



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:43 AM GMT

PDB ID : 3UBX
Title : Crystal structure of the mouse CD1d-C20:2-aGalCer-L363mAb Fab complex
Authors : Yu, E.D.; Zajonc, D.M.
Deposited on : 2011-10-25
Resolution : 3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

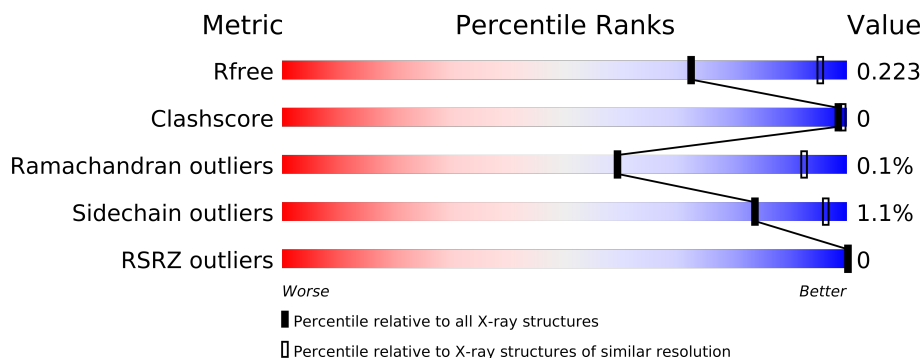
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	286	
1	D	286	
2	B	99	
2	E	99	
3	I	214	
3	L	214	
4	G	222	
4	H	222	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	09N	A	287	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	09N	D	287	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12917 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	1	0
			2233	1420	395	406	12			
1	D	276	Total	C	N	O	S	0	0	0
			2230	1419	393	406	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	HIS	-	EXPRESSION TAG	UNP P11609
A	281	HIS	-	EXPRESSION TAG	UNP P11609
A	282	HIS	-	EXPRESSION TAG	UNP P11609
A	283	HIS	-	EXPRESSION TAG	UNP P11609
A	284	HIS	-	EXPRESSION TAG	UNP P11609
A	285	HIS	-	EXPRESSION TAG	UNP P11609
A	286	HIS	-	EXPRESSION TAG	UNP P11609
D	201	HIS	ASP	SEE REMARK 999	UNP P11609
D	280	HIS	-	EXPRESSION TAG	UNP P11609
D	281	HIS	-	EXPRESSION TAG	UNP P11609
D	282	HIS	-	EXPRESSION TAG	UNP P11609
D	283	HIS	-	EXPRESSION TAG	UNP P11609
D	284	HIS	-	EXPRESSION TAG	UNP P11609
D	285	HIS	-	EXPRESSION TAG	UNP P11609
D	286	HIS	-	EXPRESSION TAG	UNP P11609

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	2	0
			832	531	142	152	7			
2	E	98	Total	C	N	O	S	0	0	0
			805	514	136	148	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	ASP	SEE REMARK 999	UNP P01887
E	85	ALA	ASP	SEE REMARK 999	UNP P01887

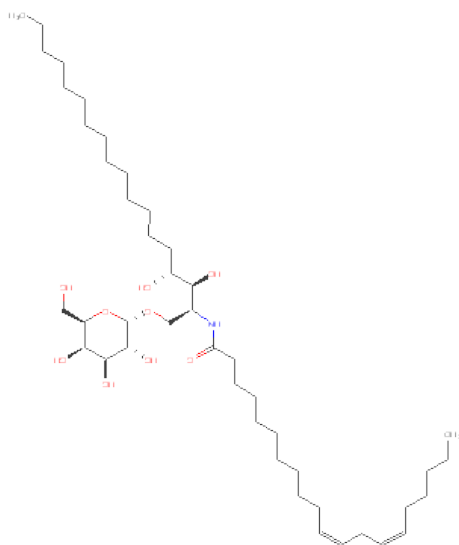
- Molecule 3 is a protein called L363 light chain (IGKV13-84*01).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1653	1027	278	341	7			
3	I	214	Total	C	N	O	S	0	0	0
			1655	1028	279	341	7			

- Molecule 4 is a protein called L363 heavy chain (IGHV9-4*02).

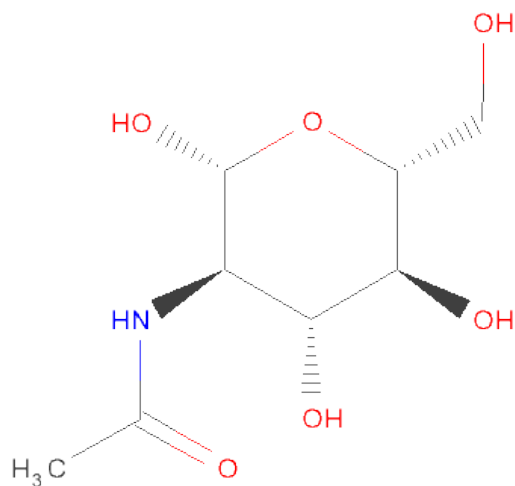
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	221	Total	C	N	O	S	0	0	0
			1660	1064	272	317	7			
4	G	221	Total	C	N	O	S	0	0	0
			1657	1063	271	316	7			

- Molecule 5 is (11Z,14Z)-N-[(2S,3S,4R)-1-(ALPHA-D-GALACTOPYRANOSYLOXY)-3,4-DIHYDROXYOCTADECAN-2-YL]ICOSA-11,14-DIENAMIDE (three-letter code: 09N) (formula: C₄₄H₈₃NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			54	44	1	9		
5	D	1	Total	C	N	O	0	0
			54	44	1	9		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	HIS	-	EXPRESSION TAG	UNP P11609

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Chain	Residue	Modelled	Actual	Comment	Reference
A	281	HIS	-	EXPRESSION TAG	UNP P11609
A	282	HIS	-	EXPRESSION TAG	UNP P11609
A	283	HIS	-	EXPRESSION TAG	UNP P11609
A	284	HIS	-	EXPRESSION TAG	UNP P11609
A	285	HIS	-	EXPRESSION TAG	UNP P11609
A	286	HIS	-	EXPRESSION TAG	UNP P11609
D	201	HIS	ASP	SEE REMARK 999	UNP P11609
D	280	HIS	-	EXPRESSION TAG	UNP P11609
D	281	HIS	-	EXPRESSION TAG	UNP P11609
D	282	HIS	-	EXPRESSION TAG	UNP P11609
D	283	HIS	-	EXPRESSION TAG	UNP P11609
D	284	HIS	-	EXPRESSION TAG	UNP P11609
D	285	HIS	-	EXPRESSION TAG	UNP P11609
D	286	HIS	-	EXPRESSION TAG	UNP P11609

3 Residue-property plots

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: Antigen-presenting glycoprotein CD1d1

Chain A: 



- Molecule 1: Antigen-presenting glycoprotein CD1d1

Chain D: 



- Molecule 2: Beta-2-microglobulin

Chain B: 



- Molecule 2: Beta-2-microglobulin

Chain E: 



- Molecule 3: L363 light chain (IGKV13-84*01)

Chain L: 



- Molecule 3: L363 light chain (IGKV13-84*01)

Chain I: 



- Molecule 4: L363 heavy chain (IGHV9-4*02)

Chain H: 



- Molecule 4: L363 heavy chain (IGHV9-4*02)

Chain G: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	234.95Å 234.95Å 99.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.89 – 3.10 37.89 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.89-3.10) 100.0 (37.89-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.6.0104	Depositor
R, R_{free}	0.202 , 0.230 0.196 , 0.223	Depositor DCC
R_{free} test set	2897 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 12.7	EDS
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 56798 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12917	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 09N

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.66	2/2303 (0.1%)	0.60	2/3130 (0.1%)
1	D	0.66	8/2299 (0.3%)	0.59	2/3125 (0.1%)
2	B	0.57	0/859	0.53	0/1167
2	E	0.57	1/831 (0.1%)	0.54	0/1129
3	I	0.50	2/1691 (0.1%)	0.55	0/2297
3	L	0.51	2/1689 (0.1%)	0.55	0/2294
4	G	0.61	5/1706 (0.3%)	0.54	0/2336
4	H	0.61	5/1709 (0.3%)	0.54	0/2341
All	All	0.60	25/13087 (0.2%)	0.56	4/17819 (0.0%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	109	TRP	CD2-CE2	5.40	1.47	1.41
1	D	23	TRP	CD2-CE2	5.35	1.47	1.41
4	H	106	TRP	CD2-CE2	5.30	1.47	1.41
1	D	40	TRP	CD2-CE2	5.29	1.47	1.41
1	D	53	TRP	CD2-CE2	5.28	1.47	1.41
4	G	161	TRP	CD2-CE2	5.26	1.47	1.41
3	L	163	TRP	CD2-CE2	5.22	1.47	1.41
3	L	35	TRP	CD2-CE2	5.21	1.47	1.41
1	D	192	TRP	CD2-CE2	5.20	1.47	1.41
4	H	109	TRP	CD2-CE2	5.18	1.47	1.41
4	G	110	TRP	CD2-CE2	5.17	1.47	1.41
1	D	63	TRP	CD2-CE2	5.15	1.47	1.41
4	G	50	TRP	CD2-CE2	5.15	1.47	1.41
3	I	92	TRP	CD2-CE2	5.14	1.47	1.41
4	H	47	TRP	CD2-CE2	5.12	1.47	1.41
4	H	195	TRP	CD2-CE2	5.12	1.47	1.41
1	A	192	TRP	CD2-CE2	5.12	1.47	1.41
4	H	161	TRP	CD2-CE2	5.10	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	142	TRP	CD2-CE2	5.08	1.47	1.41
4	G	195	TRP	CD2-CE2	5.08	1.47	1.41
3	I	163	TRP	CD2-CE2	5.06	1.47	1.41
1	D	245	TRP	CD2-CE2	5.04	1.47	1.41
1	A	40	TRP	CD2-CE2	5.03	1.47	1.41
1	D	219	TRP	CD2-CE2	5.00	1.47	1.41
2	E	95	TRP	CD2-CE2	5.00	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ARG	NE-CZ-NH1	9.43	125.01	120.30
1	A	173	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	D	173	ARG	NE-CZ-NH1	-7.81	116.39	120.30
1	D	173	ARG	NE-CZ-NH2	7.32	123.96	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2233	0	0	0	0
1	D	2230	0	0	2	0
2	B	832	0	0	0	0
2	E	805	0	0	0	0
3	I	1655	0	0	1	0
3	L	1653	0	0	1	0
4	G	1657	0	0	2	0
4	H	1660	0	0	2	0
5	A	54	0	0	0	0
5	D	54	0	0	0	0
6	A	14	0	0	0	0
6	D	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	28	0	0	0	0
7	D	28	0	0	0	0
All	All	12917	0	0	6	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 0.

All (6) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:32:ARG:NH1	4:H:103:ARG:O	2.09	0.85
3:I:32:ARG:NH1	4:G:103:ARG:O	2.12	0.82
4:H:67:ARG:NH2	4:H:90:ASP:OD2	2.36	0.58
4:G:67:ARG:NH2	4:G:90:ASP:OD2	2.37	0.58
1:D:280:HIS:CD2	1:D:281:HIS:N	2.81	0.49
1:D:14:GLN:NE2	1:D:73:TYR:CE2	2.88	0.42

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	272/286 (95%)	260 (96%)	12 (4%)	0	100	100
1	D	272/286 (95%)	258 (95%)	13 (5%)	1 (0%)	43	84
2	B	99/99 (100%)	97 (98%)	2 (2%)	0	100	100
2	E	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
3	I	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
3	L	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
4	G	217/222 (98%)	205 (94%)	11 (5%)	1 (0%)	38	81
4	H	217/222 (98%)	206 (95%)	11 (5%)	0	100	100
All	All	1597/1642 (97%)	1521 (95%)	74 (5%)	2 (0%)	59	92

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	281	HIS
4	G	41	PRO

5.3.2 Protein sidechains ⓘ

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	240/250 (96%)	238 (99%)	2 (1%)	89	97
1	D	240/250 (96%)	237 (99%)	3 (1%)	80	95
2	B	94/93 (101%)	92 (98%)	2 (2%)	66	92
2	E	91/93 (98%)	89 (98%)	2 (2%)	64	92
3	I	189/190 (100%)	185 (98%)	4 (2%)	66	92
3	L	189/190 (100%)	186 (98%)	3 (2%)	75	94
4	G	177/184 (96%)	177 (100%)	0	100	100
4	H	179/184 (97%)	179 (100%)	0	100	100
All	All	1399/1434 (98%)	1383 (99%)	16 (1%)	84	96

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	SER
1	A	215	PRO
2	B	57	SER
2	B	75	THR
1	D	157	SER
1	D	173	ARG
1	D	215	PRO
2	E	57	SER
2	E	75	THR
3	L	8	SER
3	L	78	LEU
3	L	210	ASN
3	I	8	SER
3	I	78	LEU

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Mol	Chain	Res	Type
3	I	210	ASN
3	I	212	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	$\# Z > 2$
7	NAG	A	506	1,7	12,14,15	0.72	0	15,19,21	0.85	1 (6%)
7	NAG	A	507	7	12,14,15	0.56	0	15,19,21	1.25	2 (13%)
7	NAG	D	506	1,7	12,14,15	0.66	0	15,19,21	0.97	1 (6%)
7	NAG	D	507	7	12,14,15	0.58	0	15,19,21	1.72	2 (13%)

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
7	NAG	A	506	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	507	7	-	0/6/23/26	0/1/1/1
7	NAG	D	506	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	507	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	507	NAG	O5-C5-C6	4.97	112.20	106.98
7	D	507	NAG	O5-C5-C4	-2.43	107.56	110.65
7	A	506	NAG	C3-C2-N2	-2.42	108.07	111.76
7	A	507	NAG	O5-C5-C4	2.30	113.57	110.65
7	D	506	NAG	C3-C2-N2	-2.17	108.45	111.76
7	A	507	NAG	O3-C3-C2	-2.03	104.83	109.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

4 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	09N	A	287	-	54,54,54	0.93	4 (7%)	63,63,63	0.65	0
6	NAG	A	512	1	12,14,15	0.54	0	15,19,21	0.76	0
5	09N	D	287	-	54,54,54	0.88	2 (3%)	63,63,63	0.59	0
6	NAG	D	512	1	12,14,15	0.48	0	15,19,21	0.95	1 (6%)

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	09N	A	287	-	-	0/52/72/72	0/1/1/1
6	NAG	A	512	1	-	0/6/23/26	0/1/1/1
5	09N	D	287	-	-	0/52/72/72	0/1/1/1
6	NAG	D	512	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	287	09N	O1-C1	2.60	1.44	1.40
5	A	287	09N	O5-C1	2.42	1.48	1.41
5	A	287	09N	CBK-CBP	-2.33	1.40	1.50
5	A	287	09N	CBF-CBG	-2.28	1.40	1.50
5	D	287	09N	CBK-CBP	-2.22	1.40	1.50
5	D	287	09N	CBF-CBG	-2.22	1.40	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	512	NAG	O5-C5-C6	2.56	109.67	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	275/286 (96%)	-0.33	0 100 100	46, 61, 86, 113	0
1	D	276/286 (96%)	-0.31	0 100 100	46, 66, 96, 125	0
2	B	99/99 (100%)	-0.28	0 100 100	46, 58, 82, 105	0
2	E	98/99 (98%)	-0.25	0 100 100	46, 64, 81, 96	0
3	I	214/214 (100%)	-0.35	0 100 100	47, 59, 84, 113	0
3	L	214/214 (100%)	-0.31	0 100 100	39, 56, 87, 118	0
4	G	221/222 (99%)	-0.32	0 100 100	51, 71, 105, 133	0
4	H	221/222 (99%)	-0.29	0 100 100	43, 72, 107, 139	0
All	All	1618/1642 (98%)	-0.31	0 100 100	39, 64, 96, 139	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	NAG	A	507	14/15	0.29	2.61	82,86,92,96	0
7	NAG	A	506	14/15	0.13	-1.10	64,67,71,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	NAG	D	506	14/15	0.10	-1.39	65,68,72,73	0
7	NAG	D	507	14/15	0.18	-19.40	74,78,83,85	0

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	09N	D	287	54/54	0.30	4.11	52,59,71,72	0
5	09N	A	287	54/54	0.28	3.51	44,49,62,67	0
6	NAG	D	512	14/15	0.19	1.30	84,87,90,91	0
6	NAG	A	512	14/15	0.14	-0.09	74,78,81,83	0

6.5 Other polymers

There are no such residues in this entry.