



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2021 – 04:25 PM EDT

PDB ID : 4FP8
Title : Crystal structure of broadly neutralizing antibody C05 bound to H3 influenza hemagglutinin, HA1 subunit
Authors : Ekiert, D.C.; Wilson, I.A.
Deposited on : 2012-06-21
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

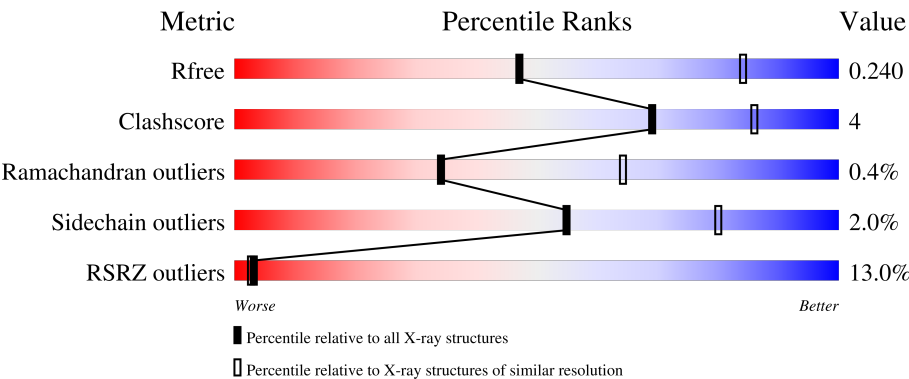
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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.



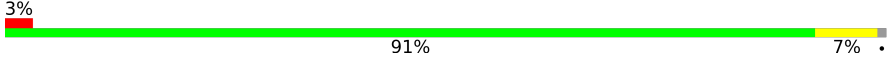

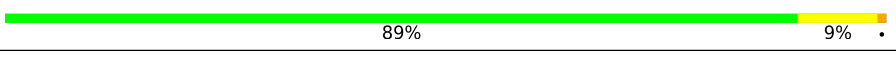
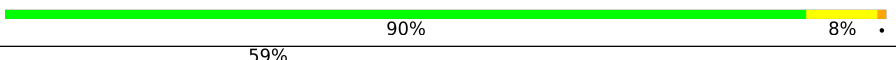

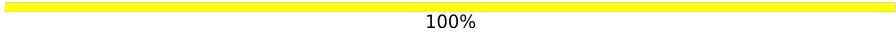
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	278	<div><div>7%</div><div>88%</div><div>8%</div><div>.</div></div>
1	B	278	<div><div>11%</div><div>92%</div><div>.</div><div>.</div></div>
1	C	278	<div><div>15%</div><div>86%</div><div>9%</div><div>5%</div></div>
1	D	278	<div><div>19%</div><div>88%</div><div>8%</div><div>.</div></div>
2	H	241	<div><div>3%</div><div>88%</div><div>10%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
2	I	241	 3% 91% 7% •
2	J	241	 5% 91% 8% •
2	K	241	 30% 88% 10% ••
3	L	214	 88% 10% •
3	M	214	 89% 9% •
3	N	214	 90% 8% •
3	O	214	 59% 87% 11% •
4	E	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22406 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	8	0
			2141	1346	375	408	12			
1	B	267	Total	C	N	O	S	0	8	0
			2141	1346	375	408	12			
1	C	265	Total	C	N	O	S	0	7	0
			2116	1330	369	405	12			
1	D	266	Total	C	N	O	S	0	8	0
			2128	1335	374	407	12			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	ALA	-	expression tag	UNP Q91MA7
A	40	ASP	-	expression tag	UNP Q91MA7
A	41	PRO	-	expression tag	UNP Q91MA7
A	42	GLY	-	expression tag	UNP Q91MA7
A	310	GLY	-	expression tag	UNP Q91MA7
A	311	HIS	-	expression tag	UNP Q91MA7
A	312	HIS	-	expression tag	UNP Q91MA7
A	313	HIS	-	expression tag	UNP Q91MA7
A	314	HIS	-	expression tag	UNP Q91MA7
A	315	HIS	-	expression tag	UNP Q91MA7
A	316	HIS	-	expression tag	UNP Q91MA7
B	39	ALA	-	expression tag	UNP Q91MA7
B	40	ASP	-	expression tag	UNP Q91MA7
B	41	PRO	-	expression tag	UNP Q91MA7
B	42	GLY	-	expression tag	UNP Q91MA7
B	310	GLY	-	expression tag	UNP Q91MA7
B	311	HIS	-	expression tag	UNP Q91MA7
B	312	HIS	-	expression tag	UNP Q91MA7
B	313	HIS	-	expression tag	UNP Q91MA7
B	314	HIS	-	expression tag	UNP Q91MA7
B	315	HIS	-	expression tag	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	316	HIS	-	expression tag	UNP Q91MA7
C	39	ALA	-	expression tag	UNP Q91MA7
C	40	ASP	-	expression tag	UNP Q91MA7
C	41	PRO	-	expression tag	UNP Q91MA7
C	42	GLY	-	expression tag	UNP Q91MA7
C	310	GLY	-	expression tag	UNP Q91MA7
C	311	HIS	-	expression tag	UNP Q91MA7
C	312	HIS	-	expression tag	UNP Q91MA7
C	313	HIS	-	expression tag	UNP Q91MA7
C	314	HIS	-	expression tag	UNP Q91MA7
C	315	HIS	-	expression tag	UNP Q91MA7
C	316	HIS	-	expression tag	UNP Q91MA7
D	39	ALA	-	expression tag	UNP Q91MA7
D	40	ASP	-	expression tag	UNP Q91MA7
D	41	PRO	-	expression tag	UNP Q91MA7
D	42	GLY	-	expression tag	UNP Q91MA7
D	310	GLY	-	expression tag	UNP Q91MA7
D	311	HIS	-	expression tag	UNP Q91MA7
D	312	HIS	-	expression tag	UNP Q91MA7
D	313	HIS	-	expression tag	UNP Q91MA7
D	314	HIS	-	expression tag	UNP Q91MA7
D	315	HIS	-	expression tag	UNP Q91MA7
D	316	HIS	-	expression tag	UNP Q91MA7

- Molecule 2 is a protein called Antibody C05, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
2	I	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
2	J	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
2	K	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			

- Molecule 3 is a protein called Antibody C05, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			

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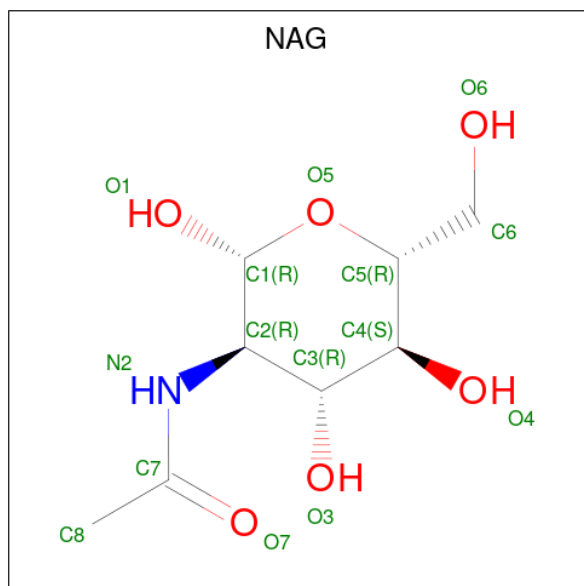
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
3	N	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
3	O	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

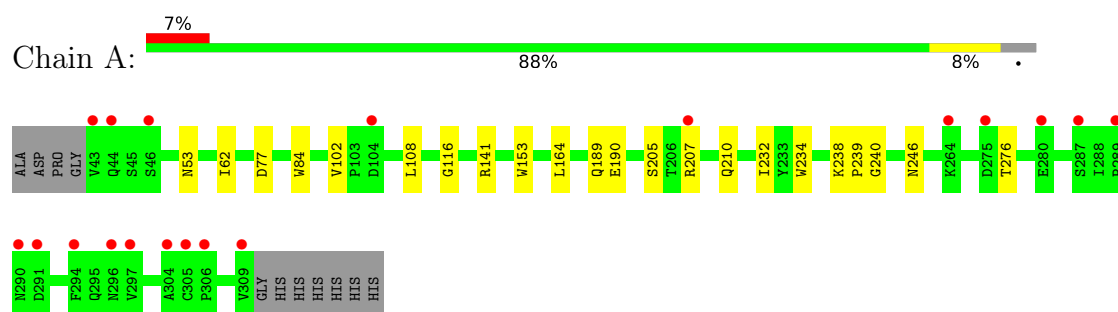
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total 1	Zn 1	0	0
6	L	2	Total 2	Zn 2	0	0
6	M	1	Total 1	Zn 1	0	0
6	J	1	Total 1	Zn 1	0	0
6	N	2	Total 2	Zn 2	0	0
6	O	1	Total 1	Zn 1	0	0

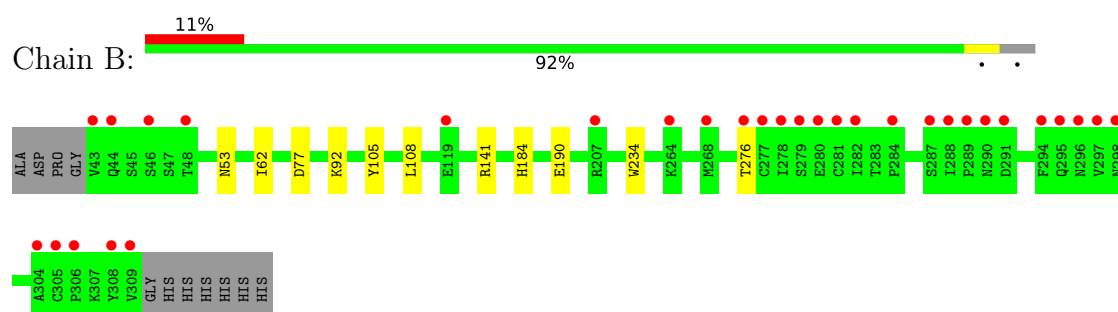
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

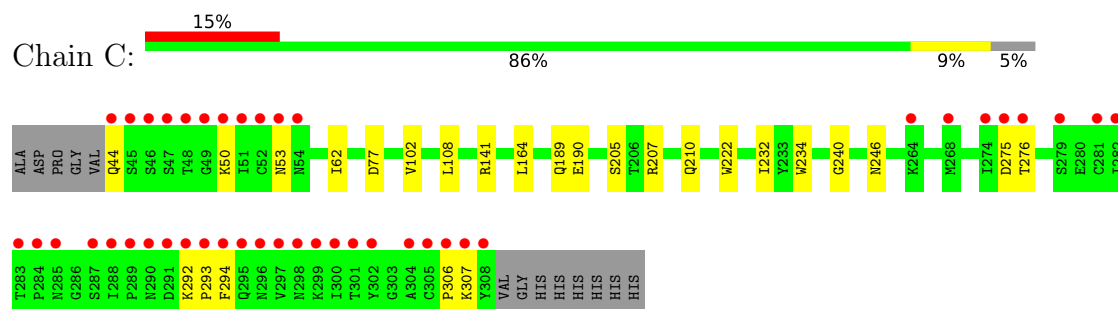
- Molecule 1: Hemagglutinin HA1 chain



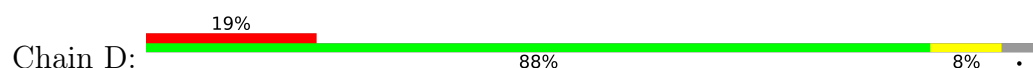
- Molecule 1: Hemagglutinin HA1 chain

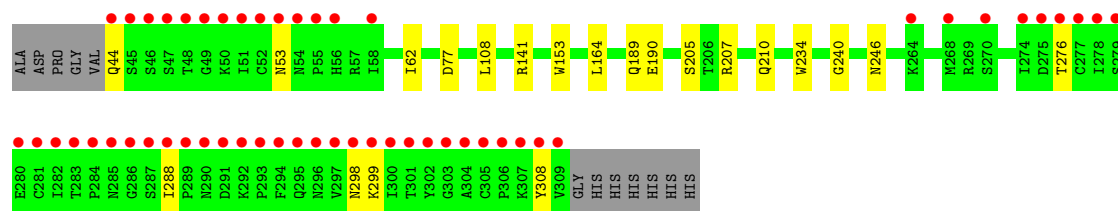


- Molecule 1: Hemagglutinin HA1 chain

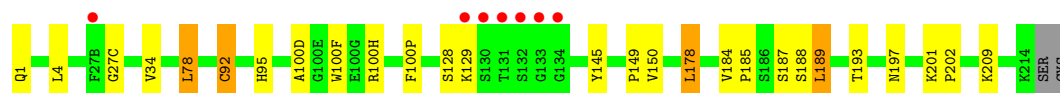
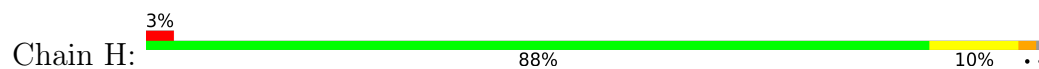


- Molecule 1: Hemagglutinin HA1 chain

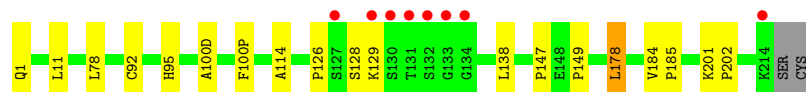




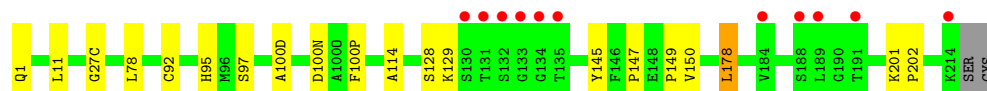
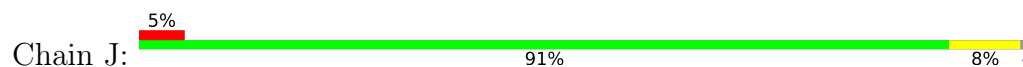
• Molecule 2: Antibody C05, heavy chain



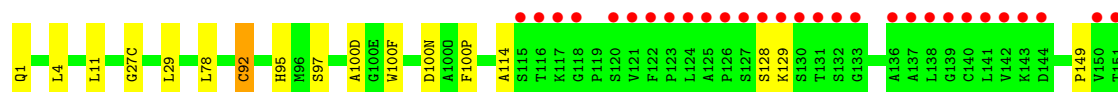
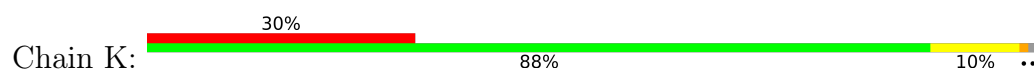
• Molecule 2: Antibody C05, heavy chain



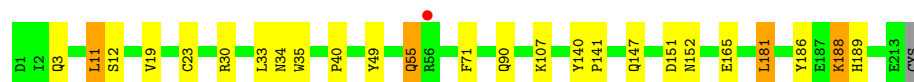
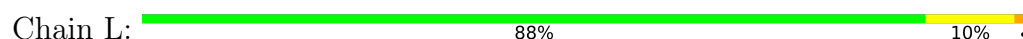
• Molecule 2: Antibody C05, heavy chain




• Molecule 2: Antibody C05, heavy chain



• Molecule 3: Antibody C05, light chain




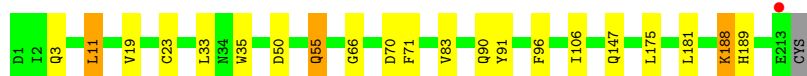
• Molecule 3: Antibody C05, light chain

Chain M:  89% 9%




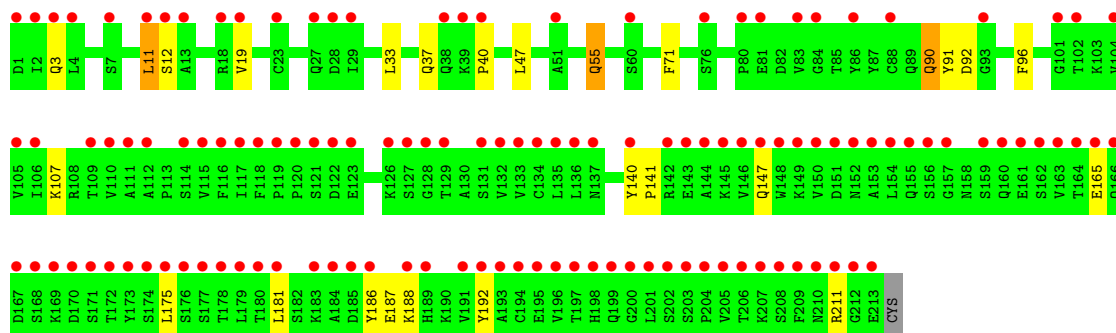
- Molecule 3: Antibody C05, light chain

Chain N:  90% 8%



- Molecule 3: Antibody C05, light chain

Chain O:  59% 87% 11%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.79Å 247.72Å 95.38Å 90.00° 91.33° 90.00°	Depositor
Resolution (Å)	44.49 – 2.95 44.49 – 2.95	Depositor EDS
% Data completeness (in resolution range)	95.1 (44.49-2.95) 95.0 (44.49-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.212 , 0.241 0.210 , 0.240	Depositor DCC
R_{free} test set	4191 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for l,k,-h 0.028 for h,-k,-l 0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22406	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.30	0/2195	0.58	0/2990
1	B	0.29	0/2195	0.57	0/2990
1	C	0.29	0/2170	0.59	0/2956
1	D	0.31	0/2181	0.58	0/2971
2	H	0.31	0/1837	0.58	1/2500 (0.0%)
2	I	0.28	0/1837	0.54	0/2500
2	J	0.28	0/1837	0.54	0/2500
2	K	0.26	0/1837	0.51	0/2500
3	L	0.34	0/1682	0.59	0/2280
3	M	0.32	0/1682	0.57	0/2280
3	N	0.30	0/1682	0.56	0/2280
3	O	0.26	0/1682	0.52	0/2280
All	All	0.30	0/22817	0.56	1/31027 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	100(H)	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2141	0	2074	13	0
1	B	2141	0	2075	12	0
1	C	2116	0	2044	21	0
1	D	2128	0	2058	18	0
2	H	1806	0	1749	16	0
2	I	1806	0	1749	13	0
2	J	1806	0	1749	13	0
2	K	1806	0	1749	20	0
3	L	1648	0	1614	19	0
3	M	1648	0	1614	15	0
3	N	1648	0	1614	12	0
3	O	1648	0	1614	15	0
4	E	28	0	25	0	0
5	A	14	0	13	0	0
5	D	14	0	13	0	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	L	2	0	0	0	0
6	M	1	0	0	0	0
6	N	2	0	0	0	0
6	O	1	0	0	0	0
All	All	22406	0	21754	165	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 4.

All (165) 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:C:205:SER:HB3	1:C:210:GLN:HG3	1.64	0.80
1:A:77:ASP:OD2	1:A:141:ARG:NH1	2.16	0.78
3:M:11:LEU:HD12	3:M:11:LEU:C	2.09	0.72
1:D:299:LYS:HA	1:D:308:TYR:CG	2.28	0.69
1:D:210:GLN:HB3	3:M:12:SER:HB2	1.77	0.65
2:J:11:LEU:HD21	2:J:114:ALA:O	1.96	0.65
1:C:77:ASP:OD2	1:C:141:ARG:NH1	2.22	0.64
3:O:11:LEU:C	3:O:11:LEU:HD12	2.18	0.64
1:D:205:SER:HB3	1:D:210:GLN:HG3	1.80	0.62
1:C:293:PRO:HG2	1:C:294:PHE:CD2	2.35	0.61
2:J:11:LEU:HB2	2:J:147:PRO:HG3	1.82	0.61
1:B:190:GLU:HG3	2:I:100(D):ALA:HB2	1.81	0.60
1:A:189:GLN:HG3	2:H:27(C):GLY:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:GLU:HG3	2:J:100(D):ALA:HB2	1.84	0.60
1:D:190:GLU:HG3	2:K:100(D):ALA:HB2	1.84	0.60
3:N:33:LEU:HD22	3:N:71:PHE:CG	2.38	0.58
3:L:11:LEU:C	3:L:11:LEU:HD12	2.25	0.57
3:N:11:LEU:HD21	3:N:19:VAL:HG13	1.85	0.57
3:N:83:VAL:HG12	3:N:106:ILE:HG12	1.87	0.56
2:J:95:HIS:CE1	2:J:100(P):PHE:CE2	2.92	0.56
3:M:33:LEU:HD22	3:M:71:PHE:CG	2.40	0.56
3:M:91:TYR:HB2	3:M:96:PHE:CE1	2.40	0.56
3:O:90:GLN:OE1	3:O:92:ASP:N	2.39	0.56
3:L:11:LEU:HD21	3:L:19:VAL:HG13	1.88	0.56
3:N:83:VAL:CG1	3:N:106:ILE:HG12	2.37	0.55
2:K:11:LEU:HD21	2:K:114:ALA:O	2.07	0.55
3:L:151:ASP:OD1	3:L:189:HIS:HB3	2.06	0.55
2:I:178:LEU:C	2:I:178:LEU:HD23	2.27	0.55
2:J:178:LEU:C	2:J:178:LEU:HD23	2.27	0.55
1:D:276:THR:O	1:D:276:THR:HG23	2.07	0.55
2:H:128:SER:O	2:H:129:LYS:HB3	2.05	0.55
1:A:207[B]:ARG:NH1	1:A:240:GLY:O	2.38	0.55
1:D:77:ASP:OD2	1:D:141:ARG:NH1	2.37	0.55
2:I:128:SER:O	2:I:129:LYS:HB3	2.07	0.55
1:C:294:PHE:N	1:C:306:PRO:HB3	2.22	0.55
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.42	0.54
3:N:11:LEU:C	3:N:11:LEU:HD12	2.27	0.54
3:N:50:ASP:OD1	3:N:91:TYR:OH	2.19	0.54
1:A:276:THR:HG23	1:A:276:THR:O	2.08	0.54
2:I:11:LEU:HD21	2:I:114:ALA:O	2.08	0.54
2:K:178:LEU:C	2:K:178:LEU:HD23	2.27	0.54
2:H:178:LEU:C	2:H:178:LEU:HD23	2.27	0.54
1:B:190:GLU:CG	2:I:100(D):ALA:HB2	2.37	0.54
1:D:44:GLN:HG2	1:D:288:ILE:HB	1.88	0.54
3:M:151:ASP:OD2	3:M:189:HIS:HB3	2.08	0.54
3:O:33:LEU:HD22	3:O:71:PHE:CG	2.42	0.54
1:B:77:ASP:OD2	1:B:141:ARG:NH1	2.32	0.54
1:C:276:THR:O	1:C:276:THR:HG23	2.08	0.54
2:H:4:LEU:HD13	2:H:92:CYS:SG	2.47	0.54
1:C:189:GLN:HG3	2:J:27(C):GLY:O	2.08	0.54
2:J:128:SER:O	2:J:129:LYS:HB3	2.07	0.54
1:B:276:THR:HG23	1:B:276:THR:O	2.07	0.53
3:L:12:SER:HB3	3:L:107:LYS:HE3	1.90	0.53
2:I:11:LEU:HB2	2:I:147:PRO:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:128:SER:O	2:K:129:LYS:HB3	2.09	0.53
3:L:30:ARG:N	3:L:30:ARG:HD2	2.23	0.52
3:O:11:LEU:HD21	3:O:19:VAL:HG13	1.91	0.52
2:K:184:VAL:HG11	2:K:194:TYR:CE1	2.45	0.52
2:J:97:SER:OG	2:J:100(N):ASP:OD2	2.25	0.52
3:N:188:LYS:HB3	3:N:189:HIS:CD2	2.45	0.51
1:C:50:LYS:HD3	1:C:275[B]:ASP:OD2	2.11	0.51
3:M:40:PRO:CB	3:M:165:GLU:HG3	2.40	0.51
2:K:184:VAL:HG11	2:K:194:TYR:CZ	2.46	0.51
3:N:23:CYS:HB2	3:N:35:TRP:CH2	2.45	0.51
3:O:37:GLN:HB2	3:O:47:LEU:HD11	1.94	0.51
1:D:189:GLN:HG3	2:K:27(C):GLY:O	2.10	0.50
3:L:140:TYR:CG	3:L:141:PRO:HA	2.47	0.50
3:M:11:LEU:HD21	3:M:19:VAL:HG13	1.94	0.50
3:M:188:LYS:HB3	3:M:189:HIS:CD2	2.47	0.49
1:A:190:GLU:HG3	2:H:100(D):ALA:HB2	1.95	0.49
1:A:108:LEU:HB2	1:A:234[A]:TRP:CZ3	2.47	0.49
2:K:95:HIS:CE1	2:K:100(P):PHE:CE2	3.01	0.49
2:K:201:LYS:N	2:K:202:PRO:CD	2.75	0.49
1:B:184:HIS:HE1	3:L:152:ASN:HD22	1.59	0.49
2:H:34:VAL:HG11	2:H:78:LEU:HD22	1.95	0.48
2:H:201:LYS:N	2:H:202:PRO:CD	2.76	0.48
1:C:294:PHE:HD1	1:C:307:LYS:HB2	1.78	0.48
1:D:108:LEU:HB2	1:D:234[A]:TRP:CZ3	2.49	0.48
1:B:184:HIS:HE1	3:L:152:ASN:ND2	2.12	0.47
1:C:190:GLU:CG	2:J:100(D):ALA:HB2	2.44	0.47
1:C:294:PHE:CD1	1:C:307:LYS:HB2	2.48	0.47
3:O:40:PRO:CB	3:O:165:GLU:HG3	2.44	0.47
1:D:299:LYS:HA	1:D:308:TYR:CB	2.45	0.47
1:D:190:GLU:CG	2:K:100(D):ALA:HB2	2.43	0.47
2:K:4:LEU:HD13	2:K:92:CYS:SG	2.55	0.47
3:M:11:LEU:HD21	3:M:19:VAL:CG1	2.45	0.47
2:J:145:TYR:CE2	2:J:150:VAL:HG13	2.49	0.47
3:N:91:TYR:HB2	3:N:96:PHE:CE1	2.50	0.47
3:O:55:GLN:HE21	3:O:55:GLN:HA	1.80	0.47
3:L:40:PRO:CB	3:L:165:GLU:HG3	2.45	0.47
1:C:293:PRO:C	1:C:306:PRO:HB3	2.36	0.46
1:D:153:TRP:CH2	2:K:100(F):TRP:HB2	2.50	0.46
2:H:128:SER:O	2:H:129:LYS:CB	2.64	0.46
3:M:12:SER:HB3	3:M:107:LYS:HE3	1.97	0.45
3:M:80:PRO:HA	3:M:106:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:97:SER:OG	2:K:100(N):ASP:OD2	2.25	0.45
2:I:201:LYS:HB2	2:I:202:PRO:HD3	1.98	0.45
2:H:129:LYS:O	2:H:129:LYS:HG2	2.17	0.45
3:L:40:PRO:HB3	3:L:165:GLU:HG3	1.98	0.45
3:L:181:LEU:CD1	3:L:186:TYR:HB2	2.47	0.45
2:K:188:SER:O	2:K:189:LEU:C	2.55	0.45
1:B:92:LYS:HB2	1:C:222:TRP:CE3	2.52	0.44
3:O:12:SER:HB3	3:O:107:LYS:HE3	1.99	0.44
3:M:40:PRO:HB3	3:M:165:GLU:HG3	1.98	0.44
3:M:55:GLN:HE21	3:M:55:GLN:HA	1.81	0.44
3:O:11:LEU:HD21	3:O:19:VAL:CG1	2.48	0.44
2:H:34:VAL:HB	2:H:78:LEU:HD21	2.00	0.44
2:H:145:TYR:CE2	2:H:150:VAL:HG13	2.52	0.44
2:I:128:SER:O	2:I:129:LYS:CB	2.65	0.44
1:B:108:LEU:HB2	1:B:234[A]:TRP:CZ3	2.53	0.44
1:A:190:GLU:CG	2:H:100(D):ALA:HB2	2.47	0.44
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.98	0.44
1:C:44:GLN:HB2	1:C:292:LYS:HD2	1.98	0.44
3:M:140:TYR:CG	3:M:141:PRO:HA	2.53	0.43
3:O:140:TYR:CG	3:O:141:PRO:HA	2.54	0.43
1:A:238:LYS:HB3	1:A:239:PRO:HD2	2.00	0.43
1:D:189:GLN:NE2	2:K:27(C):GLY:O	2.46	0.43
2:J:128:SER:O	2:J:129:LYS:CB	2.66	0.43
1:C:207:ARG:NH1	1:C:240:GLY:O	2.52	0.43
1:C:294:PHE:CA	1:C:306:PRO:HB3	2.48	0.43
3:L:188:LYS:HB3	3:L:189:HIS:CD2	2.54	0.43
2:K:184:VAL:O	2:K:185:PRO:C	2.57	0.43
3:O:187:GLU:O	3:O:211:ARG:NH2	2.51	0.43
1:B:184:HIS:CE1	3:L:152:ASN:HD22	2.36	0.43
1:D:164:LEU:O	1:D:246:ASN:HA	2.19	0.43
3:N:55:GLN:HE21	3:N:55:GLN:HA	1.83	0.43
2:H:95:HIS:CE1	2:H:100(P):PHE:CE2	3.06	0.43
3:L:23:CYS:HB2	3:L:35:TRP:CH2	2.54	0.43
1:A:205:SER:HB3	1:A:210:GLN:HG3	2.01	0.42
1:B:184:HIS:CE1	3:L:152:ASN:ND2	2.87	0.42
2:J:129:LYS:HG2	2:J:129:LYS:O	2.20	0.42
3:O:90:GLN:CD	3:O:90:GLN:C	2.78	0.42
1:D:207[B]:ARG:NH1	1:D:240:GLY:O	2.52	0.42
1:A:164:LEU:O	1:A:246:ASN:HA	2.20	0.42
3:M:151:ASP:CG	3:M:189:HIS:HB3	2.39	0.42
2:K:129:LYS:HG2	2:K:129:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:184:VAL:O	2:I:185:PRO:C	2.58	0.42
2:J:201:LYS:HB2	2:J:202:PRO:HD3	2.02	0.42
1:C:50:LYS:CD	1:C:275[B]:ASP:OD2	2.68	0.42
2:K:4:LEU:HD21	2:K:29:LEU:HD13	2.02	0.42
2:H:188:SER:O	2:H:189:LEU:C	2.59	0.42
3:L:34:ASN:OD1	3:L:49:TYR:HA	2.19	0.42
2:I:95:HIS:CE1	2:I:100(P):PHE:CE2	3.08	0.42
2:I:129:LYS:O	2:I:129:LYS:HG2	2.19	0.42
2:K:128:SER:O	2:K:129:LYS:CB	2.67	0.42
1:C:108:LEU:HB2	1:C:234[A]:TRP:CZ3	2.54	0.41
3:L:55:GLN:HE21	3:L:55:GLN:HA	1.85	0.41
1:D:298:ASN:C	1:D:308:TYR:CD1	2.93	0.41
3:N:66:GLY:HA3	3:N:70:ASP:O	2.20	0.41
1:D:299:LYS:HB3	1:D:308:TYR:CD2	2.56	0.41
3:L:11:LEU:HD21	3:L:19:VAL:CG1	2.51	0.41
1:B:105:TYR:CD1	1:B:105:TYR:C	2.94	0.41
1:B:190:GLU:CD	2:I:100(D):ALA:HB2	2.41	0.41
1:C:164:LEU:O	1:C:246:ASN:HA	2.21	0.41
1:A:102:VAL:HG22	1:A:232:ILE:HB	2.02	0.41
1:C:293:PRO:HB2	1:C:294:PHE:CE2	2.56	0.41
1:D:190:GLU:CD	2:K:100(D):ALA:HB2	2.41	0.41
2:H:184:VAL:O	2:H:185:PRO:C	2.59	0.41
3:O:175:LEU:C	3:O:175:LEU:HD23	2.41	0.41
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.56	0.41
3:O:186:TYR:HA	3:O:192:TYR:OH	2.21	0.41
1:A:153:TRP:CH2	2:H:100(F):TRP:HB2	2.56	0.40
2:I:126:PRO:HD3	2:I:138:LEU:HB3	2.04	0.40
3:N:175:LEU:HD23	3:N:175:LEU:C	2.41	0.40
3:O:91:TYR:HB2	3:O:96:PHE:CE1	2.57	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 X-ray entries followed by that with respect to entries of similar resolution.

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	273/278 (98%)	266 (97%)	6 (2%)	1 (0%)	34	64
1	B	273/278 (98%)	266 (97%)	6 (2%)	1 (0%)	34	64
1	C	270/278 (97%)	264 (98%)	5 (2%)	1 (0%)	34	64
1	D	272/278 (98%)	265 (97%)	6 (2%)	1 (0%)	34	64
2	H	241/241 (100%)	234 (97%)	5 (2%)	2 (1%)	19	49
2	I	241/241 (100%)	234 (97%)	6 (2%)	1 (0%)	34	64
2	J	241/241 (100%)	235 (98%)	5 (2%)	1 (0%)	34	64
2	K	241/241 (100%)	233 (97%)	6 (2%)	2 (1%)	19	49
3	L	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
3	M	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
3	N	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
3	O	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
All	All	2900/2932 (99%)	2827 (98%)	63 (2%)	10 (0%)	34	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	189	LEU
2	K	189	LEU
1	A	62	ILE
1	B	62	ILE
1	C	62	ILE
1	D	62	ILE
2	J	149	PRO
2	I	149	PRO
2	K	149	PRO
2	H	149	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/244 (100%)	243 (100%)	1 (0%)	91	97
1	B	244/244 (100%)	243 (100%)	1 (0%)	91	97
1	C	241/244 (99%)	240 (100%)	1 (0%)	91	97
1	D	242/244 (99%)	241 (100%)	1 (0%)	91	97
2	H	202/200 (101%)	195 (96%)	7 (4%)	36	67
2	I	202/200 (101%)	199 (98%)	3 (2%)	65	85
2	J	202/200 (101%)	199 (98%)	3 (2%)	65	85
2	K	202/200 (101%)	198 (98%)	4 (2%)	55	80
3	L	187/187 (100%)	180 (96%)	7 (4%)	34	65
3	M	187/187 (100%)	180 (96%)	7 (4%)	34	65
3	N	187/187 (100%)	180 (96%)	7 (4%)	34	65
3	O	187/187 (100%)	180 (96%)	7 (4%)	34	65
All	All	2527/2524 (100%)	2478 (98%)	49 (2%)	55	81

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	B	53	ASN
1	C	53	ASN
1	D	53	ASN
2	H	78	LEU
2	H	92	CYS
2	H	178	LEU
2	H	187	SER
2	H	193	THR
2	H	197	ASN
2	H	209	LYS
3	L	3	GLN
3	L	11	LEU
3	L	55	GLN
3	L	90	GLN
3	L	147	GLN
3	L	181	LEU
3	L	188	LYS
2	I	78	LEU

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Mol	Chain	Res	Type
2	I	92	CYS
2	I	178	LEU
3	M	3	GLN
3	M	11	LEU
3	M	55	GLN
3	M	90	GLN
3	M	147	GLN
3	M	181	LEU
3	M	188	LYS
2	J	78	LEU
2	J	92	CYS
2	J	178	LEU
3	N	3	GLN
3	N	11	LEU
3	N	55	GLN
3	N	90	GLN
3	N	147	GLN
3	N	181	LEU
3	N	188	LYS
2	K	78	LEU
2	K	92	CYS
2	K	178	LEU
2	K	196	CYS
3	O	3	GLN
3	O	11	LEU
3	O	55	GLN
3	O	90	GLN
3	O	147	GLN
3	O	181	LEU
3	O	188	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	54	ASN
1	B	53	ASN
1	B	54	ASN
1	C	53	ASN
1	C	54	ASN
1	D	53	ASN
1	D	54	ASN

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Mol	Chain	Res	Type
1	D	210	GLN
1	D	211	GLN
2	H	13	GLN
2	H	192	GLN
3	L	55	GLN
3	L	137	ASN
3	L	138	ASN
3	L	152	ASN
3	L	189	HIS
3	L	199	GLN
3	M	55	GLN
3	M	199	GLN
3	N	55	GLN
3	N	189	HIS
3	N	199	GLN
3	O	55	GLN
3	O	189	HIS
3	O	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	PCA	J	1	2	7,8,9	2.16	2 (28%)	9,10,12	2.22	5 (55%)
2	PCA	K	1	2	7,8,9	2.18	2 (28%)	9,10,12	2.21	5 (55%)
2	PCA	I	1	2	7,8,9	2.16	2 (28%)	9,10,12	2.23	5 (55%)
2	PCA	H	1	2	7,8,9	2.15	2 (28%)	9,10,12	2.20	5 (55%)

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	PCA	J	1	2	-	0/0/11/13	0/1/1/1
2	PCA	K	1	2	-	0/0/11/13	0/1/1/1
2	PCA	I	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	PCA	CD-N	4.66	1.46	1.34
2	J	1	PCA	CD-N	4.65	1.46	1.34
2	I	1	PCA	CD-N	4.63	1.46	1.34
2	H	1	PCA	CD-N	4.54	1.46	1.34
2	H	1	PCA	CA-N	3.26	1.50	1.46
2	K	1	PCA	CA-N	3.23	1.50	1.46
2	J	1	PCA	CA-N	3.17	1.50	1.46
2	I	1	PCA	CA-N	3.13	1.50	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	PCA	CA-N-CD	-3.26	102.43	113.58
2	J	1	PCA	CA-N-CD	-3.16	102.75	113.58
2	H	1	PCA	CA-N-CD	-3.16	102.77	113.58
2	J	1	PCA	OE-CD-CG	-3.10	121.35	126.76
2	K	1	PCA	OE-CD-CG	-3.10	121.36	126.76
2	I	1	PCA	OE-CD-CG	-3.07	121.41	126.76
2	K	1	PCA	CA-N-CD	-3.06	103.09	113.58
2	I	1	PCA	CB-CA-N	3.06	112.07	103.30
2	H	1	PCA	OE-CD-CG	-3.00	121.53	126.76
2	H	1	PCA	CB-CA-N	2.94	111.74	103.30
2	J	1	PCA	CB-CA-N	2.90	111.62	103.30
2	K	1	PCA	CB-CA-C	-2.89	108.73	112.70
2	K	1	PCA	CB-CA-N	2.76	111.23	103.30
2	J	1	PCA	CG-CD-N	2.59	115.10	108.39
2	I	1	PCA	CG-CD-N	2.59	115.10	108.39
2	H	1	PCA	CG-CD-N	2.56	115.01	108.39
2	J	1	PCA	CB-CA-C	-2.52	109.23	112.70
2	K	1	PCA	CG-CD-N	2.50	114.87	108.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	CB-CA-C	-2.36	109.45	112.70
2	I	1	PCA	CB-CA-C	-2.28	109.56	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

2 monosaccharides 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	$\# Z > 2$
4	NAG	E	1	4,1	14,14,15	0.55	0	17,19,21	0.91	1 (5%)
4	NAG	E	2	4	14,14,15	0.52	0	17,19,21	0.72	1 (5%)

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
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	O5-C1-C2	-2.94	106.65	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	O5-C5-C6	2.15	110.57	107.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
5	NAG	A	701	1	14,14,15	0.59	0	17,19,21	0.91	1 (5%)
5	NAG	D	701	1	14,14,15	0.57	0	17,19,21	0.88	1 (5%)

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
5	NAG	A	701	1	-	0/6/23/26	0/1/1/1
5	NAG	D	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	A	701	NAG	O5-C1-C2	-3.12	106.37	111.29
5	D	701	NAG	O5-C1-C2	-3.03	106.50	111.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	267/278 (96%)	0.32	19 (7%) 16 14	30, 54, 125, 181	0
1	B	267/278 (96%)	0.44	31 (11%) 4 4	29, 60, 146, 202	0
1	C	265/278 (95%)	0.81	43 (16%) 1 1	33, 59, 237, 285	0
1	D	266/278 (95%)	1.20	53 (19%) 1 1	31, 62, 281, 438	0
2	H	238/241 (98%)	0.09	7 (2%) 51 51	31, 50, 97, 265	0
2	I	238/241 (98%)	0.25	8 (3%) 45 43	31, 63, 133, 250	0
2	J	238/241 (98%)	0.27	11 (4%) 32 32	35, 68, 131, 246	0
2	K	238/241 (98%)	2.34	73 (30%) 0 0	36, 100, 312, 488	0
3	L	213/214 (99%)	-0.02	1 (0%) 91 91	30, 46, 75, 106	0
3	M	213/214 (99%)	-0.00	1 (0%) 91 91	27, 46, 86, 147	0
3	N	213/214 (99%)	0.11	1 (0%) 91 91	49, 69, 113, 140	0
3	O	213/214 (99%)	3.18	126 (59%) 0 0	89, 178, 276, 356	0
All	All	2869/2932 (97%)	0.74	374 (13%) 3 3	27, 62, 228, 488	0

All (374) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	182	VAL	22.9
2	K	138	LEU	22.1
2	K	139	GLY	16.0
2	K	140	CYS	15.4
2	K	158	ALA	14.0
1	D	294	PHE	13.5
2	K	181	VAL	13.5
2	K	180	SER	13.3
2	K	127	SER	12.4
2	I	130	SER	12.3
3	O	135	LEU	12.3

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Mol	Chain	Res	Type	RSRZ
2	K	141	LEU	11.8
2	K	198	VAL	11.7
2	K	136	ALA	11.2
2	K	130	SER	11.1
3	O	176	SER	11.0
2	K	131	THR	10.9
2	K	193	THR	10.8
2	K	132	SER	10.8
1	D	293	PRO	10.7
2	K	183	THR	10.4
2	K	133	GLY	10.4
1	D	297	VAL	10.3
3	O	111	ALA	10.2
2	K	159	LEU	10.2
3	O	133	VAL	10.2
3	O	174	SER	10.0
3	O	116	PHE	9.9
1	D	281	CYS	9.8
2	K	155	ASN	9.6
3	O	196	VAL	9.4
1	D	288	ILE	9.3
3	O	162	SER	9.1
2	K	206	LYS	9.1
1	D	308	TYR	9.1
2	K	184	VAL	9.0
3	O	194	CYS	8.8
2	K	142	VAL	8.7
2	K	128	SER	8.6
3	O	152	ASN	8.5
1	D	296	ASN	8.5
1	D	289	PRO	8.4
3	O	109	THR	8.4
3	O	117	ILE	8.3
1	D	301	THR	8.3
1	C	299	LYS	8.3
1	D	290	ASN	8.2
1	D	284	PRO	8.1
3	O	198	HIS	8.0
1	D	291	ASP	8.0
2	K	122	PHE	8.0
3	O	207	LYS	8.0
1	C	46	SER	7.9

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Mol	Chain	Res	Type	RSRZ
2	K	129	LYS	7.9
3	O	122	ASP	7.8
3	O	142	ARG	7.7
3	O	195	GLU	7.7
1	D	48	THR	7.7
2	H	133	GLY	7.6
2	K	190	GLY	7.6
1	C	291	ASP	7.5
1	C	48	THR	7.4
2	J	132	SER	7.4
3	O	144	ALA	7.3
1	D	282	ILE	7.3
3	O	161	GLU	7.3
2	K	151	THR	7.2
1	D	52	CYS	7.2
2	I	132	SER	7.2
1	C	289	PRO	7.2
1	B	43	VAL	7.1
2	K	152	VAL	7.1
1	C	300	ILE	7.1
3	O	132	VAL	7.1
2	K	161[A]	SER	7.1
1	D	47	SER	7.0
3	O	120	PRO	7.0
1	D	275[A]	ASP	7.0
2	K	179	SER	7.0
1	D	274[A]	ILE	7.0
2	K	213	PRO	7.0
2	H	131	THR	7.0
3	O	201	LEU	7.0
2	H	130	SER	6.9
1	C	294	PHE	6.8
3	O	145	LYS	6.8
3	O	119	PRO	6.8
3	O	202	SER	6.8
3	O	172	THR	6.8
2	J	133	GLY	6.7
3	O	106	ILE	6.7
3	O	150	VAL	6.7
2	K	214	LYS	6.7
1	D	302	TYR	6.6
2	K	117	LYS	6.5

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Mol	Chain	Res	Type	RSRZ
1	D	53	ASN	6.4
3	O	169	LYS	6.4
3	O	206	THR	6.3
1	D	300	ILE	6.3
3	O	200	GLY	6.3
1	C	301	THR	6.2
1	D	276	THR	6.2
1	D	45	SER	6.2
2	K	191	THR	6.2
2	J	130	SER	6.1
2	K	126	PRO	6.0
1	C	279	SER	6.0
3	O	156	SER	5.9
1	C	297	VAL	5.9
1	C	52	CYS	5.9
2	K	153	SER	5.9
1	C	45	SER	5.8
1	D	279	SER	5.8
1	B	297	VAL	5.8
3	O	153	ALA	5.7
3	O	155	GLN	5.7
1	D	287	SER	5.7
1	C	290	ASN	5.7
3	O	175	LEU	5.7
1	C	293	PRO	5.6
2	I	131	THR	5.6
3	O	147	GLN	5.6
2	K	212	GLU	5.6
3	O	203	SER	5.6
1	D	309	VAL	5.6
3	O	184	ALA	5.6
3	O	164	THR	5.5
2	I	129	LYS	5.5
2	K	192	GLN	5.5
1	C	284	PRO	5.5
1	C	296	ASN	5.4
2	K	121	VAL	5.4
3	O	208	SER	5.4
3	O	112	ALA	5.4
1	D	298	ASN	5.3
1	B	291	ASP	5.3
1	D	304	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	49	GLY	5.3
3	O	180	THR	5.2
3	O	179	LEU	5.2
1	D	51	ILE	5.2
2	K	116	THR	5.2
1	D	50	LYS	5.1
1	C	307	LYS	5.1
2	I	133	GLY	5.0
3	O	186	TYR	5.0
3	O	134	CYS	5.0
1	C	47	SER	5.0
1	D	264	LYS	4.9
3	O	83	VAL	4.9
3	O	211	ARG	4.9
1	C	288	ILE	4.9
3	O	181	LEU	4.9
3	O	170	ASP	4.9
1	D	280	GLU	4.9
1	B	280	GLU	4.8
2	I	214	LYS	4.8
2	K	137	ALA	4.8
3	O	163	VAL	4.8
1	D	270	SER	4.7
3	O	165	GLU	4.7
1	C	308	TYR	4.7
2	K	208	ASP	4.7
3	O	148	TRP	4.7
3	O	80	PRO	4.7
3	O	146	VAL	4.7
1	D	306	PRO	4.6
1	C	282	ILE	4.6
2	I	134	GLY	4.6
1	C	44	GLN	4.6
3	O	160	GLN	4.6
1	D	49	GLY	4.6
2	K	210	ARG	4.6
1	C	298	ASN	4.6
1	D	295	GLN	4.5
3	O	127	SER	4.5
1	D	277	CYS	4.5
2	J	214	LYS	4.5
3	O	126	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
3	O	140	TYR	4.5
2	K	125	ALA	4.5
1	C	281	CYS	4.5
3	O	136	LEU	4.5
2	K	154	TRP	4.5
3	O	197	THR	4.4
1	C	305	CYS	4.4
1	D	44	GLN	4.4
2	H	134	GLY	4.4
3	O	143	GLU	4.3
1	D	278	ILE	4.3
1	A	297	VAL	4.3
3	O	137	ASN	4.2
3	O	123	GLU	4.2
1	C	53	ASN	4.2
2	K	163	VAL	4.2
3	O	151	ASP	4.2
3	O	189	HIS	4.1
3	O	110	VAL	4.1
3	O	121	SER	4.1
2	K	195	ILE	4.1
1	D	46	SER	4.1
1	D	54	ASN	4.0
2	K	123	PRO	4.0
2	K	160	THR	4.0
1	C	304	ALA	4.0
3	O	149	LYS	3.9
1	C	285	ASN	3.9
1	D	305	CYS	3.9
2	J	189	LEU	3.9
2	K	150	VAL	3.9
3	O	128	GLY	3.9
1	C	292	LYS	3.9
3	O	192	TYR	3.9
1	D	292	LYS	3.9
1	C	275[A]	ASP	3.8
2	K	201	LYS	3.8
1	D	283	THR	3.8
2	J	131	THR	3.8
3	O	178	THR	3.8
1	A	43	VAL	3.8
3	O	185	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
2	K	118	GLY	3.7
2	J	134	GLY	3.7
3	O	13	ALA	3.7
3	O	114	SER	3.7
3	O	199	GLN	3.6
3	O	171	SER	3.5
3	O	210	ASN	3.5
1	D	299	LYS	3.5
1	B	289	PRO	3.5
3	O	212	GLY	3.5
1	C	295	GLN	3.5
1	C	287	SER	3.5
3	O	167	ASP	3.5
2	K	189	LEU	3.4
2	H	132	SER	3.4
3	O	159	SER	3.4
3	O	84	GLY	3.4
2	K	178	LEU	3.4
1	A	294	PHE	3.4
3	O	28	ASP	3.4
1	B	288	ILE	3.4
1	C	283	THR	3.3
3	O	209	PHE	3.3
1	C	264	LYS	3.3
2	K	143	LYS	3.3
3	O	76	SER	3.3
3	O	118	PHE	3.3
3	O	213	GLU	3.3
1	C	302	TYR	3.3
2	K	170	LEU	3.3
1	D	307	LYS	3.3
1	B	295	GLN	3.3
1	B	282	ILE	3.3
3	O	4	LEU	3.3
3	O	157	GLY	3.3
1	B	294	PHE	3.2
1	A	309	VAL	3.2
1	B	268	MET	3.2
1	C	276	THR	3.2
3	O	12	SER	3.2
2	J	188	SER	3.2
2	H	27(B)	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	46	SER	3.1
1	D	303	GLY	3.1
3	O	115	VAL	3.1
1	B	46	SER	3.1
2	K	194	TYR	3.1
1	B	309	VAL	3.1
2	K	164	HIS	3.1
3	O	154	LEU	3.1
1	C	50	LYS	3.0
1	C	306	PRO	3.0
3	O	51	ALA	3.0
3	O	1	ASP	3.0
2	J	135	THR	3.0
1	A	290	ASN	3.0
2	K	202	PRO	2.9
3	O	183	LYS	2.9
3	O	131	SER	2.9
2	J	191	THR	2.9
3	O	173	TYR	2.9
1	C	274[A]	ILE	2.9
2	K	115	SER	2.8
2	I	127	SER	2.8
1	B	305	CYS	2.8
3	O	205	VAL	2.8
3	O	27	GLN	2.8
2	K	120	SER	2.7
1	B	290	ASN	2.7
1	B	119	GLU	2.7
1	B	287	SER	2.7
2	K	167	PRO	2.7
2	K	200	HIS	2.7
3	O	168	SER	2.7
1	A	305	CYS	2.7
2	K	199	ASN	2.7
3	O	11	LEU	2.7
1	D	56	HIS	2.7
1	A	289	PRO	2.6
3	O	105	VAL	2.6
1	A	291	ASP	2.6
2	K	168	ALA	2.6
1	A	304	ALA	2.6
3	O	193	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	296	ASN	2.6
2	K	124	LEU	2.5
3	O	101	GLY	2.5
2	K	209	LYS	2.5
1	D	285	ASN	2.5
3	O	204	PRO	2.5
3	O	88	CYS	2.5
3	O	177	SER	2.5
2	K	197	ASN	2.5
1	A	207[A]	ARG	2.5
3	O	29	ILE	2.5
1	D	58	ILE	2.5
2	K	211	VAL	2.5
1	B	44	GLN	2.5
3	O	129	THR	2.5
1	B	306	PRO	2.4
3	O	102	THR	2.4
1	A	104	ASP	2.4
1	C	54	ASN	2.4
3	O	60	SER	2.4
3	O	23	CYS	2.4
3	O	19	VAL	2.4
1	A	287	SER	2.4
2	K	157	GLY	2.3
1	C	268	MET	2.3
1	B	279	SER	2.3
3	O	188	LYS	2.3
1	B	48	THR	2.3
3	N	213	GLU	2.3
2	K	204	ASN	2.3
1	D	268	MET	2.3
1	B	298	ASN	2.3
1	A	306	PRO	2.3
1	C	51	ILE	2.3
1	B	277	CYS	2.3
2	H	129	LYS	2.3
1	D	55	PRO	2.2
1	B	207[A]	ARG	2.2
3	O	18[A]	ARG	2.2
3	O	7	SER	2.2
3	O	81	GLU	2.2
3	O	3	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	264	LYS	2.2
3	M	126	LYS	2.2
1	B	281	CYS	2.2
1	A	264	LYS	2.2
1	A	280	GLU	2.2
2	K	196	CYS	2.2
1	B	276	THR	2.2
3	O	104	VAL	2.2
2	K	144	ASP	2.2
1	A	296	ASN	2.1
3	O	39	LYS	2.1
1	D	286	GLY	2.1
3	O	93	GLY	2.1
1	B	278	ILE	2.1
3	O	2	ILE	2.1
3	O	86	TYR	2.1
1	A	44	GLN	2.1
3	O	191	VAL	2.1
1	B	304	ALA	2.1
1	A	275[A]	ASP	2.1
1	B	308	TYR	2.1
3	O	40	PRO	2.1
1	B	284	PRO	2.0
3	L	56	ARG	2.0
3	O	38	GLN	2.0
3	O	166	GLN	2.0
2	J	184	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PCA	K	1	8/9	0.82	0.20	122,139,147,148	0
2	PCA	J	1	8/9	0.87	0.19	86,98,103,106	0
2	PCA	I	1	8/9	0.92	0.20	61,81,87,88	0
2	PCA	H	1	8/9	0.95	0.22	79,96,104,105	0

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	E	1	14/15	0.80	0.32	109,120,130,136	0
4	NAG	E	2	14/15	0.82	0.31	120,125,127,128	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	701	14/15	0.70	0.28	122,134,148,154	0
6	ZN	H	301	1/1	0.84	0.18	134,134,134,134	0
5	NAG	D	701	14/15	0.85	0.27	100,115,129,135	0
6	ZN	L	301	1/1	0.94	0.09	106,106,106,106	0
6	ZN	L	302	1/1	0.94	0.14	72,72,72,72	0
6	ZN	J	301	1/1	0.94	0.04	143,143,143,143	0
6	ZN	N	302	1/1	0.94	0.07	104,104,104,104	0
6	ZN	N	301	1/1	0.95	0.12	102,102,102,102	0
6	ZN	O	301	1/1	0.95	0.12	133,133,133,133	0
6	ZN	M	301	1/1	0.98	0.09	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.