



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2023 – 06:45 AM EDT

PDB ID : 7MYZ
Title : Structure of the full length 5-TM receptor CD47 bound to Fab B6H12
Authors : Fenalti, G.; Villanueva, N.
Deposited on : 2021-05-22
Resolution : 3.40 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

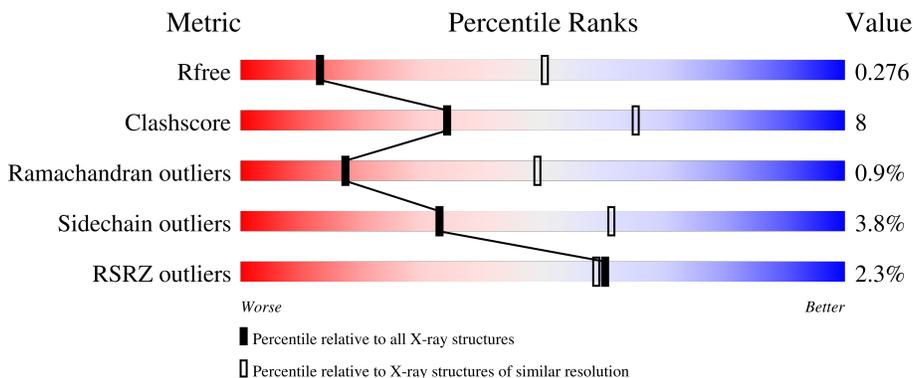
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	C	421	
1	D	421	
2	H	220	
2	I	220	
3	L	213	

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Mol	Chain	Length	Quality of chain
3	M	213	 80% 19%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 9181 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 Fusion protein of Leukocyte surface antigen CD47 an Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	263	1911	1258	299	345	9	0	0	0
1	D	117	872	556	136	175	5	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	147L	TRP	MET	conflict	UNP P0ABE7
C	151C	ILE	HIS	conflict	UNP P0ABE7
C	151G	LEU	-	linker	UNP P0ABE7
C	306	HIS	-	expression tag	UNP Q08722
C	307	HIS	-	expression tag	UNP Q08722
C	308	HIS	-	expression tag	UNP Q08722
C	309	HIS	-	expression tag	UNP Q08722
C	310	HIS	-	expression tag	UNP Q08722
C	311	HIS	-	expression tag	UNP Q08722
C	312	HIS	-	expression tag	UNP Q08722
C	313	HIS	-	expression tag	UNP Q08722
C	314	HIS	-	expression tag	UNP Q08722
C	315	HIS	-	expression tag	UNP Q08722
D	159	TRP	MET	conflict	UNP P0ABE7
D	254	ILE	HIS	conflict	UNP P0ABE7
D	258	LEU	-	linker	UNP P0ABE7
D	412	HIS	-	expression tag	UNP Q08722
D	413	HIS	-	expression tag	UNP Q08722
D	414	HIS	-	expression tag	UNP Q08722
D	415	HIS	-	expression tag	UNP Q08722
D	416	HIS	-	expression tag	UNP Q08722
D	417	HIS	-	expression tag	UNP Q08722
D	418	HIS	-	expression tag	UNP Q08722
D	419	HIS	-	expression tag	UNP Q08722

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Chain	Residue	Modelled	Actual	Comment	Reference
D	420	HIS	-	expression tag	UNP Q08722
D	421	HIS	-	expression tag	UNP Q08722

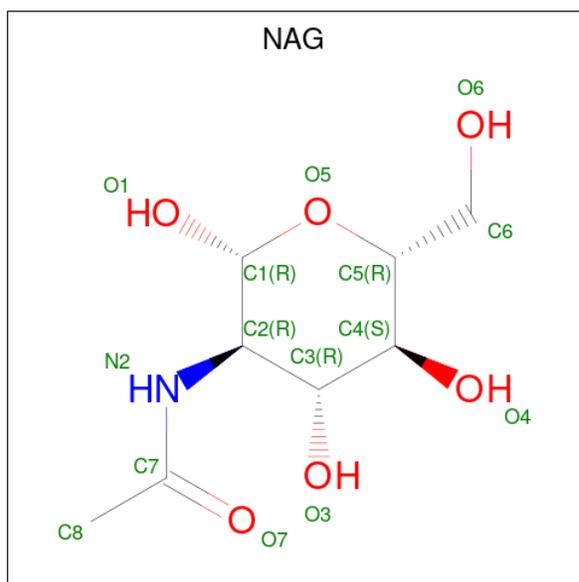
- Molecule 2 is a protein called B6H12 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	214	Total 1551	C 988	N 253	O 304	S 6	0	0	0
2	I	214	Total 1554	C 992	N 254	O 302	S 6	0	0	0

- Molecule 3 is a protein called B6H12 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	213	Total 1591	C 1000	N 269	O 317	S 5	0	1	0
3	M	213	Total 1595	C 1001	N 274	O 315	S 5	0	1	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



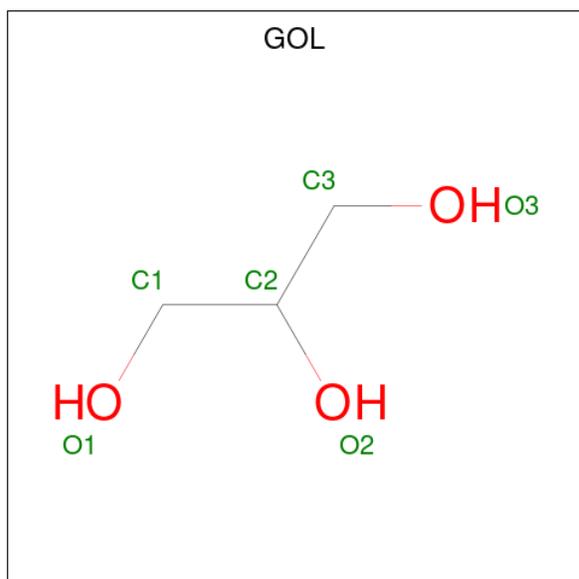
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	C	1	Total 14	C 8	N 1	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



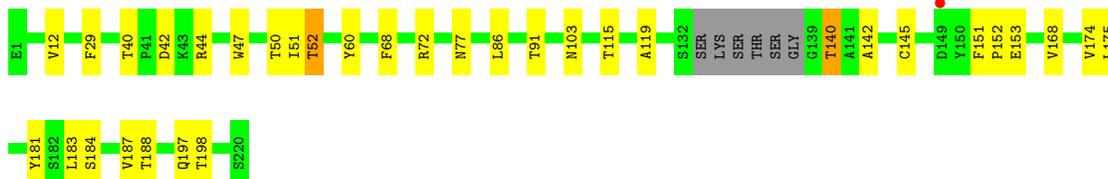
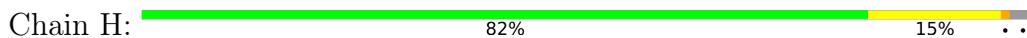
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

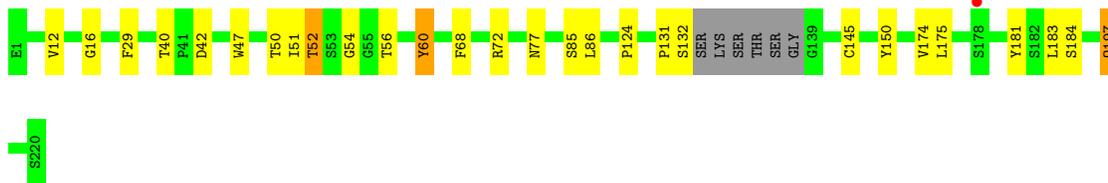
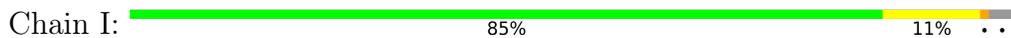
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	2	Total	O	0	0
			2	2		
6	L	1	Total	O	0	0
			1	1		

LEU ALA GLN LEU LEU LEU VAL TYR MET LYS PHE VAL ALA SER ASN GLN LYS THR ILE GLN PRO PRO ARG LYS ALA VAL VAL GLU PRO LEU ASN ALA PHE LYS LYS SER LYS GLY MET MET MET ASN ASP GLU HIS HIS HIS HIS HIS HIS HIS

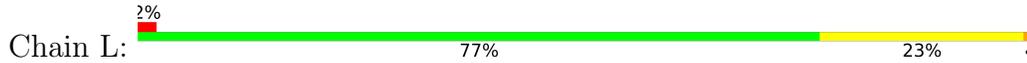
• Molecule 2: B6H12 Fab heavy chain



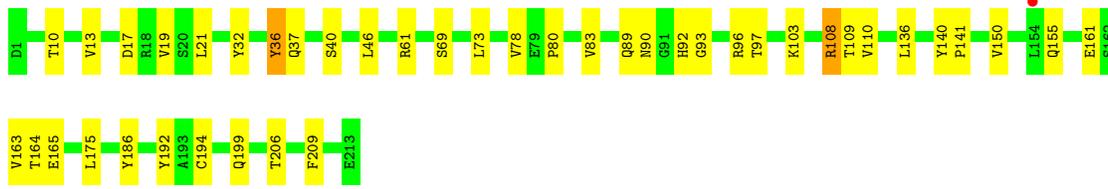
• Molecule 2: B6H12 Fab heavy chain



• Molecule 3: B6H12 Fab light chain



• Molecule 3: B6H12 Fab light chain



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	141.53Å 53.73Å 181.70Å 90.00° 92.88° 90.00°	Depositor
Resolution (Å)	48.68 – 3.40 48.63 – 3.40	Depositor EDS
% Data completeness (in resolution range)	91.6 (48.68-3.40) 91.7 (48.63-3.40)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.253 , 0.277 0.253 , 0.276	Depositor DCC
R_{free} test set	1781 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	79.0	Xtrriage
Anisotropy	0.110	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.074 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9181	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.49% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.70	0/1945	0.80	0/2661
1	D	0.72	0/886	0.82	0/1207
2	H	0.70	0/1588	0.88	0/2174
2	I	0.71	0/1591	0.89	0/2176
3	L	0.68	0/1630	0.83	0/2220
3	M	0.68	0/1634	0.85	0/2224
All	All	0.70	0/9274	0.85	0/12662

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	C	1911	0	1865	39	0
1	D	872	0	809	17	0
2	H	1551	0	1448	21	0
2	I	1554	0	1461	20	0
3	L	1591	0	1487	33	0
3	M	1595	0	1504	29	0
4	C	56	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	42	0	39	3	0
5	L	6	0	8	3	0
6	I	2	0	0	0	0
6	L	1	0	0	1	0
All	All	9181	0	8673	149	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 8.

The worst 5 of 149 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:H:12:VAL:HG21	2:H:86:LEU:HD13	1.63	0.80
3:L:36:TYR:CE2	3:L:46:LEU:HD13	2.17	0.79
2:I:12:VAL:HG21	2:I:86:LEU:HD13	1.66	0.77
3:M:36:TYR:CE2	3:M:46:LEU:HD13	2.19	0.77
3:L:110:VAL:HG21	3:L:199:GLN:HE21	1.53	0.73

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	C	257/421 (61%)	228 (89%)	22 (9%)	7 (3%)	5 26
1	D	115/421 (27%)	110 (96%)	4 (4%)	1 (1%)	17 49
2	H	210/220 (96%)	204 (97%)	6 (3%)	0	100 100
2	I	210/220 (96%)	202 (96%)	7 (3%)	1 (0%)	29 61
3	L	212/213 (100%)	197 (93%)	13 (6%)	2 (1%)	17 49
3	M	212/213 (100%)	195 (92%)	17 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1216/1708 (71%)	1136 (93%)	69 (6%)	11 (1%)	17 49

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	118	TRP
1	C	180	VAL
1	D	17	ASP
1	C	275	ALA
1	C	276	SER

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	C	191/359 (53%)	183 (96%)	8 (4%)	30 59
1	D	90/359 (25%)	86 (96%)	4 (4%)	28 58
2	H	158/185 (85%)	152 (96%)	6 (4%)	33 61
2	I	158/185 (85%)	152 (96%)	6 (4%)	33 61
3	L	170/188 (90%)	163 (96%)	7 (4%)	30 59
3	M	172/188 (92%)	167 (97%)	5 (3%)	42 69
All	All	939/1464 (64%)	903 (96%)	36 (4%)	33 61

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	69	SER
3	M	108	ARG
3	L	125	LEU
3	M	37	GLN
2	H	52	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	138	ASN
3	L	152	ASN
3	M	199	GLN
3	M	90	ASN
3	M	138	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](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
5	GOL	L	301	-	5,5,5	0.15	0	5,5,5	0.40	0
4	NAG	C	403	1	14,14,15	0.79	0	17,19,21	2.05	5 (29%)
4	NAG	C	401	1	14,14,15	0.51	0	17,19,21	1.96	6 (35%)
4	NAG	D	502	1	14,14,15	0.59	0	17,19,21	2.25	8 (47%)
4	NAG	D	503	1	14,14,15	0.69	0	17,19,21	1.87	4 (23%)
4	NAG	C	402	1	14,14,15	0.91	1 (7%)	17,19,21	1.89	3 (17%)
4	NAG	D	501	1	14,14,15	0.62	0	17,19,21	2.41	5 (29%)
4	NAG	C	404	1	14,14,15	0.69	0	17,19,21	1.42	1 (5%)

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	GOL	L	301	-	-	2/4/4/4	-
4	NAG	C	403	1	-	2/6/23/26	0/1/1/1
4	NAG	C	401	1	-	2/6/23/26	0/1/1/1
4	NAG	D	502	1	-	5/6/23/26	0/1/1/1
4	NAG	D	503	1	-	2/6/23/26	0/1/1/1
4	NAG	C	402	1	-	2/6/23/26	0/1/1/1
4	NAG	D	501	1	-	4/6/23/26	0/1/1/1
4	NAG	C	404	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	NAG	C1-C2	2.86	1.56	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	NAG	C1-O5-C5	7.94	122.95	112.19
4	D	502	NAG	C2-N2-C7	5.18	130.28	122.90
4	D	503	NAG	C1-O5-C5	4.47	118.25	112.19
4	C	402	NAG	O5-C1-C2	4.38	118.20	111.29
4	C	403	NAG	C4-C3-C2	-4.19	104.87	111.02

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	401	NAG	C3-C2-N2-C7
4	D	501	NAG	C3-C2-N2-C7
4	D	502	NAG	O5-C5-C6-O6
4	C	402	NAG	O5-C5-C6-O6
4	D	501	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	301	GOL	3	0
4	C	401	NAG	1	0
4	D	502	NAG	1	0
4	D	503	NAG	1	0
4	D	501	NAG	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 [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	C	263/421 (62%)	0.17	13 (4%) 29 29	56, 133, 196, 217	0
1	D	117/421 (27%)	0.51	7 (5%) 21 23	61, 104, 160, 177	0
2	H	214/220 (97%)	-0.23	1 (0%) 91 90	37, 61, 93, 118	0
2	I	214/220 (97%)	-0.08	1 (0%) 91 90	33, 67, 98, 127	0
3	L	213/213 (100%)	0.07	5 (2%) 60 59	42, 74, 111, 134	0
3	M	213/213 (100%)	-0.07	1 (0%) 91 90	44, 75, 110, 128	0
All	All	1234/1708 (72%)	0.03	28 (2%) 60 59	33, 77, 168, 217	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	VAL	3.5
1	C	10	VAL	3.2
1	C	113	TYR	3.1
3	L	194	CYS	3.1
1	C	162	LEU	3.0

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](#)

There are no monosaccharides in this entry.

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. 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	B-factors(Å ²)	Q<0.9
5	GOL	L	301	6/6	0.75	0.26	79,93,99,99	0
4	NAG	D	502	14/15	0.80	0.21	112,133,147,150	0
4	NAG	C	404	14/15	0.81	0.49	118,137,142,148	0
4	NAG	D	501	14/15	0.86	0.24	126,140,143,145	0
4	NAG	C	402	14/15	0.88	0.25	78,120,129,137	0
4	NAG	C	401	14/15	0.90	0.18	96,109,118,120	0
4	NAG	D	503	14/15	0.90	0.17	84,96,107,107	0
4	NAG	C	403	14/15	0.90	0.18	79,82,107,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.