



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Apr 24, 2017 – 12:15 PM EDT

PDB ID : 5X58
EMDB ID: : EMD-6703
Title : Prefusion structure of SARS-CoV spike glycoprotein, conformation 1
Authors : Yuan, Y.; Cao, D.; Zhang, Y.; Ma, J.; Qi, J.; Wang, Q.; Lu, G.; Wu, Y.; Yan, J.; Shi, Y.; Zhang, X.; Gao, G.F.
Deposited on : 2017-02-15
Resolution : 3.20 Å(reported)
Based on PDB ID : 5X4S, 2AJF

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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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-20029077

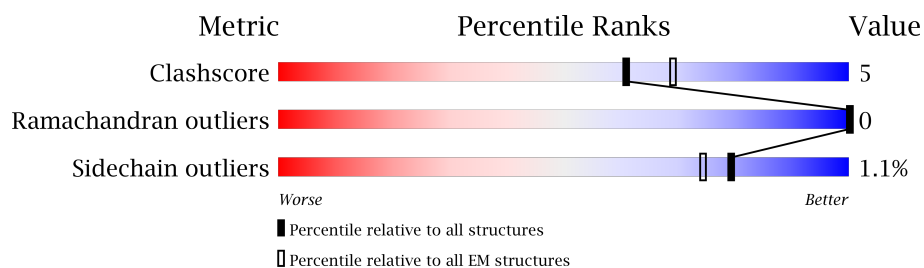
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	1228	
1	B	1228	
1	C	1228	

2 Entry composition [i](#)

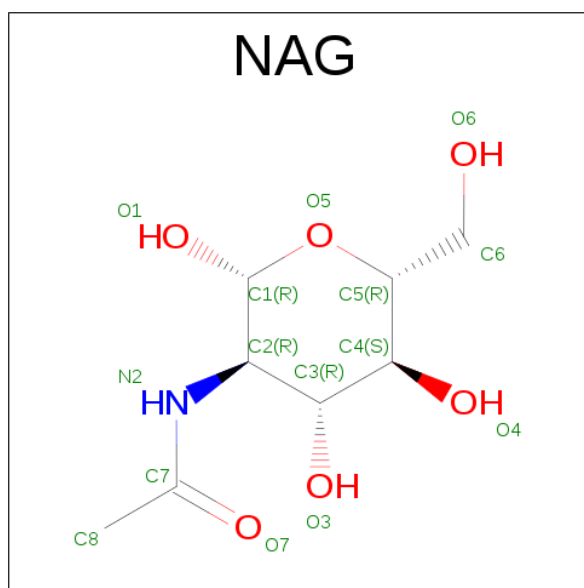
There are 2 unique types of molecules in this entry. The entry contains 25265 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1054	Total	C	N	O	S	0	0
			8234	5260	1363	1567	44		
1	B	1053	Total	C	N	O	S	0	0
			8226	5256	1362	1564	44		
1	C	1052	Total	C	N	O	S	0	0
			8217	5250	1360	1563	44		

- 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
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	

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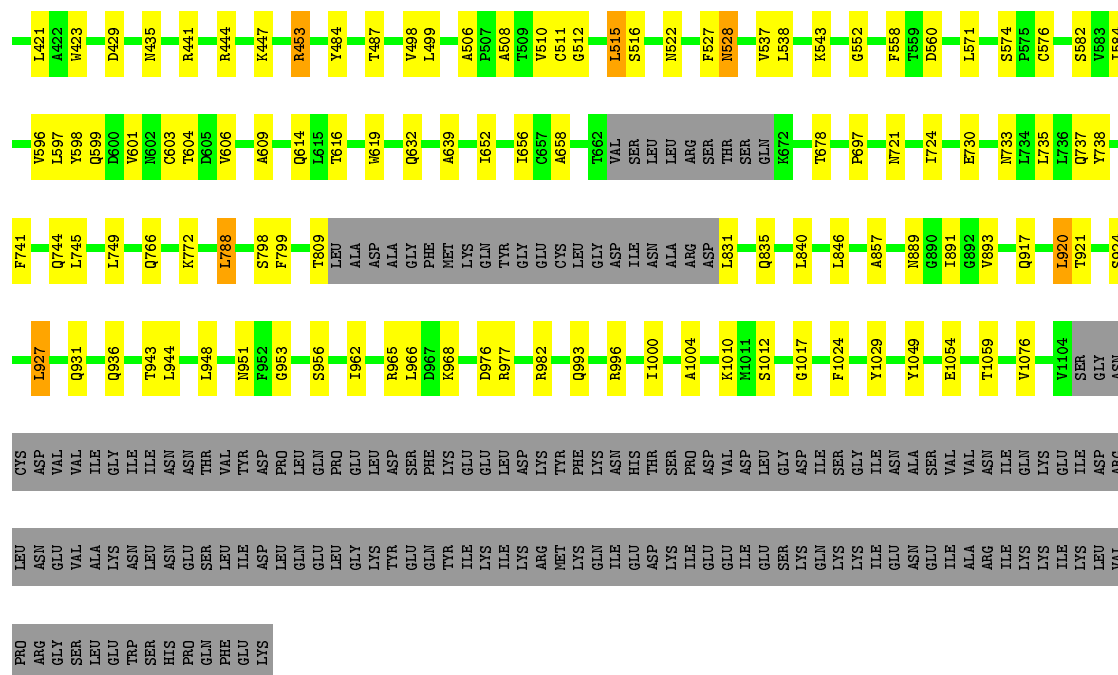
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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	A	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	

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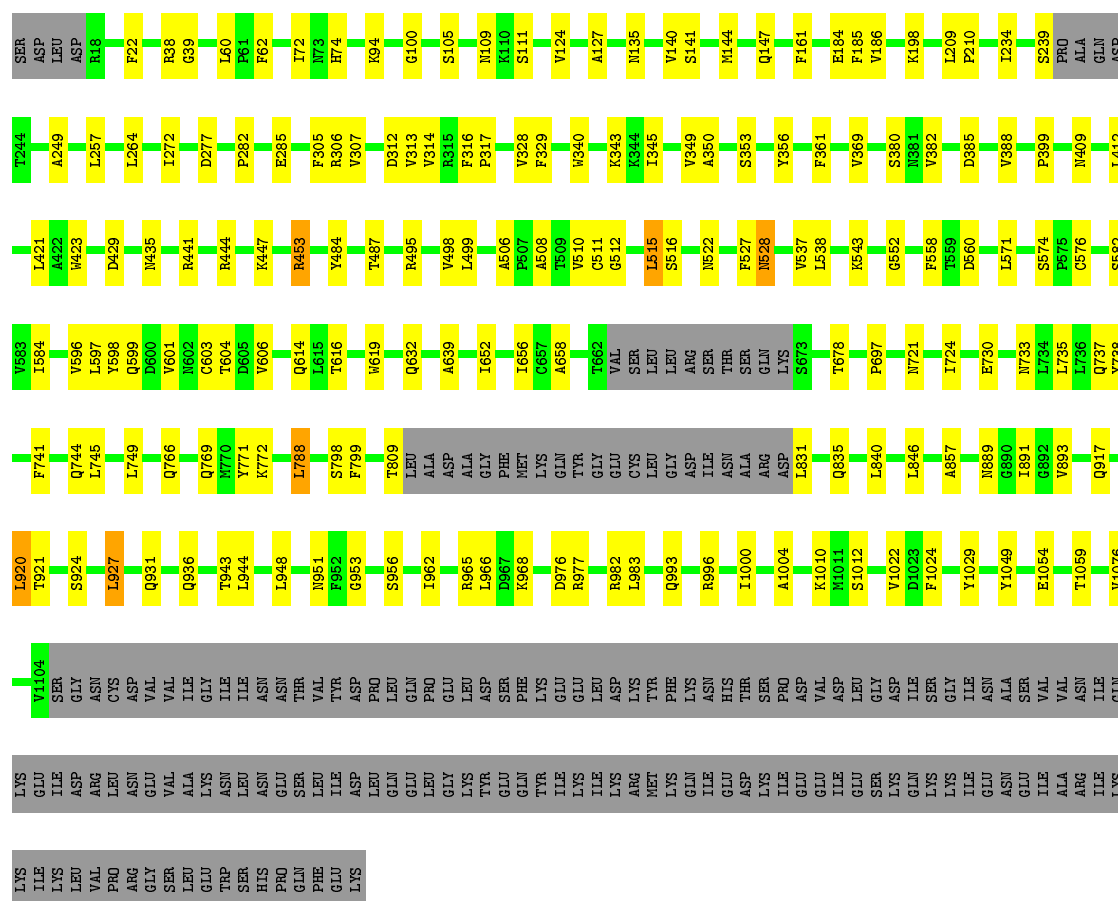
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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	B	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	
2	C	1	Total	C	N	O	0
			196	112	14	70	



• Molecule 1: Spike glycoprotein

Chain C: 71% 14% 14%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.38	0/8432	0.62	8/11475 (0.1%)
1	B	0.38	0/8424	0.62	8/11464 (0.1%)
1	C	0.38	0/8415	0.62	8/11453 (0.1%)
All	All	0.38	0/25271	0.62	24/34392 (0.1%)

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	4
1	B	0	4
1	C	0	4
All	All	0	12

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	515	LEU	CA-CB-CG	8.31	134.43	115.30
1	C	515	LEU	CA-CB-CG	8.31	134.42	115.30
1	B	515	LEU	CA-CB-CG	8.31	134.40	115.30
1	A	920	LEU	CA-CB-CG	7.47	132.49	115.30
1	B	920	LEU	CA-CB-CG	7.46	132.46	115.30
1	C	920	LEU	CA-CB-CG	7.45	132.44	115.30
1	C	927	LEU	CA-CB-CG	6.82	130.98	115.30
1	B	927	LEU	CA-CB-CG	6.81	130.97	115.30
1	A	927	LEU	CA-CB-CG	6.81	130.96	115.30
1	A	788	LEU	CA-CB-CG	5.58	128.14	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	788	LEU	CA-CB-CG	5.56	128.09	115.30
1	C	788	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	749	LEU	CA-CB-CG	5.52	128.00	115.30
1	B	749	LEU	CA-CB-CG	5.51	127.97	115.30
1	C	749	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	735	LEU	CA-CB-CG	5.29	127.46	115.30
1	C	735	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	735	LEU	CA-CB-CG	5.25	127.39	115.30
1	B	745	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	745	LEU	CA-CB-CG	5.18	127.22	115.30
1	C	745	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	846	LEU	CA-CB-CG	5.08	126.99	115.30
1	B	846	LEU	CA-CB-CG	5.07	126.95	115.30
1	C	846	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316	PHE	Peptide
1	A	512	GLY	Peptide
1	A	616	THR	Peptide
1	A	741	PHE	Peptide
1	B	316	PHE	Peptide
1	B	512	GLY	Peptide
1	B	616	THR	Peptide
1	B	741	PHE	Peptide
1	C	316	PHE	Peptide
1	C	512	GLY	Peptide
1	C	616	THR	Peptide
1	C	741	PHE	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	8234	0	8002	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8226	0	7997	95	0
1	C	8217	0	7984	94	0
2	A	196	0	180	3	0
2	B	196	0	180	3	0
2	C	196	0	180	3	0
All	All	25265	0	24523	264	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 5.

All (264) 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:953:GLY:HA3	1:A:977:ARG:HH11	1.61	0.66
1:C:953:GLY:HA3	1:C:977:ARG:HH11	1.61	0.66
1:B:891:ILE:HD12	1:B:1029:TYR:HB3	1.78	0.65
1:C:891:ILE:HD12	1:C:1029:TYR:HB3	1.78	0.65
1:A:891:ILE:HD12	1:A:1029:TYR:HB3	1.78	0.63
1:B:953:GLY:HA3	1:B:977:ARG:HH11	1.61	0.63
1:A:831:LEU:HB3	1:C:632:GLN:HE22	1.64	0.63
1:A:632:GLN:HE22	1:B:831:LEU:HB3	1.64	0.61
1:B:385:ASP:HB2	1:B:498:VAL:HB	1.83	0.60
1:B:632:GLN:HE22	1:C:831:LEU:HB3	1.64	0.60
1:C:385:ASP:HB2	1:C:498:VAL:HB	1.83	0.59
1:A:385:ASP:HB2	1:A:498:VAL:HB	1.83	0.59
1:B:38:ARG:NH1	1:B:184:GLU:OE2	2.36	0.59
1:A:349:VAL:HG13	1:A:511:CYS:HB3	1.85	0.59
1:A:38:ARG:NH1	1:A:184:GLU:OE2	2.36	0.59
1:C:317:PRO:HG2	1:C:511:CYS:HB2	1.85	0.58
1:B:349:VAL:HG13	1:B:511:CYS:HB3	1.85	0.58
1:C:38:ARG:NH1	1:C:184:GLU:OE2	2.36	0.58
1:A:317:PRO:HG2	1:A:511:CYS:HB2	1.85	0.58
1:C:349:VAL:HG13	1:C:511:CYS:HB3	1.85	0.58
1:B:317:PRO:HG2	1:B:511:CYS:HB2	1.85	0.57
1:C:62:PHE:HD2	1:C:277:ASP:HB2	1.69	0.57
1:B:62:PHE:HD2	1:B:277:ASP:HB2	1.69	0.57
1:C:421:LEU:HD13	1:C:499:LEU:HD13	1.88	0.56
1:A:62:PHE:HD2	1:A:277:ASP:HB2	1.69	0.56
1:C:599:GLN:HG3	1:C:606:VAL:HG11	1.87	0.56
1:C:380:SER:HA	1:C:508:ALA:HA	1.88	0.56
1:B:340:TRP:O	1:B:453:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LEU:HD13	1:B:499:LEU:HD13	1.87	0.56
1:A:599:GLN:HG3	1:A:606:VAL:HG11	1.87	0.56
1:A:380:SER:HA	1:A:508:ALA:HA	1.88	0.55
1:A:409:ASN:HD21	1:A:441:ARG:HB2	1.71	0.55
1:B:599:GLN:HG3	1:B:606:VAL:HG11	1.87	0.55
1:C:314:VAL:HA	1:C:516:SER:HB2	1.88	0.55
1:A:340:TRP:O	1:A:453:ARG:NH1	2.39	0.55
1:B:380:SER:HA	1:B:508:ALA:HA	1.88	0.55
1:B:314:VAL:HA	1:B:516:SER:HB2	1.88	0.55
1:C:409:ASN:HD21	1:C:441:ARG:HB2	1.71	0.55
1:C:340:TRP:O	1:C:453:ARG:NH1	2.39	0.55
1:A:421:LEU:HD13	1:A:499:LEU:HD13	1.88	0.54
1:B:409:ASN:HD21	1:B:441:ARG:HB2	1.72	0.54
1:C:936:GLN:HG2	1:C:996:ARG:HE	1.72	0.54
1:A:282:PRO:HG2	1:A:597:LEU:HD11	1.89	0.54
1:A:314:VAL:HA	1:A:516:SER:HB2	1.88	0.54
1:A:285:GLU:HB2	1:A:619:TRP:HE1	1.73	0.54
1:B:766:GLN:NE2	1:B:1012:SER:OG	2.41	0.54
1:A:766:GLN:NE2	1:A:1012:SER:OG	2.41	0.53
1:B:282:PRO:HG2	1:B:597:LEU:HD11	1.89	0.53
1:A:936:GLN:HG2	1:A:996:ARG:HE	1.72	0.53
1:C:282:PRO:HG2	1:C:597:LEU:HD11	1.89	0.53
1:B:936:GLN:HG2	1:B:996:ARG:HE	1.72	0.53
1:C:766:GLN:NE2	1:C:1012:SER:OG	2.41	0.53
1:A:798:SER:OG	1:A:799:PHE:N	2.42	0.53
1:B:285:GLU:HB2	1:B:619:TRP:HE1	1.73	0.53
1:A:329:PHE:HZ	1:A:499:LEU:HD11	1.74	0.53
1:B:329:PHE:HZ	1:B:499:LEU:HD11	1.74	0.53
1:A:109:ASN:ND2	2:A:1314:NAG:O3	2.42	0.53
1:B:798:SER:OG	1:B:799:PHE:N	2.42	0.52
1:C:798:SER:OG	1:C:799:PHE:N	2.42	0.52
1:C:329:PHE:HZ	1:C:499:LEU:HD11	1.74	0.52
1:C:285:GLU:HB2	1:C:619:TRP:HE1	1.73	0.52
1:A:948:LEU:HD13	1:C:558:PHE:HE2	1.75	0.52
1:B:558:PHE:HE2	1:C:948:LEU:HD13	1.75	0.52
1:A:965:ARG:HB2	1:C:369:VAL:HA	1.93	0.51
1:B:109:ASN:ND2	2:B:1314:NAG:O3	2.43	0.51
1:A:558:PHE:HE2	1:B:948:LEU:HD13	1.75	0.51
1:C:127:ALA:HB3	1:C:161:PHE:HB3	1.93	0.51
1:C:353:SER:HA	1:C:356:TYR:HB3	1.92	0.51
1:A:369:VAL:HA	1:B:965:ARG:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:VAL:HG13	1:A:257:LEU:HD11	1.93	0.51
1:B:353:SER:HA	1:B:356:TYR:HB3	1.92	0.51
1:B:543:LYS:NZ	1:B:560:ASP:OD2	2.44	0.51
1:C:543:LYS:NZ	1:C:560:ASP:OD2	2.44	0.51
1:A:538:LEU:HD12	1:A:571:LEU:HD13	1.93	0.51
1:A:543:LYS:NZ	1:A:560:ASP:OD2	2.44	0.50
1:C:186:VAL:HG13	1:C:257:LEU:HD11	1.93	0.50
1:A:185:PHE:HE1	1:A:198:LYS:HG3	1.75	0.50
1:A:353:SER:HA	1:A:356:TYR:HB3	1.92	0.50
1:A:39:GLY:HA3	1:A:60:LEU:HB3	1.93	0.50
1:C:39:GLY:HA3	1:C:60:LEU:HB3	1.93	0.50
1:B:127:ALA:HB3	1:B:161:PHE:HB3	1.93	0.50
1:B:185:PHE:HE1	1:B:198:LYS:HG3	1.75	0.50
1:A:312:ASP:O	1:A:528:ASN:N	2.41	0.50
1:B:186:VAL:HG13	1:B:257:LEU:HD11	1.93	0.50
1:C:1000:ILE:O	1:C:1004:ALA:N	2.45	0.50
1:B:312:ASP:O	1:B:528:ASN:N	2.41	0.50
1:A:127:ALA:HB3	1:A:161:PHE:HB3	1.93	0.50
1:B:39:GLY:HA3	1:B:60:LEU:HB3	1.93	0.50
1:C:185:PHE:HE1	1:C:198:LYS:HG3	1.75	0.50
1:B:1000:ILE:O	1:B:1004:ALA:N	2.45	0.49
1:B:369:VAL:HA	1:C:965:ARG:HB2	1.93	0.49
1:C:109:ASN:ND2	2:C:1314:NAG:O3	2.44	0.49
1:C:788:LEU:HD13	1:C:857:ALA:HB2	1.95	0.49
1:A:1010:LYS:NZ	1:A:1024:PHE:O	2.46	0.49
1:A:788:LEU:HD13	1:A:857:ALA:HB2	1.95	0.49
1:C:538:LEU:HD12	1:C:571:LEU:HD13	1.93	0.49
1:B:1010:LYS:NZ	1:B:1024:PHE:O	2.46	0.49
1:B:788:LEU:HD13	1:B:857:ALA:HB2	1.95	0.49
1:C:1010:LYS:NZ	1:C:1024:PHE:O	2.46	0.49
1:A:484:TYR:HB2	1:A:487:THR:HG23	1.95	0.49
1:B:100:GLY:HA3	1:B:234:ILE:HB	1.95	0.49
1:B:538:LEU:HD12	1:B:571:LEU:HD13	1.93	0.49
1:A:603:CYS:SG	1:A:604:THR:N	2.85	0.48
1:B:484:TYR:HB2	1:B:487:THR:HG23	1.95	0.48
1:C:603:CYS:SG	1:C:604:THR:N	2.85	0.48
1:A:100:GLY:HA3	1:A:234:ILE:HB	1.95	0.48
1:B:603:CYS:SG	1:B:604:THR:N	2.85	0.48
1:C:840:LEU:HD11	1:C:944:LEU:HD23	1.96	0.48
1:C:312:ASP:O	1:C:528:ASN:N	2.41	0.48
1:C:724:ILE:O	1:C:982:ARG:NH1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:GLY:HA3	1:C:234:ILE:HB	1.95	0.48
1:B:140:VAL:HG22	1:B:147:GLN:HA	1.96	0.48
1:C:345:ILE:HD13	1:C:382:VAL:HG23	1.96	0.48
1:B:313:VAL:HA	1:B:528:ASN:HB3	1.96	0.48
1:C:313:VAL:HA	1:C:528:ASN:HB3	1.96	0.48
1:C:484:TYR:HB2	1:C:487:THR:HG23	1.95	0.48
1:A:313:VAL:HA	1:A:528:ASN:HB3	1.96	0.48
1:C:527:PHE:HB3	1:C:538:LEU:HD21	1.95	0.48
1:B:345:ILE:HD13	1:B:382:VAL:HG23	1.96	0.47
1:B:891:ILE:HB	1:B:893:VAL:HG12	1.96	0.47
1:C:140:VAL:HG22	1:C:147:GLN:HA	1.96	0.47
1:A:328:VAL:HG22	1:A:343:LYS:HD3	1.96	0.47
1:A:94:LYS:NZ	1:A:249:ALA:O	2.48	0.47
1:A:361:PHE:HA	1:A:423:TRP:HB3	1.96	0.47
1:B:527:PHE:HB3	1:B:538:LEU:HD21	1.95	0.47
1:C:105:SER:HB2	1:C:111:SER:HB2	1.97	0.47
1:C:328:VAL:HG22	1:C:343:LYS:HD3	1.96	0.47
1:A:527:PHE:HB3	1:A:538:LEU:HD21	1.95	0.47
1:B:141:SER:HB3	1:B:144:MET:HB2	1.95	0.47
1:A:1000:ILE:O	1:A:1004:ALA:N	2.45	0.47
1:A:724:ILE:O	1:A:982:ARG:NH1	2.45	0.47
1:B:1059:THR:OG1	1:B:1076:VAL:O	2.32	0.47
1:B:105:SER:HB2	1:B:111:SER:HB2	1.97	0.47
1:B:840:LEU:HD11	1:B:944:LEU:HD23	1.96	0.47
1:A:141:SER:HB3	1:A:144:MET:HB2	1.96	0.47
1:C:141:SER:HB3	1:C:144:MET:HB2	1.95	0.47
1:A:140:VAL:HG22	1:A:147:GLN:HA	1.96	0.47
1:B:94:LYS:NZ	1:B:249:ALA:O	2.48	0.47
1:A:380:SER:HB3	1:A:506:ALA:HB3	1.97	0.47
1:A:738:TYR:OH	1:A:976:ASP:OD1	2.31	0.47
1:B:361:PHE:HA	1:B:423:TRP:HB3	1.96	0.47
1:C:965:ARG:HG3	1:C:966:LEU:HD12	1.97	0.47
1:A:105:SER:HB2	1:A:111:SER:HB2	1.97	0.47
1:A:965:ARG:HG3	1:A:966:LEU:HD12	1.97	0.47
1:C:584:ILE:HB	1:C:596:VAL:HG22	1.97	0.47
1:A:744:GLN:HG3	1:C:943:THR:HG21	1.97	0.47
1:A:345:ILE:HD13	1:A:382:VAL:HG23	1.96	0.46
1:A:840:LEU:HD11	1:A:944:LEU:HD23	1.96	0.46
1:B:724:ILE:O	1:B:982:ARG:NH1	2.45	0.46
1:B:965:ARG:HG3	1:B:966:LEU:HD12	1.97	0.46
1:C:306:ARG:HB3	1:C:576:CYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:LYS:NZ	1:C:249:ALA:O	2.48	0.46
1:C:1059:THR:OG1	1:C:1076:VAL:O	2.32	0.46
1:A:1059:THR:OG1	1:A:1076:VAL:O	2.32	0.46
1:A:943:THR:HG21	1:B:744:GLN:HG3	1.97	0.46
1:A:891:ILE:HB	1:A:893:VAL:HG12	1.96	0.46
1:B:328:VAL:HG22	1:B:343:LYS:HD3	1.96	0.46
1:C:891:ILE:HB	1:C:893:VAL:HG12	1.96	0.46
1:C:917:GLN:O	1:C:921:THR:OG1	2.34	0.46
1:A:993:GLN:OE1	1:A:996:ARG:NH1	2.49	0.46
1:C:361:PHE:HA	1:C:423:TRP:HB3	1.96	0.45
1:A:306:ARG:HB3	1:A:576:CYS:HB3	1.97	0.45
1:A:596:VAL:HG21	1:A:639:ALA:HB2	1.98	0.45
1:B:306:ARG:HB3	1:B:576:CYS:HB3	1.97	0.45
1:B:444:ARG:NH2	2:C:1310:NAG:O7	2.45	0.45
1:C:380:SER:HB3	1:C:506:ALA:HB3	1.97	0.45
1:B:584:ILE:HB	1:B:596:VAL:HG22	1.97	0.45
1:C:993:GLN:OE1	1:C:996:ARG:NH1	2.49	0.45
1:A:584:ILE:HB	1:A:596:VAL:HG22	1.97	0.45
1:B:596:VAL:HG21	1:B:639:ALA:HB2	1.98	0.45
1:B:993:GLN:OE1	1:B:996:ARG:NH1	2.49	0.45
1:B:943:THR:HG21	1:C:744:GLN:HG3	1.97	0.45
1:B:380:SER:HB3	1:B:506:ALA:HB3	1.97	0.45
1:C:596:VAL:HG21	1:C:639:ALA:HB2	1.98	0.44
1:C:738:TYR:OH	1:C:976:ASP:OD1	2.31	0.44
1:B:582:SER:O	1:B:598:TYR:N	2.50	0.44
1:B:956:SER:H	1:B:962:ILE:HD11	1.83	0.44
1:B:738:TYR:OH	1:B:976:ASP:OD1	2.31	0.44
1:A:582:SER:O	1:A:598:TYR:N	2.51	0.44
1:A:956:SER:H	1:A:962:ILE:HD11	1.83	0.44
1:B:124:VAL:HG21	2:B:1312:NAG:H82	2.00	0.44
1:C:399:PRO:HD3	1:C:412:LEU:HD23	2.00	0.44
1:A:917:GLN:O	1:A:921:THR:OG1	2.33	0.44
1:A:737:GLN:HB2	1:C:951:ASN:HB3	2.00	0.44
1:C:956:SER:H	1:C:962:ILE:HD11	1.83	0.44
1:A:264:LEU:HD22	1:A:272:ILE:HD13	2.00	0.44
1:B:399:PRO:HD3	1:B:412:LEU:HD23	2.00	0.44
1:C:582:SER:O	1:C:598:TYR:N	2.50	0.44
1:B:951:ASN:HB3	1:C:737:GLN:HB2	2.00	0.43
1:C:1029:TYR:HB2	1:C:1049:TYR:HB3	2.00	0.43
1:A:124:VAL:HG21	2:A:1312:NAG:H82	1.99	0.43
1:B:264:LEU:HD22	1:B:272:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ILE:HA	1:B:678:THR:HA	2.01	0.43
1:A:601:VAL:HG22	1:B:835:GLN:HE22	1.82	0.43
1:A:835:GLN:HE22	1:C:601:VAL:HG22	1.82	0.43
1:B:601:VAL:HG22	1:C:835:GLN:HE22	1.82	0.43
1:A:951:ASN:HB3	1:B:737:GLN:HB2	2.00	0.43
1:A:444:ARG:NH2	2:B:1310:NAG:O7	2.45	0.43
1:B:652:ILE:HD11	1:B:658:ALA:HB2	2.01	0.43
1:C:769:GLN:NE2	1:C:771:TYR:OH	2.48	0.43
1:A:399:PRO:HD3	1:A:412:LEU:HD23	2.00	0.43
1:A:730:GLU:HG3	1:A:968:LYS:HD3	2.01	0.43
1:B:1029:TYR:HB2	1:B:1049:TYR:HB3	2.01	0.43
1:B:917:GLN:O	1:B:921:THR:OG1	2.34	0.43
1:C:264:LEU:HD22	1:C:272:ILE:HD13	2.00	0.43
1:A:1029:TYR:HB2	1:A:1049:TYR:HB3	2.00	0.43
2:A:1310:NAG:O7	1:C:444:ARG:NH2	2.45	0.43
1:C:652:ILE:HD11	1:C:658:ALA:HB2	2.01	0.43
1:A:209:LEU:HD12	1:A:210:PRO:HD2	2.01	0.43
1:B:305:PHE:HD1	1:B:305:PHE:HA	1.76	0.43
1:A:552:GLY:O	1:A:560:ASP:N	2.50	0.42
1:C:124:VAL:HG21	2:C:1312:NAG:H82	2.00	0.42
1:A:652:ILE:HD11	1:A:658:ALA:HB2	2.01	0.42
1:C:656:ILE:HA	1:C:678:THR:HA	2.01	0.42
1:B:22:PHE:H	1:B:135:ASN:HD22	1.68	0.42
1:B:209:LEU:HD12	1:B:210:PRO:HD2	2.01	0.42
1:C:350:ALA:HB3	1:C:510:VAL:HG13	2.02	0.42
1:A:22:PHE:H	1:A:135:ASN:HD22	1.67	0.42
1:B:537:VAL:N	1:B:574:SER:O	2.44	0.42
1:A:444:ARG:NH1	1:A:447:LYS:O	2.53	0.42
1:B:730:GLU:HG3	1:B:968:LYS:HD3	2.01	0.42
1:A:656:ILE:HA	1:A:678:THR:HA	2.01	0.42
1:B:444:ARG:NH1	1:B:447:LYS:O	2.53	0.42
1:C:209:LEU:HD12	1:C:210:PRO:HD2	2.01	0.42
1:C:444:ARG:NH1	1:C:447:LYS:O	2.53	0.42
1:C:552:GLY:O	1:C:560:ASP:N	2.50	0.42
1:C:730:GLU:HG3	1:C:968:LYS:HD3	2.01	0.42
1:A:140:VAL:O	1:A:239:SER:N	2.53	0.42
1:A:307:VAL:N	1:A:614:GLN:O	2.53	0.42
1:C:22:PHE:H	1:C:135:ASN:HD22	1.68	0.42
1:A:350:ALA:HB3	1:A:510:VAL:HG13	2.02	0.41
1:A:924:SER:HB2	1:A:927:LEU:HG	2.02	0.41
1:B:72:ILE:HG23	1:B:74:HIS:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:VAL:N	1:C:614:GLN:O	2.53	0.41
1:B:140:VAL:O	1:B:239:SER:N	2.53	0.41
1:C:72:ILE:HG23	1:C:74:HIS:H	1.86	0.41
1:A:1022:VAL:HG21	1:B:1017:GLY:HA3	2.02	0.41
1:B:924:SER:HB2	1:B:927:LEU:HG	2.02	0.41
1:C:697:PRO:HA	1:C:1054:GLU:HA	2.03	0.41
1:C:924:SER:HB2	1:C:927:LEU:HG	2.03	0.41
1:A:697:PRO:HA	1:A:1054:GLU:HA	2.03	0.41
1:B:609:ALA:HB1	1:B:614:GLN:HB2	2.03	0.41
1:A:72:ILE:HG23	1:A:74:HIS:H	1.86	0.41
1:A:429:ASP:O	1:A:435:ASN:ND2	2.54	0.41
1:B:697:PRO:HA	1:B:1054:GLU:HA	2.03	0.41
1:B:552:GLY:O	1:B:560:ASP:N	2.50	0.41
1:A:609:ALA:HB1	1:A:614:GLN:HB2	2.03	0.41
1:B:429:ASP:O	1:B:435:ASN:ND2	2.54	0.41
1:B:307:VAL:N	1:B:614:GLN:O	2.53	0.41
1:C:429:ASP:O	1:C:435:ASN:ND2	2.54	0.41
1:A:809:THR:H	1:A:931:GLN:HE22	1.69	0.40
1:C:809:THR:H	1:C:931:GLN:HE22	1.69	0.40
1:C:983:LEU:HA	1:C:983:LEU:HD13	1.95	0.40
1:A:582:SER:H	1:A:598:TYR:HB2	1.86	0.40
1:B:809:THR:H	1:B:931:GLN:HE22	1.69	0.40
1:C:388:VAL:HG22	1:C:495:ARG:HG2	2.03	0.40
1:A:91:ALA:HA	1:A:252:TYR:HA	2.03	0.40
1:A:388:VAL:HG22	1:A:495:ARG:HG2	2.03	0.40
1:B:350:ALA:HB3	1:B:510:VAL:HG13	2.02	0.40
1:C:140:VAL:O	1:C:239:SER:N	2.53	0.40
1:C:537:VAL:N	1:C:574:SER:O	2.44	0.40
1:A:1017:GLY:HA3	1:C:1022:VAL:HG21	2.02	0.40
1:B:105:SER:OG	1:B:227:ASN:O	2.34	0.40
1:B:582:SER:H	1:B:598:TYR:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1046/1228 (85%)	950 (91%)	96 (9%)	0	100	100
1	B	1045/1228 (85%)	950 (91%)	95 (9%)	0	100	100
1	C	1044/1228 (85%)	948 (91%)	96 (9%)	0	100	100
All	All	3135/3684 (85%)	2848 (91%)	287 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	914/1073 (85%)	904 (99%)	10 (1%)	78	92
1	B	913/1073 (85%)	903 (99%)	10 (1%)	78	92
1	C	912/1073 (85%)	902 (99%)	10 (1%)	78	92
All	All	2739/3219 (85%)	2709 (99%)	30 (1%)	79	92

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	PHE
1	A	453	ARG
1	A	515	LEU
1	A	522	ASN
1	A	528	ASN
1	A	721	ASN
1	A	733	ASN
1	A	772	LYS
1	A	889	ASN
1	A	920	LEU
1	B	305	PHE
1	B	453	ARG
1	B	515	LEU

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Mol	Chain	Res	Type
1	B	522	ASN
1	B	528	ASN
1	B	721	ASN
1	B	733	ASN
1	B	772	LYS
1	B	889	ASN
1	B	920	LEU
1	C	305	PHE
1	C	453	ARG
1	C	515	LEU
1	C	522	ASN
1	C	528	ASN
1	C	721	ASN
1	C	733	ASN
1	C	772	LYS
1	C	889	ASN
1	C	920	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	135	ASN
1	A	409	ASN
1	A	522	ASN
1	A	528	ASN
1	A	549	GLN
1	A	599	GLN
1	A	614	GLN
1	A	632	GLN
1	A	641	HIS
1	A	661	HIS
1	A	721	ASN
1	A	733	ASN
1	A	766	GLN
1	A	835	GLN
1	A	917	GLN
1	A	937	ASN
1	A	1090	ASN
1	A	1101	ASN
1	B	70	HIS
1	B	135	ASN

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Mol	Chain	Res	Type
1	B	409	ASN
1	B	522	ASN
1	B	528	ASN
1	B	549	GLN
1	B	599	GLN
1	B	614	GLN
1	B	632	GLN
1	B	641	HIS
1	B	661	HIS
1	B	721	ASN
1	B	733	ASN
1	B	766	GLN
1	B	917	GLN
1	B	937	ASN
1	B	1090	ASN
1	B	1101	ASN
1	C	70	HIS
1	C	135	ASN
1	C	201	GLN
1	C	409	ASN
1	C	522	ASN
1	C	528	ASN
1	C	549	GLN
1	C	599	GLN
1	C	614	GLN
1	C	632	GLN
1	C	641	HIS
1	C	661	HIS
1	C	721	ASN
1	C	733	ASN
1	C	766	GLN
1	C	835	GLN
1	C	917	GLN
1	C	937	ASN
1	C	1090	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

42 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	-	14,14,15	0.54	0	15,19,21	1.01	1 (6%)
2	NAG	A	1302	1	14,14,15	0.76	0	15,19,21	1.09	2 (13%)
2	NAG	A	1303	1	14,14,15	0.35	0	15,19,21	1.01	1 (6%)
2	NAG	A	1304	1	14,14,15	1.49	2 (14%)	15,19,21	1.94	2 (13%)
2	NAG	A	1305	1	14,14,15	0.41	0	15,19,21	1.06	1 (6%)
2	NAG	A	1306	1	14,14,15	0.45	0	15,19,21	0.43	0
2	NAG	A	1307	1	14,14,15	0.44	0	15,19,21	0.68	0
2	NAG	A	1308	1	14,14,15	0.48	0	15,19,21	0.68	1 (6%)
2	NAG	A	1309	1	14,14,15	0.36	0	15,19,21	0.39	0
2	NAG	A	1310	1	14,14,15	0.32	0	15,19,21	0.57	0
2	NAG	A	1311	1	14,14,15	0.38	0	15,19,21	0.63	0
2	NAG	A	1312	1	14,14,15	0.66	1 (7%)	15,19,21	0.61	0
2	NAG	A	1313	1	14,14,15	0.41	0	15,19,21	0.58	0
2	NAG	A	1314	-	14,14,15	0.39	0	15,19,21	0.45	0
2	NAG	B	1301	1	14,14,15	0.86	1 (7%)	15,19,21	1.18	2 (13%)
2	NAG	B	1302	1	14,14,15	0.80	2 (14%)	15,19,21	1.09	2 (13%)
2	NAG	B	1303	1	14,14,15	0.35	0	15,19,21	1.00	1 (6%)
2	NAG	B	1304	1	14,14,15	1.49	2 (14%)	15,19,21	1.94	3 (20%)
2	NAG	B	1305	1	14,14,15	0.34	0	15,19,21	1.05	1 (6%)
2	NAG	B	1306	1	14,14,15	0.45	0	15,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1307	1	14,14,15	0.44	0	15,19,21	0.67	0
2	NAG	B	1308	1	14,14,15	0.46	0	15,19,21	0.69	1 (6%)
2	NAG	B	1309	1	14,14,15	0.37	0	15,19,21	0.39	0
2	NAG	B	1310	1	14,14,15	0.32	0	15,19,21	0.56	0
2	NAG	B	1311	1	14,14,15	0.36	0	15,19,21	0.65	0
2	NAG	B	1312	1	14,14,15	0.65	0	15,19,21	0.61	0
2	NAG	B	1313	1	14,14,15	0.40	0	15,19,21	0.59	0
2	NAG	B	1314	-	14,14,15	0.38	0	15,19,21	0.47	0
2	NAG	C	1301	1	14,14,15	0.90	1 (7%)	15,19,21	1.25	2 (13%)
2	NAG	C	1302	1	14,14,15	0.75	0	15,19,21	1.09	2 (13%)
2	NAG	C	1303	1	14,14,15	0.33	0	15,19,21	1.00	1 (6%)
2	NAG	C	1304	1	14,14,15	1.49	2 (14%)	15,19,21	1.95	3 (20%)
2	NAG	C	1305	1	14,14,15	0.34	0	15,19,21	1.05	1 (6%)
2	NAG	C	1306	1	14,14,15	0.43	0	15,19,21	0.43	0
2	NAG	C	1307	1	14,14,15	0.43	0	15,19,21	0.67	0
2	NAG	C	1308	1	14,14,15	0.47	0	15,19,21	0.66	1 (6%)
2	NAG	C	1309	1	14,14,15	0.37	0	15,19,21	0.39	0
2	NAG	C	1310	1	14,14,15	0.32	0	15,19,21	0.56	0
2	NAG	C	1311	1	14,14,15	0.36	0	15,19,21	0.64	0
2	NAG	C	1312	1	14,14,15	0.66	0	15,19,21	0.62	0
2	NAG	C	1313	1	14,14,15	0.41	0	15,19,21	0.58	0
2	NAG	C	1314	-	14,14,15	0.38	0	15,19,21	0.44	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	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1312	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1314	-	-	0/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1314	-	-	0/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1314	-	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1302	NAG	O5-C1	2.04	1.47	1.43
2	B	1302	NAG	C1-C2	2.05	1.55	1.52
2	A	1312	NAG	C1-C2	2.07	1.55	1.52
2	B	1301	NAG	C1-C2	2.73	1.56	1.52
2	C	1301	NAG	C1-C2	2.90	1.56	1.52
2	A	1304	NAG	O5-C1	3.76	1.49	1.43
2	B	1304	NAG	O5-C1	3.78	1.49	1.43
2	C	1304	NAG	C1-C2	3.79	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1304	NAG	O5-C1	3.84	1.50	1.43
2	B	1304	NAG	C1-C2	3.85	1.57	1.52
2	A	1304	NAG	C1-C2	3.86	1.57	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1304	NAG	C3-C4-C5	2.05	113.83	110.22
2	B	1302	NAG	C1-O5-C5	2.08	115.03	112.17
2	C	1304	NAG	C3-C4-C5	2.08	113.89	110.22
2	A	1302	NAG	C1-O5-C5	2.09	115.05	112.17
2	C	1302	NAG	C1-O5-C5	2.09	115.05	112.17
2	B	1301	NAG	C2-N2-C7	2.10	126.01	122.94
2	C	1308	NAG	C1-O5-C5	2.11	115.07	112.17
2	C	1301	NAG	C2-N2-C7	2.13	126.05	122.94
2	A	1308	NAG	C1-O5-C5	2.17	115.15	112.17
2	B	1308	NAG	C1-O5-C5	2.20	115.20	112.17
2	C	1304	NAG	C4-C3-C2	2.71	114.99	111.02
2	B	1304	NAG	C4-C3-C2	2.75	115.04	111.02
2	A	1304	NAG	C4-C3-C2	2.75	115.05	111.02
2	C	1303	NAG	C2-N2-C7	2.87	127.13	122.94
2	B	1303	NAG	C2-N2-C7	2.87	127.13	122.94
2	A	1303	NAG	C2-N2-C7	2.91	127.19	122.94
2	A	1301	NAG	C2-N2-C7	2.96	127.27	122.94
2	B	1302	NAG	C2-N2-C7	2.99	127.31	122.94
2	C	1302	NAG	C2-N2-C7	2.99	127.31	122.94
2	A	1302	NAG	C2-N2-C7	3.02	127.35	122.94
2	C	1305	NAG	C2-N2-C7	3.05	127.40	122.94
2	B	1305	NAG	C2-N2-C7	3.06	127.40	122.94
2	A	1305	NAG	C2-N2-C7	3.09	127.45	122.94
2	B	1301	NAG	C1-O5-C5	3.47	116.95	112.17
2	C	1301	NAG	C1-O5-C5	3.75	117.34	112.17
2	A	1304	NAG	C1-O5-C5	6.52	121.16	112.17
2	B	1304	NAG	C1-O5-C5	6.54	121.18	112.17
2	C	1304	NAG	C1-O5-C5	6.56	121.21	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1310	NAG	1	0
2	A	1312	NAG	1	0
2	A	1314	NAG	1	0
2	B	1310	NAG	1	0
2	B	1312	NAG	1	0
2	B	1314	NAG	1	0
2	C	1310	NAG	1	0
2	C	1312	NAG	1	0
2	C	1314	NAG	1	0

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.