



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:57 AM GMT

PDB ID : 3GML
Title : Structure of mouse CD1d in complex with C6Ph
Authors : Schiefner, A.; Wilson, I.A.
Deposited on : 2009-03-14
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure 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/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

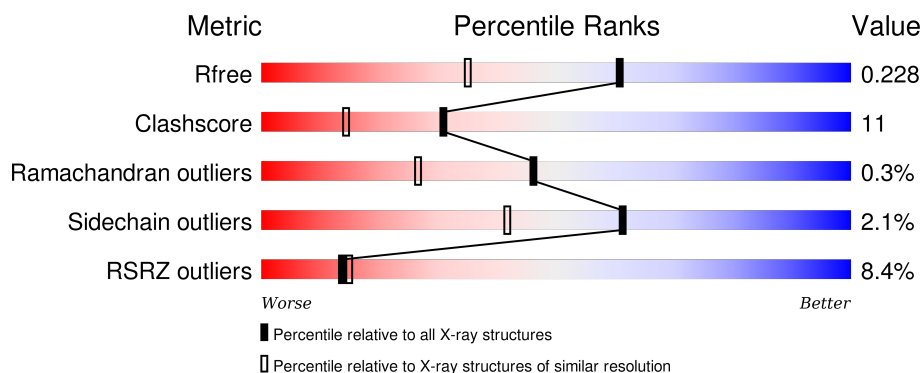
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	287	
2	B	99	

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
4	MAN	A	292	-	-	-	X
5	MAN	A	297	-	-	-	X
7	PLM	A	301	-	-	-	X
8	EDO	A	302	-	-	-	X
8	EDO	A	304[A]	-	-	-	X
8	EDO	A	304[B]	-	-	-	X
8	EDO	B	100	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3606 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 T-cell surface glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	6	0
			2211	1404	384	410	13			

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
2	B	99	Total	C	N	O	S	0	2	0
			833	531	140	155	7			

- 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		

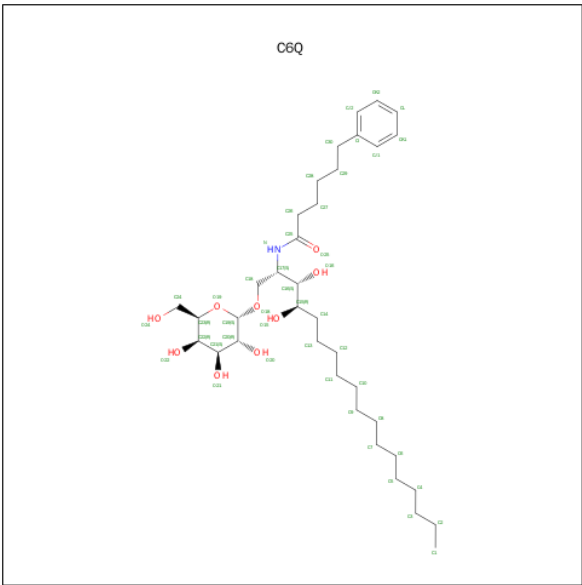
- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

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

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

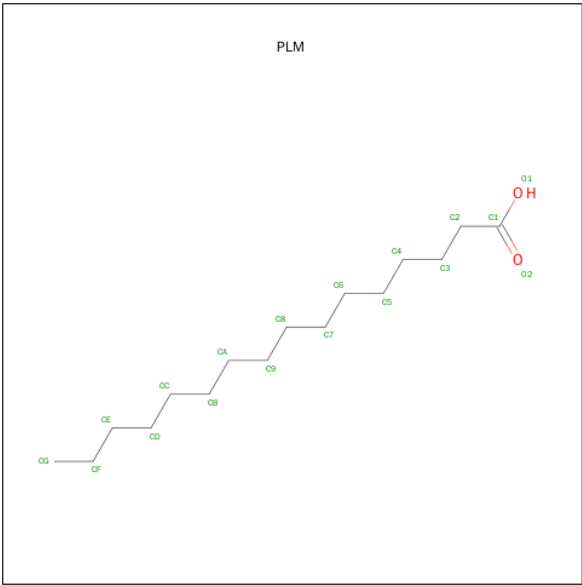
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 6 is N-[(1S,2S,3R)-1-[(ALPHA-D-GALACTOPYRANOSYLOXY)METHYL]-2,3-DIHYDROXYHEPTADECYL]-6-PHENYLHEXANAMIDE (three-letter code: C6Q) (formula: C₃₆H₆₃NO₉).



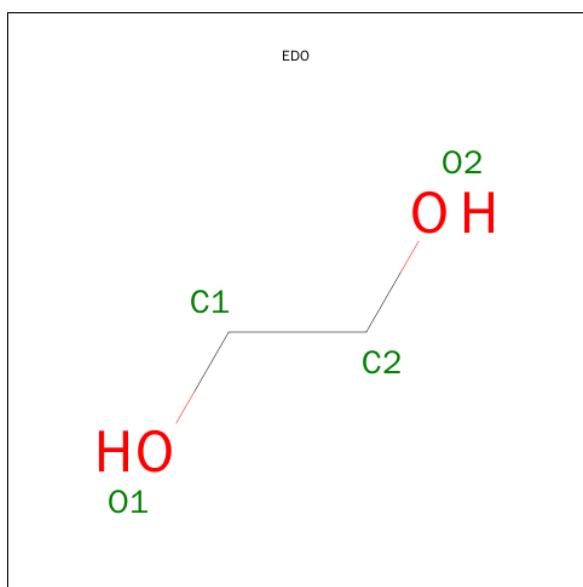
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			46	36	1	9		

- 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	A	1	Total	C	O	0	1
			8	4	4		
8	B	1	Total	C	O	0	0
			4	2	2		

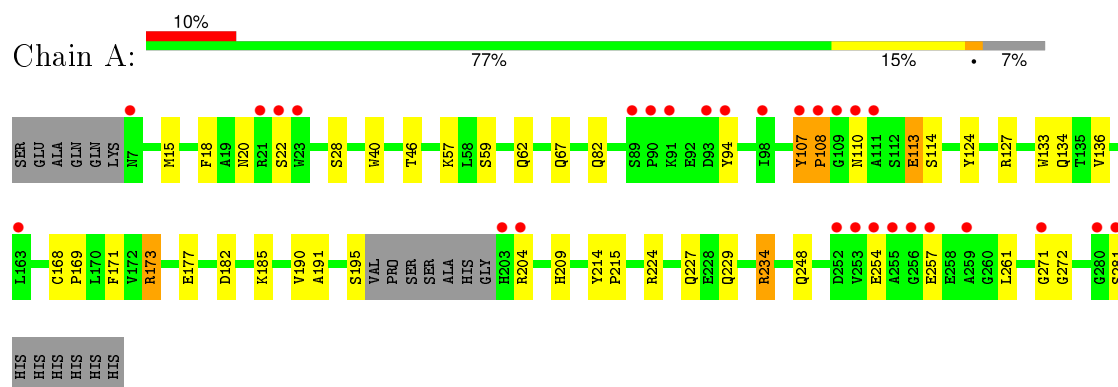
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	232	Total	O	0	5
			237	237		
9	B	94	Total	O	0	1
			95	95		

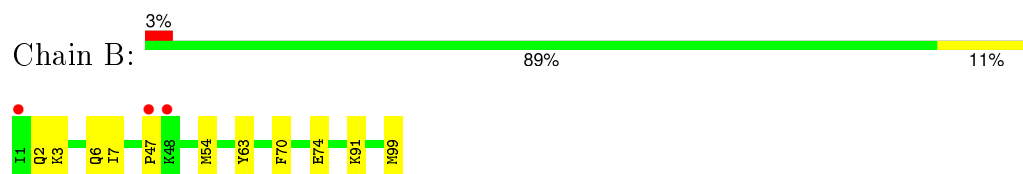
3 Residue-property plots

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



- Molecule 2: Beta-2 microglobulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.66Å 97.63Å 55.27Å 90.00° 106.50° 90.00°	Depositor
Resolution (Å)	28.27 – 1.70 28.27 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (28.27-1.70) 99.6 (28.27-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.177 , 0.216 0.183 , 0.228	Depositor DCC
R_{free} test set	2344 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 46351 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3606	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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, EDO, C6Q, 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	1.04	0/2274	0.95	1/3087 (0.0%)
2	B	1.13	2/859 (0.2%)	1.00	0/1164
All	All	1.07	2/3133 (0.1%)	0.96	1/4251 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	MET	CG-SD	-6.45	1.64	1.81
2	B	63	TYR	CD2-CE2	5.20	1.47	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	GLY	N-CA-C	-5.42	99.55	113.10

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	2211	0	2101	50	1
2	B	833	0	806	16	0
3	A	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	61	0	52	4	1
5	A	71	0	61	0	0
6	A	46	0	63	1	0
7	A	18	0	31	2	0
8	A	16	0	24	3	0
8	B	4	0	6	0	0
9	A	237	0	0	6	0
9	B	95	0	0	10	0
All	All	3606	0	3157	70	1

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 11.

All (70) 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:B:6:GLN:NE2	9:B:342:HOH:O	1.75	1.18
1:A:234:ARG:HH11	1:A:234:ARG:HG2	1.15	1.08
1:A:173:ARG:NH1	1:A:173:ARG:HG2	1.48	1.08
2:B:99:MET:CE	9:B:355:HOH:O	2.02	1.07
2:B:99:MET:HE1	9:B:355:HOH:O	1.54	1.02
1:A:173:ARG:CG	1:A:173:ARG:HH11	1.75	0.99
1:A:248:GLN:HG3	8:A:303:EDO:H21	1.44	0.99
1:A:173:ARG:HH11	1:A:173:ARG:HG2	0.82	0.96
1:A:248:GLN:OE1	2:B:99:MET:HG2	1.72	0.89
1:A:234:ARG:NH1	1:A:234:ARG:HG2	1.93	0.81
2:B:2:GLN:HG2	9:B:268:HOH:O	1.82	0.79
1:A:127:ARG:HG2	1:A:134[B]:GLN:HG2	1.63	0.79
1:A:134[B]:GLN:HG3	1:A:134[B]:GLN:O	1.83	0.78
1:A:173:ARG:NH1	1:A:173:ARG:CG	2.37	0.75
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.68	0.74
2:B:2:GLN:NE2	9:B:268:HOH:O	1.95	0.74
1:A:59:SER:OG	1:A:62:GLN:HG3	1.90	0.72
1:A:248:GLN:HG3	8:A:303:EDO:C2	2.17	0.71
1:A:127:ARG:CG	1:A:134[B]:GLN:HG2	2.21	0.69
2:B:99:MET:SD	9:B:355:HOH:O	2.49	0.68
1:A:257:GLU:O	1:A:257:GLU:HG3	1.96	0.66
4:A:292:MAN:C1	4:A:293:MAN:H5	2.26	0.65
2:B:2:GLN:CG	9:B:268:HOH:O	2.44	0.61
4:A:289:NAG:H61	4:A:290:NAG:C1	2.32	0.60
1:A:234:ARG:HB2	9:A:532:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:HE	1:A:134[B]:GLN:CD	2.06	0.58
1:A:110:ASN:HA	1:A:173:ARG:HH21	1.67	0.58
1:A:110:ASN:HA	1:A:173:ARG:NH2	2.19	0.57
1:A:227[B]:GLN:HE21	1:A:229:GLN:HE22	1.50	0.57
2:B:6:GLN:CD	9:B:342:HOH:O	2.26	0.56
1:A:134[B]:GLN:CG	1:A:134[B]:GLN:O	2.54	0.56
1:A:272:GLY:O	9:A:367:HOH:O	2.18	0.55
1:A:227[A]:GLN:OE1	1:A:227[A]:GLN:HA	2.08	0.54
4:A:290:NAG:H81	9:A:492:HOH:O	2.08	0.53
2:B:74:GLU:HA	2:B:74:GLU:OE1	2.09	0.53
1:A:168:CYS:HB3	1:A:169:PRO:CD	2.40	0.52
1:A:18:PHE:HB3	1:A:94:TYR:CE2	2.45	0.52
1:A:254:GLU:O	1:A:257:GLU:HG2	2.11	0.51
1:A:107:TYR:CB	1:A:108:PRO:HD2	2.34	0.51
1:A:182:ASP:O	1:A:185:LYS:HG2	2.11	0.50
2:B:6:GLN:HG2	9:B:107:HOH:O	2.10	0.50
1:A:82:GLN:HG2	9:A:496:HOH:O	2.13	0.49
2:B:7:ILE:HD12	2:B:91:LYS:HD3	1.95	0.48
4:A:291:BMA:H3	4:A:293:MAN:O6	2.14	0.47
1:A:57:LYS:HE3	1:A:177:GLU:OE2	2.14	0.47
1:A:224:ARG:NH2	1:A:261:LEU:HD21	2.29	0.47
1:A:110:ASN:CA	1:A:173:ARG:HH21	2.27	0.47
1:A:127:ARG:HG2	1:A:134[B]:GLN:CG	2.40	0.47
1:A:257:GLU:O	1:A:257:GLU:CG	2.56	0.47
1:A:195:SER:OG	1:A:204:ARG:NH1	2.48	0.47
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.97	0.46
1:A:20:ASN:HA	1:A:94:TYR:CD1	2.50	0.45
2:B:47:PRO:O	9:B:261:HOH:O	2.20	0.45
7:A:301:PLM:HA2	7:A:301:PLM:H71	1.60	0.45
1:A:28[A]:SER:OG	1:A:40:TRP:HB3	2.17	0.45
2:B:7:ILE:CD1	2:B:91:LYS:HD3	2.48	0.44
1:A:22:SER:CB	3:A:288:NAG:H82	2.47	0.44
1:A:248:GLN:OE1	2:B:99:MET:CG	2.55	0.44
1:A:234:ARG:HD2	9:A:469:HOH:O	2.16	0.43
1:A:46:THR:HB	1:A:67:GLN:OE1	2.18	0.43
8:A:304[B]:EDO:H22	9:A:517:HOH:O	2.19	0.43
1:A:18:PHE:HB3	1:A:94:TYR:HE2	1.85	0.42
1:A:191:ALA:HA	1:A:209:HIS:O	2.20	0.41
1:A:133:TRP:CH2	6:A:300:C6Q:H9A	2.55	0.41
1:A:214:TYR:CG	1:A:215:PRO:HA	2.55	0.41
1:A:124:TYR:CZ	1:A:136:VAL:HG11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PHE:CE2	7:A:301:PLM:H91	2.56	0.40
1:A:113:GLU:HG3	1:A:114:SER:N	2.35	0.40
2:B:3:LYS:HB3	2:B:3:LYS:HE2	1.80	0.40
1:A:127:ARG:HG3	1:A:134[B]:GLN:HG2	2.02	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:VAL:CG2	4:A:292:MAN:O3[2_445]	2.15	0.05

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	270/287 (94%)	263 (97%)	6 (2%)	1 (0%)	39	20
2	B	99/99 (100%)	97 (98%)	2 (2%)	0	100	100
All	All	369/386 (96%)	360 (98%)	8 (2%)	1 (0%)	46	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	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%)	234 (98%)	6 (2%)	55	34
2	B	95/93 (102%)	94 (99%)	1 (1%)	80	69
All	All	335/343 (98%)	328 (98%)	7 (2%)	61	42

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	107	TYR
1	A	113	GLU
1	A	173	ARG
1	A	234	ARG
1	A	281	SER
2	B	70	PHE

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

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](#)

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	14,14,15	0.79	1 (7%)	15,19,21	1.95	7 (46%)
4	NAG	A	290	4	14,14,15	0.61	0	15,19,21	1.41	3 (20%)
4	BMA	A	291	4	11,11,12	0.57	0	14,15,17	2.22	4 (28%)
4	MAN	A	292	4	11,11,12	0.61	0	14,15,17	1.30	1 (7%)
4	MAN	A	293	4	11,11,12	0.56	0	14,15,17	1.35	2 (14%)
5	NAG	A	294	1,5	14,14,15	0.61	0	15,19,21	1.69	3 (20%)
5	NAG	A	295	5	14,14,15	0.59	0	15,19,21	1.36	3 (20%)
5	BMA	A	296	5	11,11,12	0.73	0	14,15,17	2.03	5 (35%)
5	MAN	A	297	5	11,11,12	0.77	1 (9%)	14,15,17	1.20	1 (7%)
5	MAN	A	298	5	11,11,12	0.57	0	14,15,17	2.05	7 (50%)
5	FUC	A	299	5	10,10,11	0.80	0	14,14,16	2.12	7 (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)
4	A	289	NAG	O3-C3	-2.16	1.37	1.43
5	A	297	MAN	O5-C1	-2.15	1.40	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	291	BMA	C1-O5-C5	-4.19	106.94	112.25
5	A	299	FUC	O5-C1-C2	-3.76	104.76	110.86
4	A	291	BMA	C3-C4-C5	-3.59	103.95	110.20
5	A	298	MAN	C3-C4-C5	-3.37	104.31	110.20
5	A	299	FUC	C6-C5-C4	-3.37	106.44	113.08
4	A	290	NAG	C2-N2-C7	-3.35	118.73	123.04
5	A	296	BMA	O2-C2-C3	-3.31	103.46	110.12
4	A	289	NAG	C3-C4-C5	-3.17	104.67	110.20
4	A	289	NAG	C6-C5-C4	-2.99	105.65	113.02
4	A	292	MAN	O4-C4-C3	-2.89	103.83	110.34
5	A	298	MAN	C2-C3-C4	-2.87	106.16	111.04
4	A	293	MAN	C1-O5-C5	-2.86	108.62	112.25
5	A	298	MAN	C1-C2-C3	-2.81	106.22	109.54
5	A	297	MAN	O3-C3-C4	-2.69	104.28	110.34
4	A	290	NAG	C3-C4-C5	-2.68	105.52	110.20
5	A	299	FUC	C2-C3-C4	-2.58	106.65	111.04
5	A	296	BMA	O6-C6-C5	-2.55	102.91	111.33
5	A	294	NAG	O7-C7-C8	-2.44	117.58	122.06
5	A	298	MAN	O2-C2-C1	-2.44	104.31	109.21
4	A	289	NAG	O4-C4-C5	-2.29	103.17	109.24
5	A	295	NAG	O7-C7-C8	-2.27	117.91	122.06
5	A	295	NAG	C2-N2-C7	-2.26	120.13	123.04
5	A	296	BMA	O3-C3-C4	-2.25	105.28	110.34
4	A	290	NAG	C3-C2-N2	-2.21	105.27	110.56
5	A	296	BMA	O2-C2-C1	-2.17	104.85	109.21
4	A	289	NAG	O7-C7-C8	-2.14	118.13	122.06
5	A	299	FUC	O5-C5-C4	2.02	113.03	109.53
5	A	299	FUC	O3-C3-C2	2.04	113.69	110.00
4	A	289	NAG	C4-C3-C2	2.12	114.53	111.23
5	A	298	MAN	O3-C3-C2	2.15	113.89	110.00
5	A	295	NAG	C1-O5-C5	2.42	115.31	112.25
5	A	298	MAN	O3-C3-C4	2.54	116.06	110.34
5	A	299	FUC	O3-C3-C4	2.57	116.12	110.34
5	A	299	FUC	C1-O5-C5	2.67	116.50	112.38
5	A	298	MAN	C1-O5-C5	2.71	115.69	112.25
4	A	289	NAG	C8-C7-N2	2.76	121.38	116.11
4	A	291	BMA	O5-C5-C6	3.24	114.37	107.35
4	A	293	MAN	O5-C5-C6	3.51	114.96	107.35
5	A	294	NAG	C1-O5-C5	3.54	116.75	112.25
5	A	294	NAG	C8-C7-N2	3.58	122.97	116.11
4	A	289	NAG	O5-C5-C6	3.88	115.74	107.35
5	A	296	BMA	C1-O5-C5	4.59	118.07	112.25
4	A	291	BMA	C1-C2-C3	4.92	115.36	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	289	NAG	1	0
4	A	290	NAG	2	0
4	A	291	BMA	1	0
4	A	292	MAN	1	1
4	A	293	MAN	2	0

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	14,14,15	0.82	1 (7%)	15,19,21	1.20	3 (20%)
6	C6Q	A	300	-	46,47,47	0.82	2 (4%)	54,58,58	1.49	11 (20%)
7	PLM	A	301	-	14,17,17	0.42	0	14,17,17	0.98	1 (7%)
8	EDO	A	302	-	3,3,3	0.60	0	2,2,2	0.41	0
8	EDO	A	303	-	3,3,3	0.69	0	2,2,2	0.36	0
8	EDO	A	304[A]	-	3,3,3	0.55	0	2,2,2	0.78	0
8	EDO	A	304[B]	-	3,3,3	0.60	0	2,2,2	0.57	0
8	EDO	B	100	-	3,3,3	0.75	0	2,2,2	0.52	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	C6Q	A	300	-	-	0/41/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PLM	A	301	-	-	0/13/15/15	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	A	304[A]	-	-	0/1/1/1	0/0/0/0
8	EDO	A	304[B]	-	-	0/1/1/1	0/0/0/0
8	EDO	B	100	-	-	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)
3	A	288	NAG	C1-C2	2.02	1.55	1.52
6	A	300	C6Q	C18-C17	2.07	1.56	1.52
6	A	300	C6Q	O18-C19	3.45	1.46	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	300	C6Q	O19-C19-C20	-3.53	103.03	110.28
7	A	301	PLM	C4-C3-C2	-2.66	102.67	113.90
6	A	300	C6Q	C24-C23-C22	-2.37	107.16	113.02
6	A	300	C6Q	C13-C14-C15	-2.14	110.38	114.20
6	A	300	C6Q	O25-C25-N	-2.10	119.44	123.01
3	A	288	NAG	O3-C3-C2	-2.05	105.06	109.11
6	A	300	C6Q	C29-C30-CI	-2.04	105.96	113.71
3	A	288	NAG	C1-O5-C5	-2.02	109.68	112.25
6	A	300	C6Q	O24-C24-C23	-2.01	104.70	111.33
6	A	300	C6Q	O19-C23-C22	2.05	113.53	109.68
3	A	288	NAG	C4-C3-C2	2.07	114.44	111.23
6	A	300	C6Q	O18-C19-C20	2.14	110.74	108.04
6	A	300	C6Q	O25-C25-C26	2.17	125.73	121.98
6	A	300	C6Q	C19-O19-C23	3.19	119.94	113.75
6	A	300	C6Q	C18-O18-C19	3.90	122.02	113.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	288	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	300	C6Q	1	0
7	A	301	PLM	2	0
8	A	303	EDO	2	0
8	A	304[B]	EDO	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

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%)	0.52	28 (10%) 8 9	13, 19, 39, 56	0
2	B	99/99 (100%)	0.04	3 (3%) 54 58	13, 19, 31, 36	0
All	All	367/386 (95%)	0.39	31 (8%) 14 15	13, 19, 37, 56	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	PRO	8.8
1	A	203	HIS	6.7
1	A	255	ALA	6.7
1	A	110	ASN	6.3
1	A	280	GLY	6.3
1	A	281	SER	6.2
1	A	109	GLY	5.3
1	A	111	ALA	4.5
1	A	93	ASP	4.2
1	A	7	ASN	4.1
1	A	107	TYR	3.8
1	A	254	GLU	3.5
2	B	47	PRO	3.5
1	A	253	VAL	3.4
2	B	48	LYS	3.3
1	A	90	PRO	3.2
1	A	256	GLY	3.2
1	A	22	SER	3.2
1	A	204	ARG	3.1
1	A	252	ASP	2.7
1	A	21	ARG	2.7
2	B	1	ILE	2.6
1	A	259	ALA	2.5
1	A	271	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	257	GLU	2.2
1	A	94	TYR	2.2
1	A	91	LYS	2.2
1	A	89	SER	2.1
1	A	98	ILE	2.1
1	A	163	LEU	2.0
1	A	23	TRP	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
4	MAN	A	292	11/12	0.77	0.27	9.08	38,42,53,56	0
5	MAN	A	297	11/12	0.89	0.22	2.06	34,39,43,45	0
5	FUC	A	299	10/11	0.73	0.20	1.66	38,40,44,47	0
4	NAG	A	289	14/15	0.94	0.11	0.02	31,41,47,48	0
5	NAG	A	294	14/15	0.93	0.07	-0.51	25,29,31,34	0
5	NAG	A	295	14/15	0.93	0.14	-	31,36,39,40	0
4	NAG	A	290	14/15	0.78	0.36	-	53,59,61,64	0
5	BMA	A	296	11/12	0.80	0.25	-	37,39,44,49	0
4	BMA	A	291	11/12	0.76	0.42	-	56,62,66,70	0
4	MAN	A	293	11/12	0.59	0.43	-	65,69,71,73	0
5	MAN	A	298	11/12	0.82	0.30	-	56,59,60,63	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(\AA^2)	Q<0.9
7	PLM	A	301	18/18	0.83	0.24	3.91	35,41,44,45	0
8	EDO	B	100	4/4	0.94	0.16	3.15	23,25,27,32	0
8	EDO	A	304[A]	4/4	0.91	0.17	2.47	30,32,33,37	4
8	EDO	A	304[B]	4/4	0.91	0.17	2.33	25,27,27,30	4
8	EDO	A	302	4/4	0.95	0.18	2.12	25,25,27,31	0
6	C6Q	A	300	46/46	0.92	0.14	1.02	22,31,42,53	0
8	EDO	A	303	4/4	0.92	0.12	0.71	24,33,33,39	0
3	NAG	A	288	14/15	0.63	0.45	-	57,64,73,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.