wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:38 PM GMT

PDB ID	:	3UBX
Title	:	Crystal structure of the mouse CD1d-C20:2-aGalCer-L363 mAb Fab complex
Authors	:	Yu, E.D.; Zajonc, D.M.
Deposited on	:	2011-10-25
Resolution	:	3.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

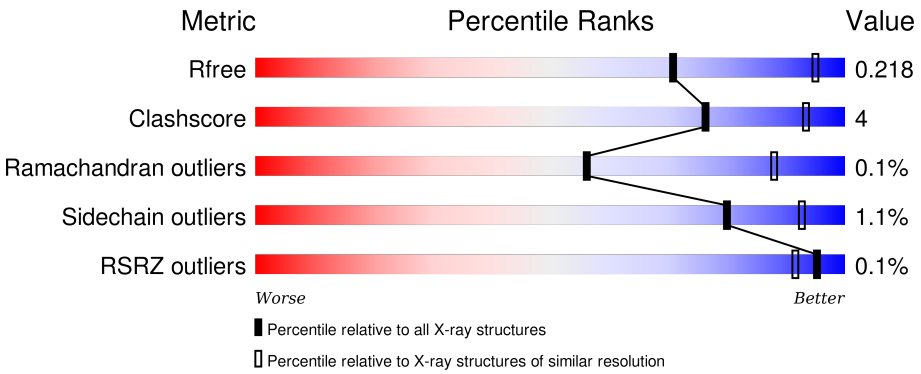
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	286	82% 14% •
1	D	286	81% 14% • •
2	B	99	87% 13%
2	E	99	87% 12% •
3	I	214	91% 9%

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Mol	Chain	Length	Quality of chain
3	L	214	90% 9%
4	G	222	90% 9%
4	H	222	91% 9%

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
5	09N	A	287	-	-	-	X
5	09N	D	287	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12917 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 Antigen-presenting glycoprotein CD1d1.

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

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
			Total	C	N	O	S			
2	B	99	832	531	142	152	7	0	2	0
2	E	98	805	514	136	148	7	0	0	0

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

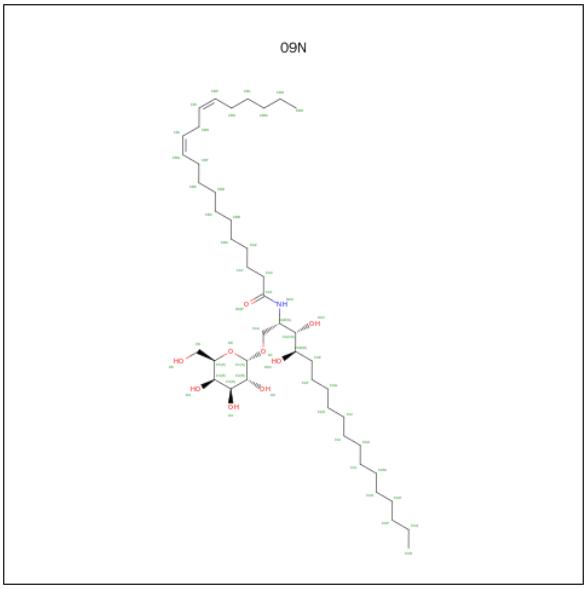
- Molecule 3 is a protein called L363 light chain (IGKV13-84*01).

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

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

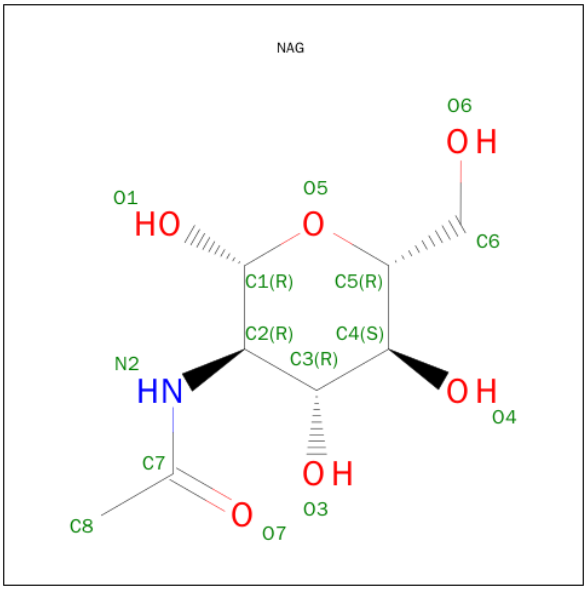
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	221	1660	1064	272	317	7	0	0	0
4	G	221	1657	1063	271	316	7	0	0	0

- 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: $C_{44}H_{83}NO_9$).



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

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



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

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

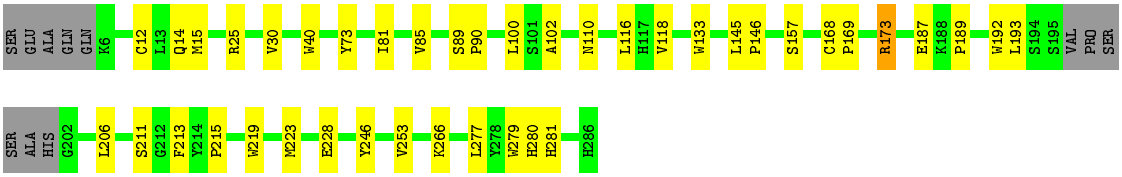
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	2	28	16	2	10	0	0
7	D	2	28	16	2	10	0	0

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.

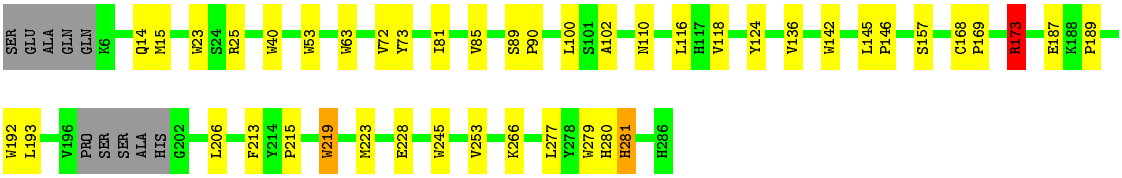
- Molecule 1: Antigen-presenting glycoprotein CD1d1

Chain A:



- Molecule 1: Antigen-presenting glycoprotein CD1d1

Chain D:

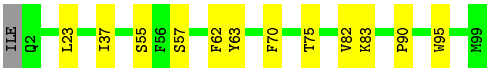


- Molecule 2: Beta-2-microglobulin

Chain B:

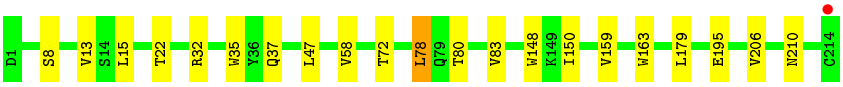
- Molecule 2: Beta-2-microglobulin

Chain E:



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

Chain L:

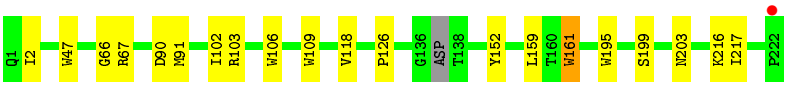


- Molecule 3: L363 light chain (IGKV13-84*01)

Chain I:

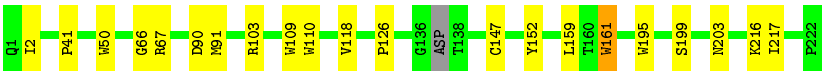
- Molecule 4: L363 heavy chain (IGHV9-4*02)

Chain H:



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

Chain G:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.63 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.6.0104	Depositor
R, R_{free}	0.202 , 0.230 0.192 , 0.218	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 , 13.6	EDS
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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 (i)

5.1 Standard geometry (i)

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%)

The worst 5 of 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

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 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	2233	0	2106	28	0
1	D	2230	0	2109	24	0
2	B	832	0	799	7	0
2	E	805	0	772	5	0
3	I	1655	0	1581	9	0
3	L	1653	0	1580	10	0
4	G	1657	0	1595	10	0
4	H	1660	0	1605	11	0
5	A	54	0	83	5	0
5	D	54	0	83	1	0
6	A	14	0	13	0	0
6	D	14	0	13	0	0
7	A	28	0	25	1	0
7	D	28	0	25	1	0
All	All	12917	0	12389	97	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.

The worst 5 of 97 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)
4:H:91:MET:HG3	4:H:118:VAL:H	1.40	0.86
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
1:D:280:HIS:CD2	1:D:281:HIS:H	1.96	0.82
4:G:91:MET:HG3	4:G:118:VAL:H	1.44	0.80

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	272/286 (95%)	260 (96%)	12 (4%)	0	100	100
1	D	272/286 (95%)	258 (95%)	13 (5%)	1 (0%)	39	75
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%)	34	72
4	H	217/222 (98%)	206 (95%)	11 (5%)	0	100	100
All	All	1597/1642 (97%)	1521 (95%)	74 (5%)	2 (0%)	56	88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	281	HIS
4	G	41	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	240/250 (96%)	238 (99%)	2 (1%)	86	94
1	D	240/250 (96%)	237 (99%)	3 (1%)	76	91
2	B	94/93 (101%)	92 (98%)	2 (2%)	61	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	91/93 (98%)	89 (98%)	2 (2%)	60	85
3	I	189/190 (100%)	185 (98%)	4 (2%)	61	86
3	L	189/190 (100%)	186 (98%)	3 (2%)	70	89
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%)	80	93

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	57	SER
2	E	75	THR
3	I	8	SER
1	D	215	PRO
3	I	78	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	282	HIS
3	I	31	ASN
1	D	286	HIS
2	B	29	GLN
2	E	29	GLN

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)

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	14,14,15	0.53	0	15,19,21	1.12	1 (6%)
7	NAG	A	507	7	14,14,15	0.45	0	15,19,21	1.70	2 (13%)
7	NAG	D	506	1,7	14,14,15	0.51	0	15,19,21	1.42	1 (6%)
7	NAG	D	507	7	14,14,15	0.52	0	15,19,21	1.11	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
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.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	507	NAG	O3-C3-C2	-2.16	104.83	109.11
7	D	507	NAG	C3-C4-C5	-2.00	106.71	110.20
7	D	507	NAG	O5-C5-C6	2.24	112.20	107.35
7	A	506	NAG	C1-O5-C5	3.48	116.66	112.25
7	D	506	NAG	C1-O5-C5	4.45	117.90	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
7	A	506	NAG	1	0
7	D	506	NAG	1	0

5.6 Ligand geometry (i)

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	-	53,54,54	0.93	4 (7%)	59,63,63	0.65	0
6	NAG	A	512	1	14,14,15	0.42	0	15,19,21	1.26	1 (6%)
5	09N	D	287	-	53,54,54	0.87	2 (3%)	59,63,63	0.61	0
6	NAG	D	512	1	14,14,15	0.41	0	15,19,21	1.43	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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	287	09N	CBK-CBP	-2.29	1.40	1.50
5	A	287	09N	CBF-CBG	-2.24	1.40	1.50
5	D	287	09N	CBK-CBP	-2.18	1.40	1.50
5	D	287	09N	CBF-CBG	-2.18	1.40	1.50
5	A	287	09N	O5-C1	2.42	1.48	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	512	NAG	C1-O5-C5	4.12	117.47	112.25
6	D	512	NAG	C1-O5-C5	4.81	118.35	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	287	09N	5	0
5	D	287	09N	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	A	275/286 (96%)	-0.45	0	100	100	46, 61, 86, 113	0
1	D	276/286 (96%)	-0.40	0	100	100	46, 66, 96, 125	0
2	B	99/99 (100%)	-0.34	0	100	100	46, 58, 82, 105	0
2	E	98/99 (98%)	-0.27	0	100	100	46, 64, 81, 96	0
3	I	214/214 (100%)	-0.49	0	100	100	47, 59, 84, 113	0
3	L	214/214 (100%)	-0.42	1 (0%)	91	83	39, 56, 87, 118	0
4	G	221/222 (99%)	-0.40	0	100	100	51, 71, 105, 133	0
4	H	221/222 (99%)	-0.35	1 (0%)	91	83	43, 72, 107, 139	0
All	All	1618/1642 (98%)	-0.40	2 (0%)	95	91	39, 64, 96, 139	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	222	PRO	2.5
3	L	214	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, 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(Å^2)	Q<0.9
7	NAG	A	507	14/15	0.89	0.30	-	82,86,92,96	0
7	NAG	A	506	14/15	0.95	0.15	-	64,67,71,75	0
7	NAG	D	506	14/15	0.95	0.10	-	65,68,72,73	0
7	NAG	D	507	14/15	0.85	0.18	-	74,78,83,85	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, 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(Å^2)	Q<0.9
5	09N	D	287	54/54	0.95	0.27	2.90	52,59,71,72	0
5	09N	A	287	54/54	0.96	0.24	2.21	44,49,62,67	0
6	NAG	D	512	14/15	0.91	0.18	-	84,87,90,91	0
6	NAG	A	512	14/15	0.91	0.15	-	74,78,81,83	0

6.5 Other polymers (i)

There are no such residues in this entry.