Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:26 PM GMT

PDB ID	:	1AU1
Title	:	HUMAN INTERFERON-BETA CRYSTAL STRUCTURE
Authors	:	Karpusas, M.; Nolte, M.; Lipscomb, W.
Deposited on	:	1997-09-09
Resolution	:	2.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

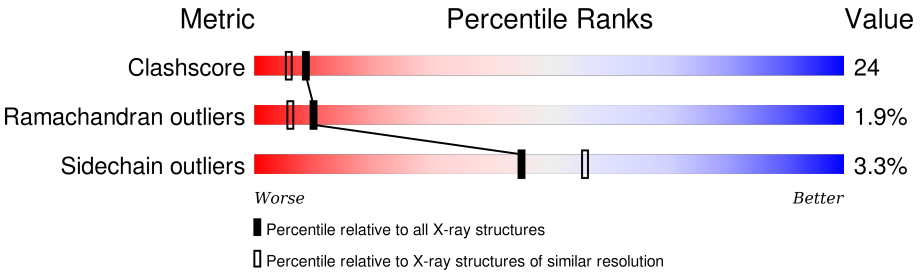
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	166	73% 22%
1	B	166	70% 26%

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
3	G6D	B	168	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3866 atoms, of which 890 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 INTERFERON-BETA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	166	Total	C	H	N	O	S	0	0	0
			1782	908	369	246	252	7			
1	B	163	Total	C	H	N	O	S	0	0	0
			1728	888	344	243	246	7			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	7	Total	C	H	O	0	0
			87	42	11	34		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	2	Total	C	H	O	0	0
			25	12	4	9		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	29	Total	H	O	0	0
			87	58	29		
5	B	52	Total	H	O	0	0
			156	104	52		

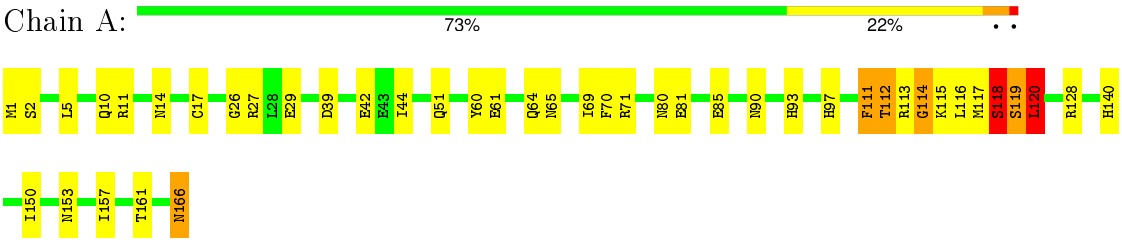
3 Residue-property plots (i)

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.

Note EDS was not executed.

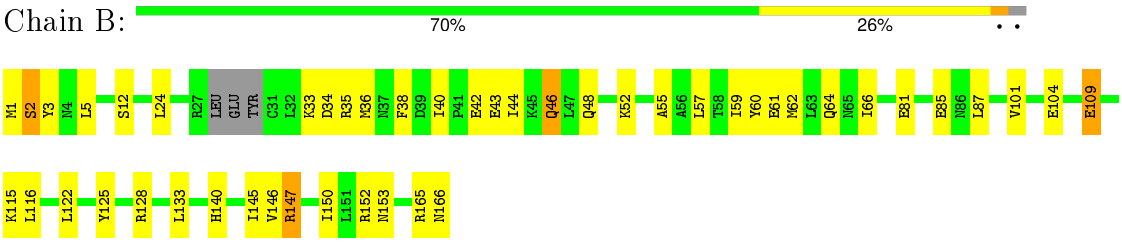
- Molecule 1: INTERFERON-BETA

Chain A:



- Molecule 1: INTERFERON-BETA

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.30Å 65.90Å 121.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20	Depositor
% Data completeness (in resolution range)	83.1 (30.00-2.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.81	Depositor
R, R_{free}	0.223 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3866	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BGC, G6D

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	0.66	0/1443	0.82	2/1940 (0.1%)
1	B	0.65	1/1412 (0.1%)	0.76	1/1896 (0.1%)
All	All	0.66	1/2855 (0.0%)	0.79	3/3836 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	B	1	0
All	All	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2	SER	CA-CB	5.39	1.61	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	26	GLY	N-CA-C	-5.55	99.22	113.10
1	A	128	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	116	LEU	CA-CB-CG	5.15	127.14	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	168	G6D	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	PHE	Sidechain

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	1413	369	1405	91	11
1	B	1384	344	1382	79	11
2	A	76	11	64	1	0
3	B	21	4	19	0	0
4	B	1	0	0	0	0
5	A	29	58	0	6	0
5	B	52	104	0	1	0
All	All	2976	890	2870	136	11

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 24.

All (136) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:CD2	1:B:5:LEU:HD23	1.19	1.60
1:A:115:LYS:HG3	1:A:118:SER:CB	1.27	1.60
1:A:116:LEU:CD1	1:B:2:SER:HB2	1.35	1.51
1:A:115:LYS:CG	1:A:118:SER:HB2	1.39	1.50
1:A:113:ARG:CZ	1:B:104:GLU:OE1	1.72	1.36
1:B:33:LYS:NZ	1:B:36:MET:HG3	1.49	1.26
1:A:113:ARG:NH1	1:B:104:GLU:OE1	1.66	1.24
1:A:116:LEU:CD2	1:B:5:LEU:CD2	2.16	1.24
1:A:116:LEU:HD12	1:B:2:SER:CB	1.67	1.22
1:A:115:LYS:CD	1:A:118:SER:HB2	1.68	1.19
1:A:113:ARG:CZ	1:B:2:SER:OG	1.92	1.17
1:A:116:LEU:CD1	1:B:2:SER:CB	2.23	1.16
1:B:33:LYS:HZ1	1:B:36:MET:CA	1.59	1.16
1:A:113:ARG:NE	1:B:104:GLU:OE2	1.81	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD22	1:B:5:LEU:CD2	1.76	1.13
1:A:116:LEU:HD23	1:B:5:LEU:HD23	1.31	1.09
1:A:115:LYS:HD3	1:A:119:SER:OG	1.46	1.08
1:B:33:LYS:NZ	1:B:36:MET:HA	1.67	1.08
1:B:33:LYS:NZ	1:B:36:MET:CG	2.16	1.08
1:A:116:LEU:O	1:A:116:LEU:HD23	1.56	1.06
1:A:61:GLU:OE1	1:A:115:LYS:HD2	1.42	1.06
1:A:113:ARG:CZ	1:B:104:GLU:CD	2.26	1.04
1:B:33:LYS:NZ	1:B:36:MET:CB	2.21	1.02
1:B:33:LYS:HZ1	1:B:36:MET:HA	0.86	1.01
1:B:33:LYS:HZ3	1:B:36:MET:CG	1.71	1.01
1:A:113:ARG:NH2	1:B:2:SER:OG	1.93	1.00
1:B:33:LYS:HZ3	1:B:36:MET:CB	1.75	0.99
1:A:115:LYS:CG	1:A:118:SER:CB	2.12	0.98
1:A:61:GLU:OE1	1:A:115:LYS:CD	2.07	0.98
1:A:116:LEU:HD22	1:B:5:LEU:HD23	0.99	0.96
1:A:116:LEU:HD21	1:B:5:LEU:HD23	1.47	0.93
1:A:115:LYS:HG3	1:A:118:SER:CA	1.99	0.92
1:A:116:LEU:HD11	1:B:2:SER:HB2	1.51	0.89
1:B:33:LYS:NZ	1:B:36:MET:CA	2.28	0.88
1:A:113:ARG:HH22	1:B:101:VAL:HG13	1.40	0.87
1:A:113:ARG:NE	1:B:104:GLU:CD	2.26	0.87
1:B:33:LYS:HZ3	1:B:36:MET:HG3	1.27	0.85
1:A:115:LYS:HE3	1:A:118:SER:CB	2.05	0.85
1:A:115:LYS:HG3	1:A:118:SER:HB2	0.89	0.85
1:A:115:LYS:HG3	1:A:118:SER:OG	1.77	0.84
1:A:115:LYS:HD3	1:A:119:SER:HG	1.44	0.82
1:A:116:LEU:HD12	1:B:2:SER:HB2	0.81	0.80
1:A:116:LEU:C	1:A:116:LEU:HD23	2.01	0.80
1:B:33:LYS:HZ2	1:B:36:MET:HG3	1.47	0.75
1:A:113:ARG:CZ	1:B:104:GLU:OE2	2.33	0.74
1:A:113:ARG:NE	1:B:104:GLU:OE1	2.19	0.74
1:B:33:LYS:HZ3	1:B:36:MET:HB2	1.52	0.74
1:A:116:LEU:HD13	1:B:2:SER:HA	1.70	0.74
1:A:115:LYS:CD	1:A:118:SER:CB	2.57	0.73
1:A:2:SER:HB2	1:A:166:ASN:OD1	1.89	0.73
1:A:113:ARG:NH2	1:B:101:VAL:HG22	2.06	0.70
1:A:115:LYS:CG	1:A:118:SER:CA	2.58	0.69
1:B:125:TYR:HA	1:B:128:ARG:NH1	2.08	0.69
1:B:33:LYS:HG2	1:B:35:ARG:H	1.59	0.67
1:A:120:LEU:HD23	1:A:120:LEU:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:HG3	1:A:161:THR:HG21	1.79	0.65
1:A:80:ASN:ND2	2:A:167:BGC:H6C1	2.12	0.64
1:A:17:CYS:SG	1:A:90:ASN:ND2	2.70	0.64
1:A:60:TYR:O	1:A:64:GLN:HG3	1.97	0.64
1:A:113:ARG:NH1	1:B:2:SER:OG	2.30	0.64
1:A:11:ARG:NH2	5:A:201:HOH:O	2.21	0.64
1:A:116:LEU:C	1:A:116:LEU:CD2	2.67	0.62
1:A:111:PHE:HD2	1:A:113:ARG:H	1.48	0.62
1:B:33:LYS:CE	1:B:36:MET:HA	2.30	0.62
1:B:109:GLU:HB2	1:B:115:LYS:NZ	2.15	0.62
1:A:116:LEU:CD1	1:B:2:SER:HA	2.30	0.61
1:B:24:LEU:HB2	1:B:147:ARG:NH1	2.15	0.61
1:B:38:PHE:O	1:B:128:ARG:NH1	2.35	0.60
1:B:46:GLN:OE1	1:B:48:GLN:NE2	2.35	0.59
1:A:116:LEU:CD1	1:B:2:SER:CA	2.79	0.59
1:A:115:LYS:CE	1:A:118:SER:CB	2.65	0.58
1:A:113:ARG:HH21	1:B:101:VAL:HG22	1.67	0.58
1:B:81:GLU:O	1:B:85:GLU:HG2	2.03	0.58
1:A:120:LEU:HD23	1:A:120:LEU:N	2.20	0.57
1:B:24:LEU:HB2	1:B:147:ARG:HH11	1.69	0.57
1:A:27:ARG:NH2	1:A:29:GLU:OE1	2.37	0.57
1:B:3:TYR:CD2	1:B:52:LYS:HE2	2.40	0.56
1:B:24:LEU:O	1:B:147:ARG:NH1	2.37	0.56
1:A:116:LEU:HD23	1:B:5:LEU:CD2	2.10	0.55
1:A:115:LYS:HD2	1:A:118:SER:HB2	1.77	0.55
1:B:60:TYR:O	1:B:64:GLN:HG3	2.08	0.54
1:B:133:LEU:HD21	1:B:146:VAL:HG21	1.88	0.54
1:A:1:MET:HG3	1:A:5:LEU:HD23	1.90	0.53
1:B:33:LYS:HZ1	1:B:36:MET:CB	1.97	0.53
1:A:113:ARG:CD	1:B:104:GLU:OE1	2.55	0.53
1:A:51:GLN:HE22	1:B:1:MET:HG3	1.73	0.53
1:B:33:LYS:O	1:B:34:ASP:HB2	2.09	0.53
1:A:81:GLU:O	1:A:85:GLU:HG2	2.08	0.53
1:A:113:ARG:HG2	1:A:113:ARG:O	2.10	0.52
1:A:93:HIS:O	1:A:97:HIS:HB2	2.10	0.51
1:A:70:PHE:HE1	1:A:150:ILE:HG13	1.76	0.51
1:A:65:ASN:O	1:A:69:ILE:HG12	2.10	0.50
1:A:116:LEU:HD21	5:A:175:HOH:O	2.10	0.50
1:A:113:ARG:HD2	1:B:104:GLU:OE1	2.12	0.50
1:B:44:ILE:HD11	1:B:122:LEU:CD2	2.42	0.50
1:A:44:ILE:HD13	1:A:117:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:CE	1:A:118:SER:HB2	2.21	0.49
1:B:33:LYS:CE	1:B:36:MET:CA	2.89	0.49
1:A:10:GLN:NE2	5:A:196:HOH:O	2.46	0.49
1:B:33:LYS:HZ1	1:B:36:MET:CG	2.08	0.48
1:A:2:SER:HB2	1:A:166:ASN:CG	2.34	0.47
1:A:150:ILE:O	1:A:153:ASN:HB2	2.14	0.47
1:A:115:LYS:HE3	1:A:118:SER:HB3	1.95	0.47
1:A:113:ARG:CD	1:B:104:GLU:CD	2.84	0.47
1:A:111:PHE:O	1:A:112:THR:OG1	2.30	0.46
1:A:112:THR:C	1:A:114:GLY:N	2.68	0.46
1:B:44:ILE:HD11	1:B:122:LEU:HD22	1.97	0.46
1:A:113:ARG:HH22	1:B:101:VAL:CG1	2.20	0.45
1:B:43:GLU:H	1:B:43:GLU:HG2	1.54	0.45
1:B:42:GLU:HG2	1:B:46:GLN:HG3	1.99	0.44
1:B:43:GLU:HA	1:B:46:GLN:NE2	2.32	0.44
1:A:2:SER:CB	1:A:166:ASN:OD1	2.63	0.44
1:A:113:ARG:CZ	1:B:2:SER:CB	2.89	0.44
1:B:57:LEU:O	1:B:61:GLU:HG3	2.17	0.44
1:A:14:ASN:HD21	1:A:157:ILE:HG22	1.83	0.44
1:A:153:ASN:O	1:A:157:ILE:HG13	2.17	0.44
1:B:34:ASP:H	1:B:145:ILE:HD11	1.84	0.43
1:B:150:ILE:O	1:B:153:ASN:HB2	2.19	0.43
1:A:116:LEU:O	1:A:120:LEU:HD21	2.18	0.43
1:A:112:THR:O	1:A:113:ARG:C	2.58	0.43
1:A:111:PHE:HD2	1:A:113:ARG:N	2.13	0.42
1:A:11:ARG:NH1	5:A:201:HOH:O	2.51	0.42
1:B:55:ALA:O	1:B:59:ILE:HG13	2.19	0.42
1:B:61:GLU:HB3	5:B:180:HOH:O	2.18	0.42
1:B:62:MET:O	1:B:66:ILE:HG13	2.19	0.42
1:B:165:ARG:O	1:B:166:ASN:HB2	2.19	0.42
1:B:3:TYR:HB2	1:B:166:ASN:O	2.20	0.42
1:B:1:MET:N	1:B:166:ASN:O	2.53	0.41
1:A:11:ARG:CG	1:A:161:THR:HG21	2.47	0.41
1:B:133:LEU:CD2	1:B:146:VAL:HG21	2.50	0.41
1:A:116:LEU:CD2	5:A:175:HOH:O	2.67	0.41
1:A:42:GLU:HG3	5:A:183:HOH:O	2.20	0.40
1:B:40:ILE:HD11	1:B:152:ARG:HD2	2.03	0.40
1:A:118:SER:O	1:A:119:SER:C	2.59	0.40
1:A:44:ILE:HD13	1:A:117:MET:HE1	2.04	0.40
1:A:44:ILE:HD13	1:A:117:MET:HE2	2.03	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the

symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:NH2	1:B:104:GLU:CG[3_645]	1.25	0.95
1:A:71:ARG:HH12	1:B:104:GLU:CA[3_645]	0.73	0.87
1:A:71:ARG:NH1	1:B:104:GLU:CA[3_645]	1.46	0.74
1:A:71:ARG:HH22	1:B:104:GLU:CG[3_645]	0.90	0.70
1:A:71:ARG:HH22	1:B:104:GLU:CB[3_645]	1.30	0.30
1:A:71:ARG:HH12	1:B:104:GLU:N[3_645]	1.41	0.19
1:A:71:ARG:NH2	1:B:104:GLU:CB[3_645]	2.02	0.18
1:A:71:ARG:HH21	1:B:104:GLU:CG[3_645]	1.47	0.13
1:A:71:ARG:CZ	1:B:104:GLU:CA[3_645]	2.08	0.12
1:A:71:ARG:NH1	1:B:104:GLU:N[3_645]	2.10	0.10
1:A:71:ARG:HH12	1:B:104:GLU:C[3_645]	1.54	0.06

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	164/166 (99%)	151 (92%)	7 (4%)	6 (4%)	4 1
1	B	159/166 (96%)	154 (97%)	5 (3%)	0	100 100
All	All	323/332 (97%)	305 (94%)	12 (4%)	6 (2%)	10 6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	THR
1	A	114	GLY
1	A	118	SER
1	A	119	SER
1	A	120	LEU
1	A	39	ASP

5.3.2 Protein sidechains (i)

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	154/154 (100%)	150 (97%)	4 (3%)	54 66
1	B	151/154 (98%)	145 (96%)	6 (4%)	38 47
All	All	305/308 (99%)	295 (97%)	10 (3%)	45 56

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	SER
1	A	120	LEU
1	A	140	HIS
1	A	166	ASN
1	B	12	SER
1	B	46	GLN
1	B	87	LEU
1	B	109	GLU
1	B	140	HIS
1	B	147	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	48	GLN
1	A	51	GLN
1	A	90	ASN
1	A	94	GLN
1	B	46	GLN
1	B	48	GLN
1	B	86	ASN
1	B	121	HIS

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

9 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	$\#\|Z\| > 2$
2	BGC	A	167	1,2	11,11,12	1.30	2 (18%)	14,15,17	2.23	7 (50%)
2	BGC	A	168	2	11,11,12	1.66	1 (9%)	14,15,17	3.21	7 (50%)
2	G6D	A	169	2	10,10,11	1.19	1 (10%)	14,14,16	2.37	3 (21%)
2	BGC	A	170	2	11,11,12	2.33	4 (36%)	14,15,17	3.05	8 (57%)
2	BGC	A	171	2	11,11,12	2.15	4 (36%)	14,15,17	3.72	7 (50%)
2	BGC	A	172	2	11,11,12	1.58	4 (36%)	14,15,17	3.67	4 (28%)
2	BGC	A	173	2	11,11,12	2.38	3 (27%)	14,15,17	2.45	6 (42%)
3	BGC	B	167	1,3	11,11,12	1.30	1 (9%)	14,15,17	3.21	6 (42%)
3	G6D	B	168	3	10,10,11	1.65	3 (30%)	14,14,16	2.26	5 (35%)

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	BGC	A	167	1,2	-	0/2/19/22	0/1/1/1
2	BGC	A	168	2	-	0/2/19/22	0/1/1/1
2	G6D	A	169	2	-	0/0/17/20	0/1/1/1
2	BGC	A	170	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	A	171	2	-	0/2/19/22	0/1/1/1
2	BGC	A	172	2	-	0/2/19/22	0/1/1/1
2	BGC	A	173	2	-	0/2/19/22	0/1/1/1
3	BGC	B	167	1,3	-	0/2/19/22	0/1/1/1
3	G6D	B	168	3	1/1/4/5	0/0/17/20	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	172	BGC	C4-C3	2.05	1.57	1.52
2	A	172	BGC	C1-C2	2.11	1.57	1.52
2	A	167	BGC	C1-C2	2.19	1.57	1.52
3	B	168	G6D	C4A-C3A	2.20	1.58	1.52
2	A	171	BGC	C4-C3	2.37	1.58	1.52
2	A	170	BGC	C1-C2	2.43	1.58	1.52
3	B	168	G6D	C4A-C5A	2.44	1.58	1.52
2	A	172	BGC	C4-C5	2.59	1.58	1.53
2	A	169	G6D	C1-C2	2.85	1.59	1.52
2	A	167	BGC	C2-C3	2.94	1.56	1.52
2	A	172	BGC	C2-C3	3.00	1.56	1.52
2	A	173	BGC	C1-C2	3.08	1.59	1.52
3	B	168	G6D	C1-C2	3.24	1.60	1.52
2	A	171	BGC	C4-C5	3.27	1.60	1.53
2	A	171	BGC	C1-C2	3.35	1.60	1.52
2	A	170	BGC	C4-C3	3.56	1.61	1.52
3	B	167	BGC	C1-C2	3.57	1.60	1.52
2	A	173	BGC	C4-C5	3.78	1.61	1.53
2	A	170	BGC	C4-C5	3.98	1.61	1.53
2	A	168	BGC	C4-C5	4.20	1.62	1.53
2	A	170	BGC	C2-C3	4.39	1.58	1.52
2	A	171	BGC	C2-C3	4.55	1.58	1.52
2	A	173	BGC	C2-C3	5.36	1.59	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	167	BGC	O5-C5-C6	-5.56	95.30	107.35
2	A	170	BGC	O4-C4-C3	-5.16	98.73	110.34
2	A	169	G6D	O2-C2-C3A	-4.80	100.46	110.12
2	A	173	BGC	O2-C2-C1	-4.56	100.06	109.21
2	A	171	BGC	O4-C4-C3	-4.40	100.42	110.34
2	A	169	G6D	O4A-C4A-C3A	-4.33	100.58	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	167	BGC	C6-C5-C4	-4.27	102.48	113.02
2	A	167	BGC	C6-C5-C4	-3.33	104.80	113.02
2	A	167	BGC	C2-C3-C4	-3.29	105.46	111.04
2	A	170	BGC	O2-C2-C1	-3.16	102.87	109.21
3	B	167	BGC	O3-C3-C4	-3.09	103.39	110.34
2	A	167	BGC	C1-C2-C3	-3.06	105.92	109.54
2	A	168	BGC	O4-C4-C3	-3.06	103.44	110.34
2	A	170	BGC	C6-C5-C4	-3.00	105.62	113.02
2	A	168	BGC	C1-C2-C3	-2.92	106.09	109.54
3	B	168	G6D	O4A-C4A-C3A	-2.70	104.26	110.34
2	A	170	BGC	O3-C3-C4	-2.63	104.42	110.34
3	B	167	BGC	O2-C2-C1	-2.55	104.09	109.21
2	A	172	BGC	O2-C2-C1	-2.50	104.20	109.21
3	B	168	G6D	O2-C2-C3A	-2.40	105.29	110.12
2	A	173	BGC	O4-C4-C3	-2.35	105.04	110.34
2	A	173	BGC	O3-C3-C4	-2.21	105.36	110.34
2	A	171	BGC	O2-C2-C1	-2.10	105.00	109.21
2	A	168	BGC	O5-C5-C6	2.07	111.82	107.35
3	B	167	BGC	O4-C4-C5	2.14	114.91	109.24
2	A	170	BGC	O5-C5-C6	2.14	111.99	107.35
2	A	173	BGC	O4-C4-C5	2.16	114.97	109.24
2	A	167	BGC	O4-C4-C5	2.24	115.18	109.24
2	A	167	BGC	O2-C2-C3	2.30	114.75	110.12
2	A	170	BGC	C3-C4-C5	2.43	114.43	110.20
2	A	167	BGC	C1-O5-C5	2.65	115.62	112.25
2	A	173	BGC	C1-C2-C3	2.75	112.79	109.54
3	B	168	G6D	C1-O5-C5A	2.79	116.69	112.38
2	A	172	BGC	O4-C4-C5	2.96	117.09	109.24
3	B	168	G6D	C2-C3A-C4A	3.07	116.25	111.04
2	A	171	BGC	C1-C2-C3	3.15	113.27	109.54
2	A	168	BGC	C3-C4-C5	3.22	115.80	110.20
2	A	168	BGC	C2-C3-C4	3.38	116.78	111.04
2	A	167	BGC	O5-C1-C2	3.41	116.40	110.86
2	A	171	BGC	C2-C3-C4	3.86	117.60	111.04
2	A	168	BGC	O5-C1-C2	3.92	117.22	110.86
2	A	169	G6D	C2-C3A-C4A	4.86	119.30	111.04
2	A	171	BGC	O2-C2-C3	5.19	120.55	110.12
2	A	170	BGC	C2-C3-C4	5.31	120.06	111.04
2	A	173	BGC	C1-O5-C5	5.50	119.23	112.25
3	B	168	G6D	O5-C1-C2	5.64	120.01	110.86
2	A	170	BGC	C1-O5-C5	5.82	119.64	112.25
2	A	172	BGC	O5-C1-C2	5.93	120.47	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	171	BGC	O5-C1-C2	7.14	122.44	110.86
2	A	171	BGC	C1-O5-C5	7.35	121.58	112.25
3	B	167	BGC	C1-O5-C5	8.13	122.57	112.25
2	A	168	BGC	C1-O5-C5	8.34	122.83	112.25
2	A	172	BGC	C1-O5-C5	11.14	126.38	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	168	G6D	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	167	BGC	1	0

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.