W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 27, 2014 – 09:27 PM GMT

PDB ID   :   3HS0
Title   :   Cobra Venom Factor (CVF) in complex with human factor B
Authors   :   Janssen, B.J.C.; Gomes, L.; Koning, R.I.; Svergun, D.I.; Koster, A.J.; Fritzinger, D.C.; Vogel, C.-W.; Gros, P.
Deposited on   :   2009-06-10
Resolution   :   3.00 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Rfree		0.236
Clashscore		3
Ramachandran outliers		1.6%
Sidechain outliers		2.5%
RSRZ outliers		0.4%

Worse　　　　　　　　　　　　　　　Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
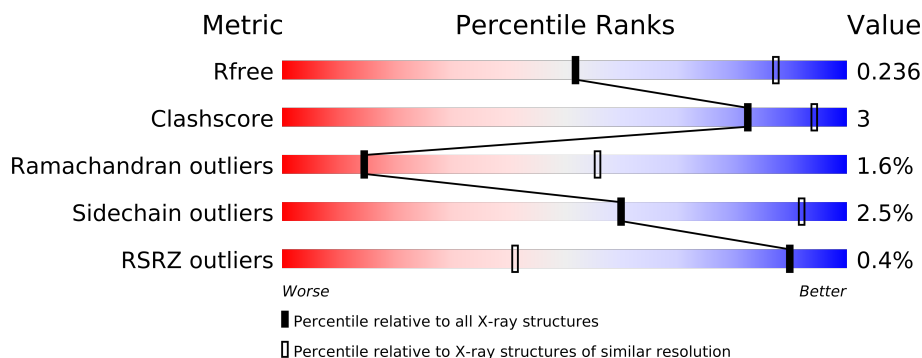
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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	627	
1	F	627	
2	B	252	
2	G	252	
3	C	379	
3	H	379	
4	D	741	
4	I	741	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	C	9324	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	D	9117	-	X
5	NAG	D	9353	-	X
5	NAG	H	9324	-	X
5	NAG	I	9117	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 30435 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 Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total 4794	C 3069	N 804	O 906	S 15	0	0	0
1	F	617	Total 4826	C 3085	N 811	O 915	S 15	0	0	0

- Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total 1856	C 1194	N 311	O 346	S 5	0	0	0
2	G	233	Total 1856	C 1194	N 311	O 346	S 5	0	0	0

- Molecule 3 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	359	Total 2900	C 1831	N 484	O 566	S 19	0	0	0
3	H	366	Total 2957	C 1864	N 496	O 578	S 19	0	0	0

- Molecule 4 is a protein called Complement factor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	699	Total 5513	C 3474	N 954	O 1052	S 33	0	0	0
4	I	704	Total 5567	C 3506	N 972	O 1056	S 33	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	254	GLY	ASP	ENGINEERED	UNP P00751
D	260	ASP	ASN	ENGINEERED	UNP P00751
D	740	ALA	-	INSERTION	UNP P00751
D	741	ALA	-	INSERTION	UNP P00751
I	254	GLY	ASP	ENGINEERED	UNP P00751
I	260	ASP	ASN	ENGINEERED	UNP P00751
I	740	ALA	-	INSERTION	UNP P00751
I	741	ALA	-	INSERTION	UNP P00751

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
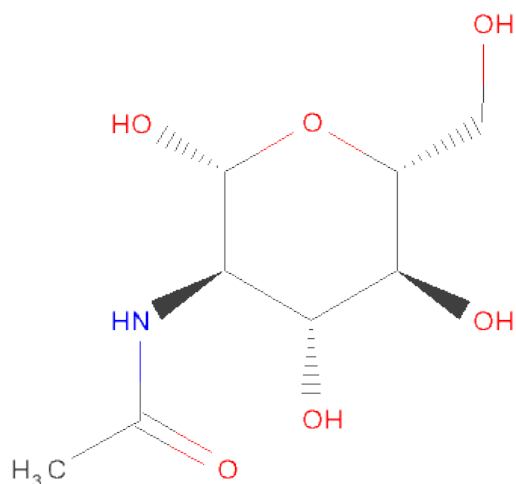
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	1	Total 1	Mg 1	0	0
6	A	1	Total 1	Mg 1	0	0
6	D	1	Total 1	Mg 1	0	0
6	F	1	Total 1	Mg 1	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	2	Total 28	C 16	N 2	O 10	0	0
7	I	2	Total 28	C 16	N 2	O 10	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	254	GLY	ASP	ENGINEERED	UNP P00751
D	260	ASP	ASN	ENGINEERED	UNP P00751
D	740	ALA	-	INSERTION	UNP P00751
D	741	ALA	-	INSERTION	UNP P00751
I	254	GLY	ASP	ENGINEERED	UNP P00751
I	260	ASP	ASN	ENGINEERED	UNP P00751
I	740	ALA	-	INSERTION	UNP P00751
I	741	ALA	-	INSERTION	UNP P00751

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total 2	O 2	0	0
8	C	1	Total 1	O 1	0	0
8	D	1	Total 1	O 1	0	0
8	F	2	Total 2	O 2	0	0
8	H	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	1	Total	O	0	0
			1	1		

wwPDB X-ray Structure Validation Summary Report

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
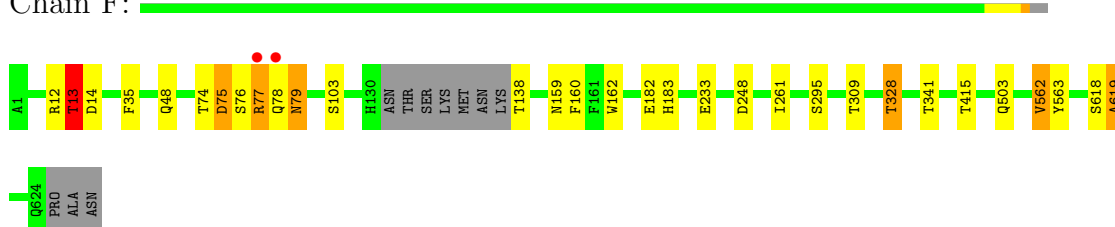
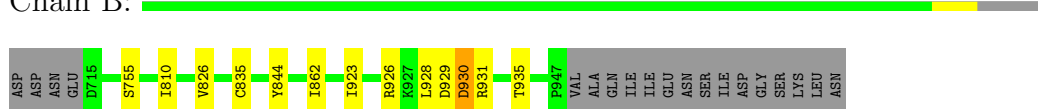- Molecule 1: Cobra venom factor

Chain A:
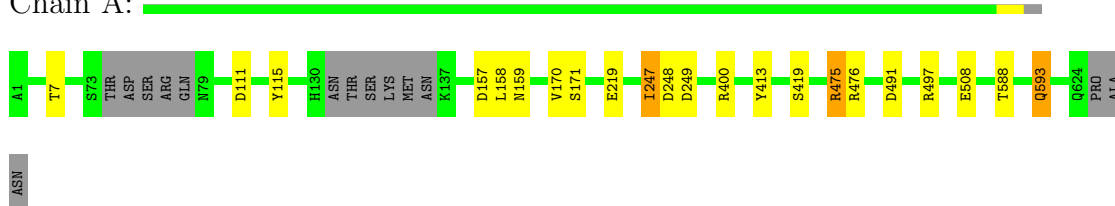
- Molecule 1: Cobra venom factor
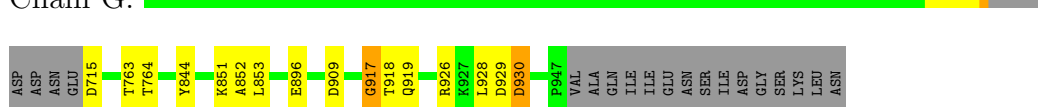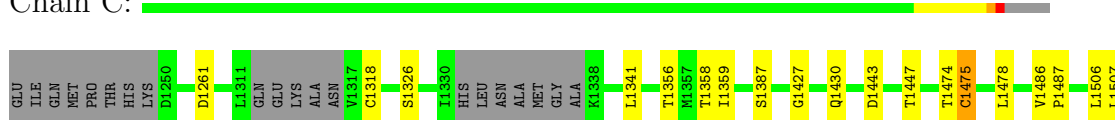
Chain F:

- Molecule 2: Cobra venom factor
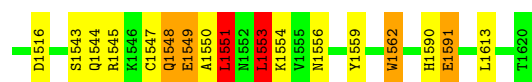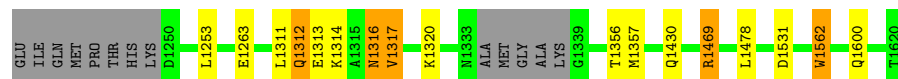
Chain B:

- Molecule 2: Cobra venom factor

Chain G:

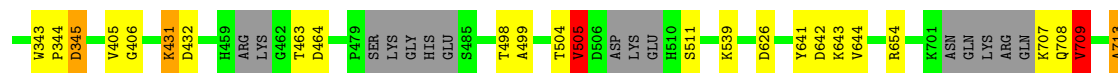- Molecule 3: Cobra venom factor

Chain C:

D1516 S1543 Q1544 R1545 K1546 C1547 Q1548 E1549 A1550 L1551 N1552 L1553 K1554 V1555 N1556 Y1559 W1562 H1590 E1591 L1613 T1620

• Molecule 3: Cobra venom factor

Chain H:

GLU ILE GLN MET PRO THR HIS LYS D1250 L1253 E1263 L1311 Q1312 E1313 K1314 A1315 N1316 V1317 K1320 N1333 ALA MET GLY ALA LYS G1339 T1356 M1357 Q1430 R1469 L1478 D1531 W1562 Q1600 T1620

• Molecule 4: Complement factor B

Chain D:

THR PRO TRP SER LEU ALA ARG PRO GLN GLY S11 K20 L27 Y35 Y44 P45 V46 Q47 T48 C51 S58 D64 R74 V98 T111 S175 Q203 T216 ILE GLU GLY VAL ASP ALA GLU ASP GLY HIS GLY PRO GLU GLU GLN GLN K233 A290

W343 P344 D345 V405 G406 K431 D432 H459 ARG LYS G462 T463 D464 P479 SER LYS GLY HIS GLU S485 T498 A499 T504 V505 D506 ASP LYS GLU H510 S511 K539 D626 Y641 D642 K643 V644 R654 K701 ASN GLN LYS ARG GLN K707 Q708 V709 A713

R714 L724 P725 K728 G737 F738 L739 A740 ALA

• Molecule 4: Complement factor B

Chain I:

THR PRO TRP SER LEU ALA ARG PRO GLN GLY S11 C12 S13 L14 E15 G16 V17 E18 I19 K20 G21 L26 E29 G30 P38 T50 C51 R52 S53 T54 W57 K61 T62 T111 E182 F209 T216 ILE GLU GLY VAL ASP ALA GLU ASP GLY HIS GLY PRO GLY

GLU GLN GLN K233 A290 D303 S304 S305 N306 S342 W343 P344 ASP ASP V347 W352 N353 T363 D364 G406 P407 L408 M443 E446 S447 Q448 S449 L450 S451 L452 K461 G462 T463 D464 Y465 H466 K467 Q468 R478 PRO SER LYS GLY H483 T504 V505 ASP ASP LYS

GLU H510 D522 I544 P545 R654 K701 N702 Q703 K704 R705 Q706 K707 E734 D735 L736 G737 A740 ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	134.03Å 136.97Å 283.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.88 – 3.00 34.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.88-3.00) 99.8 (34.88-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.189 , 0.243 0.179 , 0.236	Depositor DCC
R_{free} test set	2095 reflections (2.00%)	DCC
Wilson B-factor (Å^2)	72.0	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 26.3	EDS
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
L-test for twinning	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	1 of 104864 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	30435	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities 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: MG, 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	0.27	0/4902	0.46	0/6668
1	F	0.27	0/4935	0.49	2/6715 (0.0%)
2	B	0.27	0/1894	0.46	0/2570
2	G	0.28	0/1894	0.51	1/2570 (0.0%)
3	C	0.26	0/2950	0.51	1/3989 (0.0%)
3	H	0.26	0/3009	0.47	0/4071
4	D	0.26	0/5636	0.48	2/7629 (0.0%)
4	I	0.25	0/5691	0.46	0/7699
All	All	0.26	0/30911	0.48	6/41911 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	1	0
3	C	0	1
All	All	1	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1553	LEU	N-CA-C	5.97	127.12	111.00
1	F	13	THR	C-N-CA	5.71	135.96	121.70
4	D	739	LEU	CA-CB-CG	5.49	127.93	115.30
2	G	917	GLY	N-CA-C	5.23	126.18	113.10
1	F	13	THR	CA-C-N	5.19	128.62	117.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	13	THR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	1551	LEU	Peptide

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	4794	0	0	8	0
1	F	4826	0	0	14	0
2	B	1856	0	7	3	0
2	G	1856	0	7	5	0
3	C	2900	0	3	13	0
3	H	2957	0	3	8	0
4	D	5513	0	0	19	0
4	I	5567	0	0	27	0
5	A	14	0	13	0	0
5	C	14	0	13	0	0
5	D	28	0	0	0	0
5	F	14	0	13	0	0
5	H	14	0	13	0	0
5	I	14	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	I	1	0	0	0	0
7	D	28	0	0	0	0
7	I	28	0	0	0	0
8	A	2	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1	0	0	0	0
8	I	1	0	0	0	0
All	All	30435	0	72	94	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 3.

The worst 5 of 94 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:I:701:LYS:N	4:I:702:ASN:O	2.20	0.74
4:I:449:SER:O	4:I:451:SER:N	2.22	0.73
4:I:446:GLU:O	4:I:448:GLN:N	2.22	0.72
3:H:1312:GLN:O	3:H:1314:LYS:N	2.24	0.71
4:I:447:SER:O	4:I:448:GLN:CB	2.39	0.70

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	607/627 (97%)	577 (95%)	26 (4%)	4 (1%)	30	78
1	F	613/627 (98%)	571 (93%)	36 (6%)	6 (1%)	22	70
2	B	231/252 (92%)	218 (94%)	13 (6%)	0	100	100
2	G	231/252 (92%)	218 (94%)	12 (5%)	1 (0%)	43	87
3	C	353/379 (93%)	318 (90%)	29 (8%)	6 (2%)	14	54
3	H	362/379 (96%)	333 (92%)	24 (7%)	5 (1%)	16	60
4	D	687/741 (93%)	608 (88%)	63 (9%)	16 (2%)	10	43
4	I	694/741 (94%)	605 (87%)	65 (9%)	24 (4%)	6	30
All	All	3778/3998 (94%)	3448 (91%)	268 (7%)	62 (2%)	14	56

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	ILE
4	D	44	TYR
4	D	46	VAL
4	D	344	PRO
4	D	505	VAL

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	535/548 (98%)	529 (99%)	6 (1%)	84	97
1	F	539/548 (98%)	528 (98%)	11 (2%)	68	94
2	B	210/227 (92%)	200 (95%)	10 (5%)	35	79
2	G	210/227 (92%)	202 (96%)	8 (4%)	44	85
3	C	329/345 (95%)	314 (95%)	15 (5%)	37	80
3	H	335/345 (97%)	326 (97%)	9 (3%)	57	91
4	D	610/643 (95%)	596 (98%)	14 (2%)	63	93
4	I	615/643 (96%)	605 (98%)	10 (2%)	75	95
All	All	3383/3526 (96%)	3300 (98%)	83 (2%)	60	92

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	175	SER
1	F	138	THR
4	I	342	SER
4	D	203	GLN
4	D	728	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 ⓘ

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

5.5 Carbohydrates ⓘ

4 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	#$|Z| > 2$
7	NAG	D	9097	4,7	12,14,15	0.60	0	15,19,21	1.89	4 (26%)
7	NAG	D	9098	7	12,14,15	0.60	0	15,19,21	1.07	1 (6%)
7	NAG	I	9097	4,7	12,14,15	0.60	0	15,19,21	1.06	1 (6%)
7	NAG	I	9098	7	12,14,15	0.56	0	15,19,21	1.78	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
7	NAG	D	9097	4,7	-	0/6/23/26	0/1/1/1
7	NAG	D	9098	7	-	2/6/23/26	0/1/1/1
7	NAG	I	9097	4,7	-	0/6/23/26	0/1/1/1
7	NAG	I	9098	7	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	9098	NAG	O5-C5-C6	6.61	113.92	106.98
7	D	9097	NAG	O5-C5-C4	4.54	116.41	110.65
7	D	9098	NAG	O5-C5-C6	3.26	110.40	106.98
7	D	9097	NAG	C3-C4-C5	2.83	115.26	110.20
7	D	9097	NAG	C3-C2-N2	2.67	115.82	111.76

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	9098	NAG	C3-C2-N2-C7
7	D	9098	NAG	C8-C7-N2-C2
7	D	9098	NAG	O7-C7-N2-C2

There are no ring outliers.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	9187	1	12,14,15	0.54	0	15,19,21	1.18	2 (13%)
5	NAG	C	9324	3	12,14,15	0.59	0	15,19,21	0.88	1 (6%)
5	NAG	D	9117	4	12,14,15	0.48	0	15,19,21	1.60	1 (6%)
5	NAG	D	9353	4	12,14,15	0.63	0	15,19,21	0.82	0
5	NAG	F	9187	1	12,14,15	0.51	0	15,19,21	1.51	3 (20%)
5	NAG	H	9324	3	12,14,15	0.62	0	15,19,21	0.89	1 (6%)
5	NAG	I	9117	4	12,14,15	0.58	0	15,19,21	0.89	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	A	9187	1	-	0/6/23/26	0/1/1/1
5	NAG	C	9324	3	-	0/6/23/26	0/1/1/1
5	NAG	D	9117	4	-	0/6/23/26	0/1/1/1
5	NAG	D	9353	4	-	0/6/23/26	0/1/1/1
5	NAG	F	9187	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	H	9324	3	-	0/6/23/26	0/1/1/1
5	NAG	I	9117	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	9117	NAG	O5-C5-C4	5.36	117.46	110.65
5	F	9187	NAG	O5-C5-C6	3.29	110.43	106.98
5	F	9187	NAG	O5-C5-C4	3.26	114.79	110.65
5	A	9187	NAG	O5-C5-C6	2.87	109.99	106.98
5	H	9324	NAG	O5-C5-C6	2.41	109.51	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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	613/627 (97%)	-0.44	0	100	100	31, 68, 125, 182	0
1	F	617/627 (98%)	-0.41	2 (0%)	91	48	37, 75, 132, 187	0
2	B	233/252 (92%)	-0.49	0	100	100	34, 63, 111, 123	0
2	G	233/252 (92%)	-0.47	0	100	100	33, 66, 115, 151	0
3	C	359/379 (94%)	-0.30	0	100	100	40, 94, 210, 291	0
3	H	366/379 (96%)	-0.42	0	100	100	33, 81, 135, 216	0
4	D	699/741 (94%)	-0.27	2 (0%)	91	48	35, 88, 189, 233	0
4	I	704/741 (95%)	-0.25	11 (1%)	68	16	37, 91, 191, 244	0
All	All	3824/3998 (95%)	-0.36	15 (0%)	90	41	31, 79, 168, 291	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	30	GLY	4.5
4	I	29	GLU	4.2
4	I	51	CYS	3.8
4	I	16	GLY	3.7
4	I	26	LEU	3.2

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

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

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
7	NAG	I	9097	14/15	0.27	3.78	126,139,157,173	0
7	NAG	D	9097	14/15	0.24	2.32	136,146,153,163	0
7	NAG	D	9098	14/15	0.50	-	161,168,182,183	0
7	NAG	I	9098	14/15	0.68	-	173,184,194,201	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
5	NAG	I	9117	14/15	0.35	4.02	116,129,142,143	0
5	NAG	D	9117	14/15	0.23	3.41	98,117,131,132	0
5	NAG	C	9324	14/15	0.28	3.35	111,123,130,134	0
5	NAG	H	9324	14/15	0.38	3.01	129,140,144,146	0
5	NAG	D	9353	14/15	0.29	2.04	122,136,142,146	0
5	NAG	A	9187	14/15	0.18	0.46	87,102,110,114	0
5	NAG	F	9187	14/15	0.30	0.46	106,116,125,127	0
6	MG	I	742	1/1	0.13	-0.72	97,97,97,97	0
6	MG	D	742	1/1	0.10	-1.85	107,107,107,107	0
6	MG	A	628	1/1	0.08	-2.22	105,105,105,105	0
6	MG	F	628	1/1	0.04	-3.08	73,73,73,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.