



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:37 PM GMT

PDB ID : 3GMM
Title : Structure of mouse CD1d in complex with C8Ph
Authors : Schiefner, A.; Wilson, I.A.
Deposited on : 2009-03-14
Resolution : 1.80 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>

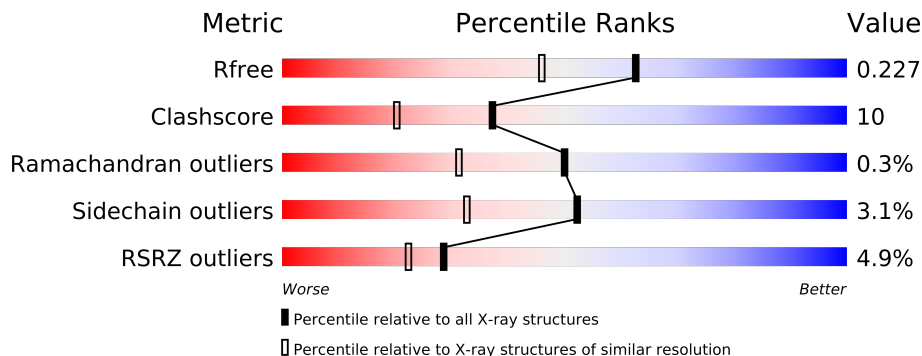
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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	287	
2	B	99	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	288	-	X
7	PLM	A	301	-	X
8	EDO	B	101[A]	-	X
8	EDO	B	101[B]	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3590 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 T-cell surface glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	268	2205	1401	383	408	13	0	5	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	GLY	-	EXPRESSION TAG	UNP P11609
A	281	SER	-	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
A	287	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	833	531	140	155	7	0	2	0

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	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		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	GLY	-	EXPRESSION TAG	UNP P11609
A	281	SER	-	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
A	287	HIS	-	EXPRESSION TAG	UNP P11609

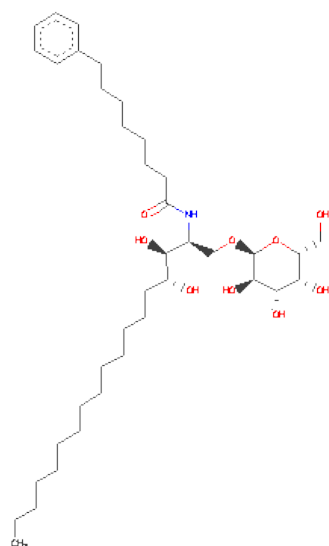
- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	6	Total	C	N	O	0	0
			71	40	2	29		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	GLY	-	EXPRESSION TAG	UNP P11609
A	281	SER	-	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
A	287	HIS	-	EXPRESSION TAG	UNP P11609

- Molecule 6 is N-{(1S,2S,3R)-1-[(ALPHA-D-GALACTOPYRANOSYLOXY)METHYL]-2,3-DIHYDROXYHEPTADECYL}-8-PHENYLOCTANAMIDE (three-letter code: C8P) (formula: C₃₈H₆₇NO₉).



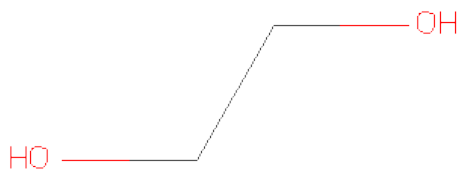
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			48	38	1	9		

- Molecule 7 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			18	16	2		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	1
			8	4	4		

- Molecule 9 is water.

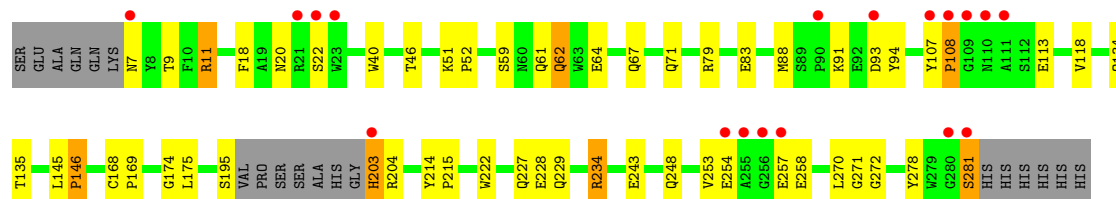
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	218	Total	O	0	5
			223	223		
9	B	96	Total	O	0	1
			97	97		

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.

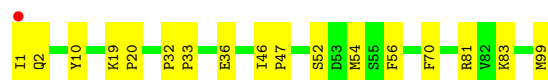
- Molecule 1: T-cell surface glycoprotein CD1d1

Chain A: 



- Molecule 2: Beta-2 microglobulin

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.74Å 97.90Å 55.42Å 90.00° 106.57° 90.00°	Depositor
Resolution (Å)	29.77 – 1.80 29.77 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.77-1.80) 99.6 (29.77-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.175 , 0.219 0.182 , 0.227	Depositor DCC
R_{free} test set	1993 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 39341 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3590	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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: C8P, BMA, NAG, EDO, FUC, PLM, 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	1.09	2/2268 (0.1%)	0.98	2/3079 (0.1%)
2	B	1.22	3/859 (0.3%)	1.03	0/1164
All	All	1.13	5/3127 (0.2%)	0.99	2/4243 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	MET	CG-SD	-7.23	1.62	1.81
2	B	10	TYR	CD1-CE1	5.79	1.48	1.39
2	B	56	PHE	CE2-CZ	5.34	1.47	1.37
1	A	40	TRP	CE3-CZ3	5.20	1.47	1.38
1	A	222	TRP	CB-CG	5.03	1.59	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	GLY	N-CA-C	-5.29	99.89	113.10
1	A	175	LEU	CB-CG-CD2	5.18	119.81	111.00

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	2205	0	2097	48	0
2	B	833	0	806	14	1
3	A	14	0	13	1	0
4	A	61	0	52	2	0
5	A	71	0	61	1	0
6	A	48	0	67	2	0
7	A	18	0	31	2	0
8	A	8	0	12	1	0
8	B	12	0	18	2	0
9	A	223	0	0	12	0
9	B	97	0	0	6	1
All	All	3590	0	3157	65	1

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 10.

All (65) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:234:ARG:HH11	1:A:234:ARG:HG2	1.14	1.08
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.26	1.08
1:A:59:SER:OG	1:A:62:GLN:HG3	1.69	0.91
1:A:107:TYR:HB3	1:A:108:PRO:CD	2.00	0.91
1:A:228:GLU:HG3	9:A:397:HOH:O	1.73	0.86
1:A:234:ARG:NH1	1:A:234:ARG:HG2	1.93	0.81
1:A:248:GLN:OE1	2:B:99:MET:HG2	1.81	0.81
1:A:234:ARG:HD2	9:A:459:HOH:O	1.81	0.81
1:A:11[A]:ARG:HD2	9:A:408:HOH:O	1.81	0.79
1:A:272:GLY:O	9:A:367:HOH:O	2.09	0.69
2:B:36[B]:GLU:HG3	9:B:303:HOH:O	1.95	0.67
1:A:107:TYR:CB	1:A:108:PRO:HD2	2.01	0.66
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.79	0.64
2:B:19:LYS:HE3	9:B:138:HOH:O	1.99	0.62
1:A:248:GLN:HG3	8:A:303:EDO:H21	1.83	0.61
1:A:257:GLU:O	1:A:257:GLU:HG3	2.01	0.59
1:A:46:THR:HB	1:A:67:GLN:OE1	2.02	0.58
2:B:2:GLN:HG2	9:B:268:HOH:O	2.03	0.58
1:A:234:ARG:CD	9:A:459:HOH:O	2.43	0.58
1:A:248:GLN:OE1	2:B:99:MET:CG	2.51	0.57
1:A:18:PHE:HB3	1:A:94:TYR:CE2	2.39	0.57
1:A:257:GLU:O	1:A:257:GLU:CG	2.51	0.56
1:A:227[B]:GLN:HG2	1:A:229:GLN:NE2	2.19	0.56
1:A:83:GLU:OE1	9:A:369:HOH:O	2.18	0.56
1:A:195:SER:OG	1:A:204:ARG:NH1	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1:ILE:HG13	2:B:2:GLN:N	2.24	0.52
5:A:294:NAG:C7	9:A:330:HOH:O	2.57	0.52
6:A:300:C8P:H31A	7:A:301:PLM:HF1	1.92	0.51
1:A:7:ASN:HD21	1:A:107:TYR:HD1	1.57	0.50
1:A:88:MET:O	1:A:91:LYS:HB2	2.12	0.50
1:A:7:ASN:ND2	1:A:107:TYR:HD1	2.10	0.49
1:A:107:TYR:CB	1:A:108:PRO:CD	2.70	0.48
2:B:32:PRO:HB2	2:B:33:PRO:HD2	1.93	0.48
1:A:168:CYS:HB3	1:A:169:PRO:CD	2.43	0.48
2:B:52:SER:OG	8:B:101[A]:EDO:H21	2.13	0.48
1:A:254:GLU:N	1:A:257:GLU:OE1	2.38	0.47
4:A:292:MAN:C1	4:A:293:MAN:H5	2.43	0.47
1:A:20:ASN:HA	1:A:94:TYR:CD1	2.49	0.47
1:A:18:PHE:HB3	1:A:94:TYR:HE2	1.80	0.47
1:A:174:GLY:HA3	9:A:313:HOH:O	2.14	0.46
1:A:234:ARG:HH11	1:A:234:ARG:CG	2.04	0.46
1:A:134[B]:GLN:HG2	1:A:135:THR:O	2.16	0.46
2:B:83:LYS:HG3	9:B:120:HOH:O	2.16	0.45
1:A:278:TYR:O	1:A:281:SER:HB2	2.18	0.44
1:A:214:TYR:CG	1:A:215:PRO:HA	2.52	0.44
2:B:52:SER:CB	8:B:101[A]:EDO:H21	2.48	0.44
1:A:79:ARG:O	1:A:83:GLU:HG2	2.17	0.44
2:B:81:ARG:NH1	9:B:145:HOH:O	2.30	0.43
2:B:19:LYS:HA	2:B:20:PRO:HD3	1.93	0.43
4:A:290:NAG:H81	9:A:482:HOH:O	2.19	0.42
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.76	0.42
1:A:9:THR:HG22	1:A:11[A]:ARG:HG3	2.02	0.42
1:A:203:HIS:C	1:A:203:HIS:CD2	2.92	0.42
1:A:64:GLU:HG2	9:A:500:HOH:O	2.19	0.42
1:A:22:SER:HB2	3:A:288:NAG:H82	2.01	0.41
2:B:46:ILE:HA	2:B:47:PRO:HD2	1.86	0.41
1:A:118:VAL:HG11	6:A:300:C8P:H5A	2.02	0.41
1:A:243:GLU:HG3	9:A:476[B]:HOH:O	2.21	0.41
1:A:7:ASN:ND2	1:A:107:TYR:CD1	2.89	0.41
2:B:2:GLN:NE2	9:B:268:HOH:O	2.23	0.41
7:A:301:PLM:H72	7:A:301:PLM:H42	1.76	0.41
1:A:71:GLN:HG2	9:A:517:HOH:O	2.19	0.41
1:A:145:LEU:HB3	1:A:146:PRO:HD3	2.03	0.41
1:A:51:LYS:HB3	1:A:52:PRO:HD2	2.03	0.41
1:A:253:VAL:HG21	1:A:258:GLU:HG2	2.03	0.40

All (1) 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	Distance(Å)	Clash(Å)
2:B:1:ILE:CD1	9:B:392:HOH:O[1_655]	1.33	0.87

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	269/287 (94%)	262 (97%)	6 (2%)	1 (0%)	43	25
2	B	99/99 (100%)	96 (97%)	3 (3%)	0	100	100
All	All	368/386 (95%)	358 (97%)	9 (2%)	1 (0%)	50	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	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	239/250 (96%)	229 (96%)	10 (4%)	40	20
2	B	95/93 (102%)	94 (99%)	1 (1%)	84	77
All	All	334/343 (97%)	323 (97%)	11 (3%)	52	30

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11[A]	ARG
1	A	11[B]	ARG
1	A	61	GLN
1	A	62	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	93	ASP
1	A	113	GLU
1	A	146	PRO
1	A	203	HIS
1	A	234	ARG
1	A	281	SER
2	B	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	HIS

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 ⓘ

11 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	289	1,4	12,14,15	0.97	1 (8%)	15,19,21	2.52	7 (46%)
4	NAG	A	290	4	12,14,15	0.77	0	15,19,21	1.74	3 (20%)
4	BMA	A	291	4	10,11,12	0.72	0	11,15,17	1.86	2 (18%)
4	MAN	A	292	4	10,11,12	0.72	0	11,15,17	1.78	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	A	293	4	10,11,12	0.73	0	11,15,17	2.14	2 (18%)
5	NAG	A	294	1,5	12,14,15	1.07	1 (8%)	15,19,21	2.02	5 (33%)
5	NAG	A	295	5	12,14,15	0.64	0	15,19,21	1.67	5 (33%)
5	BMA	A	296	5	10,11,12	0.82	0	11,15,17	1.34	2 (18%)
5	MAN	A	297	5	10,11,12	0.62	0	11,15,17	1.46	2 (18%)
5	MAN	A	298	5	10,11,12	0.73	0	11,15,17	2.30	4 (36%)
5	FUC	A	299	5	9,10,11	0.89	0	10,14,16	2.35	5 (50%)

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	289	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	290	4	-	0/6/23/26	0/1/1/1
4	BMA	A	291	4	-	0/2/19/22	0/1/1/1
4	MAN	A	292	4	-	0/2/19/22	0/1/1/1
4	MAN	A	293	4	-	0/2/19/22	0/1/1/1
5	NAG	A	294	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	295	5	-	0/6/23/26	0/1/1/1
5	BMA	A	296	5	-	0/2/19/22	0/1/1/1
5	MAN	A	297	5	-	0/2/19/22	0/1/1/1
5	MAN	A	298	5	-	0/2/19/22	0/1/1/1
5	FUC	A	299	5	-	0/0/17/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	294	NAG	O5-C5	-3.30	1.39	1.45
4	A	289	NAG	O3-C3	-2.24	1.37	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	293	MAN	O5-C5-C6	6.51	113.82	106.98
4	A	289	NAG	C3-C4-C5	-6.11	99.29	110.20
4	A	289	NAG	O5-C5-C6	4.92	112.14	106.98
5	A	298	MAN	C4-C3-C2	-4.85	104.00	110.50
4	A	291	BMA	O5-C5-C6	4.78	112.00	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	290	NAG	C3-C2-N2	-4.15	105.44	111.76
4	A	292	MAN	O5-C5-C6	4.03	111.21	106.98
5	A	294	NAG	C8-C7-N2	3.93	123.78	116.11
5	A	298	MAN	O5-C5-C6	3.79	110.96	106.98
4	A	290	NAG	O5-C5-C6	3.75	110.91	106.98
5	A	299	FUC	C6-C5-C4	-3.51	107.35	113.06
5	A	299	FUC	O3-C3-C2	3.33	116.04	109.94
5	A	299	FUC	O3-C3-C4	3.32	117.79	110.35
5	A	294	NAG	C2-N2-C7	-3.30	117.56	123.09
5	A	294	NAG	O7-C7-C8	-3.21	115.79	122.04
4	A	291	BMA	O5-C5-C4	-3.03	106.81	110.65
5	A	299	FUC	C4-C3-C2	-3.00	106.48	110.50
5	A	295	NAG	C6-C5-C4	-2.94	105.90	113.00
5	A	295	NAG	C2-N2-C7	-2.88	118.26	123.09
5	A	297	MAN	O5-C5-C6	2.78	109.90	106.98
5	A	294	NAG	O5-C5-C4	-2.49	107.49	110.65
5	A	295	NAG	O7-C7-C8	-2.43	117.31	122.04
4	A	289	NAG	O7-C7-C8	-2.42	117.31	122.04
4	A	289	NAG	O6-C6-C5	-2.39	103.13	111.36
5	A	294	NAG	O5-C5-C6	2.37	109.47	106.98
4	A	292	MAN	O4-C4-C3	-2.37	105.05	110.35
5	A	298	MAN	O3-C3-C2	2.31	114.15	109.94
4	A	289	NAG	C8-C7-N2	2.29	120.57	116.11
5	A	295	NAG	O4-C4-C3	2.28	115.47	110.35
5	A	296	BMA	O6-C6-C5	-2.26	103.58	111.36
4	A	290	NAG	C2-N2-C7	-2.25	119.31	123.09
4	A	289	NAG	O5-C5-C4	-2.24	107.81	110.65
5	A	297	MAN	O3-C3-C4	-2.23	105.35	110.35
5	A	295	NAG	O4-C4-C5	-2.22	103.44	109.28
5	A	299	FUC	O4-C4-C3	2.21	115.30	110.35
5	A	298	MAN	O3-C3-C4	2.14	115.15	110.35
5	A	296	BMA	O2-C2-C3	-2.12	105.59	110.18
4	A	293	MAN	O5-C5-C4	-2.00	108.11	110.65
4	A	289	NAG	O4-C4-C5	-2.00	104.01	109.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

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	$\# Z > 2$
3	NAG	A	288	1	12,14,15	0.91	1 (8%)	15,19,21	1.71	2 (13%)
6	C8P	A	300	-	49,49,49	0.81	2 (4%)	60,60,60	1.40	9 (15%)
7	PLM	A	301	-	17,17,17	0.39	0	17,17,17	1.05	1 (5%)
8	EDO	A	302	-	3,3,3	0.59	0	2,2,2	0.55	0
8	EDO	A	303	-	3,3,3	0.88	0	2,2,2	0.58	0
8	EDO	B	100	-	3,3,3	0.78	0	2,2,2	0.75	0
8	EDO	B	101[A]	-	3,3,3	0.59	0	2,2,2	0.67	0
8	EDO	B	101[B]	-	3,3,3	0.64	0	2,2,2	0.59	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
3	NAG	A	288	1	-	0/6/23/26	0/1/1/1
6	C8P	A	300	-	-	0/43/63/63	0/2/2/2
7	PLM	A	301	-	-	0/15/15/15	0/0/0/0
8	EDO	A	302	-	-	0/1/1/1	0/0/0/0
8	EDO	A	303	-	-	0/1/1/1	0/0/0/0
8	EDO	B	100	-	-	0/1/1/1	0/0/0/0
8	EDO	B	101[A]	-	-	0/1/1/1	0/0/0/0
8	EDO	B	101[B]	-	-	0/1/1/1	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	300	C8P	O18-C19	3.03	1.45	1.40
3	A	288	NAG	O5-C5	-2.64	1.40	1.45
6	A	300	C8P	C18-C17	2.26	1.56	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	288	NAG	O5-C5-C4	-4.66	104.75	110.65
6	A	300	C8P	C18-C17-N	-3.22	105.22	109.74
6	A	300	C8P	O20-C20-C21	-2.95	103.73	110.35
3	A	288	NAG	C3-C2-N2	-2.91	107.33	111.76
6	A	300	C8P	O19-C23-C22	2.83	115.00	109.76
7	A	301	PLM	O1-C1-C2	2.80	124.11	114.22
6	A	300	C8P	O16-C16-C17	-2.59	102.79	109.07
6	A	300	C8P	C15-C16-C17	2.56	117.46	113.61
6	A	300	C8P	C28-C27-C26	-2.52	103.79	113.28
6	A	300	C8P	O22-C22-C21	-2.52	104.71	110.35
6	A	300	C8P	C8-C9-C10	-2.41	101.59	114.61
6	A	300	C8P	C18-O18-C19	2.31	118.42	113.81

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	268/287 (93%)	0.16	18 (6%) 17 12	13, 21, 42, 57	0
2	B	99/99 (100%)	-0.18	1 (1%) 79 76	14, 20, 31, 40	0
All	All	367/386 (95%)	0.07	19 (5%) 28 20	13, 21, 40, 57	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	PRO	5.3
1	A	203	HIS	5.2
1	A	109	GLY	5.2
1	A	255	ALA	4.9
1	A	280	GLY	4.1
1	A	281	SER	4.1
1	A	110	ASN	3.9
1	A	111	ALA	3.8
1	A	93	ASP	3.4
1	A	256	GLY	3.4
1	A	7	ASN	3.3
2	B	1	ILE	2.8
1	A	107	TYR	2.7
1	A	21	ARG	2.5
1	A	22	SER	2.5
1	A	257	GLU	2.4
1	A	23	TRP	2.3
1	A	90	PRO	2.2
1	A	254	GLU	2.2

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
4	MAN	A	293	11/12	0.42	48.54	75,78,81,82	0
5	MAN	A	298	11/12	0.28	11.80	63,67,68,71	0
4	MAN	A	292	11/12	0.26	8.98	46,54,63,68	0
4	NAG	A	290	14/15	0.31	7.72	62,65,69,71	0
5	MAN	A	297	11/12	0.20	1.46	41,45,50,52	0
5	FUC	A	299	10/11	0.15	0.69	39,42,45,45	0
5	NAG	A	295	14/15	0.09	0.67	35,37,41,42	0
5	BMA	A	296	11/12	0.21	0.63	42,45,52,57	0
4	NAG	A	289	14/15	0.12	0.17	33,42,48,52	0
5	NAG	A	294	14/15	0.07	-1.02	26,30,33,35	0
4	BMA	A	291	11/12	0.43	-	67,71,74,76	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(Å ²)	Q<0.9
3	NAG	A	288	14/15	0.40	5.29	59,66,74,75	0
7	PLM	A	301	18/18	0.28	4.63	41,46,52,53	0
8	EDO	B	101[B]	4/4	0.15	2.77	21,22,25,29	4
8	EDO	B	101[A]	4/4	0.15	2.36	30,31,31,38	4
8	EDO	A	302	4/4	0.14	1.77	27,28,29,33	0
8	EDO	B	100	4/4	0.11	1.25	22,28,30,32	0
8	EDO	A	303	4/4	0.14	0.98	24,34,36,45	0
6	C8P	A	300	48/48	0.12	0.22	23,33,42,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.