2	NAG	A	1317	1	14,14,15	0.21	0	17,19,21	0.52	0
2	NAG	A	1318	1	14,14,15	0.35	0	17,19,21	1.23	1 (5%)
2	NAG	A	1319	1	14,14,15	0.34	0	17,19,21	0.71	1 (5%)
2	NAG	B	1301	1	14,14,15	0.46	0	17,19,21	0.77	1 (5%)
2	NAG	B	1302	1	14,14,15	0.33	0	17,19,21	0.76	1 (5%)
2	NAG	B	1303	1	14,14,15	0.33	0	17,19,21	0.61	0
2	NAG	B	1304	1	14,14,15	0.42	0	17,19,21	1.45	3 (17%)
2	NAG	B	1305	1,2	14,14,15	0.38	0	17,19,21	0.85	0
2	NAG	B	1306	2	14,14,15	0.30	0	17,19,21	0.72	0
2	NAG	B	1307	1,2	14,14,15	0.31	0	17,19,21	0.52	0
2	NAG	B	1308	2	14,14,15	0.33	0	17,19,21	0.62	1 (5%)
2	NAG	B	1309	1,2	14,14,15	0.25	0	17,19,21	0.47	0
2	NAG	B	1310	2	14,14,15	0.25	0	17,19,21	0.39	0
2	NAG	B	1311	1,2	14,14,15	0.36	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	1312	2	14,14,15	0.19	0	17,19,21	0.40	0
2	NAG	B	1313	1,2	14,14,15	0.25	0	17,19,21	0.41	0
2	NAG	B	1314	2	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	B	1315	1	14,14,15	0.30	0	17,19,21	0.44	0
2	NAG	B	1316	1	14,14,15	0.30	0	17,19,21	0.57	0
2	NAG	B	1317	1	14,14,15	0.47	0	17,19,21	0.69	1 (5%)
2	NAG	B	1318	1	14,14,15	0.27	0	17,19,21	0.46	0
2	NAG	B	1319	1	14,14,15	0.34	0	17,19,21	1.25	2 (11%)
2	NAG	B	1320	1,2	14,14,15	0.43	0	17,19,21	1.36	2 (11%)
2	NAG	B	1321	2	14,14,15	0.30	0	17,19,21	1.12	3 (17%)
2	NAG	C	1301	1,2	14,14,15	0.32	0	17,19,21	0.71	0
2	NAG	C	1302	2	14,14,15	0.28	0	17,19,21	0.54	0
2	NAG	C	1303	1,2	14,14,15	0.32	0	17,19,21	0.75	0
2	NAG	C	1304	2	14,14,15	0.32	0	17,19,21	0.78	0
2	NAG	C	1305	1,2	14,14,15	0.53	0	17,19,21	0.62	1 (5%)
2	NAG	C	1306	2	14,14,15	0.40	0	17,19,21	1.26	2 (11%)
2	NAG	C	1307	1,2	14,14,15	0.36	0	17,19,21	0.82	0
2	NAG	C	1308	2	14,14,15	0.29	0	17,19,21	0.77	0
2	NAG	C	1309	1,2	14,14,15	0.26	0	17,19,21	0.43	0
2	NAG	C	1310	2	14,14,15	0.73	0	17,19,21	0.57	0
2	NAG	C	1311	1,2	14,14,15	0.31	0	17,19,21	0.75	0
2	NAG	C	1312	2	14,14,15	0.27	0	17,19,21	0.70	0
2	NAG	C	1313	1	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	C	1314	1	14,14,15	0.28	0	17,19,21	0.66	0
2	NAG	C	1315	1	14,14,15	0.53	0	17,19,21	1.24	2 (11%)
2	NAG	C	1316	1	14,14,15	0.22	0	17,19,21	0.58	0
2	NAG	C	1317	1	14,14,15	0.33	0	17,19,21	0.69	1 (5%)
2	NAG	C	1318	1	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	C	1319	1	14,14,15	0.31	0	17,19,21	0.50	0
2	NAG	C	1320	1	14,14,15	0.84	2 (14%)	17,19,21	0.74	1 (5%)
2	NAG	C	1321	1	14,14,15	0.24	0	17,19,21	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1305	1,2	-	1/6/23/26	0/1/1/1
2	NAG	A	1306	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1307	1,2	-	2/6/23/26	0/1/1/1
2	NAG	A	1308	2	-	1/6/23/26	0/1/1/1
2	NAG	A	1309	1,2	-	4/6/23/26	0/1/1/1
2	NAG	A	1310	2	-	3/6/23/26	0/1/1/1
2	NAG	A	1311	1,2	-	1/6/23/26	0/1/1/1
2	NAG	A	1312	2	-	4/6/23/26	0/1/1/1
2	NAG	A	1313	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1314	2	-	2/6/23/26	0/1/1/1
2	NAG	A	1315	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1316	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1317	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1318	1	-	5/6/23/26	0/1/1/1
2	NAG	A	1319	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1305	1,2	-	3/6/23/26	0/1/1/1
2	NAG	B	1306	2	-	3/6/23/26	0/1/1/1
2	NAG	B	1307	1,2	-	3/6/23/26	0/1/1/1
2	NAG	B	1308	2	-	2/6/23/26	0/1/1/1
2	NAG	B	1309	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	1310	2	-	2/6/23/26	0/1/1/1
2	NAG	B	1311	1,2	-	1/6/23/26	0/1/1/1
2	NAG	B	1312	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1313	1,2	-	1/6/23/26	0/1/1/1
2	NAG	B	1314	2	-	2/6/23/26	0/1/1/1
2	NAG	B	1315	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1316	1	-	5/6/23/26	0/1/1/1
2	NAG	B	1317	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1318	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1319	1	-	5/6/23/26	0/1/1/1
2	NAG	B	1320	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1321	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1301	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1302	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1303	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1304	2	-	5/6/23/26	0/1/1/1
2	NAG	C	1305	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	1306	2	-	5/6/23/26	0/1/1/1
2	NAG	C	1307	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	1308	2	-	3/6/23/26	0/1/1/1
2	NAG	C	1309	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	1310	2	-	2/6/23/26	0/1/1/1
2	NAG	C	1311	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	1312	2	-	4/6/23/26	0/1/1/1
2	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1314	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1315	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1317	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1318	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1319	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1320	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1321	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1304	NAG	O5-C1	2.20	1.47	1.43
2	C	1320	NAG	O5-C1	-2.06	1.40	1.43
2	C	1320	NAG	C1-C2	-2.02	1.49	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1304	NAG	C2-N2-C7	4.47	129.33	122.92
2	A	1318	NAG	C2-N2-C7	4.31	129.10	122.92
2	B	1319	NAG	C2-N2-C7	4.27	129.04	122.92
2	C	1306	NAG	C2-N2-C7	4.23	128.98	122.92
2	C	1315	NAG	C2-N2-C7	4.12	128.83	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1320	NAG	C2-N2-C7	-3.35	118.12	122.92
2	B	1304	NAG	C4-C3-C2	-2.70	107.05	111.02
2	A	1316	NAG	C4-C3-C2	-2.59	107.23	111.02
2	B	1320	NAG	O5-C1-C2	-2.58	107.31	111.36
2	A	1302	NAG	C4-C3-C2	-2.29	107.67	111.02
2	B	1321	NAG	C2-N2-C7	-2.26	119.68	122.92
2	C	1320	NAG	C4-C3-C2	-2.25	107.72	111.02
2	B	1317	NAG	C4-C3-C2	-2.24	107.74	111.02
2	A	1319	NAG	C4-C3-C2	-2.23	107.75	111.02
2	B	1302	NAG	C4-C3-C2	-2.21	107.78	111.02
2	B	1301	NAG	C4-C3-C2	-2.19	107.81	111.02
2	A	1301	NAG	C1-O5-C5	2.17	115.15	112.20
2	B	1321	NAG	O5-C1-C2	-2.16	107.96	111.36
2	B	1304	NAG	C1-C2-N2	2.14	114.14	110.49
2	B	1308	NAG	C4-C3-C2	-2.11	107.93	111.02
2	B	1321	NAG	C4-C3-C2	-2.09	107.96	111.02
2	C	1317	NAG	C4-C3-C2	-2.08	107.97	111.02
2	C	1306	NAG	C1-C2-N2	2.08	114.04	110.49
2	A	1303	NAG	C4-C3-C2	-2.07	107.98	111.02
2	C	1305	NAG	C1-O5-C5	2.05	114.99	112.20
2	A	1304	NAG	C4-C3-C2	-2.05	108.02	111.02
2	B	1319	NAG	C1-C2-N2	2.02	113.94	110.49
2	C	1315	NAG	C1-C2-N2	2.00	113.91	110.49

There are no chirality outliers.

All (129) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1316	NAG	C8-C7-N2-C2
2	B	1316	NAG	O7-C7-N2-C2
2	B	1306	NAG	C3-C2-N2-C7
2	C	1304	NAG	C8-C7-N2-C2
2	C	1304	NAG	O7-C7-N2-C2
2	C	1314	NAG	C3-C2-N2-C7
2	C	1314	NAG	C8-C7-N2-C2
2	C	1314	NAG	O7-C7-N2-C2
2	C	1311	NAG	C8-C7-N2-C2
2	C	1311	NAG	O7-C7-N2-C2
2	B	1305	NAG	C3-C2-N2-C7
2	B	1305	NAG	C8-C7-N2-C2
2	B	1305	NAG	O7-C7-N2-C2
2	B	1315	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	C	1307	NAG	C1-C2-N2-C7
2	C	1307	NAG	C8-C7-N2-C2
2	C	1307	NAG	O7-C7-N2-C2
2	B	1321	NAG	C8-C7-N2-C2
2	B	1321	NAG	O7-C7-N2-C2
2	A	1310	NAG	C8-C7-N2-C2
2	A	1310	NAG	O7-C7-N2-C2
2	C	1308	NAG	C3-C2-N2-C7
2	C	1308	NAG	C8-C7-N2-C2
2	C	1308	NAG	O7-C7-N2-C2
2	B	1306	NAG	C8-C7-N2-C2
2	B	1306	NAG	O7-C7-N2-C2
2	A	1312	NAG	C8-C7-N2-C2
2	A	1312	NAG	O7-C7-N2-C2
2	A	1307	NAG	C8-C7-N2-C2
2	A	1307	NAG	O7-C7-N2-C2
2	C	1305	NAG	O5-C5-C6-O6
2	A	1316	NAG	C4-C5-C6-O6
2	B	1301	NAG	O5-C5-C6-O6
2	B	1307	NAG	O5-C5-C6-O6
2	B	1319	NAG	O5-C5-C6-O6
2	A	1317	NAG	C4-C5-C6-O6
2	C	1306	NAG	C4-C5-C6-O6
2	C	1309	NAG	O5-C5-C6-O6
2	B	1307	NAG	C4-C5-C6-O6
2	B	1308	NAG	O5-C5-C6-O6
2	B	1314	NAG	O5-C5-C6-O6
2	A	1316	NAG	O5-C5-C6-O6
2	A	1315	NAG	O5-C5-C6-O6
2	C	1319	NAG	O5-C5-C6-O6
2	C	1319	NAG	C4-C5-C6-O6
2	C	1305	NAG	C4-C5-C6-O6
2	C	1306	NAG	O5-C5-C6-O6
2	A	1304	NAG	O5-C5-C6-O6
2	B	1314	NAG	C4-C5-C6-O6
2	C	1312	NAG	C1-C2-N2-C7
2	B	1301	NAG	C4-C5-C6-O6
2	B	1319	NAG	C4-C5-C6-O6
2	A	1304	NAG	C4-C5-C6-O6
2	B	1308	NAG	C4-C5-C6-O6
2	B	1302	NAG	O5-C5-C6-O6
2	B	1304	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	B	1304	NAG	O7-C7-N2-C2
2	A	1318	NAG	C8-C7-N2-C2
2	A	1318	NAG	O7-C7-N2-C2
2	C	1306	NAG	C8-C7-N2-C2
2	C	1306	NAG	O7-C7-N2-C2
2	A	1309	NAG	C8-C7-N2-C2
2	B	1310	NAG	C8-C7-N2-C2
2	B	1310	NAG	O7-C7-N2-C2
2	C	1315	NAG	C8-C7-N2-C2
2	C	1315	NAG	O7-C7-N2-C2
2	C	1302	NAG	C8-C7-N2-C2
2	B	1319	NAG	C8-C7-N2-C2
2	B	1319	NAG	O7-C7-N2-C2
2	B	1320	NAG	C4-C5-C6-O6
2	A	1318	NAG	O5-C5-C6-O6
2	C	1313	NAG	O5-C5-C6-O6
2	A	1317	NAG	O5-C5-C6-O6
2	B	1320	NAG	O5-C5-C6-O6
2	A	1318	NAG	C4-C5-C6-O6
2	A	1314	NAG	O5-C5-C6-O6
2	B	1309	NAG	O5-C5-C6-O6
2	A	1301	NAG	O5-C5-C6-O6
2	C	1309	NAG	C4-C5-C6-O6
2	C	1313	NAG	C4-C5-C6-O6
2	C	1321	NAG	O5-C5-C6-O6
2	B	1302	NAG	C4-C5-C6-O6
2	A	1314	NAG	C4-C5-C6-O6
2	A	1301	NAG	C4-C5-C6-O6
2	C	1321	NAG	C4-C5-C6-O6
2	C	1320	NAG	O5-C5-C6-O6
2	C	1310	NAG	C4-C5-C6-O6
2	A	1309	NAG	O7-C7-N2-C2
2	C	1302	NAG	O7-C7-N2-C2
2	A	1310	NAG	C1-C2-N2-C7
2	C	1315	NAG	O5-C5-C6-O6
2	B	1316	NAG	C1-C2-N2-C7
2	A	1305	NAG	O5-C5-C6-O6
2	C	1304	NAG	O5-C5-C6-O6
2	A	1303	NAG	O5-C5-C6-O6
2	A	1311	NAG	O5-C5-C6-O6
2	B	1311	NAG	O5-C5-C6-O6
2	B	1313	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	1317	NAG	O5-C5-C6-O6
2	C	1310	NAG	O5-C5-C6-O6
2	A	1315	NAG	C4-C5-C6-O6
2	C	1304	NAG	C1-C2-N2-C7
2	C	1312	NAG	C8-C7-N2-C2
2	A	1302	NAG	C4-C5-C6-O6
2	B	1316	NAG	C4-C5-C6-O6
2	A	1309	NAG	C4-C5-C6-O6
2	A	1302	NAG	O5-C5-C6-O6
2	C	1311	NAG	C1-C2-N2-C7
2	B	1309	NAG	C4-C5-C6-O6
2	B	1316	NAG	O5-C5-C6-O6
2	A	1309	NAG	O5-C5-C6-O6
2	C	1312	NAG	O7-C7-N2-C2
2	B	1301	NAG	C3-C2-N2-C7
2	A	1312	NAG	C3-C2-N2-C7
2	B	1302	NAG	C3-C2-N2-C7
2	C	1311	NAG	C3-C2-N2-C7
2	A	1308	NAG	C3-C2-N2-C7
2	C	1312	NAG	C3-C2-N2-C7
2	C	1319	NAG	C3-C2-N2-C7
2	C	1307	NAG	C3-C2-N2-C7
2	B	1319	NAG	C3-C2-N2-C7
2	A	1312	NAG	C1-C2-N2-C7
2	C	1320	NAG	C4-C5-C6-O6
2	C	1304	NAG	C3-C2-N2-C7
2	B	1304	NAG	C3-C2-N2-C7
2	A	1318	NAG	C3-C2-N2-C7
2	C	1306	NAG	C3-C2-N2-C7
2	B	1307	NAG	C3-C2-N2-C7
2	C	1315	NAG	C3-C2-N2-C7

There are no ring outliers.

23 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	NAG	1	0
2	A	1307	NAG	1	0
2	A	1308	NAG	2	0
2	A	1310	NAG	5	0
2	A	1311	NAG	3	0
2	A	1316	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1318	NAG	1	0
2	B	1304	NAG	1	0
2	B	1305	NAG	3	0
2	B	1306	NAG	3	0
2	B	1311	NAG	1	0
2	B	1315	NAG	5	0
2	B	1319	NAG	1	0
2	C	1301	NAG	1	0
2	C	1302	NAG	1	0
2	C	1304	NAG	1	0
2	C	1305	NAG	2	0
2	C	1306	NAG	1	0
2	C	1307	NAG	1	0
2	C	1308	NAG	2	0
2	C	1311	NAG	4	0
2	C	1312	NAG	2	0
2	C	1315	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.