Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:17 PM GMT

PDB ID	:	3WO3
Title	:	Crystal structure of IL-18 in complex with IL-18 receptor alpha
Authors	:	Tsutsumi, N.; Kimura, T.; Arita, K.; Ariyoshi, M.; Ohnishi, H.; Kondo, N.; Shirakawa, M.; Kato, Z.; Tochio, H.
Deposited on	:	2013-12-19
Resolution	:	3.10 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 (1)) were used in the production of this report:

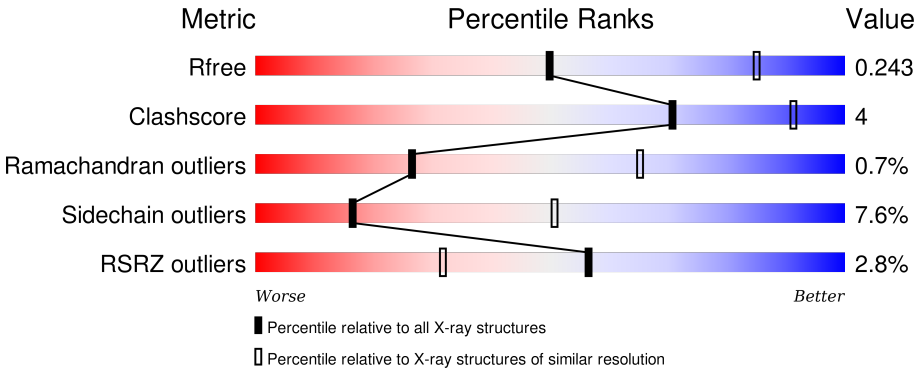
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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.

Mol	Chain	Length	Quality of chain
1	A	157	% 82% 17% ••
1	C	157	85% 13% ••
1	E	157	85% 15% •
1	G	157	83% 15% ••
1	I	157	% 83% 14% ••

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Mol	Chain	Length	Quality of chain
1	K	157	82% 15%
2	B	312	2% 76% 17% 6%
2	D	312	% 75% 17% 7%
2	F	312	2% 75% 16% 8%
2	H	312	2% 75% 15% 8%
2	J	312	8% 72% 13% 13%
2	L	312	9% 67% 14% 18%

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	SO4	B	821	-	-	-	X
3	SO4	C	204	-	-	-	X
3	SO4	D	419	-	-	-	X
3	SO4	D	421	-	-	-	X
3	SO4	E	203	-	-	-	X
3	SO4	F	821	-	-	-	X
3	SO4	F	824	-	-	-	X
3	SO4	H	817	-	-	-	X
3	SO4	H	818	-	-	-	X
4	NAG	F	903	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22047 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 Interleukin-18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1245	783	207	245	10			
1	C	156	Total	C	N	O	S	0	0	0
			1258	791	209	248	10			
1	E	157	Total	C	N	O	S	0	1	0
			1255	787	208	250	10			
1	G	156	Total	C	N	O	S	0	0	0
			1240	782	208	240	10			
1	I	156	Total	C	N	O	S	0	0	0
			1179	739	195	235	10			
1	K	156	Total	C	N	O	S	0	0	0
			1180	737	197	236	10			

- Molecule 2 is a protein called Interleukin-18 receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	294	Total	C	N	O	S	0	1	0
			2336	1477	403	442	14			
2	D	290	Total	C	N	O	S	0	0	0
			2316	1470	395	437	14			
2	F	288	Total	C	N	O	S	0	1	0
			2280	1445	392	429	14			
2	H	288	Total	C	N	O	S	0	0	0
			2284	1445	391	434	14			
2	J	272	Total	C	N	O	S	0	0	0
			2037	1286	341	397	13			
2	L	255	Total	C	N	O	S	0	0	0
			1923	1213	327	370	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	EXPRESSION TAG	UNP Q13478

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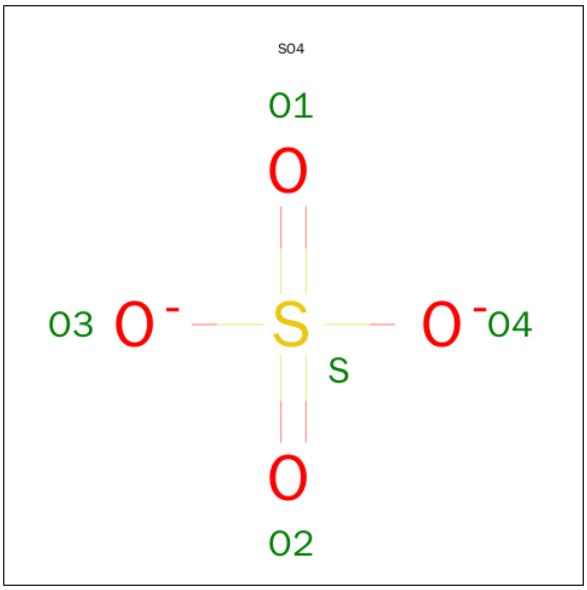
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	PRO	-	EXPRESSION TAG	UNP Q13478
D	-2	GLY	-	EXPRESSION TAG	UNP Q13478
D	-1	PRO	-	EXPRESSION TAG	UNP Q13478
F	-2	GLY	-	EXPRESSION TAG	UNP Q13478
F	-1	PRO	-	EXPRESSION TAG	UNP Q13478
H	-2	GLY	-	EXPRESSION TAG	UNP Q13478
H	-1	PRO	-	EXPRESSION TAG	UNP Q13478
J	-2	GLY	-	EXPRESSION TAG	UNP Q13478
J	-1	PRO	-	EXPRESSION TAG	UNP Q13478
L	-2	GLY	-	EXPRESSION TAG	UNP Q13478
L	-1	PRO	-	EXPRESSION TAG	UNP Q13478

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

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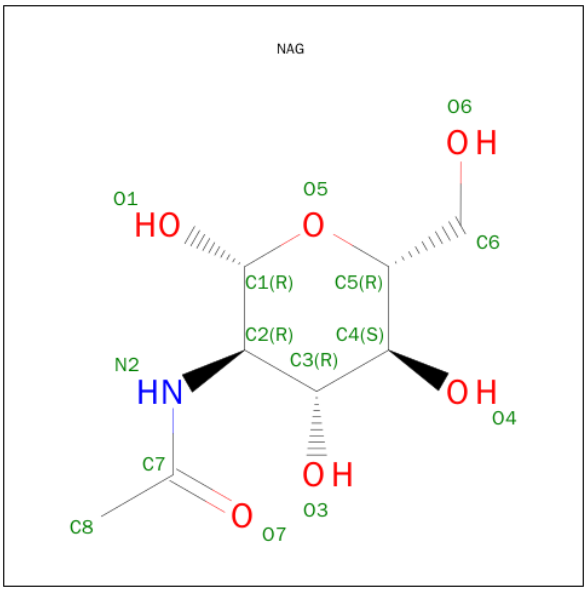
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0

- 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	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	H	1	Total C N O 14 8 1 5	0	0
4	H	1	Total C N O 14 8 1 5	0	0
4	J	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total C N O 38 22 2 14	0	0
5	B	3	Total C N O 38 22 2 14	0	0
5	J	3	Total C N O 38 22 2 14	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	6	Total C N O 72 40 2 30	0	0
6	F	6	Total C N O 72 40 2 30	0	0

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

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

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

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	3	Total C N O 39 22 2 15	0	0
8	D	3	Total C N O 39 22 2 15	0	0
8	D	3	Total C N O 39 22 2 15	0	0
8	F	3	Total C N O 39 22 2 15	0	0
8	H	3	Total C N O 39 22 2 15	0	0
8	J	3	Total C N O 39 22 2 15	0	0
8	J	3	Total C N O 39 22 2 15	0	0
8	L	3	Total C N O 39 22 2 15	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	2	Total C N O 24 14 1 9	0	0

- Molecule 10 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	5	Total C N O 61 34 2 25	0	0
10	H	5	Total C N O 61 34 2 25	0	0

- Molecule 11 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	4	Total	C	N	O	0	0
			49	28	2	19		
11	H	4	Total	C	N	O	0	0
			49	28	2	19		
11	L	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 12 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	F	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 13 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	F	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	15	Total	O	0	0
			15	15		
14	B	10	Total	O	0	0
			10	10		
14	C	9	Total	O	0	0
			9	9		
14	D	18	Total	O	0	0
			18	18		
14	E	5	Total	O	0	0
			5	5		
14	F	12	Total	O	0	0
			12	12		
14	G	3	Total	O	0	0
			3	3		
14	H	11	Total	O	0	0
			11	11		
14	I	6	Total	O	0	0
			6	6		
14	J	3	Total	O	0	0
			3	3		

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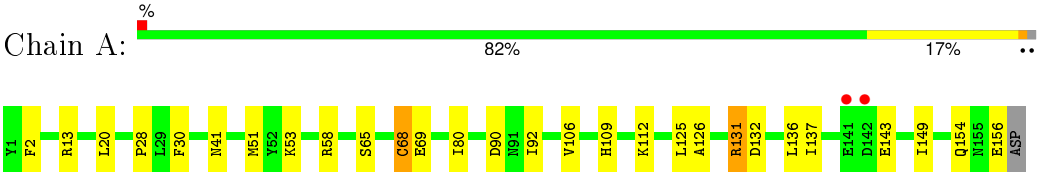
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	K	1	Total O 1 1	0	0
14	L	6	Total O 6 6	0	0

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.

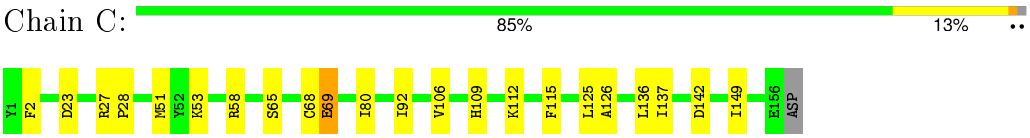
- Molecule 1: Interleukin-18

Chain A:



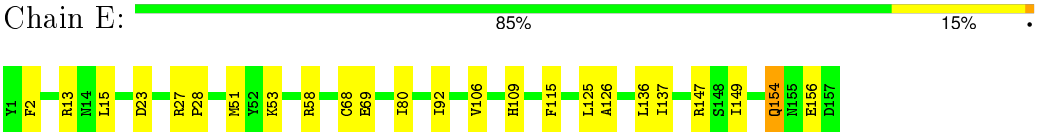
- Molecule 1: Interleukin-18

Chain C:



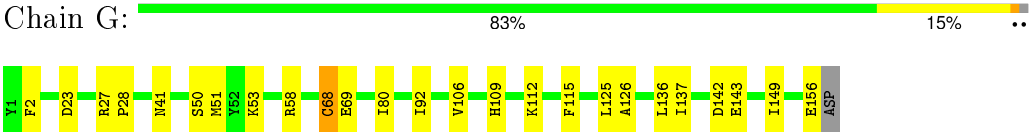
- Molecule 1: Interleukin-18

Chain E:



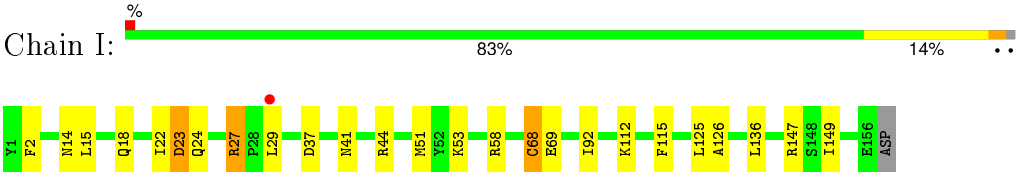
- Molecule 1: Interleukin-18

Chain G:



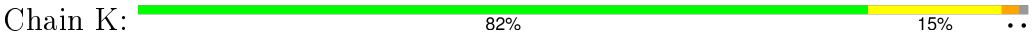
- Molecule 1: Interleukin-18

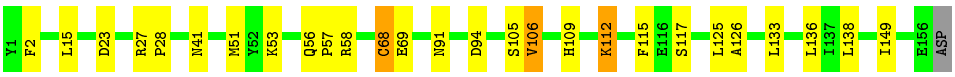
Chain I:



- Molecule 1: Interleukin-18

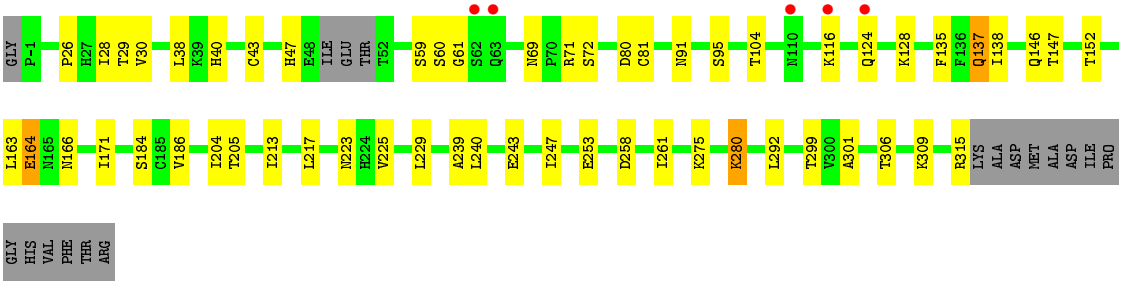
Chain K:





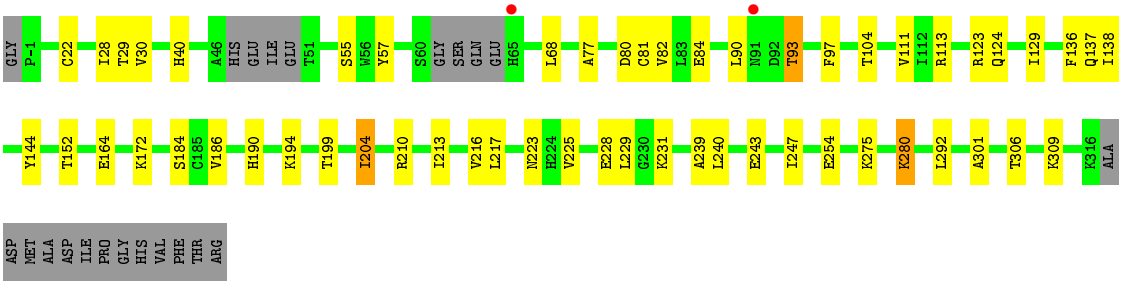
• Molecule 2: Interleukin-18 receptor 1

Chain B:



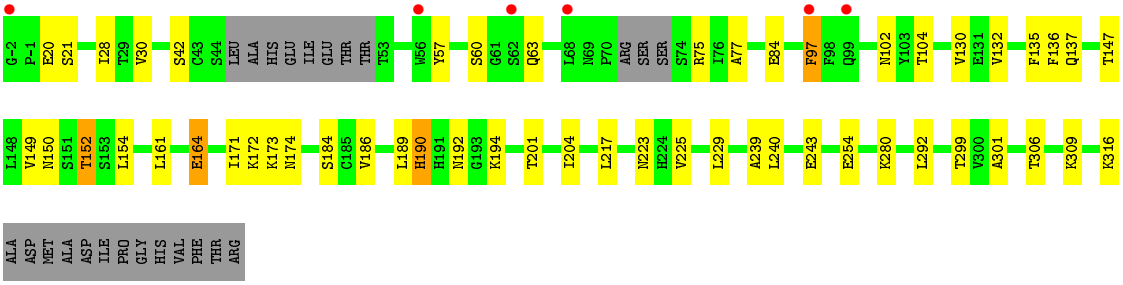
• Molecule 2: Interleukin-18 receptor 1

Chain D:



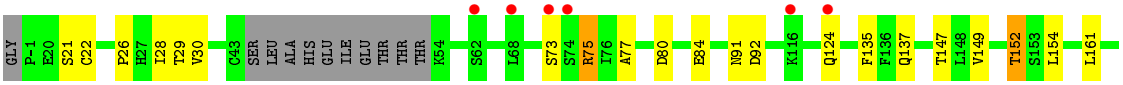
• Molecule 2: Interleukin-18 receptor 1

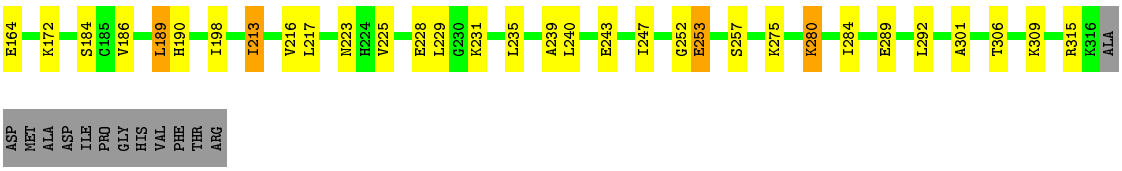
Chain F:



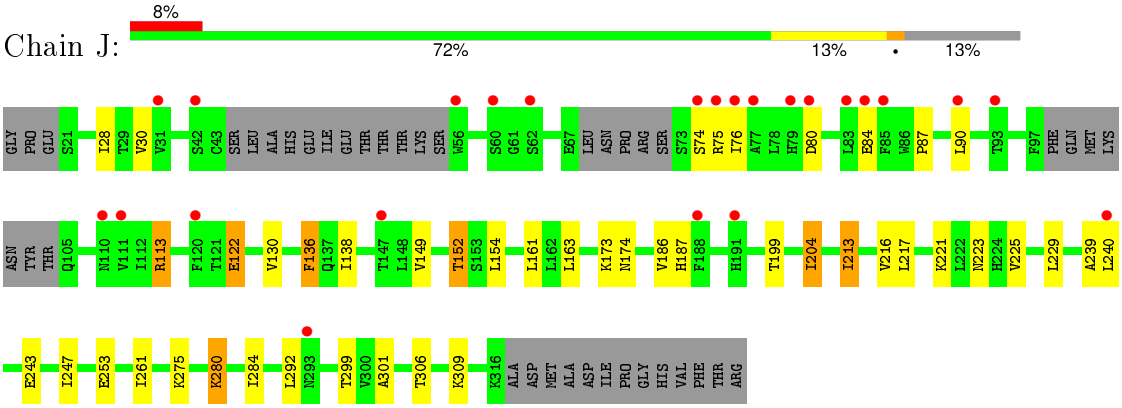
• Molecule 2: Interleukin-18 receptor 1

Chain H:

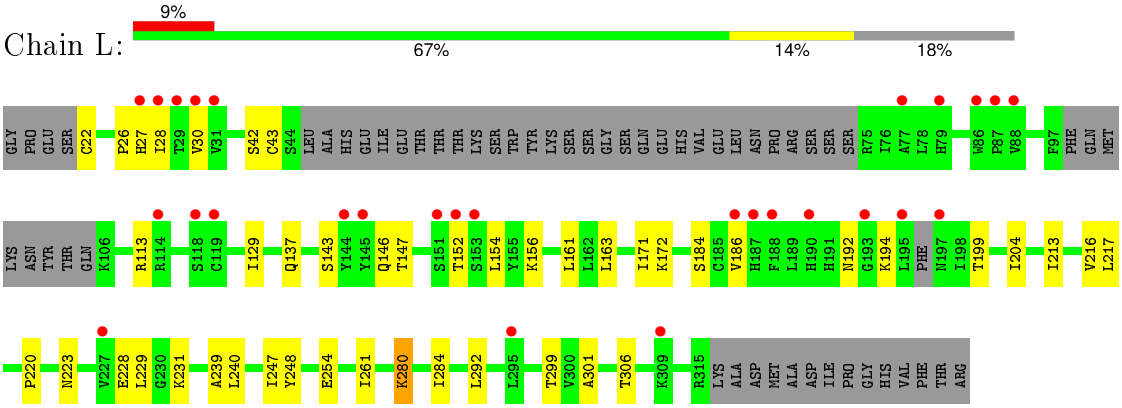




• Molecule 2: Interleukin-18 receptor 1



• Molecule 2: Interleukin-18 receptor 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	135.49Å 174.81Å 183.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.25 – 3.10 43.85 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (31.25-3.10) 99.4 (43.85-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.191 , 0.222 0.210 , 0.243	Depositor DCC
R_{free} test set	3973 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	69.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 84.5	EDS
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 79134 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22047	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MAN, SO4, BMA, NAG, FUC

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	0.49	0/1266	0.65	0/1701
1	C	0.50	0/1279	0.68	0/1717
1	E	0.46	0/1279	0.66	0/1719
1	G	0.52	0/1261	0.66	0/1695
1	I	0.43	0/1200	0.64	0/1625
1	K	0.44	0/1200	0.63	0/1622
2	B	0.46	0/2390	0.68	0/3244
2	D	0.47	0/2368	0.69	0/3209
2	F	0.45	0/2335	0.69	0/3166
2	H	0.46	0/2337	0.67	0/3174
2	J	0.43	0/2077	0.69	0/2830
2	L	0.42	0/1964	0.65	0/2677
All	All	0.46	0/20956	0.67	0/28379

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1245	0	1207	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1258	0	1233	11	0
1	E	1255	0	1206	11	0
1	G	1240	0	1210	13	0
1	I	1179	0	1066	13	0
1	K	1180	0	1074	15	0
2	B	2336	0	2208	18	0
2	D	2316	0	2233	22	0
2	F	2280	0	2166	16	0
2	H	2284	0	2154	22	0
2	J	2037	0	1832	19	0
2	L	1923	0	1715	16	0
3	A	10	0	0	0	0
3	B	25	0	0	0	0
3	C	25	0	0	0	0
3	D	35	0	0	0	0
3	E	15	0	0	0	0
3	F	25	0	0	1	0
3	G	10	0	0	0	0
3	H	25	0	0	1	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
4	B	28	0	26	0	0
4	D	14	0	13	0	0
4	F	28	0	26	0	0
4	H	28	0	26	0	0
4	J	14	0	13	0	0
5	B	76	0	68	0	0
5	J	38	0	34	0	0
6	B	72	0	61	1	0
6	F	72	0	61	3	0
7	B	28	0	25	0	0
7	H	28	0	25	0	0
7	J	28	0	25	0	0
7	L	56	0	50	0	0
8	B	39	0	34	0	0
8	D	78	0	68	0	0
8	F	39	0	34	0	0
8	H	39	0	34	0	0
8	J	78	0	68	1	0
8	L	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	24	0	22	1	0
10	D	61	0	52	0	0
10	H	61	0	52	1	0
11	D	49	0	43	0	0
11	H	49	0	43	0	0
11	L	49	0	43	2	0
12	F	50	0	43	0	0
13	F	60	0	52	1	0
14	A	15	0	0	1	0
14	B	10	0	0	0	0
14	C	9	0	0	0	0
14	D	18	0	0	0	0
14	E	5	0	0	0	0
14	F	12	0	0	0	0
14	G	3	0	0	0	0
14	H	11	0	0	0	0
14	I	6	0	0	0	0
14	J	3	0	0	0	0
14	K	1	0	0	0	0
14	L	6	0	0	0	0
All	All	22047	0	20379	184	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (184) 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)
13:F:912:NAG:H83	2:J:221:LYS:HG2	1.73	0.70
2:D:90:LEU:O	2:D:93:THR:HG23	1.92	0.70
1:G:106:VAL:HG22	1:G:109:HIS:HB2	1.74	0.69
1:E:106:VAL:HG22	1:E:109:HIS:HB2	1.76	0.68
1:K:41:ASN:HD21	2:L:27:HIS:H	1.41	0.67
2:L:186:VAL:HG11	8:L:905:NAG:H82	1.78	0.66
2:J:149:VAL:HG11	2:J:152:THR:HG22	1.77	0.65
1:C:106:VAL:HG22	1:C:109:HIS:HB2	1.78	0.65
1:A:41:ASN:OD1	2:B:26:PRO:HD2	1.98	0.63
1:A:106:VAL:HG22	1:A:109:HIS:HB2	1.79	0.63
2:D:93:THR:HG22	2:D:111:VAL:HB	1.82	0.62
2:F:150:ASN:HB2	2:F:190:HIS:CE1	2.38	0.59
2:D:129:ILE:HD13	2:D:210:ARG:HH22	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:ASP:CG	1:G:143:GLU:H	2.07	0.58
2:J:152:THR:HB	2:J:187:HIS:HA	1.83	0.58
2:B:40:HIS:CE1	2:B:81:CYS:HA	2.39	0.57
2:J:261:ILE:HG12	2:J:284:ILE:HG12	1.87	0.56
2:H:252:GLY:O	2:H:257:SER:HA	2.05	0.56
1:K:41:ASN:ND2	2:L:26:PRO:HD2	2.23	0.54
2:D:93:THR:HG22	2:D:111:VAL:H	1.72	0.54
2:B:29:THR:HG22	2:B:124:GLN:HE22	1.71	0.54
1:I:37:ASP:O	1:I:41:ASN:HB2	2.08	0.53
1:A:90:ASP:HB3	14:A:315:HOH:O	2.07	0.53
1:K:106:VAL:HG22	1:K:109:HIS:HB2	1.91	0.53
2:J:186:VAL:HG11	8:J:905:NAG:H82	1.91	0.52
1:K:15:LEU:HD11	1:K:112:LYS:HG3	1.91	0.52
1:E:13:ARG:NH2	1:E:154:GLN:HE21	2.08	0.52
2:J:74:SER:HB2	2:J:87:PRO:HD2	1.91	0.52
2:B:137:GLN:HA	2:B:171:ILE:O	2.10	0.52
1:I:125:LEU:HG	1:I:136:LEU:HD11	1.93	0.51
2:B:138:ILE:HD11	2:B:204:ILE:HD13	1.92	0.51
1:E:15:LEU:HD23	1:E:147[B]:ARG:NE	2.25	0.51
1:A:13:ARG:NH2	1:A:154:GLN:OE1	2.43	0.51
1:K:125:LEU:HG	1:K:136:LEU:HD11	1.92	0.51
2:D:29:THR:HG22	2:D:124:GLN:HE22	1.74	0.51
2:B:217:LEU:HD23	2:B:239:ALA:HB2	1.93	0.51
1:C:28:PRO:HB2	1:C:136:LEU:HB3	1.92	0.50
2:H:29:THR:HG22	2:H:124:GLN:HE22	1.75	0.50
2:B:223:ASN:HD21	2:B:309:LYS:HE3	1.77	0.50
2:D:190:HIS:CE1	9:D:998:FUC:H5	2.47	0.50
2:D:217:LEU:HD23	2:D:239:ALA:HB2	1.94	0.49
2:L:228:GLU:HG3	2:L:231:LYS:HG3	1.95	0.49
2:L:217:LEU:HD23	2:L:239:ALA:HB2	1.94	0.49
2:L:229:LEU:HD11	2:L:292:LEU:HD11	1.94	0.49
1:G:126:ALA:HB2	1:G:149:ILE:HG22	1.95	0.49
1:A:125:LEU:HG	1:A:136:LEU:HD11	1.95	0.49
1:A:28:PRO:HB2	1:A:136:LEU:HB3	1.94	0.49
2:B:69:ASN:H	2:B:72:SER:HB2	1.78	0.49
2:D:223:ASN:HD21	2:D:309:LYS:HE3	1.77	0.49
1:I:2:PHE:HA	1:I:53:LYS:O	2.13	0.49
2:D:57:TYR:HB2	2:D:97:PHE:HB2	1.95	0.49
2:D:90:LEU:HD11	2:D:113:ARG:HG2	1.95	0.48
1:C:109:HIS:HB3	1:C:112:LYS:HD2	1.95	0.48
2:J:217:LEU:HD23	2:J:239:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:137:GLN:HG3	2:H:172:LYS:HG2	1.95	0.48
2:D:137:GLN:HG3	2:D:172:LYS:HG2	1.94	0.48
1:G:23:ASP:OD1	1:G:27:ARG:HG2	2.13	0.48
1:E:28:PRO:HB2	1:E:136:LEU:HB3	1.96	0.48
2:F:137:GLN:HG3	2:F:172:LYS:HG2	1.95	0.48
1:E:23:ASP:OD1	1:E:27:ARG:HG2	2.14	0.47
1:K:117:SER:HB2	1:K:138:LEU:HD11	1.95	0.47
2:F:217:LEU:HD23	2:F:239:ALA:HB2	1.95	0.47
2:H:229:LEU:HD11	2:H:292:LEU:HD11	1.96	0.47
1:E:2:PHE:HA	1:E:53:LYS:O	2.14	0.47
2:H:223:ASN:HD21	2:H:309:LYS:HE3	1.78	0.47
2:F:223:ASN:HD21	2:F:309:LYS:HE3	1.80	0.47
1:A:2:PHE:HA	1:A:53:LYS:O	2.15	0.47
2:B:116:LYS:HE2	6:F:954:MAN:H62	1.96	0.47
1:I:68:CYS:HB3	1:I:69:GLU:H	1.63	0.46
1:G:125:LEU:HG	1:G:136:LEU:HD11	1.95	0.46
2:J:229:LEU:HD11	2:J:292:LEU:HD11	1.97	0.46
1:E:69:GLU:HA	2:H:289:GLU:HB2	1.97	0.46
1:K:57:PRO:HD2	11:L:999:FUC:H62	1.96	0.46
1:C:126:ALA:HB2	1:C:149:ILE:HG22	1.96	0.46
1:G:2:PHE:HA	1:G:53:LYS:O	2.15	0.46
2:J:223:ASN:HD21	2:J:309:LYS:HE3	1.80	0.46
1:A:20:LEU:HB2	1:A:30:PHE:CE1	2.51	0.46
2:H:154:LEU:HG	2:H:161:LEU:HD12	1.98	0.46
1:G:28:PRO:HB2	1:G:136:LEU:HB3	1.98	0.46
2:D:93:THR:HG22	2:D:111:VAL:CB	2.44	0.46
1:A:109:HIS:HB3	1:A:112:LYS:HD2	1.98	0.46
1:E:125:LEU:HG	1:E:136:LEU:HD11	1.96	0.46
2:D:229:LEU:HD11	2:D:292:LEU:HD11	1.96	0.46
2:B:247:ILE:HG23	2:B:280:LYS:HG3	1.97	0.46
1:E:126:ALA:HB2	1:E:149:ILE:HG22	1.98	0.46
2:B:213:ILE:HG12	2:B:275:LYS:HG2	1.96	0.46
2:L:161:LEU:HD13	2:L:171:ILE:HD11	1.98	0.46
2:L:186:VAL:HG22	2:L:199:THR:HG23	1.97	0.46
1:C:2:PHE:HA	1:C:53:LYS:O	2.15	0.46
1:C:68:CYS:HB3	1:C:69:GLU:H	1.66	0.46
1:K:23:ASP:OD1	1:K:27:ARG:HG2	2.16	0.45
2:H:149:VAL:HG11	2:H:152:THR:HG22	1.98	0.45
1:K:28:PRO:HB2	1:K:136:LEU:HB3	1.97	0.45
1:G:115:PHE:HB2	1:G:125:LEU:HB2	1.98	0.45
1:I:14:ASN:ND2	1:I:18:GLN:HB2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:115:PHE:HB2	1:K:125:LEU:HB2	1.99	0.45
1:C:125:LEU:HG	1:C:136:LEU:HD11	1.99	0.45
1:I:15:LEU:HD23	1:I:147:ARG:HD2	1.98	0.45
2:B:258:ASP:HB3	2:B:261:ILE:HG13	1.98	0.45
1:G:2:PHE:HB2	1:G:92:ILE:HB	1.99	0.45
2:J:130:VAL:HG11	2:J:136:PHE:HB2	1.98	0.45
1:I:2:PHE:HB2	1:I:92:ILE:HB	1.99	0.45
2:F:77:ALA:HB3	2:F:84:GLU:HB2	1.99	0.45
2:B:229:LEU:HD11	2:B:292:LEU:HD11	1.98	0.45
1:E:2:PHE:HB2	1:E:92:ILE:HB	1.99	0.45
1:A:2:PHE:HB2	1:A:92:ILE:HB	1.99	0.44
2:D:247:ILE:HG23	2:D:280:LYS:HG3	1.98	0.44
1:K:126:ALA:HB2	1:K:149:ILE:HG22	1.98	0.44
1:K:68:CYS:HB3	1:K:69:GLU:H	1.62	0.44
2:H:135:PHE:CE2	2:H:137:GLN:HB2	2.52	0.44
2:H:235:LEU:HD22	2:H:284:ILE:HD11	1.98	0.44
1:I:115:PHE:HB2	1:I:125:LEU:HB2	2.00	0.44
1:C:23:ASP:OD1	1:C:27:ARG:HG2	2.17	0.44
1:I:126:ALA:HB2	1:I:149:ILE:HG22	1.99	0.44
2:F:149:VAL:HG11	2:F:152:THR:HG22	1.99	0.44
2:D:77:ALA:HB3	2:D:84:GLU:HB2	1.99	0.44
1:C:2:PHE:HB2	1:C:92:ILE:HB	2.00	0.44
2:H:217:LEU:HD23	2:H:239:ALA:HB2	1.99	0.44
1:A:126:ALA:HB2	1:A:149:ILE:HG22	1.98	0.44
1:G:68:CYS:HB3	1:G:69:GLU:H	1.60	0.43
2:H:77:ALA:HB3	2:H:84:GLU:HB2	2.00	0.43
1:K:53:LYS:HB2	2:L:248:TYR:CE1	2.53	0.43
2:J:213:ILE:HG12	2:J:275:LYS:HG2	2.00	0.43
2:H:213:ILE:HG12	2:H:275:LYS:HG2	2.00	0.43
2:L:220:PRO:O	2:L:223:ASN:ND2	2.51	0.43
1:I:23:ASP:HB3	1:I:29:LEU:HD12	2.00	0.43
1:K:2:PHE:HA	1:K:53:LYS:O	2.19	0.43
2:F:301:ALA:HA	2:F:306:THR:HG22	2.00	0.43
2:F:154:LEU:HG	2:F:161:LEU:HD12	1.99	0.43
2:F:229:LEU:HD11	2:F:292:LEU:HD11	2.00	0.43
2:D:228:GLU:HG3	2:D:231:LYS:HG3	2.01	0.43
2:J:186:VAL:HG22	2:J:199:THR:HG23	2.01	0.42
2:H:186:VAL:HG11	10:H:905:NAG:H82	2.00	0.42
1:C:115:PHE:HB2	1:C:125:LEU:HB2	2.01	0.42
2:D:82:VAL:HG21	2:D:144:TYR:OH	2.19	0.42
2:J:301:ALA:HA	2:J:306:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:90:LEU:HD12	2:J:90:LEU:H	1.85	0.42
1:I:22:ILE:HG23	1:I:44:ARG:HG2	2.01	0.42
2:D:301:ALA:HA	2:D:306:THR:HG22	2.00	0.42
2:L:154:LEU:HG	2:L:161:LEU:HD12	2.00	0.42
2:B:186:VAL:HG11	6:B:905:NAG:H82	2.01	0.42
1:E:115:PHE:HB2	1:E:125:LEU:HB2	2.02	0.42
2:F:135:PHE:CE2	2:F:137:GLN:HB2	2.54	0.42
2:L:137:GLN:HG3	2:L:172:LYS:HG2	2.02	0.42
2:H:301:ALA:HA	2:H:306:THR:HG22	2.02	0.42
2:L:261:ILE:HG12	2:L:284:ILE:HG23	2.02	0.42
2:B:138:ILE:HD11	2:B:204:ILE:CD1	2.49	0.42
2:H:189:LEU:HD21	2:H:198:ILE:HD12	2.02	0.42
2:J:247:ILE:HG23	2:J:280:LYS:HG3	2.02	0.42
1:A:131:ARG:HB3	1:A:132:ASP:H	1.71	0.42
2:H:253:GLU:HB3	2:H:257:SER:HB3	2.01	0.42
1:G:106:VAL:CG2	1:G:109:HIS:HB2	2.47	0.42
2:J:113:ARG:HE	2:J:113:ARG:H	1.66	0.42
1:C:106:VAL:CG2	1:C:109:HIS:HB2	2.48	0.41
2:F:186:VAL:HG11	6:F:905:NAG:H82	2.02	0.41
2:B:59:SER:OG	2:B:95:SER:HB2	2.20	0.41
2:B:135:PHE:CE2	2:B:137:GLN:HB3	2.56	0.41
6:F:951:BMA:H3	6:F:953:MAN:H2	1.77	0.41
2:J:154:LEU:HG	2:J:161:LEU:HD12	2.01	0.41
2:D:213:ILE:HG12	2:D:275:LYS:HG2	2.02	0.41
2:H:247:ILE:HG23	2:H:280:LYS:HG3	2.02	0.41
2:D:138:ILE:HD11	2:D:204:ILE:HD13	2.03	0.41
2:B:301:ALA:HA	2:B:306:THR:HG22	2.03	0.41
2:H:252:GLY:HA2	3:H:817:SO4:S	2.61	0.41
2:D:186:VAL:HG22	2:D:199:THR:HG23	2.02	0.41
2:J:138:ILE:HD11	2:J:204:ILE:HD13	2.03	0.41
1:A:68:CYS:HB3	1:A:69:GLU:H	1.65	0.41
2:L:301:ALA:HA	2:L:306:THR:HG22	2.01	0.41
2:F:161:LEU:HD13	2:F:171:ILE:HD11	2.03	0.41
2:F:130:VAL:HG11	2:F:136:PHE:HB2	2.03	0.41
2:H:228:GLU:HG3	2:H:231:LYS:HG3	2.03	0.41
1:I:24:GLN:HA	1:I:44:ARG:HH21	1.85	0.40
2:F:57:TYR:HB2	2:F:97:PHE:HD1	1.85	0.40
2:F:254:GLU:HB2	3:F:821:SO4:O4	2.21	0.40
2:D:40:HIS:CD2	2:D:81:CYS:HA	2.56	0.40
1:G:106:VAL:HG13	1:G:112:LYS:O	2.21	0.40
2:H:75:ARG:NH2	2:H:92:ASP:OD2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:156:LYS:HB2	2:L:161:LEU:HD11	2.02	0.40
1:I:23:ASP:OD1	1:I:27:ARG:HB2	2.22	0.40
2:L:247:ILE:HG23	2:L:280:LYS:HG3	2.03	0.40
2:J:173:LYS:HE2	2:J:174:ASN:O	2.21	0.40
2:F:173:LYS:HE2	2:F:174:ASN:O	2.22	0.40
1:G:41:ASN:OD1	2:H:26:PRO:HD2	2.19	0.40
1:K:56:GLN:HA	11:L:999:FUC:H4	2.04	0.40

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	154/157 (98%)	145 (94%)	9 (6%)	0	100	100
1	C	154/157 (98%)	145 (94%)	8 (5%)	1 (1%)	30	68
1	E	156/157 (99%)	148 (95%)	8 (5%)	0	100	100
1	G	154/157 (98%)	144 (94%)	10 (6%)	0	100	100
1	I	154/157 (98%)	143 (93%)	11 (7%)	0	100	100
1	K	154/157 (98%)	143 (93%)	11 (7%)	0	100	100
2	B	291/312 (93%)	278 (96%)	10 (3%)	3 (1%)	19	58
2	D	284/312 (91%)	274 (96%)	9 (3%)	1 (0%)	39	75
2	F	283/312 (91%)	266 (94%)	13 (5%)	4 (1%)	14	48
2	H	284/312 (91%)	270 (95%)	12 (4%)	2 (1%)	26	65
2	J	264/312 (85%)	240 (91%)	21 (8%)	3 (1%)	17	55
2	L	247/312 (79%)	237 (96%)	6 (2%)	4 (2%)	12	44
All	All	2579/2814 (92%)	2433 (94%)	128 (5%)	18 (1%)	26	65

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	61	GLY
2	B	164	GLU
2	F	42	SER
1	C	142	ASP
2	F	20	GLU
2	H	164	GLU
2	J	75	ARG
2	L	192	ASN
2	D	254	GLU
2	F	164	GLU
2	L	42	SER
2	L	43	CYS
2	B	47	HIS
2	H	73	SER
2	L	194	LYS
2	F	63	GLN
2	J	80	ASP
2	J	122	GLU

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	141/148 (95%)	132 (94%)	9 (6%)	22	57
1	C	145/148 (98%)	139 (96%)	6 (4%)	37	74
1	E	142/148 (96%)	135 (95%)	7 (5%)	31	68
1	G	140/148 (95%)	133 (95%)	7 (5%)	30	67
1	I	124/148 (84%)	118 (95%)	6 (5%)	31	69
1	K	125/148 (84%)	116 (93%)	9 (7%)	18	53
2	B	259/288 (90%)	233 (90%)	26 (10%)	9	34
2	D	262/288 (91%)	242 (92%)	20 (8%)	16	51
2	F	253/288 (88%)	228 (90%)	25 (10%)	10	34
2	H	254/288 (88%)	234 (92%)	20 (8%)	15	49
2	J	212/288 (74%)	194 (92%)	18 (8%)	13	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	199/288 (69%)	181 (91%)	18 (9%)	12 41
All	All	2256/2616 (86%)	2085 (92%)	171 (8%)	16 51

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	MET
1	A	58	ARG
1	A	65	SER
1	A	68	CYS
1	A	80	ILE
1	A	131	ARG
1	A	137	ILE
1	A	143	GLU
1	A	156	GLU
2	B	28	ILE
2	B	30	VAL
2	B	38	LEU
2	B	43	CYS
2	B	60	SER
2	B	71	ARG
2	B	80	ASP
2	B	91	ASN
2	B	104	THR
2	B	128	LYS
2	B	137	GLN
2	B	146	GLN
2	B	147	THR
2	B	152	THR
2	B	163	LEU
2	B	164	GLU
2	B	166	ASN
2	B	184	SER
2	B	205	THR
2	B	225	VAL
2	B	240	LEU
2	B	243	GLU
2	B	253	GLU
2	B	280	LYS
2	B	299	THR
2	B	315	ARG
1	C	51	MET

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Mol	Chain	Res	Type
1	C	58	ARG
1	C	65	SER
1	C	69	GLU
1	C	80	ILE
1	C	137	ILE
2	D	22	CYS
2	D	28	ILE
2	D	30	VAL
2	D	55	SER
2	D	68	LEU
2	D	80	ASP
2	D	93	THR
2	D	104	THR
2	D	123	ARG
2	D	136	PHE
2	D	152	THR
2	D	164	GLU
2	D	184	SER
2	D	194	LYS
2	D	204	ILE
2	D	216	VAL
2	D	225	VAL
2	D	240	LEU
2	D	243	GLU
2	D	280	LYS
1	E	51	MET
1	E	58	ARG
1	E	68	CYS
1	E	80	ILE
1	E	137	ILE
1	E	154	GLN
1	E	156	GLU
2	F	21	SER
2	F	28	ILE
2	F	30	VAL
2	F	60	SER
2	F	75	ARG
2	F	97	PHE
2	F	102	ASN
2	F	104	THR
2	F	132	VAL
2	F	147	THR

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Mol	Chain	Res	Type
2	F	152	THR
2	F	164	GLU
2	F	184	SER
2	F	189	LEU
2	F	190	HIS
2	F	192	ASN
2	F	194	LYS
2	F	201	THR
2	F	204	ILE
2	F	225	VAL
2	F	240	LEU
2	F	243	GLU
2	F	280	LYS
2	F	299	THR
2	F	316	LYS
1	G	50	SER
1	G	51	MET
1	G	58	ARG
1	G	68	CYS
1	G	80	ILE
1	G	137	ILE
1	G	156	GLU
2	H	21	SER
2	H	22	CYS
2	H	28	ILE
2	H	30	VAL
2	H	75	ARG
2	H	80	ASP
2	H	91	ASN
2	H	147	THR
2	H	152	THR
2	H	184	SER
2	H	189	LEU
2	H	190	HIS
2	H	213	ILE
2	H	216	VAL
2	H	225	VAL
2	H	240	LEU
2	H	243	GLU
2	H	253	GLU
2	H	280	LYS
2	H	315	ARG

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Mol	Chain	Res	Type
1	I	23	ASP
1	I	27	ARG
1	I	51	MET
1	I	58	ARG
1	I	68	CYS
1	I	112	LYS
2	J	28	ILE
2	J	30	VAL
2	J	76	ILE
2	J	84	GLU
2	J	113	ARG
2	J	122	GLU
2	J	136	PHE
2	J	152	THR
2	J	163	LEU
2	J	204	ILE
2	J	213	ILE
2	J	216	VAL
2	J	225	VAL
2	J	240	LEU
2	J	243	GLU
2	J	253	GLU
2	J	280	LYS
2	J	299	THR
1	K	51	MET
1	K	58	ARG
1	K	68	CYS
1	K	91	ASN
1	K	94	ASP
1	K	105	SER
1	K	106	VAL
1	K	112	LYS
1	K	133	LEU
2	L	22	CYS
2	L	28	ILE
2	L	30	VAL
2	L	113	ARG
2	L	129	ILE
2	L	143	SER
2	L	146	GLN
2	L	147	THR
2	L	152	THR

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Mol	Chain	Res	Type
2	L	163	LEU
2	L	184	SER
2	L	204	ILE
2	L	213	ILE
2	L	216	VAL
2	L	240	LEU
2	L	254	GLU
2	L	280	LYS
2	L	299	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	40	HIS
2	B	124	GLN
2	B	137	GLN
2	B	286	ASN
1	C	114	GLN
2	D	124	GLN
2	D	190	HIS
2	D	223	ASN
1	E	154	GLN
2	F	190	HIS
2	F	192	ASN
2	H	79	HIS
2	H	124	GLN
1	I	114	GLN
1	I	154	GLN
1	K	41	ASN
2	L	223	ASN

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 (i)

88 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	B	903	2,5	14,14,15	0.30	0	15,19,21	0.69	1 (6%)
5	NAG	B	904	5	14,14,15	0.32	0	15,19,21	0.80	1 (6%)
6	NAG	B	905	2,6	14,14,15	0.26	0	15,19,21	0.85	1 (6%)
6	NAG	B	906	6	14,14,15	0.25	0	15,19,21	0.89	1 (6%)
7	NAG	B	907	2,7	14,14,15	0.25	0	15,19,21	0.69	1 (6%)
7	NAG	B	908	7	14,14,15	0.28	0	15,19,21	0.69	1 (6%)
8	NAG	B	909	8,2	14,14,15	0.33	0	15,19,21	0.52	0
8	NAG	B	910	8	14,14,15	0.30	0	15,19,21	0.76	1 (6%)
5	NAG	B	911	2,5	14,14,15	0.27	0	15,19,21	0.54	0
5	NAG	B	912	5	14,14,15	0.27	0	15,19,21	0.50	0
6	BMA	B	951	6	11,11,12	0.34	0	14,15,17	0.64	0
6	MAN	B	952	6	11,11,12	0.45	0	14,15,17	1.13	2 (14%)
6	MAN	B	953	6	11,11,12	0.45	0	14,15,17	0.98	2 (14%)
6	MAN	B	954	6	11,11,12	0.37	0	14,15,17	0.95	2 (14%)
8	BMA	B	956	8	11,11,12	0.49	0	14,15,17	1.18	2 (14%)
5	FUC	B	998	5	10,10,11	0.46	0	14,14,16	1.19	1 (7%)
5	FUC	B	999	5	10,10,11	0.42	0	14,14,16	0.87	1 (7%)
9	NAG	D	903	9,2	14,14,15	0.28	0	15,19,21	0.72	1 (6%)
10	NAG	D	905	10,2	14,14,15	0.21	0	15,19,21	0.95	1 (6%)
10	NAG	D	906	10	14,14,15	0.24	0	15,19,21	0.93	1 (6%)
8	NAG	D	907	8,2	14,14,15	0.26	0	15,19,21	0.77	1 (6%)
8	NAG	D	908	8	14,14,15	0.29	0	15,19,21	0.65	0
8	NAG	D	909	8,2	14,14,15	0.31	0	15,19,21	0.45	0
8	NAG	D	910	8	14,14,15	0.27	0	15,19,21	1.09	1 (6%)
11	NAG	D	911	11,2	14,14,15	0.30	0	15,19,21	0.57	0
11	NAG	D	912	11	14,14,15	0.31	0	15,19,21	0.50	0
10	BMA	D	951	10	11,11,12	0.32	0	14,15,17	0.83	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	MAN	D	952	10	11,11,12	0.42	0	14,15,17	0.96	1 (7%)
10	MAN	D	953	10	11,11,12	0.40	0	14,15,17	0.97	2 (14%)
8	BMA	D	955	8	11,11,12	0.35	0	14,15,17	0.65	1 (7%)
8	BMA	D	956	8	11,11,12	0.40	0	14,15,17	0.99	1 (7%)
11	BMA	D	958	11	11,11,12	0.37	0	14,15,17	0.79	1 (7%)
9	FUC	D	998	9	10,10,11	0.43	0	14,14,16	1.03	1 (7%)
11	FUC	D	999	11	10,10,11	0.42	0	14,14,16	0.77	1 (7%)
6	NAG	F	905	2,6	14,14,15	0.24	0	15,19,21	0.86	1 (6%)
6	NAG	F	906	6	14,14,15	0.26	0	15,19,21	0.83	1 (6%)
8	NAG	F	907	8,2	14,14,15	0.20	0	15,19,21	0.64	1 (6%)
8	NAG	F	908	8	14,14,15	0.26	0	15,19,21	0.53	0
12	NAG	F	909	2,12	14,14,15	0.29	0	15,19,21	0.78	1 (6%)
12	NAG	F	910	12	14,14,15	0.26	0	15,19,21	0.77	1 (6%)
13	NAG	F	911	13,2	14,14,15	0.27	0	15,19,21	0.69	0
13	NAG	F	912	13	14,14,15	0.30	0	15,19,21	0.45	0
6	BMA	F	951	6	11,11,12	0.33	0	14,15,17	0.92	1 (7%)
6	MAN	F	952	6	11,11,12	0.32	0	14,15,17	0.95	1 (7%)
6	MAN	F	953	6	11,11,12	0.50	0	14,15,17	1.34	1 (7%)
6	MAN	F	954	6	11,11,12	0.41	0	14,15,17	0.94	2 (14%)
8	BMA	F	955	8	11,11,12	0.31	0	14,15,17	0.53	0
12	BMA	F	956	12	11,11,12	0.41	0	14,15,17	0.92	1 (7%)
12	MAN	F	957	12	11,11,12	0.38	0	14,15,17	1.06	2 (14%)
13	BMA	F	958	13	11,11,12	0.42	0	14,15,17	0.84	1 (7%)
13	MAN	F	959	13	11,11,12	0.50	0	14,15,17	0.90	1 (7%)
13	FUC	F	999	13	10,10,11	0.37	0	14,14,16	0.89	1 (7%)
10	NAG	H	905	10,2	14,14,15	0.25	0	15,19,21	0.87	1 (6%)
10	NAG	H	906	10	14,14,15	0.23	0	15,19,21	0.79	1 (6%)
7	NAG	H	907	2,7	14,14,15	0.25	0	15,19,21	0.51	0
7	NAG	H	908	7	14,14,15	0.28	0	15,19,21	0.48	0
8	NAG	H	909	8,2	14,14,15	0.36	0	15,19,21	0.61	0
8	NAG	H	910	8	14,14,15	0.34	0	15,19,21	0.79	0
11	NAG	H	911	11,2	14,14,15	0.30	0	15,19,21	0.70	0
11	NAG	H	912	11	14,14,15	0.28	0	15,19,21	0.63	1 (6%)
10	BMA	H	951	10	11,11,12	0.26	0	14,15,17	1.03	1 (7%)
10	MAN	H	952	10	11,11,12	0.41	0	14,15,17	1.02	1 (7%)
10	MAN	H	953	10	11,11,12	0.42	0	14,15,17	0.99	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BMA	H	956	8	11,11,12	0.47	0	14,15,17	0.88	1 (7%)
11	BMA	H	958	11	11,11,12	0.48	0	14,15,17	1.06	1 (7%)
11	FUC	H	999	11	10,10,11	0.39	0	14,14,16	0.78	0
8	NAG	J	905	8,2	14,14,15	0.25	0	15,19,21	0.70	1 (6%)
8	NAG	J	906	8	14,14,15	0.29	0	15,19,21	1.05	2 (13%)
8	NAG	J	907	8,2	14,14,15	0.25	0	15,19,21	0.35	0
8	NAG	J	908	8	14,14,15	0.27	0	15,19,21	0.59	0
7	NAG	J	909	2,7	14,14,15	0.31	0	15,19,21	0.52	0
7	NAG	J	910	7	14,14,15	0.26	0	15,19,21	0.71	1 (6%)
5	NAG	J	911	2,5	14,14,15	0.27	0	15,19,21	0.69	0
5	NAG	J	912	5	14,14,15	0.28	0	15,19,21	0.51	0
8	BMA	J	951	8	11,11,12	0.31	0	14,15,17	0.83	1 (7%)
8	BMA	J	955	8	11,11,12	0.34	0	14,15,17	0.59	0
5	FUC	J	999	5	10,10,11	0.39	0	14,14,16	0.83	1 (7%)
8	NAG	L	905	8,2	14,14,15	0.25	0	15,19,21	0.76	1 (6%)
8	NAG	L	906	8	14,14,15	0.24	0	15,19,21	0.75	1 (6%)
7	NAG	L	907	2,7	14,14,15	0.28	0	15,19,21	0.72	1 (6%)
7	NAG	L	908	7	14,14,15	0.27	0	15,19,21	0.44	0
7	NAG	L	909	2,7	14,14,15	0.31	0	15,19,21	0.53	0
7	NAG	L	910	7	14,14,15	0.28	0	15,19,21	0.59	0
11	NAG	L	911	11,2	14,14,15	0.29	0	15,19,21	0.59	0
11	NAG	L	912	11	14,14,15	0.32	0	15,19,21	0.58	0
8	BMA	L	951	8	11,11,12	0.33	0	14,15,17	0.56	0
11	BMA	L	958	11	11,11,12	0.35	0	14,15,17	0.61	0
11	FUC	L	999	11	10,10,11	0.37	0	14,14,16	0.80	1 (7%)

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	B	903	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	904	5	-	0/6/23/26	0/1/1/1
6	NAG	B	905	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	906	6	-	0/6/23/26	0/1/1/1
7	NAG	B	907	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	908	7	-	0/6/23/26	0/1/1/1
8	NAG	B	909	8,2	-	0/6/23/26	0/1/1/1
8	NAG	B	910	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	911	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	912	5	-	0/6/23/26	0/1/1/1
6	BMA	B	951	6	-	0/2/19/22	0/1/1/1
6	MAN	B	952	6	-	0/2/19/22	0/1/1/1
6	MAN	B	953	6	-	0/2/19/22	0/1/1/1
6	MAN	B	954	6	-	0/2/19/22	0/1/1/1
8	BMA	B	956	8	-	0/2/19/22	0/1/1/1
5	FUC	B	998	5	-	0/0/17/20	0/1/1/1
5	FUC	B	999	5	-	0/0/17/20	0/1/1/1
9	NAG	D	903	9,2	-	0/6/23/26	0/1/1/1
10	NAG	D	905	10,2	-	0/6/23/26	0/1/1/1
10	NAG	D	906	10	-	0/6/23/26	0/1/1/1
8	NAG	D	907	8,2	-	0/6/23/26	0/1/1/1
8	NAG	D	908	8	-	0/6/23/26	0/1/1/1
8	NAG	D	909	8,2	-	0/6/23/26	0/1/1/1
8	NAG	D	910	8	-	0/6/23/26	0/1/1/1
11	NAG	D	911	11,2	-	0/6/23/26	0/1/1/1
11	NAG	D	912	11	-	0/6/23/26	0/1/1/1
10	BMA	D	951	10	-	0/2/19/22	0/1/1/1
10	MAN	D	952	10	-	0/2/19/22	1/1/1/1
10	MAN	D	953	10	-	0/2/19/22	0/1/1/1
8	BMA	D	955	8	-	0/2/19/22	0/1/1/1
8	BMA	D	956	8	-	0/2/19/22	0/1/1/1
11	BMA	D	958	11	-	0/2/19/22	0/1/1/1
9	FUC	D	998	9	-	0/0/17/20	0/1/1/1
11	FUC	D	999	11	-	0/0/17/20	0/1/1/1
6	NAG	F	905	2,6	-	0/6/23/26	0/1/1/1
6	NAG	F	906	6	-	0/6/23/26	0/1/1/1
8	NAG	F	907	8,2	-	0/6/23/26	0/1/1/1
8	NAG	F	908	8	-	0/6/23/26	0/1/1/1
12	NAG	F	909	2,12	-	0/6/23/26	0/1/1/1
12	NAG	F	910	12	-	0/6/23/26	0/1/1/1
13	NAG	F	911	13,2	-	0/6/23/26	0/1/1/1
13	NAG	F	912	13	-	0/6/23/26	0/1/1/1
6	BMA	F	951	6	-	0/2/19/22	0/1/1/1
6	MAN	F	952	6	-	0/2/19/22	0/1/1/1
6	MAN	F	953	6	-	0/2/19/22	1/1/1/1
6	MAN	F	954	6	-	0/2/19/22	0/1/1/1
8	BMA	F	955	8	-	0/2/19/22	0/1/1/1
12	BMA	F	956	12	-	0/2/19/22	0/1/1/1
12	MAN	F	957	12	-	0/2/19/22	0/1/1/1
13	BMA	F	958	13	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MAN	F	959	13	-	0/2/19/22	0/1/1/1
13	FUC	F	999	13	-	0/0/17/20	0/1/1/1
10	NAG	H	905	10,2	-	0/6/23/26	0/1/1/1
10	NAG	H	906	10	-	0/6/23/26	0/1/1/1
7	NAG	H	907	2,7	-	0/6/23/26	0/1/1/1
7	NAG	H	908	7	-	0/6/23/26	0/1/1/1
8	NAG	H	909	8,2	-	0/6/23/26	0/1/1/1
8	NAG	H	910	8	-	0/6/23/26	0/1/1/1
11	NAG	H	911	11,2	-	0/6/23/26	0/1/1/1
11	NAG	H	912	11	-	0/6/23/26	0/1/1/1
10	BMA	H	951	10	-	0/2/19/22	0/1/1/1
10	MAN	H	952	10	-	0/2/19/22	0/1/1/1
10	MAN	H	953	10	-	0/2/19/22	0/1/1/1
8	BMA	H	956	8	-	0/2/19/22	0/1/1/1
11	BMA	H	958	11	-	0/2/19/22	0/1/1/1
11	FUC	H	999	11	-	0/0/17/20	0/1/1/1
8	NAG	J	905	8,2	-	0/6/23/26	0/1/1/1
8	NAG	J	906	8	-	0/6/23/26	0/1/1/1
8	NAG	J	907	8,2	-	0/6/23/26	0/1/1/1
8	NAG	J	908	8	-	0/6/23/26	0/1/1/1
7	NAG	J	909	2,7	-	0/6/23/26	0/1/1/1
7	NAG	J	910	7	-	0/6/23/26	0/1/1/1
5	NAG	J	911	2,5	-	0/6/23/26	0/1/1/1
5	NAG	J	912	5	-	0/6/23/26	0/1/1/1
8	BMA	J	951	8	-	0/2/19/22	0/1/1/1
8	BMA	J	955	8	-	0/2/19/22	0/1/1/1
5	FUC	J	999	5	-	0/0/17/20	0/1/1/1
8	NAG	L	905	8,2	-	0/6/23/26	0/1/1/1
8	NAG	L	906	8	-	0/6/23/26	0/1/1/1
7	NAG	L	907	2,7	-	0/6/23/26	0/1/1/1
7	NAG	L	908	7	-	0/6/23/26	0/1/1/1
7	NAG	L	909	2,7	-	0/6/23/26	0/1/1/1
7	NAG	L	910	7	-	0/6/23/26	0/1/1/1
11	NAG	L	911	11,2	-	0/6/23/26	0/1/1/1
11	NAG	L	912	11	-	0/6/23/26	0/1/1/1
8	BMA	L	951	8	-	0/2/19/22	0/1/1/1
11	BMA	L	958	11	-	0/2/19/22	0/1/1/1
11	FUC	L	999	11	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	909	NAG	O4-C4-C3	-2.16	105.47	110.34
6	F	954	MAN	C1-C2-C3	2.01	111.92	109.54
6	B	953	MAN	C1-O5-C5	2.02	114.81	112.25
11	D	999	FUC	C1-O5-C5	2.06	115.56	112.38
8	D	955	BMA	C1-O5-C5	2.07	114.88	112.25
6	B	954	MAN	C1-C2-C3	2.08	112.00	109.54
11	H	912	NAG	C1-O5-C5	2.08	114.89	112.25
13	F	959	MAN	C1-C2-C3	2.09	112.01	109.54
11	D	958	BMA	C1-O5-C5	2.11	114.92	112.25
12	F	957	MAN	C1-C2-C3	2.16	112.10	109.54
10	D	953	MAN	C1-C2-C3	2.23	112.18	109.54
8	F	907	NAG	C1-O5-C5	2.26	115.12	112.25
10	D	951	BMA	O3-C3-C4	2.28	115.46	110.34
10	H	953	MAN	C1-O5-C5	2.30	115.17	112.25
8	J	906	NAG	C1-O5-C5	2.30	115.17	112.25
5	B	999	FUC	C1-O5-C5	2.32	115.96	112.38
8	H	956	BMA	C1-C2-C3	2.32	112.29	109.54
12	F	910	NAG	C1-O5-C5	2.32	115.20	112.25
12	F	956	BMA	C1-O5-C5	2.34	115.21	112.25
13	F	958	BMA	C1-O5-C5	2.35	115.24	112.25
6	B	952	MAN	C1-C2-C3	2.38	112.36	109.54
7	B	908	NAG	C1-O5-C5	2.38	115.27	112.25
8	L	906	NAG	C1-O5-C5	2.39	115.28	112.25
5	B	903	NAG	C1-O5-C5	2.40	115.30	112.25
10	H	953	MAN	C1-C2-C3	2.41	112.39	109.54
8	J	905	NAG	C1-O5-C5	2.44	115.35	112.25
8	B	910	NAG	C1-O5-C5	2.45	115.36	112.25
7	J	910	NAG	C1-O5-C5	2.47	115.39	112.25
5	J	999	FUC	C1-O5-C5	2.52	116.27	112.38
7	B	907	NAG	C1-O5-C5	2.52	115.45	112.25
6	F	951	BMA	C1-O5-C5	2.53	115.46	112.25
9	D	903	NAG	C1-O5-C5	2.54	115.47	112.25
11	L	999	FUC	C1-O5-C5	2.55	116.32	112.38
7	L	907	NAG	C1-O5-C5	2.56	115.50	112.25
10	D	953	MAN	C1-O5-C5	2.58	115.52	112.25
6	F	954	MAN	C1-O5-C5	2.59	115.53	112.25
8	B	956	BMA	C1-C2-C3	2.60	112.61	109.54
6	B	953	MAN	C1-C2-C3	2.66	112.68	109.54
6	B	954	MAN	C1-O5-C5	2.68	115.65	112.25
5	B	904	NAG	C1-O5-C5	2.69	115.66	112.25
8	L	905	NAG	C1-O5-C5	2.69	115.66	112.25
8	D	956	BMA	C1-O5-C5	2.77	115.76	112.25
10	H	906	NAG	C1-O5-C5	2.77	115.76	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	907	NAG	C1-O5-C5	2.77	115.77	112.25
8	J	951	BMA	C1-O5-C5	2.80	115.80	112.25
11	H	958	BMA	C1-C2-C3	2.91	112.99	109.54
6	F	906	NAG	C1-O5-C5	2.93	115.97	112.25
13	F	999	FUC	C1-O5-C5	2.94	116.92	112.38
12	F	957	MAN	C1-O5-C5	2.97	116.02	112.25
8	J	906	NAG	C2-N2-C7	3.03	126.94	123.04
9	D	998	FUC	C1-O5-C5	3.06	117.10	112.38
10	D	952	MAN	C1-O5-C5	3.07	116.15	112.25
6	B	905	NAG	C1-O5-C5	3.12	116.20	112.25
6	F	952	MAN	C1-O5-C5	3.12	116.21	112.25
8	B	956	BMA	C1-O5-C5	3.13	116.22	112.25
6	F	905	NAG	C1-O5-C5	3.13	116.22	112.25
10	H	905	NAG	C1-O5-C5	3.16	116.26	112.25
10	H	951	BMA	O3-C3-C4	3.18	117.51	110.34
6	B	952	MAN	C1-O5-C5	3.20	116.31	112.25
6	B	906	NAG	C1-O5-C5	3.21	116.33	112.25
10	H	952	MAN	C1-O5-C5	3.24	116.35	112.25
10	D	906	NAG	C1-O5-C5	3.32	116.46	112.25
10	D	905	NAG	C1-O5-C5	3.41	116.57	112.25
8	D	910	NAG	C1-O5-C5	3.68	116.92	112.25
5	B	998	FUC	C1-O5-C5	3.81	118.27	112.38
6	F	953	MAN	C1-O5-C5	4.58	118.06	112.25

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	952	MAN	C1-C2-C3-C4-C5-O5
6	F	953	MAN	C1-C2-C3-C4-C5-O5

11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	905	NAG	1	0
9	D	998	FUC	1	0
6	F	905	NAG	1	0
13	F	912	NAG	1	0
6	F	951	BMA	1	0
6	F	953	MAN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	954	MAN	1	0
10	H	905	NAG	1	0
8	J	905	NAG	1	0
8	L	905	NAG	1	0
11	L	999	FUC	2	0

5.6 Ligand geometry (i)

46 ligands 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	$\#\|Z\| > 2$
3	SO4	A	201	-	4,4,4	0.51	0	6,6,6	0.09	0
3	SO4	A	202	-	4,4,4	0.25	0	6,6,6	0.17	0
3	SO4	B	820	-	4,4,4	0.12	0	6,6,6	0.18	0
3	SO4	B	821	-	4,4,4	0.20	0	6,6,6	0.19	0
3	SO4	B	822	-	4,4,4	0.30	0	6,6,6	0.23	0
3	SO4	B	823	-	4,4,4	0.25	0	6,6,6	0.21	0
3	SO4	B	824	-	4,4,4	0.16	0	6,6,6	0.12	0
4	NAG	B	901	2	14,14,15	0.27	0	15,19,21	0.65	1 (6%)
4	NAG	B	902	2	14,14,15	0.29	0	15,19,21	0.91	1 (6%)
3	SO4	C	201	-	4,4,4	0.19	0	6,6,6	0.12	0
3	SO4	C	202	-	4,4,4	0.11	0	6,6,6	0.09	0
3	SO4	C	203	-	4,4,4	0.11	0	6,6,6	0.07	0
3	SO4	C	204	-	4,4,4	0.08	0	6,6,6	0.27	0
3	SO4	C	205	-	4,4,4	0.12	0	6,6,6	0.14	0
3	SO4	D	419	-	4,4,4	0.19	0	6,6,6	0.28	0
3	SO4	D	420	-	4,4,4	0.20	0	6,6,6	0.10	0
3	SO4	D	421	-	4,4,4	0.14	0	6,6,6	0.23	0
3	SO4	D	422	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	D	423	-	4,4,4	0.13	0	6,6,6	0.07	0
3	SO4	D	424	-	4,4,4	0.16	0	6,6,6	0.23	0
3	SO4	D	425	-	4,4,4	0.34	0	6,6,6	0.20	0
4	NAG	D	902	2	14,14,15	0.38	0	15,19,21	0.62	0
3	SO4	E	201	-	4,4,4	0.40	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	E	202	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	E	203	-	4,4,4	0.37	0	6,6,6	0.14	0
3	SO4	F	821	-	4,4,4	0.18	0	6,6,6	0.20	0
3	SO4	F	822	-	4,4,4	0.10	0	6,6,6	0.15	0
3	SO4	F	823	-	4,4,4	0.29	0	6,6,6	0.34	0
3	SO4	F	824	-	4,4,4	0.17	0	6,6,6	0.10	0
3	SO4	F	825	-	4,4,4	0.27	0	6,6,6	0.16	0
4	NAG	F	901	2	14,14,15	0.27	0	15,19,21	0.57	0
4	NAG	F	903	2	14,14,15	0.30	0	15,19,21	0.82	1 (6%)
3	SO4	G	201	-	4,4,4	0.12	0	6,6,6	0.34	0
3	SO4	G	202	-	4,4,4	0.24	0	6,6,6	0.16	0
3	SO4	H	817	-	4,4,4	0.19	0	6,6,6	0.11	0
3	SO4	H	818	-	4,4,4	0.14	0	6,6,6	0.26	0
3	SO4	H	819	-	4,4,4	0.22	0	6,6,6	0.14	0
3	SO4	H	820	-	4,4,4	0.13	0	6,6,6	0.16	0
3	SO4	H	821	-	4,4,4	0.28	0	6,6,6	0.16	0
4	NAG	H	901	2	14,14,15	0.27	0	15,19,21	0.77	1 (6%)
4	NAG	H	903	2	14,14,15	0.26	0	15,19,21	0.78	1 (6%)
3	SO4	I	201	-	4,4,4	0.24	0	6,6,6	0.19	0
3	SO4	J	413	-	4,4,4	0.13	0	6,6,6	0.22	0
4	NAG	J	903	2	14,14,15	0.28	0	15,19,21	0.45	0
3	SO4	K	201	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	L	412	-	4,4,4	0.18	0	6,6,6	0.11	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
3	SO4	A	201	-	-	0/0/0/0	0/0/0/0
3	SO4	A	202	-	-	0/0/0/0	0/0/0/0
3	SO4	B	820	-	-	0/0/0/0	0/0/0/0
3	SO4	B	821	-	-	0/0/0/0	0/0/0/0
3	SO4	B	822	-	-	0/0/0/0	0/0/0/0
3	SO4	B	823	-	-	0/0/0/0	0/0/0/0
3	SO4	B	824	-	-	0/0/0/0	0/0/0/0
4	NAG	B	901	2	-	0/6/23/26	0/1/1/1
4	NAG	B	902	2	-	0/6/23/26	0/1/1/1
3	SO4	C	201	-	-	0/0/0/0	0/0/0/0
3	SO4	C	202	-	-	0/0/0/0	0/0/0/0
3	SO4	C	203	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	204	-	-	0/0/0/0	0/0/0/0
3	SO4	C	205	-	-	0/0/0/0	0/0/0/0
3	SO4	D	419	-	-	0/0/0/0	0/0/0/0
3	SO4	D	420	-	-	0/0/0/0	0/0/0/0
3	SO4	D	421	-	-	0/0/0/0	0/0/0/0
3	SO4	D	422	-	-	0/0/0/0	0/0/0/0
3	SO4	D	423	-	-	0/0/0/0	0/0/0/0
3	SO4	D	424	-	-	0/0/0/0	0/0/0/0
3	SO4	D	425	-	-	0/0/0/0	0/0/0/0
4	NAG	D	902	2	-	0/6/23/26	0/1/1/1
3	SO4	E	201	-	-	0/0/0/0	0/0/0/0
3	SO4	E	202	-	-	0/0/0/0	0/0/0/0
3	SO4	E	203	-	-	0/0/0/0	0/0/0/0
3	SO4	F	821	-	-	0/0/0/0	0/0/0/0
3	SO4	F	822	-	-	0/0/0/0	0/0/0/0
3	SO4	F	823	-	-	0/0/0/0	0/0/0/0
3	SO4	F	824	-	-	0/0/0/0	0/0/0/0
3	SO4	F	825	-	-	0/0/0/0	0/0/0/0
4	NAG	F	901	2	-	0/6/23/26	0/1/1/1
4	NAG	F	903	2	-	0/6/23/26	0/1/1/1
3	SO4	G	201	-	-	0/0/0/0	0/0/0/0
3	SO4	G	202	-	-	0/0/0/0	0/0/0/0
3	SO4	H	817	-	-	0/0/0/0	0/0/0/0
3	SO4	H	818	-	-	0/0/0/0	0/0/0/0
3	SO4	H	819	-	-	0/0/0/0	0/0/0/0
3	SO4	H	820	-	-	0/0/0/0	0/0/0/0
3	SO4	H	821	-	-	0/0/0/0	0/0/0/0
4	NAG	H	901	2	-	0/6/23/26	0/1/1/1
4	NAG	H	903	2	-	0/6/23/26	0/1/1/1
3	SO4	I	201	-	-	0/0/0/0	0/0/0/0
3	SO4	J	413	-	-	0/0/0/0	0/0/0/0
4	NAG	J	903	2	-	0/6/23/26	0/1/1/1
3	SO4	K	201	-	-	0/0/0/0	0/0/0/0
3	SO4	L	412	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	901	NAG	C1-O5-C5	2.26	115.11	112.25
4	H	901	NAG	C1-O5-C5	2.67	115.64	112.25
4	H	903	NAG	C1-O5-C5	2.82	115.83	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	903	NAG	C1-O5-C5	2.95	116.00	112.25
4	B	902	NAG	C1-O5-C5	3.33	116.48	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	821	SO4	1	0
3	H	817	SO4	1	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

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, 95^{th} 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	156/157 (99%)	-0.24	2 (1%) 79 62	38, 57, 90, 110	0
1	C	156/157 (99%)	-0.27	0 100 100	32, 58, 85, 109	0
1	E	157/157 (100%)	-0.20	0 100 100	35, 64, 92, 129	0
1	G	156/157 (99%)	-0.31	0 100 100	34, 53, 80, 95	0
1	I	156/157 (99%)	-0.10	1 (0%) 90 80	75, 99, 132, 145	0
1	K	156/157 (99%)	-0.04	0 100 100	71, 96, 121, 130	0
2	B	294/312 (94%)	0.09	5 (1%) 73 52	32, 68, 111, 139	0
2	D	290/312 (92%)	0.02	2 (0%) 89 78	36, 67, 102, 136	0
2	F	288/312 (92%)	0.07	6 (2%) 67 44	36, 72, 129, 152	0
2	H	288/312 (92%)	0.10	6 (2%) 67 44	35, 68, 121, 161	0
2	J	272/312 (87%)	0.56	24 (8%) 12 4	54, 94, 165, 191	0
2	L	255/312 (81%)	0.63	28 (10%) 7 2	69, 101, 137, 163	0
All	All	2624/2814 (93%)	0.08	74 (2%) 56 32	32, 76, 128, 191	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	63	GLN	4.6
2	B	62	SER	4.6
2	L	151	SER	4.1
2	L	88	VAL	3.9
2	L	227	VAL	3.8
1	A	141	GLU	3.8
2	J	62	SER	3.7
2	J	76	ILE	3.5
2	F	68	LEU	3.5
2	J	56	TRP	3.5
2	L	87	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	J	111	VAL	3.3
2	L	29	THR	3.2
2	J	79	HIS	3.1
2	L	30	VAL	3.0
1	I	29	LEU	3.0
1	A	142	ASP	3.0
2	L	79	HIS	2.9
2	H	73	SER	2.9
2	J	75	ARG	2.9
2	J	293	ASN	2.9
2	J	191	HIS	2.8
2	H	62	SER	2.8
2	L	31	VAL	2.8
2	J	80	ASP	2.8
2	F	-2	GLY	2.7
2	L	190	HIS	2.7
2	D	91	ASN	2.7
2	L	187	HIS	2.7
2	J	83	LEU	2.7
2	J	31	VAL	2.6
2	L	197	ASN	2.6
2	J	42	SER	2.6
2	J	93	THR	2.6
2	J	84	GLU	2.6
2	L	119	CYS	2.6
2	L	152	THR	2.5
2	L	86	TRP	2.5
2	L	145	TYR	2.5
2	L	195	LEU	2.4
2	J	147	THR	2.4
2	F	56	TRP	2.4
2	L	118	SER	2.4
2	L	28	ILE	2.4
2	L	188	PHE	2.4
2	J	90	LEU	2.4
2	D	65	HIS	2.3
2	L	77	ALA	2.3
2	H	74	SER	2.3
2	B	110	ASN	2.2
2	J	60	SER	2.2
2	J	240	LEU	2.2
2	L	186	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	116	LYS	2.2
2	L	295	LEU	2.2
2	J	85	PHE	2.2
2	L	27	HIS	2.2
2	F	62	SER	2.2
2	L	153	SER	2.2
2	B	116	LYS	2.1
2	L	114	ARG	2.1
2	B	124	GLN	2.1
2	F	99	GLN	2.1
2	J	110	ASN	2.1
2	H	68	LEU	2.1
2	H	124	GLN	2.0
2	J	74	SER	2.0
2	L	144	TYR	2.0
2	L	193	GLY	2.0
2	J	120	PHE	2.0
2	J	188	PHE	2.0
2	J	77	ALA	2.0
2	L	309	LYS	2.0
2	F	97	PHE	2.0

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, 95^{th} 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
8	NAG	F	907	14/15	0.92	0.27	1.07	87,90,96,104	0
11	NAG	H	911	14/15	0.95	0.23	0.17	65,70,80,91	0
11	NAG	D	911	14/15	0.96	0.24	0.10	78,82,96,101	0
7	NAG	H	907	14/15	0.92	0.20	-0.01	69,83,99,111	0
7	NAG	L	909	14/15	0.93	0.25	-0.15	100,104,110,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	NAG	B	909	14/15	0.93	0.22	-0.15	67,73,79,84	0
11	NAG	L	911	14/15	0.93	0.30	-0.16	120,128,136,145	0
6	NAG	B	905	14/15	0.97	0.26	-0.34	91,97,102,103	0
6	NAG	F	905	14/15	0.96	0.22	-0.37	88,94,105,105	0
5	NAG	B	911	14/15	0.95	0.17	-0.39	68,76,84,94	0
5	NAG	J	911	14/15	0.93	0.23	-0.42	99,105,109,115	0
8	NAG	J	905	14/15	0.92	0.25	-0.50	107,109,115,116	0
7	NAG	J	909	14/15	0.95	0.20	-0.61	86,90,96,103	0
8	NAG	H	909	14/15	0.94	0.21	-0.63	68,76,81,88	0
10	NAG	D	905	14/15	0.96	0.20	-0.68	64,74,85,89	0
8	NAG	D	907	14/15	0.92	0.19	-0.73	62,71,77,86	0
8	NAG	J	907	14/15	0.90	0.20	-0.75	109,114,121,129	0
7	NAG	L	907	14/15	0.89	0.18	-0.82	110,113,119,124	0
7	NAG	B	907	14/15	0.94	0.18	-0.99	81,88,99,110	0
12	NAG	F	909	14/15	0.94	0.18	-1.04	74,84,91,100	0
8	NAG	D	909	14/15	0.94	0.16	-1.22	63,67,74,81	0
13	NAG	F	911	14/15	0.95	0.16	-1.34	55,66,81,82	0
8	NAG	L	905	14/15	0.88	0.35	-1.39	142,147,151,152	0
10	NAG	H	905	14/15	0.97	0.18	-1.52	96,105,111,116	0
11	FUC	D	999	10/11	0.91	0.26	-	96,99,102,105	0
8	BMA	F	955	11/12	0.61	0.34	-	138,145,147,150	0
9	FUC	D	998	10/11	0.90	0.27	-	126,129,131,131	0
11	BMA	D	958	11/12	0.71	0.36	-	127,130,132,134	0
11	NAG	D	912	14/15	0.90	0.26	-	105,111,124,125	0
5	NAG	B	912	14/15	0.87	0.34	-	96,104,111,111	0
10	NAG	D	906	14/15	0.94	0.25	-	94,98,107,116	0
8	BMA	B	956	11/12	0.81	0.26	-	108,114,117,118	0
5	FUC	B	999	10/11	0.95	0.33	-	74,80,83,89	0
12	MAN	F	957	11/12	0.52	0.48	-	160,163,165,166	0
10	MAN	D	952	11/12	0.84	0.33	-	138,140,143,143	0
13	MAN	F	959	11/12	0.57	0.44	-	138,143,148,152	0
7	NAG	L	908	14/15	0.74	0.30	-	126,128,129,130	0
5	FUC	B	998	10/11	0.84	0.35	-	152,154,157,158	0
8	NAG	L	906	14/15	0.90	0.35	-	149,155,161,163	0
13	FUC	F	999	10/11	0.94	0.21	-	81,87,93,97	0
10	MAN	D	953	11/12	0.79	0.30	-	137,142,144,144	0
13	BMA	F	958	11/12	0.64	0.27	-	122,130,137,138	0
8	NAG	F	908	14/15	0.84	0.23	-	106,115,124,131	0
12	NAG	F	910	14/15	0.87	0.23	-	111,118,125,133	0
10	MAN	H	952	11/12	0.77	0.25	-	157,159,161,163	0
8	NAG	J	908	14/15	0.75	0.36	-	133,142,147,153	0
6	BMA	F	951	11/12	0.91	0.39	-	131,137,143,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MAN	B	954	11/12	0.74	0.38	-	163,166,172,174	0
8	NAG	D	910	14/15	0.88	0.14	-	91,96,105,114	0
6	MAN	F	952	11/12	0.84	0.33	-	139,144,155,159	0
5	FUC	J	999	10/11	0.95	0.22	-	106,111,114,115	0
7	NAG	B	908	14/15	0.81	0.30	-	119,125,131,131	0
5	NAG	B	904	14/15	0.46	0.61	-	164,166,172,174	0
5	NAG	J	912	14/15	0.82	0.27	-	120,125,130,133	0
6	MAN	F	953	11/12	0.75	0.32	-	150,151,157,157	0
8	BMA	J	951	11/12	0.83	0.34	-	132,135,138,139	0
7	NAG	J	910	14/15	0.82	0.24	-	113,121,124,126	0
6	MAN	B	952	11/12	0.59	0.43	-	149,151,159,161	0
11	FUC	H	999	10/11	0.93	0.30	-	79,82,85,85	0
10	BMA	H	951	11/12	0.87	0.34	-	145,152,156,156	0
11	FUC	L	999	10/11	0.94	0.36	-	130,135,140,143	0
6	NAG	F	906	14/15	0.91	0.33	-	109,111,120,127	0
8	BMA	D	955	11/12	0.61	0.34	-	121,125,128,131	0
8	NAG	B	910	14/15	0.80	0.23	-	93,100,104,110	0
6	BMA	B	951	11/12	0.84	0.24	-	129,136,144,145	0
9	NAG	D	903	14/15	0.79	0.28	-	124,128,137,138	0
8	BMA	H	956	11/12	0.76	0.31	-	119,125,132,135	0
8	BMA	J	955	11/12	0.58	0.38	-	158,159,163,163	0
8	BMA	L	951	11/12	0.83	0.42	-	165,169,171,172	0
8	BMA	D	956	11/12	0.76	0.28	-	123,130,134,134	0
11	BMA	H	958	11/12	0.65	0.33	-	123,127,131,135	0
8	NAG	J	906	14/15	0.90	0.37	-	116,125,130,132	0
11	NAG	L	912	14/15	0.88	0.36	-	150,155,161,164	0
12	BMA	F	956	11/12	0.65	0.27	-	140,148,154,157	0
11	NAG	H	912	14/15	0.89	0.43	-	92,100,111,118	0
8	NAG	H	910	14/15	0.79	0.26	-	92,101,110,118	0
7	NAG	L	910	14/15	0.81	0.24	-	116,125,132,133	0
7	NAG	H	908	14/15	0.72	0.37	-	120,125,132,133	0
13	NAG	F	912	14/15	0.92	0.23	-	83,94,108,114	0
10	NAG	H	906	14/15	0.92	0.31	-	121,126,133,139	0
8	NAG	D	908	14/15	0.88	0.18	-	93,98,109,114	0
6	MAN	F	954	11/12	0.61	0.50	-	155,162,169,172	0
10	BMA	D	951	11/12	0.88	0.30	-	122,130,136,137	0
10	MAN	H	953	11/12	0.82	0.38	-	158,163,168,169	0
6	NAG	B	906	14/15	0.93	0.25	-	104,107,117,123	0
11	BMA	L	958	11/12	0.71	0.43	-	161,165,170,171	0
5	NAG	B	903	14/15	0.84	0.40	-	149,154,157,161	0
6	MAN	B	953	11/12	0.54	0.37	-	146,151,153,154	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95^{th} 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
3	SO4	F	824	5/5	0.76	0.46	9.95	163,163,163,163	0
4	NAG	F	903	14/15	0.53	0.47	9.56	123,127,133,137	0
3	SO4	D	419	5/5	0.88	0.45	5.21	144,145,146,146	0
3	SO4	H	817	5/5	0.85	0.57	4.88	142,143,143,144	0
3	SO4	B	821	5/5	0.86	0.32	4.37	144,145,145,147	0
3	SO4	H	818	5/5	0.87	0.35	3.90	147,148,148,149	0
3	SO4	F	821	5/5	0.92	0.34	3.59	112,114,115,116	0
3	SO4	C	204	5/5	0.87	0.30	2.56	126,129,129,131	0
3	SO4	E	203	5/5	0.83	0.25	2.46	121,121,122,123	0
3	SO4	D	421	5/5	0.86	0.40	2.13	129,129,132,133	0
3	SO4	A	202	5/5	0.80	0.31	1.99	147,148,148,150	0
3	SO4	B	820	5/5	0.88	0.29	1.33	126,127,129,129	0
3	SO4	G	202	5/5	0.73	0.29	1.19	160,160,160,160	0
3	SO4	B	824	5/5	0.86	0.26	0.71	155,155,156,156	0
3	SO4	C	202	5/5	0.88	0.23	0.49	142,143,143,144	0
3	SO4	A	201	5/5	0.98	0.18	0.30	76,77,78,78	0
3	SO4	H	819	5/5	0.87	0.17	-0.14	159,159,159,160	0
3	SO4	B	822	5/5	0.87	0.17	-0.18	162,163,163,163	0
3	SO4	K	201	5/5	0.96	0.16	-0.64	123,124,124,125	0
3	SO4	G	201	5/5	0.99	0.13	-0.84	63,68,68,70	0
3	SO4	F	823	5/5	0.94	0.19	-0.90	121,122,123,123	0
3	SO4	C	201	5/5	0.97	0.13	-1.30	118,118,119,119	0
3	SO4	F	822	5/5	0.91	0.21	-1.46	119,120,121,121	0
3	SO4	I	201	5/5	0.94	0.11	-1.57	124,125,125,126	0
3	SO4	E	201	5/5	0.98	0.12	-1.58	81,82,82,83	0
3	SO4	H	820	5/5	0.80	0.50	-	142,143,144,147	0
3	SO4	D	420	5/5	0.82	0.23	-	146,147,147,148	0
3	SO4	F	825	5/5	0.79	0.17	-	158,159,161,161	0
3	SO4	D	425	5/5	0.86	0.14	-	144,146,147,147	0
4	NAG	H	901	14/15	0.83	0.30	-	124,131,134,135	0
3	SO4	C	203	5/5	0.69	0.33	-	174,175,176,176	0
4	NAG	B	901	14/15	0.70	0.44	-	145,152,156,156	0
4	NAG	D	902	14/15	0.77	0.27	-	119,125,137,138	0
4	NAG	J	903	14/15	0.55	0.47	-	144,150,154,156	0
3	SO4	B	823	5/5	0.90	0.15	-	155,157,159,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	H	903	14/15	0.70	0.34	-	127,135,140,144	0
3	SO4	H	821	5/5	0.82	0.25	-	166,169,169,171	0
3	SO4	D	423	5/5	0.69	0.23	-	158,159,159,159	0
4	NAG	F	901	14/15	0.69	0.42	-	151,155,162,163	0
3	SO4	E	202	5/5	0.54	0.38	-	185,186,186,187	0
3	SO4	C	205	5/5	0.62	0.30	-	191,191,192,192	0
4	NAG	B	902	14/15	0.76	0.24	-	128,137,143,144	0
3	SO4	D	424	5/5	0.86	0.18	-	130,130,132,133	0
3	SO4	L	412	5/5	0.89	0.18	-	157,159,159,160	0
3	SO4	J	413	5/5	0.81	0.19	-	125,126,126,127	0
3	SO4	D	422	5/5	0.74	0.20	-	171,172,173,174	0

6.5 Other polymers (i)

There are no such residues in this entry.