



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:06 AM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

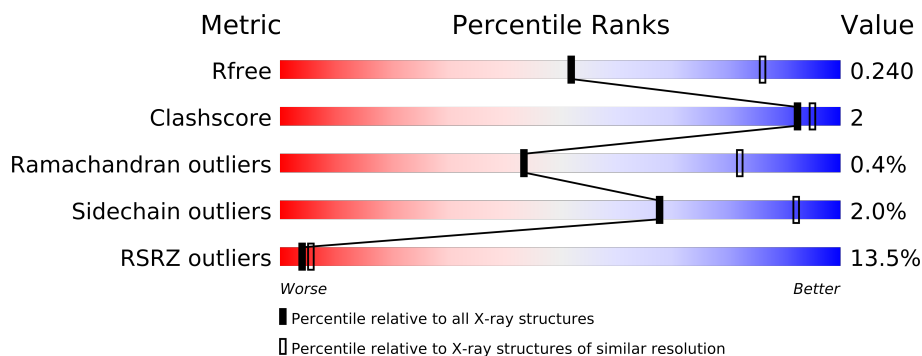
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1424 (2.98-2.90)
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RSRZ outliers	66119	1425 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	278	
1	B	278	
1	C	278	
1	D	278	
2	H	241	
2	I	241	
2	J	241	
2	K	241	
3	L	214	
3	M	214	
3	N	214	
3	O	214	

2 Entry composition

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

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.

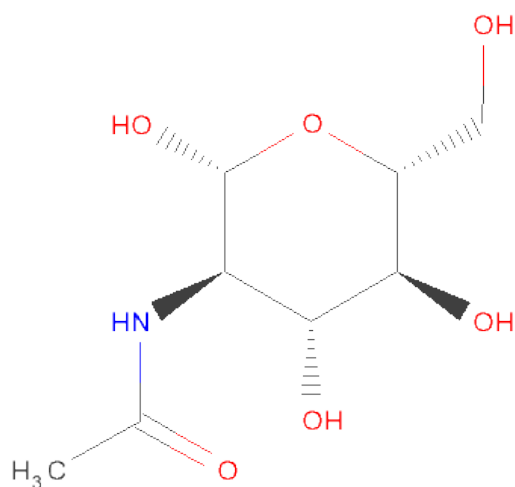
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			

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



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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	2	Total	C	N	O	0	0
			28	16	2	10		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	39	ALA	-	EXPRESSION TAG	UNP Q91MA7

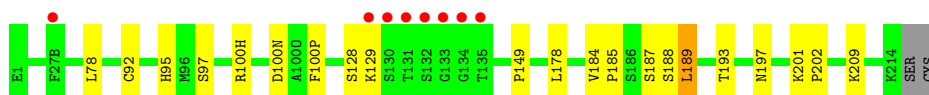
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Chain	Residue	Modelled	Actual	Comment	Reference
C	40	ASP	-	EXPRESSION TAG	UNP Q91MA7
C	41	PRO	-	EXPRESSION TAG	UNP Q91MA7
C	42	GLY	-	EXPRESSION TAG	UNP Q91MA7
C	310	GLY	-	EXPRESSION TAG	UNP Q91MA7
C	311	HIS	-	EXPRESSION TAG	UNP Q91MA7
C	312	HIS	-	EXPRESSION 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

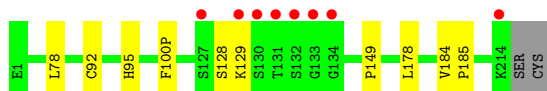
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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



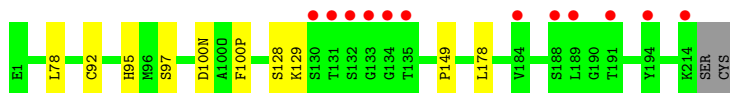
- Molecule 2: Antibody C05, heavy chain

Chain I:



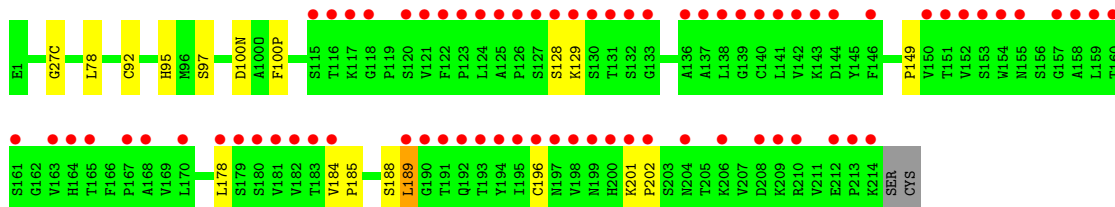
- Molecule 2: Antibody C05, heavy chain

Chain J:



- Molecule 2: Antibody C05, heavy chain

Chain K:



- Molecule 3: Antibody C05, light chain

Chain L:



- Molecule 3: Antibody C05, light chain

Chain M:



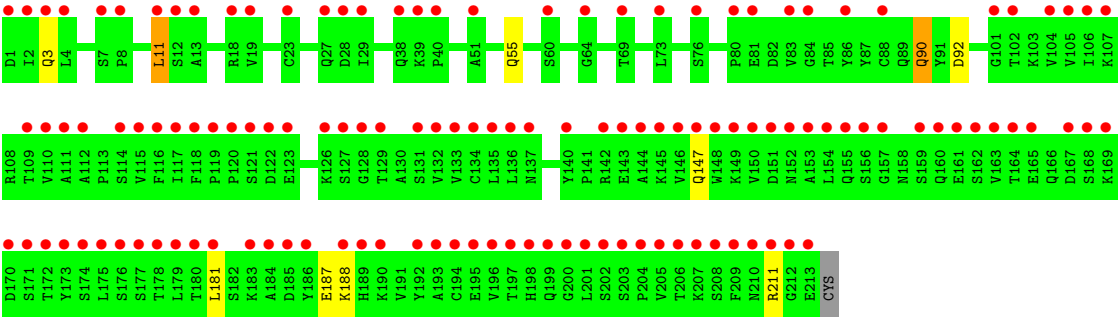
- Molecule 3: Antibody C05, light chain

Chain N:



- Molecule 3: Antibody C05, light chain

Chain O:



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	4190 reflections (4.98%)	DCC
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 , 26.9	EDS
Estimated twinning fraction	0.008 for l,k,-h 0.028 for h,-k,-l 0.021 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 84219 reflections	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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PCA, 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	0.30	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2141	0	0	2	0
1	B	2141	0	0	5	0
1	C	2116	0	0	3	0
1	D	2128	0	0	5	0
2	H	1806	0	6	6	0
2	I	1806	0	18	3	0
2	J	1806	0	18	3	0
2	K	1806	0	6	7	0
3	L	1648	0	5	2	0
3	M	1648	0	5	2	0
3	N	1648	0	5	1	0
3	O	1648	0	5	4	0
4	A	14	0	13	0	0
4	D	14	0	13	0	0
5	C	28	0	25	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	119	40	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (40) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:ASP:OD2	1:A:141:ARG:NH1	2.16	0.78
1:C:77:ASP:OD2	1:C:141:ARG:NH1	2.22	0.72
1:B:77:ASP:OD2	1:B:141:ARG:NH1	2.32	0.62
3:N:50:ASP:OD1	3:N:91:TYR:OH	2.19	0.60
1:D:77:ASP:OD2	1:D:141:ARG:NH1	2.37	0.57
2:J:95:HIS:CE1	2:J:100(P):PHE:CE2	2.92	0.56
3:O:90:GLN:OE1	3:O:92:ASP:N	2.39	0.56
1:A:207[B]:ARG:NH1	1:A:240:GLY:O	2.38	0.56
2:J:97:SER:OG	2:J:100(N):ASP:OD2	2.25	0.54
2:K:97:SER:OG	2:K:100(N):ASP:OD2	2.25	0.54
3:M:11:LEU:CD1	3:M:11:LEU:C	2.80	0.50
2:K:95:HIS:CE1	2:K:100(P):PHE:CE2	3.01	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:189:GLN:NE2	2:K:27(C):GLY:O	2.46	0.49
2:K:201:LYS:N	2:K:202:PRO:CD	2.75	0.49
1:D:101:ASP:OD2	3:M:24:GLN:NE2	2.46	0.49
2:H:201:LYS:N	2:H:202:PRO:CD	2.76	0.48
2:H:97:SER:OG	2:H:100(N):ASP:OD2	2.33	0.46
2:H:128:SER:O	2:H:129:LYS:CB	2.64	0.46
2:K:188:SER:O	2:K:189:LEU:C	2.55	0.45
3:L:39:LYS:NZ	3:L:81:GLU:O	2.50	0.44
2:I:128:SER:O	2:I:129:LYS:CB	2.65	0.44
1:B:207[B]:ARG:NH1	1:B:240:GLY:O	2.51	0.43
2:J:128:SER:O	2:J:129:LYS:CB	2.66	0.43
3:O:187:GLU:O	3:O:211:ARG:NH2	2.51	0.43
2:K:184:VAL:O	2:K:185:PRO:C	2.57	0.43
1:C:207:ARG:NH1	1:C:240:GLY:O	2.52	0.43
2:H:95:HIS:CE1	2:H:100(P):PHE:CE2	3.06	0.43
3:O:90:GLN:C	3:O:90:GLN:CD	2.78	0.42
1:B:184:HIS:CE1	3:L:152:ASN:ND2	2.87	0.42
1:D:207[B]:ARG:NH1	1:D:240:GLY:O	2.52	0.42
2:I:184:VAL:O	2:I:185:PRO:C	2.58	0.42
1:C:50:LYS:CD	1:C:275[B]:ASP:OD2	2.68	0.42
1:B:90:ARG:NH1	1:B:272:ALA:O	2.53	0.42
2:I:95:HIS:CE1	2:I:100(P):PHE:CE2	3.08	0.42
2:K:128:SER:O	2:K:129:LYS:CB	2.67	0.42
2:H:188:SER:O	2:H:189:LEU:C	2.59	0.42
1:D:298:ASN:C	1:D:308:TYR:CD1	2.93	0.41
3:O:11:LEU:CD1	3:O:11:LEU:C	2.89	0.41
1:B:105:TYR:CD1	1:B:105:TYR:C	2.94	0.41
2:H:184:VAL:O	2:H:185:PRO:C	2.59	0.41

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%)	43 82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	273/278 (98%)	266 (97%)	6 (2%)	1 (0%)	43	82
1	C	270/278 (97%)	264 (98%)	5 (2%)	1 (0%)	43	82
1	D	272/278 (98%)	265 (97%)	6 (2%)	1 (0%)	43	82
2	H	241/241 (100%)	234 (97%)	5 (2%)	2 (1%)	27	68
2	I	241/241 (100%)	234 (97%)	6 (2%)	1 (0%)	43	82
2	J	241/241 (100%)	235 (98%)	5 (2%)	1 (0%)	43	82
2	K	241/241 (100%)	233 (97%)	6 (2%)	2 (1%)	27	68
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%)	43	85

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/244 (100%)	243 (100%)	1 (0%)	95	99
1	B	244/244 (100%)	243 (100%)	1 (0%)	95	99

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	241/244 (99%)	240 (100%)	1 (0%)	95	99
1	D	242/244 (99%)	241 (100%)	1 (0%)	95	99
2	H	202/200 (101%)	195 (96%)	7 (4%)	48	84
2	I	202/200 (101%)	199 (98%)	3 (2%)	76	95
2	J	202/200 (101%)	199 (98%)	3 (2%)	76	95
2	K	202/200 (101%)	198 (98%)	4 (2%)	68	92
3	L	187/187 (100%)	180 (96%)	7 (4%)	45	83
3	M	187/187 (100%)	180 (96%)	7 (4%)	45	83
3	N	187/187 (100%)	180 (96%)	7 (4%)	45	83
3	O	187/187 (100%)	180 (96%)	7 (4%)	45	83
All	All	2527/2524 (100%)	2478 (98%)	49 (2%)	68	93

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
2	I	92	CYS
2	I	178	LEU
3	M	3	GLN
3	M	11	LEU

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	H	1	2	8,8,9	6.56	2 (25%)	8,10,12	6.10	5 (62%)
2	PCA	I	1	2	8,8,9	6.72	2 (25%)	8,10,12	6.64	5 (62%)
2	PCA	J	1	2	8,8,9	6.64	3 (37%)	8,10,12	5.80	5 (62%)
2	PCA	K	1	2	8,8,9	6.67	3 (37%)	8,10,12	5.39	3 (37%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	PCA	O-C	17.90	1.23	1.11
2	K	1	PCA	O-C	17.70	1.23	1.11
2	J	1	PCA	O-C	17.62	1.23	1.11
2	H	1	PCA	O-C	17.46	1.23	1.11
2	K	1	PCA	CD-N	5.85	1.46	1.34
2	J	1	PCA	CD-N	5.84	1.46	1.34
2	I	1	PCA	CD-N	5.81	1.46	1.34
2	H	1	PCA	CD-N	5.70	1.46	1.34
2	K	1	PCA	CA-C	2.13	1.52	1.48
2	J	1	PCA	CA-C	2.12	1.52	1.48

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	PCA	CA-N-CD	-15.28	102.43	114.37
2	J	1	PCA	CA-N-CD	-14.87	102.75	114.37
2	H	1	PCA	CA-N-CD	-14.84	102.77	114.37
2	K	1	PCA	CA-N-CD	-14.43	103.09	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	PCA	C-CA-N	-9.63	108.54	110.71
2	H	1	PCA	C-CA-N	-7.22	109.08	110.71
2	J	1	PCA	C-CA-N	-4.77	109.64	110.71
2	J	1	PCA	OE-CD-CG	-3.41	121.35	126.70
2	K	1	PCA	OE-CD-CG	-3.40	121.36	126.70
2	I	1	PCA	OE-CD-CG	-3.37	121.41	126.70
2	H	1	PCA	OE-CD-CG	-3.29	121.53	126.70
2	I	1	PCA	CB-CA-N	2.90	112.07	103.72
2	H	1	PCA	CB-CA-N	2.79	111.74	103.72
2	J	1	PCA	CB-CA-N	2.75	111.62	103.72
2	K	1	PCA	CB-CA-N	2.61	111.23	103.72
2	J	1	PCA	CG-CD-N	2.05	115.10	107.77
2	I	1	PCA	CG-CD-N	2.04	115.10	107.77
2	H	1	PCA	CG-CD-N	2.02	115.01	107.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates i

2 carbohydrates 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	$\# Z > 2$
5	NAG	C	701	1,5	12,14,15	0.67	1 (8%)	15,19,21	0.77	0
5	NAG	C	702	5	12,14,15	0.63	0	15,19,21	1.02	1 (6%)

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	C	701	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	702	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	701	NAG	O5-C5	-2.12	1.41	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	702	NAG	O5-C5-C6	3.42	110.57	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	$\# Z > 2$
4	NAG	A	701	1	12,14,15	0.74	1 (8%)	15,19,21	0.71	0
4	NAG	D	701	1	12,14,15	0.70	1 (8%)	15,19,21	0.74	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
4	NAG	A	701	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	701	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	NAG	O5-C5	-2.21	1.41	1.45
4	D	701	NAG	O5-C5	-2.14	1.41	1.45

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.

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%)	0.38	20 (7%) 14 18	30, 54, 125, 181	0
1	B	267/278 (96%)	0.50	31 (11%) 5 7	29, 60, 146, 202	0
1	C	265/278 (95%)	0.91	48 (18%) 2 3	33, 59, 237, 285	0
1	D	266/278 (95%)	1.34	55 (20%) 1 2	31, 62, 281, 438	0
2	H	239/241 (99%)	0.13	8 (3%) 44 54	31, 50, 97, 265	0
2	I	239/241 (99%)	0.26	8 (3%) 44 54	31, 63, 133, 250	0
2	J	239/241 (99%)	0.32	12 (5%) 28 35	35, 68, 131, 246	0
2	K	239/241 (99%)	2.57	74 (30%) 1 1	36, 100, 312, 488	0
3	L	213/214 (99%)	0.02	2 (0%) 81 88	30, 46, 75, 106	0
3	M	213/214 (99%)	0.03	2 (0%) 81 88	27, 46, 86, 147	0
3	N	213/214 (99%)	0.12	1 (0%) 88 94	49, 69, 113, 140	0
3	O	213/214 (99%)	3.39	129 (60%) 0 0	89, 178, 276, 356	0
All	All	2873/2932 (97%)	0.83	390 (13%) 4 5	27, 63, 228, 488	0

All (390) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	182	VAL	23.9
2	K	138	LEU	22.8
2	K	139	GLY	17.9
2	K	140	CYS	17.6
2	K	181	VAL	16.6
2	K	130	SER	16.2
2	K	198	VAL	15.9
1	D	294	PHE	15.7
2	K	158	ALA	15.3
2	K	180	SER	13.8
2	K	127	SER	13.7

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Mol	Chain	Res	Type	RSRZ
2	K	136	ALA	13.6
1	D	293	PRO	13.5
3	O	135	LEU	13.4
3	O	194	CYS	13.0
2	I	130	SER	12.6
3	O	196	VAL	12.6
2	K	141	LEU	12.3
2	K	183	THR	11.5
2	K	206	LYS	11.4
1	D	289	PRO	11.4
2	K	133	GLY	11.3
2	K	159	LEU	11.3
3	O	111	ALA	11.3
1	D	288	ILE	11.2
2	K	193	THR	11.1
3	O	133	VAL	11.0
2	K	131	THR	11.0
2	K	184	VAL	11.0
1	D	297	VAL	10.8
1	D	281	CYS	10.7
2	K	132	SER	10.5
2	K	128	SER	10.3
2	K	129	LYS	10.3
3	O	176	SER	10.0
3	O	116	PHE	9.9
3	O	174	SER	9.8
3	O	162	SER	9.7
2	H	133	GLY	9.5
1	D	296	ASN	9.4
2	K	155	ASN	9.4
1	D	282	ILE	9.2
3	O	195	GLU	9.2
3	O	152	ASN	9.2
2	K	151	THR	9.2
1	D	290	ASN	9.1
2	K	142	VAL	9.1
1	D	284	PRO	8.9
2	H	131	THR	8.8
3	O	109	THR	8.8
1	C	46	SER	8.7
1	D	308	TYR	8.7
2	K	161[A]	SER	8.7

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Mol	Chain	Res	Type	RSRZ
2	K	122	PHE	8.6
3	O	119	PRO	8.6
2	J	132	SER	8.5
1	C	299	LYS	8.5
3	O	142	ARG	8.5
3	O	161	GLU	8.5
3	O	144	ALA	8.4
1	D	291	ASP	8.4
1	B	43	VAL	8.4
3	O	198	HIS	8.3
3	O	207	LYS	8.3
1	C	300	ILE	8.2
1	D	302	TYR	8.2
1	D	275[A]	ASP	8.0
3	O	122	ASP	8.0
2	J	133	GLY	7.9
2	K	213	PRO	7.8
2	I	132	SER	7.8
2	K	214	LYS	7.7
3	O	120	PRO	7.7
1	D	48	THR	7.7
1	D	274[A]	ILE	7.6
2	K	152	VAL	7.6
2	K	190	GLY	7.6
1	C	294	PHE	7.5
3	O	117	ILE	7.5
1	D	45	SER	7.5
3	O	201	LEU	7.5
1	C	45	SER	7.5
1	C	289	PRO	7.4
2	K	191	THR	7.3
1	D	301	THR	7.2
1	D	52	CYS	7.1
1	D	53	ASN	7.1
3	O	132	VAL	7.0
1	C	297	VAL	7.0
1	C	48	THR	7.0
2	H	130	SER	6.9
1	D	276	THR	6.9
3	O	206	THR	6.9
2	K	179	SER	6.9
2	K	117	LYS	6.8

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Mol	Chain	Res	Type	RSRZ
1	C	293	PRO	6.8
3	O	172	THR	6.8
3	O	175	LEU	6.7
1	C	291	ASP	6.7
3	O	150	VAL	6.6
3	O	153	ALA	6.5
3	O	145	LYS	6.5
3	O	184	ALA	6.5
1	D	300	ILE	6.5
3	O	155	GLN	6.4
3	O	200	GLY	6.4
3	O	156	SER	6.4
3	O	106	ILE	6.3
2	J	130	SER	6.3
2	K	126	PRO	6.3
2	K	121	VAL	6.3
1	C	284	PRO	6.3
3	O	169	LYS	6.3
1	D	279	SER	6.3
2	I	131	THR	6.2
3	O	147	GLN	6.2
1	B	291	ASP	6.2
2	I	129	LYS	6.2
2	K	116	THR	6.1
1	D	47	SER	6.0
2	I	214	LYS	6.0
1	C	290	ASN	6.0
1	D	51	ILE	6.0
1	D	50	LYS	5.9
1	C	296	ASN	5.9
1	D	309	VAL	5.9
2	K	163	VAL	5.9
3	O	186	TYR	5.9
1	D	280	GLU	5.9
1	C	49	GLY	5.9
3	O	164	THR	5.9
3	O	165	GLU	5.8
1	C	52	CYS	5.7
1	C	279	SER	5.7
3	O	126	LYS	5.7
3	O	163	VAL	5.7
3	O	112	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
2	K	192	GLN	5.6
1	B	297	VAL	5.6
2	H	134	GLY	5.6
1	D	287	SER	5.6
1	D	264	LYS	5.6
1	C	288	ILE	5.5
1	C	301	THR	5.5
1	D	292	LYS	5.4
2	K	212	GLU	5.4
3	O	197	THR	5.4
3	O	180	THR	5.4
3	O	211	ARG	5.3
3	O	179	LEU	5.2
3	O	80	PRO	5.2
3	O	146	VAL	5.2
1	C	307	LYS	5.1
2	K	153	SER	5.1
3	O	143	GLU	5.1
1	D	298	ASN	5.1
3	O	148	TRP	5.1
2	I	133	GLY	5.0
3	O	127	SER	5.0
1	C	304	ALA	5.0
3	O	203	SER	5.0
1	C	53	ASN	5.0
2	K	150	VAL	4.9
3	O	170	ASP	4.9
3	O	212	GLY	4.9
3	O	202	SER	4.9
2	K	208	ASP	4.9
1	A	43	VAL	4.9
1	D	278	ILE	4.9
3	O	13	ALA	4.9
2	J	214	LYS	4.9
3	O	160	GLN	4.9
1	D	54	ASN	4.8
1	D	304	ALA	4.8
2	K	137	ALA	4.8
1	C	298	ASN	4.8
1	D	270	SER	4.8
2	K	160	THR	4.7
1	C	282	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	49	GLY	4.7
1	D	307	LYS	4.7
3	O	140	TYR	4.7
3	O	121	SER	4.7
1	D	306	PRO	4.6
1	D	295	GLN	4.6
1	C	305	CYS	4.6
3	O	151	ASP	4.6
1	B	280	GLU	4.6
1	C	308	TYR	4.6
3	O	134	CYS	4.6
3	O	110	VAL	4.6
1	C	44	GLN	4.6
2	K	123	PRO	4.5
1	D	277	CYS	4.5
1	C	275[A]	ASP	4.5
3	O	181	LEU	4.5
1	D	46	SER	4.5
2	J	134	GLY	4.4
1	D	283	THR	4.4
1	C	47	SER	4.4
2	K	154	TRP	4.4
3	O	123	GLU	4.4
3	O	208	SER	4.4
1	D	44	GLN	4.4
2	J	189	LEU	4.4
2	J	131	THR	4.3
1	D	299	LYS	4.3
2	K	195	ILE	4.3
1	A	297	VAL	4.3
2	K	189	LEU	4.3
3	O	136	LEU	4.3
3	O	192	TYR	4.3
2	I	134	GLY	4.3
2	K	210	ARG	4.3
1	A	294	PHE	4.2
1	C	281	CYS	4.2
3	O	137	ASN	4.2
2	K	125	ALA	4.2
3	O	189	HIS	4.2
2	K	201	LYS	4.1
1	C	285	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	309	VAL	4.1
3	O	178	THR	4.1
3	O	209	PHE	4.0
1	B	268	MET	4.0
3	O	83	VAL	4.0
1	C	276	THR	4.0
1	C	292	LYS	4.0
1	B	282	ILE	3.9
1	C	274[A]	ILE	3.9
1	B	289	PRO	3.9
2	H	132	SER	3.9
1	C	283	THR	3.9
2	K	194	TYR	3.8
3	O	149	LYS	3.8
3	O	118	PHE	3.8
3	O	1	ASP	3.8
2	J	135	THR	3.8
3	O	210	ASN	3.8
3	O	185	ASP	3.8
1	D	305	CYS	3.8
3	O	205	VAL	3.7
3	O	213	GLU	3.7
3	O	199	GLN	3.7
1	C	50	LYS	3.7
3	O	128	GLY	3.7
1	B	294	PHE	3.7
2	K	118	GLY	3.6
2	H	27(B)	PHE	3.6
1	A	304	ALA	3.6
1	C	302	TYR	3.6
1	C	295	GLN	3.6
2	K	164	HIS	3.6
2	K	178	LEU	3.6
1	C	264	LYS	3.5
3	O	4	LEU	3.5
3	O	167	ASP	3.5
2	K	143	LYS	3.5
3	O	28	ASP	3.5
1	D	303	GLY	3.4
3	O	114	SER	3.4
3	O	183	LYS	3.4
2	K	199	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
3	O	154	LEU	3.3
2	I	127	SER	3.3
1	B	288	ILE	3.3
1	A	207[A]	ARG	3.3
3	O	11	LEU	3.3
1	C	287	SER	3.2
3	O	27	GLN	3.2
3	O	84	GLY	3.1
2	K	202	PRO	3.1
2	J	188	SER	3.1
3	O	12	SER	3.1
2	K	170	LEU	3.1
3	O	115	VAL	3.1
1	B	290	ASN	3.0
3	O	193	ALA	3.0
3	O	105	VAL	3.0
3	O	157	GLY	3.0
2	K	204	ASN	3.0
1	B	309	VAL	3.0
1	D	58	ILE	3.0
3	O	173	TYR	3.0
1	B	305	CYS	3.0
3	O	131	SER	3.0
2	K	124	LEU	3.0
3	O	168	SER	2.9
1	C	306	PRO	2.9
2	J	191	THR	2.9
3	O	129	THR	2.9
1	A	290	ASN	2.9
1	B	295	GLN	2.9
1	D	55	PRO	2.9
2	K	168	ALA	2.9
3	O	76	SER	2.9
1	B	281	CYS	2.9
1	D	56	HIS	2.9
2	K	209	LYS	2.9
1	B	207[A]	ARG	2.9
3	O	171	SER	2.9
1	B	119	GLU	2.8
3	O	29	ILE	2.8
1	A	289	PRO	2.8
3	O	51	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	O	104	VAL	2.8
2	K	157	GLY	2.8
1	D	268	MET	2.7
1	C	268	MET	2.7
3	O	23	CYS	2.7
3	O	60	SER	2.7
1	A	305	CYS	2.7
1	C	51	ILE	2.7
2	K	196	CYS	2.7
1	B	287	SER	2.7
3	O	204	PRO	2.7
1	A	291	ASP	2.7
3	O	18[A]	ARG	2.6
3	O	102	THR	2.6
3	O	159	SER	2.6
1	A	46	SER	2.6
2	H	135	THR	2.6
3	L	56	ARG	2.6
1	B	306	PRO	2.6
3	O	88	CYS	2.6
1	B	46	SER	2.6
1	A	104	ASP	2.5
2	K	167	PRO	2.5
1	C	54	ASN	2.5
2	H	129	LYS	2.5
1	A	264	LYS	2.5
1	B	304	ALA	2.4
1	A	48	THR	2.4
3	O	190	LYS	2.4
3	O	19	VAL	2.4
1	B	276	THR	2.4
3	O	39	LYS	2.4
2	K	200	HIS	2.4
1	B	278	ILE	2.4
1	D	285	ASN	2.4
1	B	44	GLN	2.4
3	O	40	PRO	2.4
1	B	307	LYS	2.4
1	A	296	ASN	2.3
3	O	101	GLY	2.3
3	O	177	SER	2.3
1	A	280	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	N	210	ASN	2.3
3	O	7	SER	2.3
2	K	120	SER	2.3
3	O	188	LYS	2.3
1	C	119	GLU	2.2
2	K	197	ASN	2.2
1	C	278	ILE	2.2
3	O	3	GLN	2.2
3	M	56	ARG	2.2
2	K	115	SER	2.2
1	B	308	TYR	2.2
3	O	86	TYR	2.2
1	B	298	ASN	2.2
1	D	57	ARG	2.2
1	B	264	LYS	2.2
1	A	287	SER	2.1
3	O	38	GLN	2.1
1	A	300	ILE	2.1
3	O	107	LYS	2.1
2	J	194	TYR	2.1
1	A	44	GLN	2.1
2	K	165	THR	2.1
1	C	277	CYS	2.1
2	K	144	ASP	2.1
1	B	274[A]	ILE	2.1
1	B	48	THR	2.1
1	D	207[A]	ARG	2.1
1	A	51	ILE	2.1
3	O	81	GLU	2.1
1	B	279	SER	2.1
1	B	77	ASP	2.0
1	C	273	PRO	2.0
2	J	184	VAL	2.0
3	O	69	THR	2.0
3	O	2	ILE	2.0
3	L	213	GLU	2.0
1	D	286	GLY	2.0
3	M	213	GLU	2.0
1	C	270	SER	2.0
3	O	8	PRO	2.0
2	K	146	PHE	2.0
3	O	64	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
3	O	73	LEU	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PCA	I	1	8/9	0.18	-	61,81,87,88	0
2	PCA	H	1	8/9	0.21	-	79,96,104,105	0
2	PCA	K	1	8/9	0.22	-	122,139,147,148	0
2	PCA	J	1	8/9	0.17	-	86,98,103,106	0

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	C	701	14/15	0.33	-	109,120,130,136	0
5	NAG	C	702	14/15	0.32	-	120,125,127,128	0

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	ZN	H	301	1/1	0.16	-	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	D	701	14/15	0.31	-	100,115,129,135	0
6	ZN	M	301	1/1	0.08	-	94,94,94,94	0
4	NAG	A	701	14/15	0.28	-	122,134,148,154	0
6	ZN	N	302	1/1	0.07	-	104,104,104,104	0
6	ZN	L	302	1/1	0.13	-	72,72,72,72	0
6	ZN	N	301	1/1	0.13	-	102,102,102,102	0
6	ZN	O	301	1/1	0.11	-	133,133,133,133	0
6	ZN	J	301	1/1	0.05	-	143,143,143,143	0
6	ZN	L	301	1/1	0.09	-	106,106,106,106	0

6.5 Other polymers

There are no such residues in this entry.