Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:16 PM GMT

PDB ID	:	3WO4
Title	:	Crystal structure of the IL-18 signaling ternary complex
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:

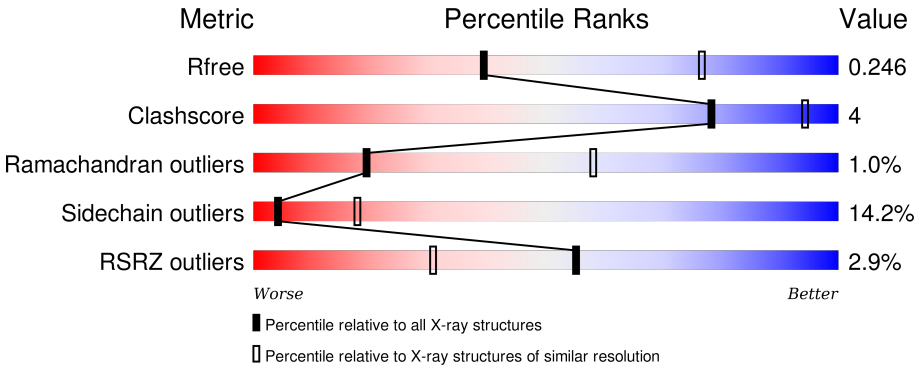
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	75% 23%
2	B	312	% 77% 16%
3	C	344	6% 64% 13% 22%

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
10	NAG	C	902	-	-	-	X
11	CL	C	908	-	-	-	X
8	NAG	B	910	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 6030 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	157	Total	C	N	O	S	0	0	0
			1266	796	209	251	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	301	Total	C	N	O	S	0	1	0
			2375	1499	406	456	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	EXPRESSION TAG	UNP Q13478
B	-1	PRO	-	EXPRESSION TAG	UNP Q13478

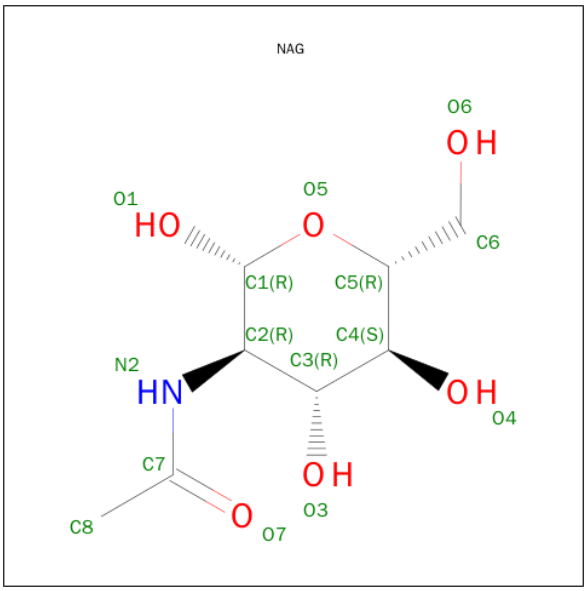
- Molecule 3 is a protein called Interleukin-18 receptor accessory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	270	Total	C	N	O	S	0	0	0
			2022	1263	347	402	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP O95256
C	-1	PRO	-	EXPRESSION TAG	UNP O95256

- 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	C	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

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	5	Total C N O 61 34 2 25	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	3	Total C N O 39 22 2 15	0	0

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 9 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	4	Total C N O 49 28 2 19	0	0

- Molecule 10 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total Cl 1 1	0	0

- Molecule 12 is water.

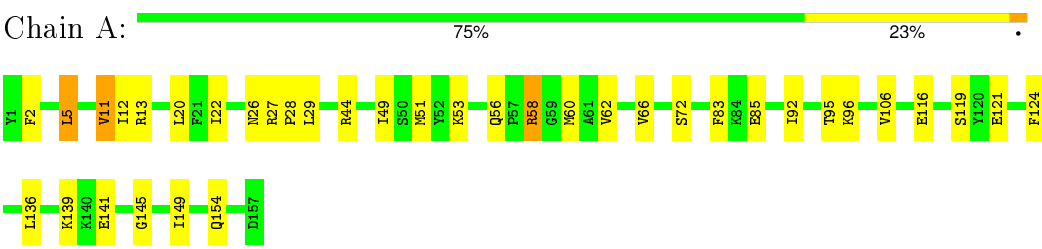
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	14	Total O 14 14	0	0
12	B	7	Total O 7 7	0	0
12	C	10	Total O 10 10	0	0

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.

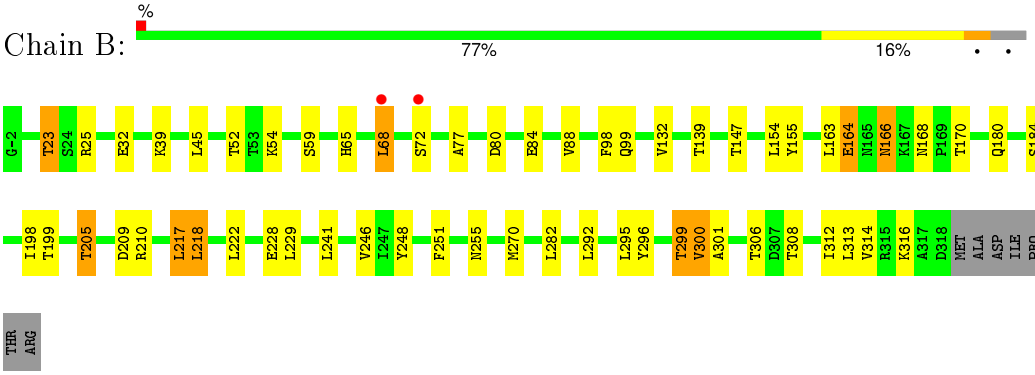
- Molecule 1: Interleukin-18

Chain A:



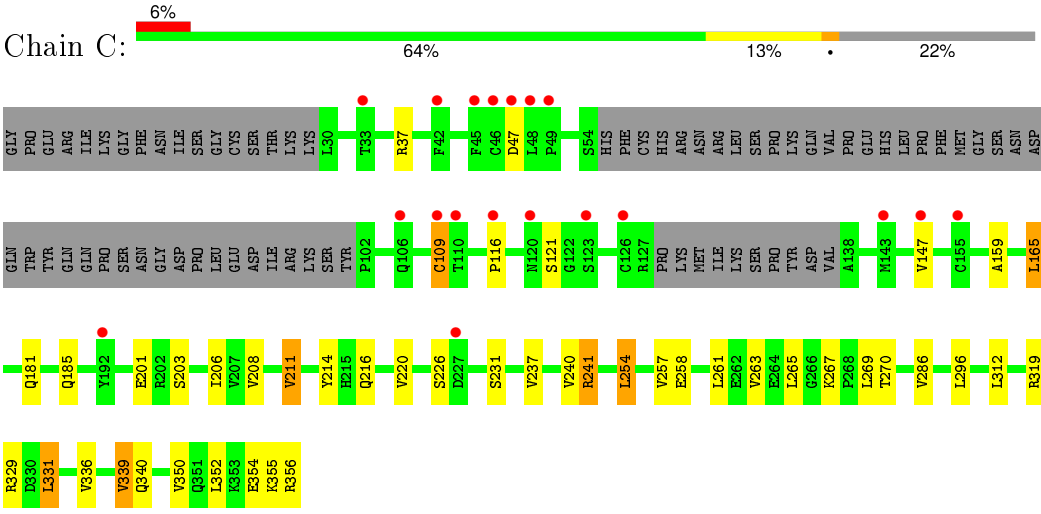
- Molecule 2: Interleukin-18 receptor 1

Chain B:



- Molecule 3: Interleukin-18 receptor accessory protein

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.56Å 111.56Å 134.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.00 – 3.10 49.34 – 3.09	Depositor EDS
% Data completeness (in resolution range)	85.0 (42.00-3.10) 84.8 (49.34-3.09)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.39 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.188 , 0.232 0.198 , 0.246	Depositor DCC
R_{free} test set	881 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	58.9	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 91.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 17449 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6030	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: FUC, MAN, BMA, NAG, CL

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	0/1287	0.71	0/1726
2	B	0.45	0/2433	0.68	0/3310
3	C	0.45	0/2057	0.72	0/2800
All	All	0.46	0/5777	0.70	0/7836

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	1266	0	1237	13	0
2	B	2375	0	2231	17	0
3	C	2022	0	1857	15	0
4	B	28	0	26	0	0
4	C	14	0	13	0	0
5	B	38	0	34	0	0
6	B	61	0	52	0	0
7	B	39	0	34	0	0
8	B	28	0	25	0	0
8	C	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	49	0	43	0	0
10	C	50	0	43	0	0
11	C	1	0	0	0	0
12	A	14	0	0	1	0
12	B	7	0	0	0	0
12	C	10	0	0	0	0
All	All	6030	0	5620	42	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 (42) 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)
2:B:295:LEU:HD12	2:B:312:ILE:HD11	1.64	0.80
2:B:180:GLN:HG3	2:B:205:THR:HA	1.77	0.67
2:B:301:ALA:HA	2:B:306:THR:HG22	1.79	0.64
3:C:216:GLN:HG3	3:C:241:ARG:HA	1.84	0.59
2:B:54:LYS:HB3	2:B:98:PHE:HE1	1.68	0.58
2:B:217:LEU:HD13	2:B:300:VAL:HG22	1.85	0.58
1:A:56:GLN:HG3	1:A:58:ARG:HH11	1.68	0.57
3:C:267:LYS:O	3:C:326:VAL:HG12	2.08	0.54
2:B:23:THR:HG23	2:B:39:LYS:H	1.71	0.53
1:A:11:VAL:HG13	1:A:154:GLN:HB3	1.91	0.53
3:C:165:LEU:HB3	3:C:211:VAL:HG21	1.91	0.53
2:B:299:THR:HG22	2:B:308:THR:HG23	1.92	0.52
3:C:286:VAL:O	3:C:339:VAL:HA	2.10	0.52
3:C:201:GLU:HG2	3:C:206:ILE:HG23	1.91	0.51
2:B:155:TYR:HB2	2:B:184:SER:HB2	1.91	0.51
1:A:28:PRO:HB3	1:A:83:PHE:HE2	1.75	0.51
3:C:263:VAL:O	3:C:354:GLU:HA	2.10	0.51
2:B:139:THR:HA	2:B:170:THR:HG22	1.94	0.50
2:B:77:ALA:HB3	2:B:84:GLU:HB2	1.93	0.49
1:A:44:ARG:NH2	12:A:202:HOH:O	2.45	0.48
1:A:2:PHE:HB2	1:A:92:ILE:HB	1.95	0.48
3:C:159:ALA:HB3	3:C:176:PRO:HA	1.97	0.47
3:C:220:VAL:HG22	3:C:237:VAL:HG22	1.96	0.46
2:B:251:PHE:HB3	2:B:296:TYR:HD1	1.80	0.46
3:C:121:SER:HB3	3:C:147:VAL:HG12	1.97	0.46
1:A:145:GLY:HA2	3:C:214:TYR:CE2	2.52	0.44
2:B:218:LEU:HD12	3:C:254:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LYS:HB3	1:A:119:SER:HA	1.98	0.44
1:A:53:LYS:HE2	2:B:248:TYR:HB2	1.98	0.44
1:A:126:ALA:HB2	1:A:149:ILE:HG22	2.00	0.43
1:A:5:LEU:HD13	1:A:53:LYS:HG3	2.01	0.43
2:B:246:VAL:HG13	2:B:301:ALA:HB3	2.01	0.42
3:C:226:SER:HA	3:C:231:SER:HA	2.02	0.42
1:A:12:ILE:HD11	1:A:49:ILE:HD11	2.01	0.42
1:A:56:GLN:HG3	1:A:58:ARG:NH1	2.34	0.41
2:B:312:ILE:HG22	2:B:314:VAL:HG23	2.03	0.41
3:C:265:LEU:HA	3:C:326:VAL:HG13	2.02	0.41
2:B:164:GLU:CD	2:B:166:ASN:HD22	2.23	0.41
2:B:68:LEU:HD13	2:B:68:LEU:HA	1.92	0.40
3:C:263:VAL:CG1	3:C:326:VAL:HG11	2.52	0.40
1:A:116:GLU:HB2	1:A:124:PHE:CE2	2.57	0.40
3:C:328:GLN:HA	3:C:331:LEU:HD22	2.03	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	155/157 (99%)	142 (92%)	12 (8%)	1 (1%)	30	68
2	B	300/312 (96%)	278 (93%)	18 (6%)	4 (1%)	15	50
3	C	264/344 (77%)	237 (90%)	25 (10%)	2 (1%)	24	63
All	All	719/813 (88%)	657 (91%)	55 (8%)	7 (1%)	19	58

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	116	PRO
2	B	72	SER

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Mol	Chain	Res	Type
2	B	80	ASP
2	B	166	ASN
2	B	209	ASP
1	A	60	MET
3	C	109	CYS

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	145/148 (98%)	124 (86%)	21 (14%)	4 16
2	B	263/288 (91%)	227 (86%)	36 (14%)	4 19
3	C	212/321 (66%)	181 (85%)	31 (15%)	4 16
All	All	620/757 (82%)	532 (86%)	88 (14%)	4 18

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	11	VAL
1	A	13	ARG
1	A	20	LEU
1	A	22	ILE
1	A	26	ASN
1	A	27	ARG
1	A	29	LEU
1	A	51	MET
1	A	58	ARG
1	A	62	VAL
1	A	66	VAL
1	A	72	SER
1	A	85	GLU
1	A	95	THR
1	A	106	VAL
1	A	121	GLU

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Mol	Chain	Res	Type
1	A	131	ARG
1	A	136	LEU
1	A	139	LYS
1	A	141	GLU
2	B	23	THR
2	B	25	ARG
2	B	32	GLU
2	B	45	LEU
2	B	52	THR
2	B	59	SER
2	B	65	HIS
2	B	68	LEU
2	B	88	VAL
2	B	99	GLN
2	B	132	VAL
2	B	147	THR
2	B	154	LEU
2	B	163	LEU
2	B	164	GLU
2	B	168	ASN
2	B	189	LEU
2	B	195	LEU
2	B	198	ILE
2	B	199	THR
2	B	205	THR
2	B	210	ARG
2	B	217	LEU
2	B	218	LEU
2	B	222	LEU
2	B	228	GLU
2	B	229	LEU
2	B	241	LEU
2	B	255	ASN
2	B	270	MET
2	B	282	LEU
2	B	292	LEU
2	B	299	THR
2	B	300	VAL
2	B	313	LEU
2	B	316	LYS
3	C	37	ARG
3	C	47	ASP

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Mol	Chain	Res	Type
3	C	109	CYS
3	C	165	LEU
3	C	166	LEU
3	C	167	LEU
3	C	181	GLN
3	C	185	GLN
3	C	203	SER
3	C	208	VAL
3	C	211	VAL
3	C	240	VAL
3	C	241	ARG
3	C	254	LEU
3	C	257	VAL
3	C	258	GLU
3	C	261	LEU
3	C	269	LEU
3	C	270	THR
3	C	296	LEU
3	C	312	LEU
3	C	319	ARG
3	C	329	ARG
3	C	331	LEU
3	C	336	VAL
3	C	339	VAL
3	C	340	GLN
3	C	350	VAL
3	C	352	LEU
3	C	355	LYS
3	C	356	ARG

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	111	ASN
1	A	114	GLN
2	B	192	ASN
2	B	212	ASN
3	C	340	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

23 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	0.28	0	15,19,21	0.56	0
5	NAG	B	904	5	14,14,15	0.27	0	15,19,21	0.56	0
6	NAG	B	905	2,6	14,14,15	0.26	0	15,19,21	0.63	1 (6%)
6	NAG	B	906	6	14,14,15	0.33	0	15,19,21	1.59	3 (20%)
7	NAG	B	907	2,7	14,14,15	0.28	0	15,19,21	0.72	1 (6%)
7	NAG	B	908	7	14,14,15	0.35	0	15,19,21	1.67	3 (20%)
8	NAG	B	909	8,2	14,14,15	0.29	0	15,19,21	0.73	0
8	NAG	B	910	8	14,14,15	0.31	0	15,19,21	0.34	0
9	NAG	B	911	9,2	14,14,15	0.28	0	15,19,21	0.69	0
9	NAG	B	912	9	14,14,15	0.30	0	15,19,21	0.39	0
6	BMA	B	951	6	11,11,12	0.32	0	14,15,17	0.97	1 (7%)
6	MAN	B	952	6	11,11,12	0.38	0	14,15,17	1.11	1 (7%)
6	MAN	B	953	6	11,11,12	0.50	0	14,15,17	1.69	2 (14%)
7	BMA	B	955	7	11,11,12	0.36	0	14,15,17	0.91	1 (7%)
9	BMA	B	958	9	11,11,12	0.34	0	14,15,17	0.67	0
5	FUC	B	998	5	10,10,11	0.43	0	14,14,16	1.22	1 (7%)
9	FUC	B	999	9	10,10,11	0.56	0	14,14,16	1.37	2 (14%)
10	NAG	C	902	10,3	14,14,15	0.30	0	15,19,21	0.65	1 (6%)
10	NAG	C	903	10	14,14,15	0.30	0	15,19,21	0.61	0
8	NAG	C	904	8,3	14,14,15	0.29	0	15,19,21	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	C	905	8	14,14,15	0.27	0	15,19,21	0.51	0
10	BMA	C	951	10	11,11,12	0.30	0	14,15,17	0.55	0
10	MAN	C	952	10	11,11,12	0.40	0	14,15,17	0.90	2 (14%)

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
9	NAG	B	911	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	912	9	-	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
7	BMA	B	955	7	-	0/2/19/22	0/1/1/1
9	BMA	B	958	9	-	0/2/19/22	0/1/1/1
5	FUC	B	998	5	-	0/0/17/20	0/1/1/1
9	FUC	B	999	9	-	0/0/17/20	0/1/1/1
10	NAG	C	902	10,3	-	0/6/23/26	0/1/1/1
10	NAG	C	903	10	-	0/6/23/26	0/1/1/1
8	NAG	C	904	8,3	-	0/6/23/26	0/1/1/1
8	NAG	C	905	8	-	0/6/23/26	0/1/1/1
10	BMA	C	951	10	-	0/2/19/22	0/1/1/1
10	MAN	C	952	10	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	907	NAG	C1-O5-C5	2.03	114.83	112.25
10	C	952	MAN	C1-C2-C3	2.14	112.08	109.54
6	B	905	NAG	C1-O5-C5	2.20	115.04	112.25
7	B	908	NAG	O4-C4-C3	2.21	115.31	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	902	NAG	C1-O5-C5	2.23	115.07	112.25
10	C	952	MAN	C1-O5-C5	2.28	115.14	112.25
6	B	906	NAG	O4-C4-C5	2.40	115.60	109.24
6	B	951	BMA	C1-O5-C5	2.75	115.74	112.25
6	B	906	NAG	O4-C4-C3	2.82	116.68	110.34
9	B	999	FUC	C1-C2-C3	2.86	112.92	109.54
7	B	955	BMA	C1-O5-C5	2.91	115.94	112.25
6	B	953	MAN	C1-C2-C3	3.01	113.11	109.54
7	B	908	NAG	O4-C4-C5	3.03	117.28	109.24
6	B	952	MAN	C1-O5-C5	3.70	116.94	112.25
9	B	999	FUC	C1-O5-C5	3.91	118.42	112.38
5	B	998	FUC	C1-O5-C5	3.94	118.47	112.38
6	B	906	NAG	C1-O5-C5	4.74	118.27	112.25
7	B	908	NAG	C1-O5-C5	4.96	118.54	112.25
6	B	953	MAN	C1-O5-C5	5.14	118.78	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	901	2	14,14,15	0.27	0	15,19,21	0.63	1 (6%)
4	NAG	B	902	2	14,14,15	0.30	0	15,19,21	0.64	1 (6%)
4	NAG	C	901	3	14,14,15	0.28	0	15,19,21	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	901	2	-	0/6/23/26	0/1/1/1
4	NAG	B	902	2	-	0/6/23/26	0/1/1/1
4	NAG	C	901	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	902	NAG	C1-O5-C5	2.14	114.96	112.25
4	B	901	NAG	C1-O5-C5	2.17	115.01	112.25

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	157/157 (100%)	-0.32	0 100 100	30, 48, 80, 109	0
2	B	301/312 (96%)	0.03	2 (0%) 89 78	36, 74, 118, 151	0
3	C	270/344 (78%)	0.28	19 (7%) 19 7	38, 80, 145, 164	0
All	All	728/813 (89%)	0.05	21 (2%) 55 31	30, 68, 136, 164	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	72	SER	4.9
3	C	120	ASN	4.7
2	B	68	LEU	3.9
3	C	45	PHE	3.5
3	C	109	CYS	3.4
3	C	227	ASP	2.9
3	C	47	ASP	2.8
3	C	48	LEU	2.7
3	C	123	SER	2.6
3	C	46	CYS	2.5
3	C	192	TYR	2.5
3	C	155	CYS	2.4
3	C	49	PRO	2.4
3	C	116	PRO	2.4
3	C	42	PHE	2.3
3	C	147	VAL	2.3
3	C	110	THR	2.3
3	C	33	THR	2.2
3	C	143	MET	2.2
3	C	106	GLN	2.1
3	C	126	CYS	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	B	910	14/15	0.74	0.45	3.74	118,126,130,131	0
10	NAG	C	902	14/15	0.73	0.33	2.60	162,167,170,171	0
7	NAG	B	907	14/15	0.91	0.17	-0.40	97,101,107,116	0
8	NAG	C	904	14/15	0.90	0.16	-0.68	94,98,103,109	0
6	NAG	B	905	14/15	0.94	0.20	-0.84	113,120,126,129	0
9	NAG	B	911	14/15	0.93	0.16	-0.94	82,88,93,101	0
8	NAG	B	909	14/15	0.92	0.17	-1.26	107,112,115,118	0
9	BMA	B	958	11/12	0.75	0.36	-	132,138,143,144	0
6	MAN	B	952	11/12	0.79	0.25	-	175,179,184,185	0
5	FUC	B	998	10/11	0.91	0.25	-	140,141,144,145	0
5	NAG	B	904	14/15	0.84	0.29	-	150,155,162,162	0
10	BMA	C	951	11/12	0.65	0.29	-	174,177,182,183	0
10	NAG	C	903	14/15	0.73	0.42	-	162,171,174,175	0
9	FUC	B	999	10/11	0.88	0.25	-	90,93,95,95	0
7	BMA	B	955	11/12	0.76	0.24	-	143,146,148,149	0
6	NAG	B	906	14/15	0.92	0.21	-	132,139,148,153	0
6	MAN	B	953	11/12	0.59	0.24	-	171,175,182,184	0
8	NAG	C	905	14/15	0.85	0.23	-	114,116,119,121	0
6	BMA	B	951	11/12	0.69	0.20	-	158,168,174,179	0
5	NAG	B	903	14/15	0.83	0.23	-	129,136,143,147	0
9	NAG	B	912	14/15	0.90	0.24	-	106,112,120,125	0
10	MAN	C	952	11/12	0.58	0.45	-	180,184,187,188	0
7	NAG	B	908	14/15	0.86	0.28	-	118,129,138,142	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
11	CL	C	908	1/1	0.98	0.28	2.68	55,55,55,55	0
4	NAG	B	901	14/15	0.73	0.56	-	146,149,153,156	0
4	NAG	B	902	14/15	0.84	0.36	-	124,132,140,143	0
4	NAG	C	901	14/15	0.70	0.55	-	180,182,186,188	0

6.5 Other polymers (i)

There are no such residues in this entry.