



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:17 AM 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)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

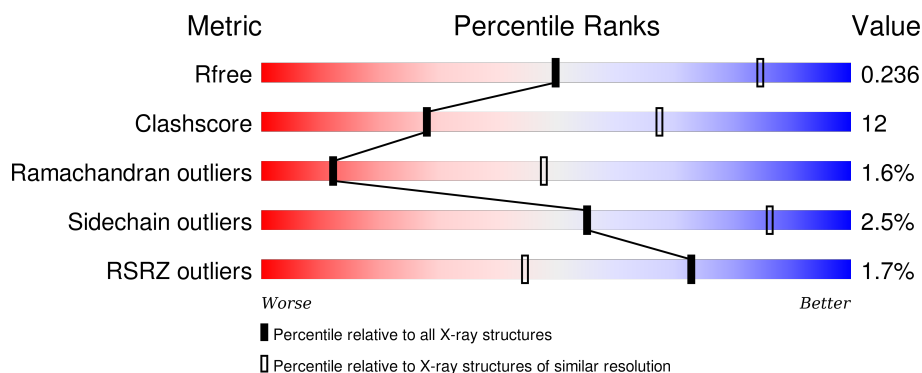
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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. 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	627	 77% 20% .
1	F	627	 76% 21% . .
2	B	252	 75% 17% . 8%
2	G	252	 72% 18% . 8%
3	C	379	 66% 26% . . 5%

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Mol	Chain	Length	Quality of chain
3	H	379	
4	D	741	
4	I	741	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	C	9324	-	-	-	X
5	NAG	D	9353	-	-	-	X
5	NAG	H	9324	-	-	-	X

2 Entry composition

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

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

- Molecule 2 is a protein called Cobra venom factor.

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

- Molecule 3 is a protein called Cobra venom factor.

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

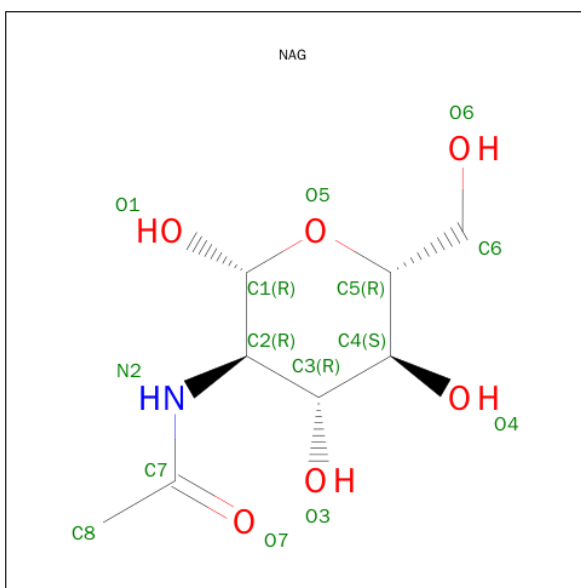
- Molecule 4 is a protein called Complement factor B.

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

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 Mg 1 1	0	0
6	A	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 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 C N O 28 16 2 10	0	0
7	I	2	Total C N O 28 16 2 10	0	0

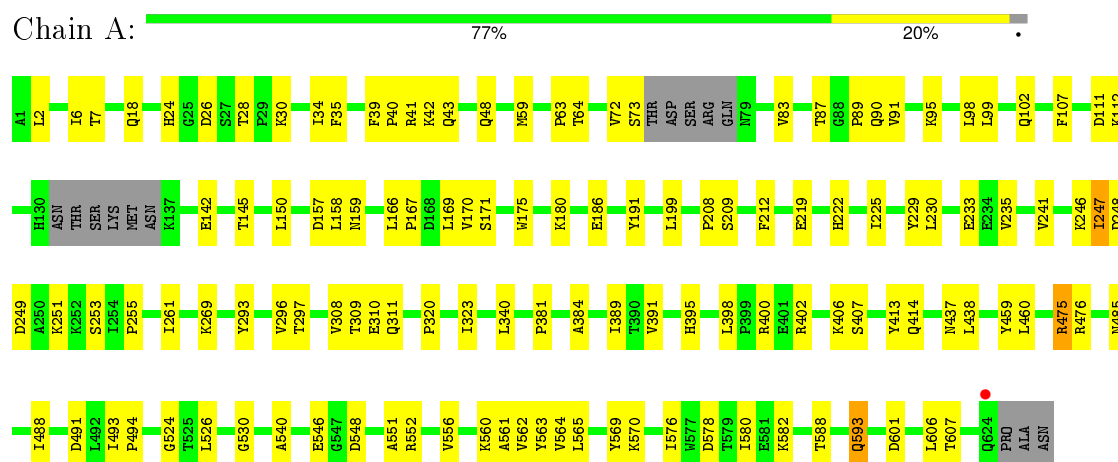
- Molecule 8 is water.

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

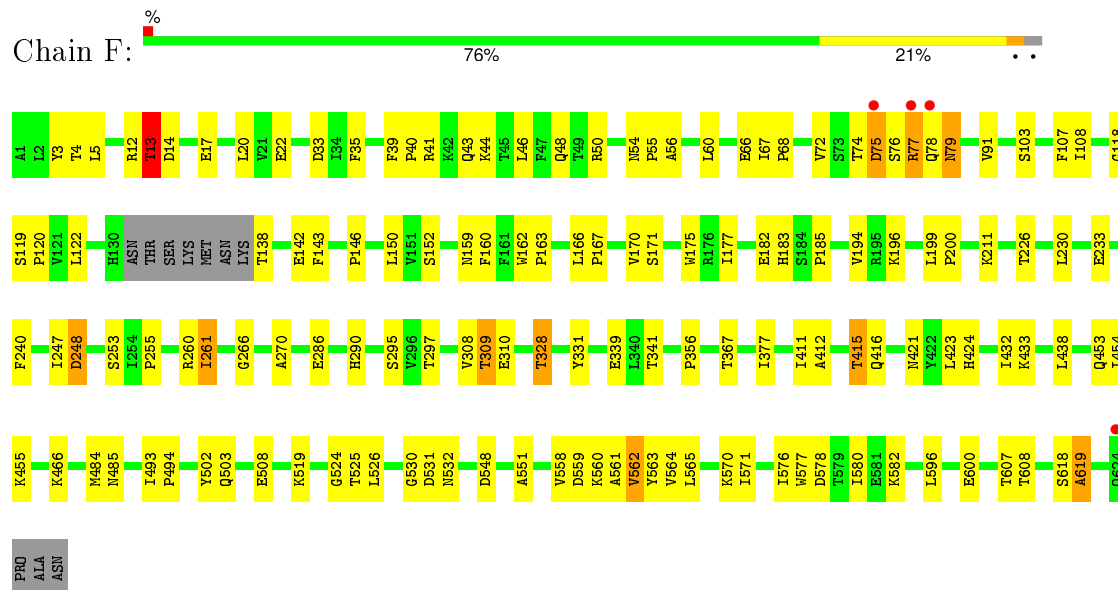
3 Residue-property plots

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

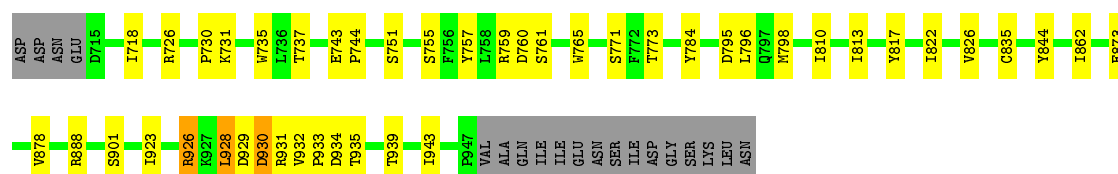


• Molecule 1: Cobra venom factor



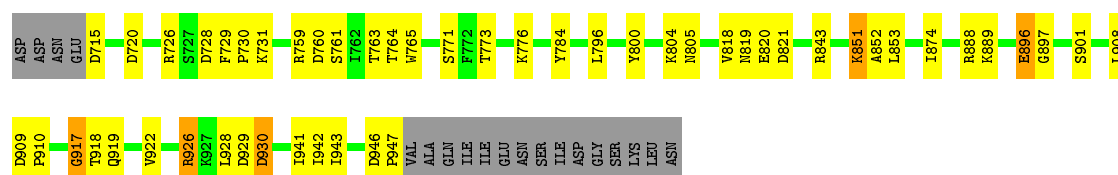
• Molecule 2: Cobra venom factor





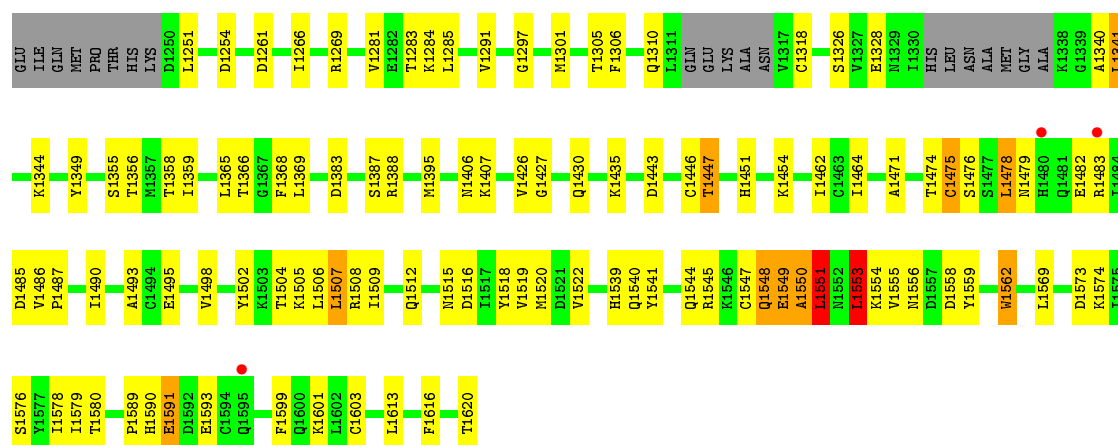
• Molecule 2: Cobra venom factor

Chain G: 72% 18% 8%



• Molecule 3: Cobra venom factor

Chain C: 66% 26% 5%



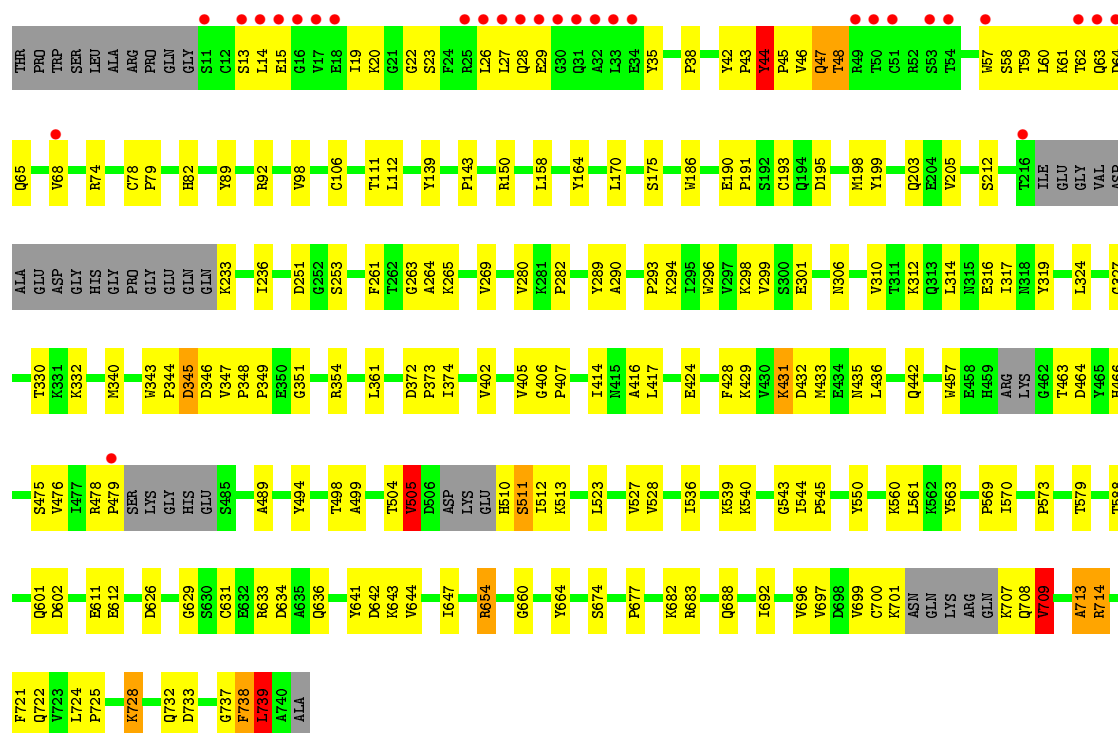
• Molecule 3: Cobra venom factor

Chain H: 78% 17% 5%

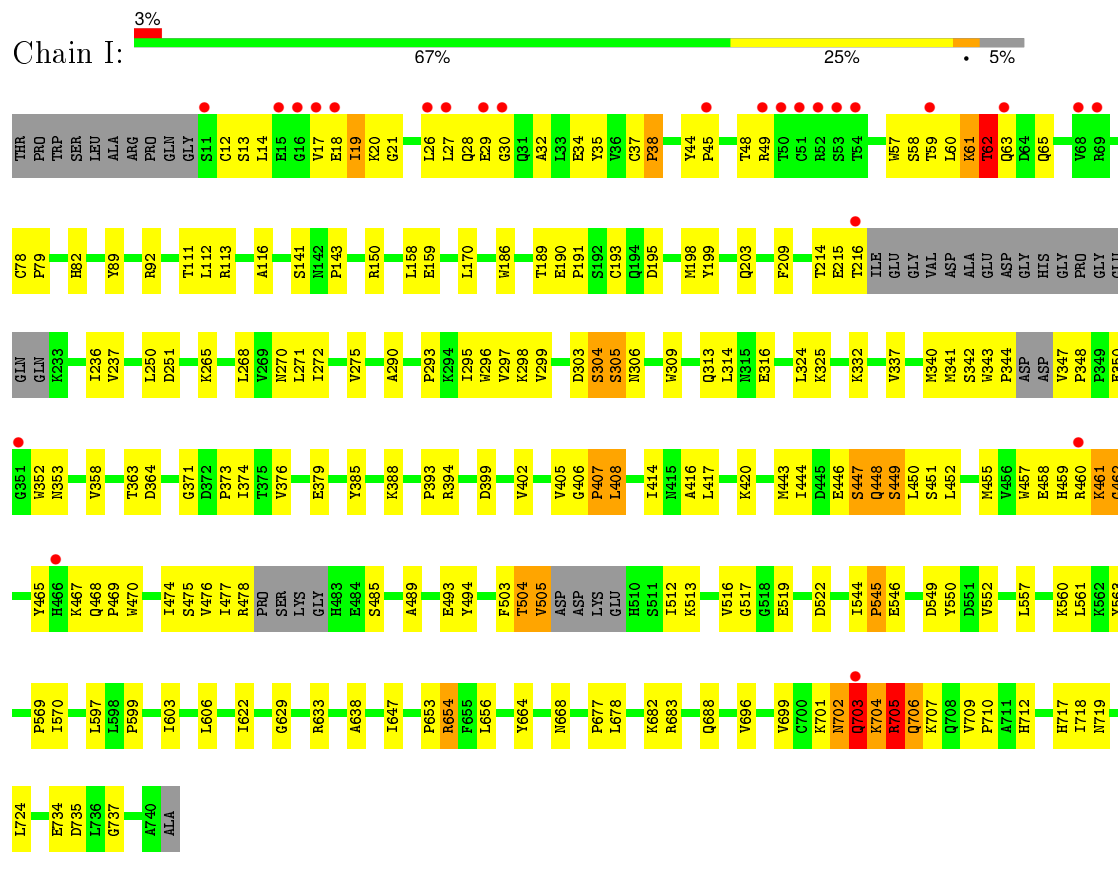


• Molecule 4: Complement factor B

Chain D: 68% 25% 6%



• Molecule 4: Complement factor B



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.189 , 0.243 0.177 , 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 , 39.3	EDS
Estimated twinning fraction	0.019 for k,h,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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(°)	Ideal(°)
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 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	4794	0	4801	90	0
1	F	4826	0	4826	111	0
2	B	1856	0	1900	37	0
2	G	1856	0	1900	40	0
3	C	2900	0	2851	101	0
3	H	2957	0	2900	62	0
4	D	5513	0	5376	153	0
4	I	5567	0	5446	160	0
5	A	14	0	13	2	0
5	C	14	0	13	0	0
5	D	28	0	26	0	0
5	F	14	0	13	0	0
5	H	14	0	13	0	0
5	I	14	0	13	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	25	0	0
7	I	28	0	25	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
8	H	1	0	0	0	0
8	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30435	0	30141	711	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 12.

The worst 5 of 711 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)
3:H:1469:ARG:HG2	3:H:1469:ARG:HH11	1.10	1.12
4:D:714:ARG:HG2	4:D:714:ARG:HH11	1.17	1.07
4:I:705:ARG:HB3	4:I:707:LYS:HG2	1.37	1.04
1:F:13:THR:HG23	1:F:14:ASP:CB	1.89	1.01
4:D:699:VAL:HG23	4:D:707:LYS:HD2	1.42	1.01

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	26	70
1	F	613/627 (98%)	571 (93%)	36 (6%)	6 (1%)	19	61
2	B	231/252 (92%)	218 (94%)	13 (6%)	0	100	100
2	G	231/252 (92%)	218 (94%)	12 (5%)	1 (0%)	39	80
3	C	353/379 (93%)	318 (90%)	29 (8%)	6 (2%)	11	46
3	H	362/379 (96%)	333 (92%)	24 (7%)	5 (1%)	14	51
4	D	687/741 (93%)	608 (88%)	63 (9%)	16 (2%)	8	36
4	I	694/741 (94%)	605 (87%)	65 (9%)	24 (4%)	4	24
All	All	3778/3998 (94%)	3448 (91%)	268 (7%)	62 (2%)	12	48

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%)	80	94
1	F	539/548 (98%)	528 (98%)	11 (2%)	63	89
2	B	210/227 (92%)	200 (95%)	10 (5%)	31	71
2	G	210/227 (92%)	202 (96%)	8 (4%)	40	78
3	C	329/345 (95%)	314 (95%)	15 (5%)	33	73
3	H	335/345 (97%)	326 (97%)	9 (3%)	52	85
4	D	610/643 (95%)	596 (98%)	14 (2%)	58	87
4	I	615/643 (96%)	605 (98%)	10 (2%)	70	92
All	All	3383/3526 (96%)	3300 (98%)	83 (2%)	55	86

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. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	593	GLN
4	D	47	GLN
4	D	601	GLN
1	F	473	GLN
4	I	468	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	14,14,15	0.49	0	15,19,21	1.98	5 (33%)
7	NAG	D	9098	7	14,14,15	0.47	0	15,19,21	1.08	2 (13%)
7	NAG	I	9097	4,7	14,14,15	0.41	0	15,19,21	1.20	1 (6%)
7	NAG	I	9098	7	14,14,15	0.47	0	15,19,21	1.12	2 (13%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	I	9097	4,7	-	0/6/23/26	0/1/1/1
7	NAG	I	9098	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	9098	NAG	C2-N2-C7	-2.14	120.30	123.04
7	D	9097	NAG	C4-C3-C2	-2.08	108.00	111.23
7	I	9098	NAG	C1-O5-C5	2.16	114.99	112.25
7	D	9097	NAG	C3-C2-N2	2.20	115.82	110.56
7	D	9098	NAG	C1-O5-C5	2.77	115.77	112.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

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	14,14,15	0.43	0	15,19,21	1.30	2 (13%)
5	NAG	C	9324	3	14,14,15	0.50	0	15,19,21	1.07	1 (6%)
5	NAG	D	9117	4	14,14,15	0.35	0	15,19,21	2.49	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	9353	4	14,14,15	0.45	0	15,19,21	0.96	1 (6%)
5	NAG	F	9187	1	14,14,15	0.42	0	15,19,21	1.43	2 (13%)
5	NAG	H	9324	3	14,14,15	0.44	0	15,19,21	0.85	1 (6%)
5	NAG	I	9117	4	14,14,15	0.43	0	15,19,21	1.18	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
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 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	9187	NAG	C2-N2-C7	-2.72	119.54	123.04
5	D	9117	NAG	C4-C3-C2	-2.43	107.45	111.23
5	H	9324	NAG	C1-O5-C5	2.05	114.84	112.25
5	F	9187	NAG	C3-C4-C5	2.42	114.42	110.20
5	D	9353	NAG	C1-O5-C5	2.82	115.82	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	9187	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.66	1 (0%) 95 87	31, 68, 125, 182	0
1	F	617/627 (98%)	-0.60	4 (0%) 90 73	37, 75, 132, 187	0
2	B	233/252 (92%)	-0.72	0 100 100	34, 63, 111, 123	0
2	G	233/252 (92%)	-0.70	0 100 100	33, 66, 115, 151	0
3	C	359/379 (94%)	-0.40	3 (0%) 87 67	40, 94, 210, 291	0
3	H	366/379 (96%)	-0.61	2 (0%) 91 76	33, 81, 135, 216	0
4	D	699/741 (94%)	-0.34	29 (4%) 41 16	35, 88, 189, 233	0
4	I	704/741 (95%)	-0.32	25 (3%) 46 20	37, 91, 191, 244	0
All	All	3824/3998 (95%)	-0.51	64 (1%) 73 45	31, 79, 168, 291	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	16	GLY	9.1
4	I	30	GLY	6.9
4	I	51	CYS	6.6
4	I	50	THR	6.2
4	I	29	GLU	5.8

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

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

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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	NAG	D	9097	14/15	0.86	0.25	1.88	136,146,153,163	0
7	NAG	I	9098	14/15	0.66	0.63	-	173,184,194,201	0
7	NAG	D	9098	14/15	0.64	0.49	-	161,168,182,183	0
7	NAG	I	9097	14/15	0.80	0.26	-	126,139,157,173	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	H	9324	14/15	0.77	0.36	2.60	129,140,144,146	0
5	NAG	D	9353	14/15	0.88	0.31	2.53	122,136,142,146	0
5	NAG	C	9324	14/15	0.82	0.25	2.19	111,123,130,134	0
5	NAG	A	9187	14/15	0.94	0.19	0.64	87,102,110,114	0
5	NAG	F	9187	14/15	0.87	0.30	0.38	106,116,125,127	0
6	MG	I	742	1/1	0.97	0.13	-0.76	97,97,97,97	0
6	MG	D	742	1/1	0.98	0.10	-1.80	107,107,107,107	0
6	MG	A	628	1/1	0.89	0.07	-2.51	105,105,105,105	0
6	MG	F	628	1/1	0.97	0.04	-4.00	73,73,73,73	0
5	NAG	I	9117	14/15	0.92	0.38	-	116,129,142,143	0
5	NAG	D	9117	14/15	0.92	0.22	-	98,117,131,132	0

6.5 Other polymers

There are no such residues in this entry.