



wwPDB X-ray Structure Validation Summary Report

Feb 1, 2016 – 03:51 PM GMT

PDB ID : 4DKF
Title : Crystal Structure of Human Interleukin-34 Bound to FAb2
Authors : Ma, X.; Chen, Y.; Stawicki, S.; Wu, Y.; Bazan, J.F.; Starovasnik, M.A.
Deposited on : 2012-02-03
Resolution : 2.61 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the  symbol.

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

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

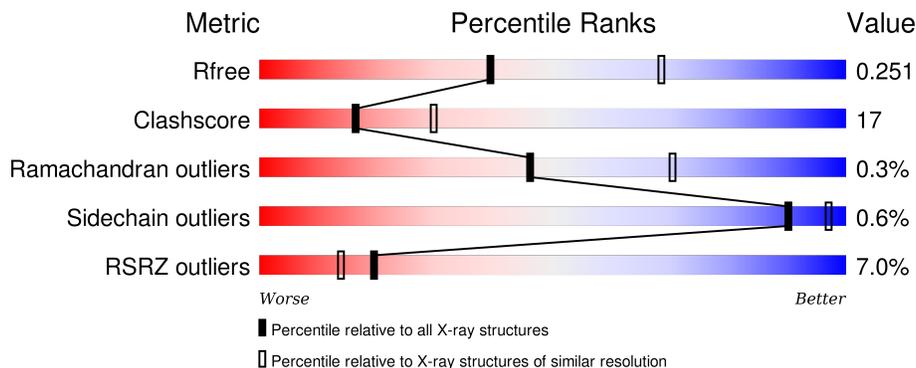
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	190	
1	B	190	
2	H	226	
2	I	226	
3	L	214	

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Mol	Chain	Length	Quality of chain
3	M	214	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '14%', a green segment in the middle labeled '66%', and a yellow segment on the right labeled '30%'. A small grey dot is visible at the far right end of the bar.</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8977 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-34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	161	1311	837	224	242	8	0	0	0
1	B	137	1118	722	192	197	7	0	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ALA	-	EXPRESSION TAG	UNP Q6ZMJ4
A	19	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
A	20	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
A	194	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
A	195	ASN	-	EXPRESSION TAG	UNP Q6ZMJ4
A	196	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
A	197	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
A	198	ASN	-	EXPRESSION TAG	UNP Q6ZMJ4
A	199	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
A	200	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	201	TYR	-	EXPRESSION TAG	UNP Q6ZMJ4
A	202	LYS	-	EXPRESSION TAG	UNP Q6ZMJ4
A	203	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	204	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	205	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	206	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	207	LYS	-	EXPRESSION TAG	UNP Q6ZMJ4
B	18	ALA	-	EXPRESSION TAG	UNP Q6ZMJ4
B	19	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
B	20	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
B	194	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
B	195	ASN	-	EXPRESSION TAG	UNP Q6ZMJ4
B	196	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
B	197	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
B	198	ASN	-	EXPRESSION TAG	UNP Q6ZMJ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	199	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
B	200	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	201	TYR	-	EXPRESSION TAG	UNP Q6ZMJ4
B	202	LYS	-	EXPRESSION TAG	UNP Q6ZMJ4
B	203	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	204	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	205	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	206	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	207	LYS	-	EXPRESSION TAG	UNP Q6ZMJ4

- Molecule 2 is a protein called FAb2 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1577	994	262	315	6			
2	I	206	Total	C	N	O	S	0	0	0
			1515	954	254	301	6			

- Molecule 3 is a protein called FAb2 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1625	1017	273	330	5			
3	M	207	Total	C	N	O	S	0	0	0
			1583	990	264	324	5			

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	14	Total	O	0	0
			14	14		

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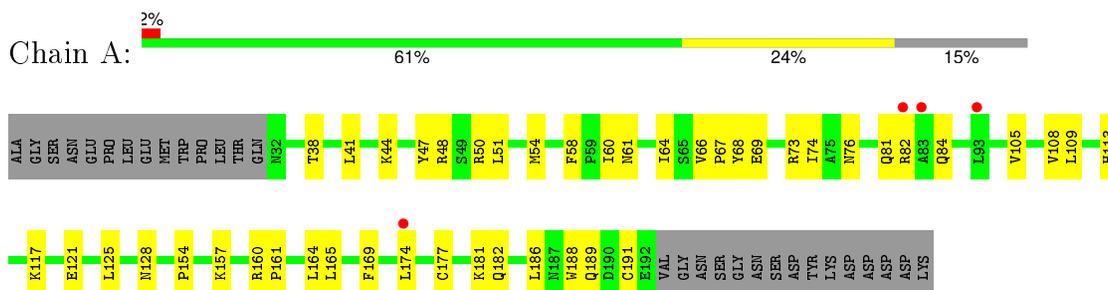
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	22	Total 22	O 22	0	0
5	L	42	Total 42	O 42	0	0
5	I	21	Total 21	O 21	0	0
5	M	20	Total 20	O 20	0	0

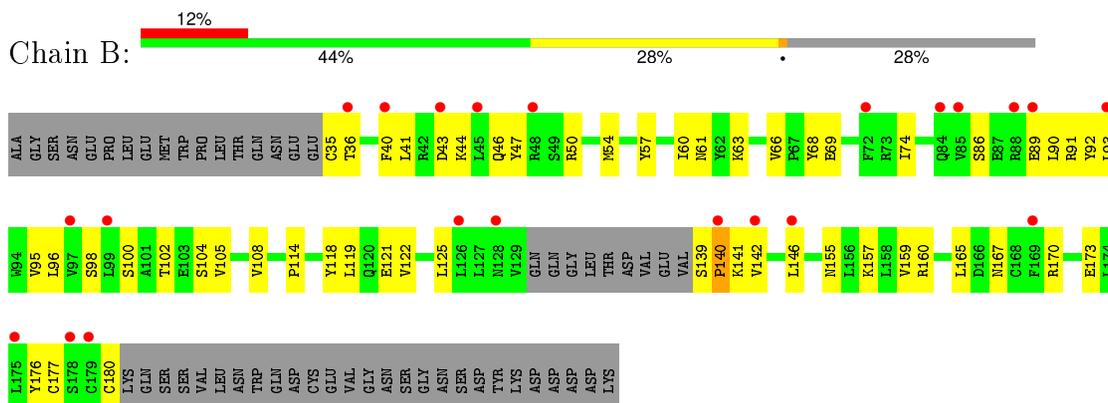
3 Residue-property plots [i](#)

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-34



- Molecule 1: Interleukin-34

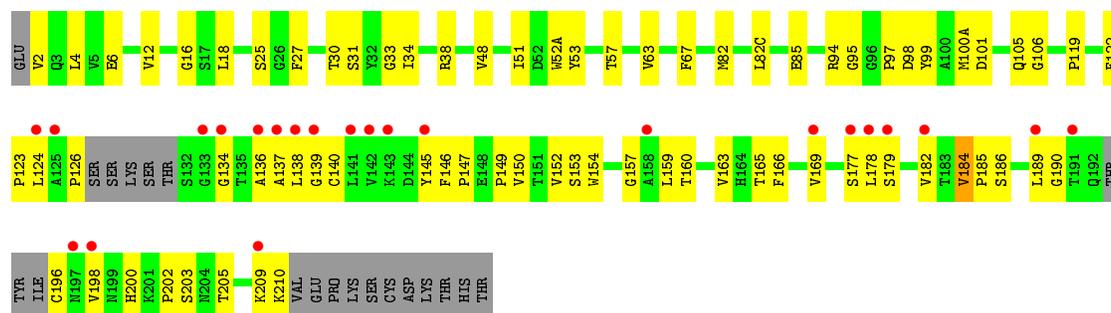


- Molecule 2: FAb2 Heavy Chain



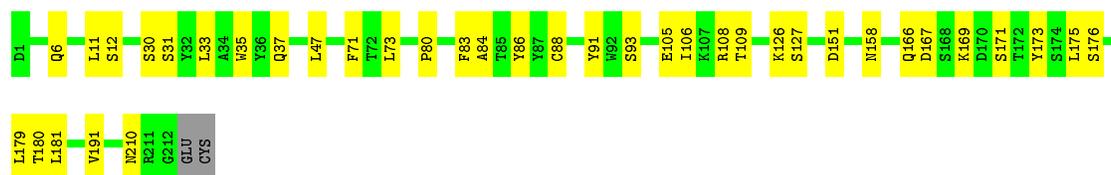
- Molecule 2: FAb2 Heavy Chain





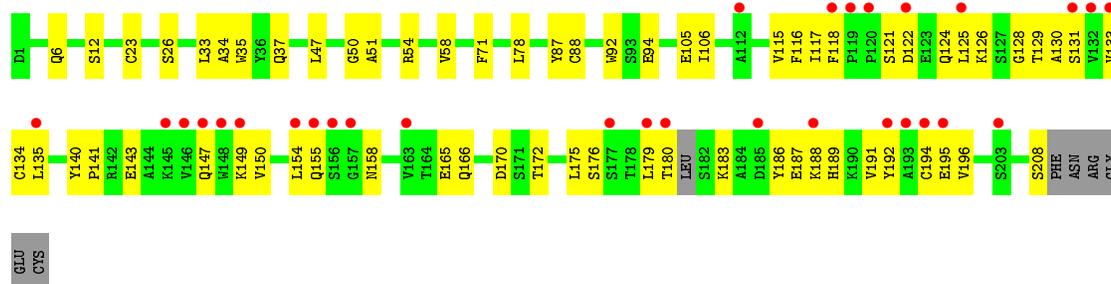
- Molecule 3: Fab2 Light Chain

Chain L: 81% 18%



- Molecule 3: Fab2 Light Chain

Chain M: 14% 66% 30%



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.92Å 181.82Å 79.25Å 90.00° 118.27° 90.00°	Depositor
Resolution (Å)	50.00 – 2.61 47.70 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.61) 98.5 (47.70-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.225 , 0.256 0.223 , 0.251	Depositor DCC
R_{free} test set	2212 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.2	EDS
Estimated twinning fraction	0.014 for 1/2*h+1/2*k+1,3/2*h-1/2*k+1,-1 0.011 for 1/2*h-1/2*k+1,-3/2*h-1/2*k-1,-1	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 44007 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8977	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.35	0/1337	0.45	0/1815
1	B	0.30	0/1141	0.43	0/1547
2	H	0.40	0/1616	0.55	0/2205
2	I	0.33	0/1551	0.49	0/2113
3	L	0.44	0/1661	0.54	0/2255
3	M	0.34	0/1617	0.48	0/2195
All	All	0.37	0/8923	0.50	0/12130

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 [i](#)

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	1311	0	1320	43	1
1	B	1118	0	1148	49	0
2	H	1577	0	1519	37	0
2	I	1515	0	1459	75	0
3	L	1625	0	1579	35	0
3	M	1583	0	1536	70	0
4	A	61	0	52	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	61	0	52	6	0
5	A	7	0	0	0	0
5	B	14	0	0	0	0
5	H	22	0	0	3	0
5	I	21	0	0	3	0
5	L	42	0	0	3	0
5	M	20	0	0	1	1
All	All	8977	0	8665	292	2

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 17.

The worst 5 of 292 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:I:85:GLU:HB2	5:I:314:HOH:O	1.52	1.08
2:H:12:VAL:HG21	2:H:18:LEU:HD22	1.34	1.06
1:A:54:MET:HG3	1:A:165:LEU:HD12	1.33	1.04
1:B:170:ARG:NH1	2:I:52(A):TRP:CH2	2.33	0.97
1:B:118:TYR:O	1:B:122:VAL:HG23	1.67	0.95

All (2) 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)
5:M:303:HOH:O	5:M:319:HOH:O[2_555]	1.98	0.22
1:A:48:ARG:NH1	1:A:48:ARG:NH1[2_656]	1.99	0.21

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	159/190 (84%)	150 (94%)	9 (6%)	0	100	100
1	B	133/190 (70%)	126 (95%)	6 (4%)	1 (1%)	24	44
2	H	210/226 (93%)	201 (96%)	8 (4%)	1 (0%)	34	58
2	I	200/226 (88%)	187 (94%)	12 (6%)	1 (0%)	34	58
3	L	210/214 (98%)	203 (97%)	7 (3%)	0	100	100
3	M	203/214 (95%)	186 (92%)	17 (8%)	0	100	100
All	All	1115/1260 (88%)	1053 (94%)	59 (5%)	3 (0%)	46	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	62	SER
1	B	140	PRO
2	I	149	PRO

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	151/176 (86%)	151 (100%)	0	100	100
1	B	128/176 (73%)	128 (100%)	0	100	100
2	H	174/186 (94%)	172 (99%)	2 (1%)	80	92
2	I	166/186 (89%)	163 (98%)	3 (2%)	66	86
3	L	185/187 (99%)	185 (100%)	0	100	100
3	M	181/187 (97%)	180 (99%)	1 (1%)	90	97
All	All	985/1098 (90%)	979 (99%)	6 (1%)	90	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	31	SER
3	M	143	GLU

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Mol	Chain	Res	Type
2	I	165	THR
2	H	186	SER
2	I	184	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	61	ASN
2	I	155	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

10 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	$\# Z > 2$
4	NAG	A	301	1,4	14,14,15	0.64	0	15,19,21	0.95	1 (6%)
4	NAG	A	302	4	14,14,15	0.53	0	15,19,21	0.86	0
4	MAN	A	303	4	11,11,12	0.52	0	14,15,17	3.12	5 (35%)
4	BMA	A	304	4	11,11,12	0.77	0	14,15,17	0.97	1 (7%)
4	MAN	A	305	4	11,11,12	0.54	0	14,15,17	1.13	2 (14%)
4	NAG	B	301	1,4	14,14,15	0.47	0	15,19,21	0.63	0
4	NAG	B	302	4	14,14,15	0.50	0	15,19,21	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	B	303	4	11,11,12	0.68	0	14,15,17	1.75	2 (14%)
4	BMA	B	304	4	11,11,12	0.54	0	14,15,17	0.75	0
4	MAN	B	305	4	11,11,12	0.57	0	14,15,17	1.20	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
4	NAG	A	301	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	302	4	-	0/6/23/26	0/1/1/1
4	MAN	A	303	4	-	0/2/19/22	0/1/1/1
4	BMA	A	304	4	-	0/2/19/22	0/1/1/1
4	MAN	A	305	4	-	0/2/19/22	1/1/1/1
4	NAG	B	301	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	302	4	-	0/6/23/26	0/1/1/1
4	MAN	B	303	4	-	0/2/19/22	0/1/1/1
4	BMA	B	304	4	-	0/2/19/22	1/1/1/1
4	MAN	B	305	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	MAN	C3-C4-C5	-7.22	97.62	110.20
4	A	303	MAN	C2-C3-C4	-3.16	105.67	111.04
4	B	303	MAN	C3-C4-C5	-2.93	105.09	110.20
4	A	301	NAG	C1-O5-C5	-2.20	109.46	112.25
4	A	305	MAN	C1-C2-C3	2.25	112.20	109.54

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	305	MAN	C1-C2-C3-C4-C5-O5
4	B	304	BMA	C1-C2-C3-C4-C5-O5

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	NAG	1	0
4	A	302	NAG	2	0
4	A	303	MAN	4	0
4	A	305	MAN	1	0
4	B	301	NAG	1	0
4	B	302	NAG	3	0
4	B	303	MAN	2	0
4	B	304	BMA	1	0
4	B	305	MAN	1	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	161/190 (84%)	0.16	4 (2%) 61 55	44, 62, 87, 91	0
1	B	137/190 (72%)	0.89	22 (16%) 3 1	58, 83, 104, 106	0
2	H	214/226 (94%)	0.04	1 (0%) 91 90	35, 55, 65, 70	0
2	I	206/226 (91%)	0.56	23 (11%) 7 4	45, 64, 105, 111	0
3	L	212/214 (99%)	0.03	0 100 100	26, 40, 57, 61	0
3	M	207/214 (96%)	0.67	30 (14%) 3 2	38, 59, 118, 125	0
All	All	1137/1260 (90%)	0.37	80 (7%) 19 14	26, 58, 106, 125	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	138	LEU	6.0
2	I	197	ASN	5.3
1	B	126	LEU	4.8
3	M	145	LYS	4.7
1	B	40	PHE	4.4

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	301	14/15	0.93	0.15	-0.69	65,71,75,76	0
4	NAG	B	301	14/15	0.94	0.14	-1.64	82,87,90,91	0
4	BMA	A	304	11/12	0.79	0.21	-	88,99,103,105	0
4	MAN	A	303	11/12	0.85	0.15	-	80,85,88,89	0
4	NAG	B	302	14/15	0.92	0.21	-	84,89,91,94	0
4	MAN	B	305	11/12	0.85	0.16	-	91,97,104,106	0
4	MAN	B	303	11/12	0.69	0.18	-	92,97,102,104	0
4	BMA	B	304	11/12	0.72	0.22	-	101,107,112,113	0
4	MAN	A	305	11/12	0.82	0.14	-	76,84,88,92	0
4	NAG	A	302	14/15	0.94	0.14	-	68,76,81,84	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.