



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:27 AM GMT

PDB ID : 3GMR  
Title : Structure of mouse CD1d in complex with C8Ph, different space group  
Authors : Schiefner, A.; Wilson, I.A.  
Deposited on : 2009-03-14  
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

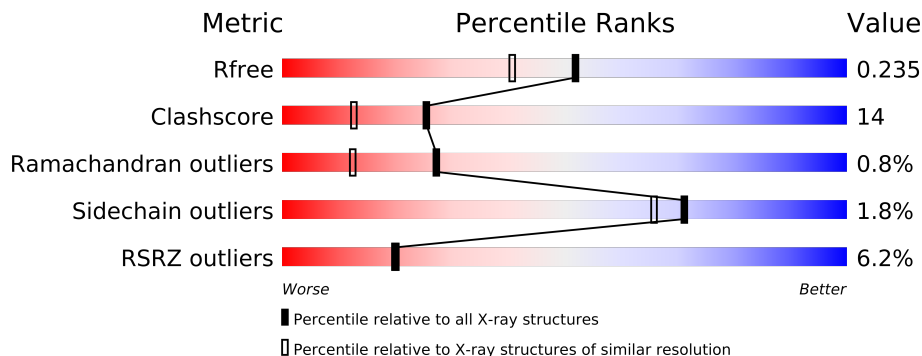
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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  $\geq 3$ , 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
6	PLM	A	299	-	X
7	EDO	A	301	-	X
7	EDO	A	302[A]	-	X
7	EDO	A	302[B]	-	X
8	PG4	B	100	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3613 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	273	2252	1430	390	419	13	0	8	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	827	528	140	152	7	0	1	0

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

There are 18 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
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

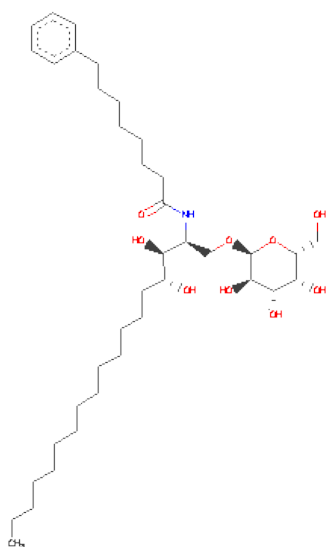
- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	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 5 is N-{(1S,2S,3R)-1-[(ALPHA-D-GALACTOPYRANOSYLOXY)METHYL]-2,3-DIHYDROXYHEPTADECYL}-8-PHENYLOCTANAMIDE (three-letter code: C8P) (formula: C<sub>38</sub>H<sub>67</sub>NO<sub>9</sub>).



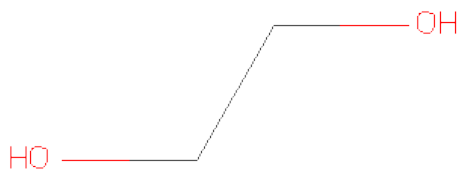
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			48	38	1	9		

- Molecule 6 is PALMITIC ACID (three-letter code: PLM) (formula:  $C_{16}H_{32}O_2$ ).



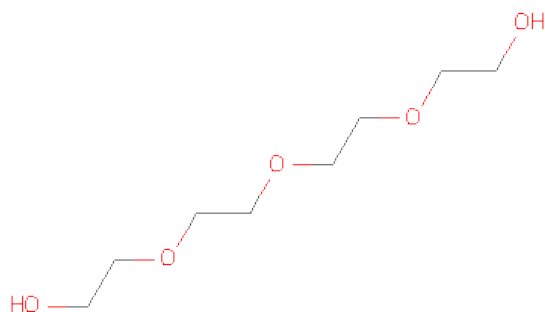
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			18	16	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is water.

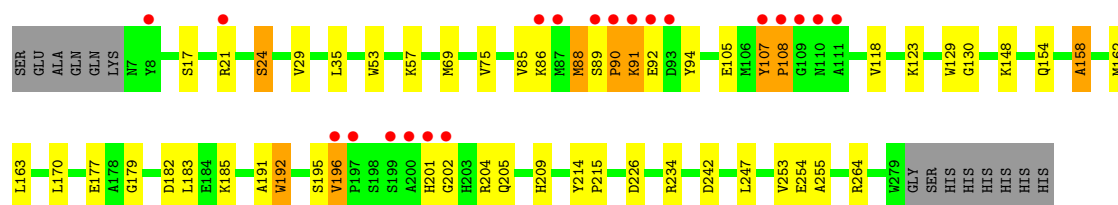
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	205	Total	O	0	0
			205	205		
9	B	103	Total	O	0	0
			103	103		

### 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.

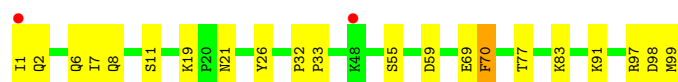
- Molecule 1: T-cell surface glycoprotein CD1d1

Chain A: 



- Molecule 2: Beta-2 microglobulin

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.27Å 107.23Å 109.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 39.43 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-1.90) 99.2 (39.43-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.97 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.186 , 0.230 0.195 , 0.235	Depositor DCC
$R_{free}$ test set	1995 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 31.2	EDS
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 39777 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3613	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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, PG4, 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	1.08	3/2323 (0.1%)	0.95	5/3157 (0.2%)
2	B	1.13	1/853 (0.1%)	0.98	1/1156 (0.1%)
All	All	1.09	4/3176 (0.1%)	0.95	6/4313 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	ALA	CA-CB	6.22	1.65	1.52
1	A	75	VAL	CB-CG1	5.87	1.65	1.52
2	B	26	TYR	CD2-CE2	5.84	1.48	1.39
1	A	192	TRP	CE3-CZ3	5.66	1.48	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	A	264	ARG	NE-CZ-NH1	8.11	124.36	120.30
2	B	59	ASP	CB-CG-OD1	7.05	124.65	118.30
1	A	242	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	170	LEU	CB-CG-CD1	-5.56	101.55	111.00
1	A	253	VAL	CG1-CB-CG2	-5.11	102.72	110.90

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	2252	0	2147	57	0
2	B	827	0	804	21	0
3	A	56	0	50	0	0
4	A	71	0	61	13	0
5	A	48	0	67	2	0
6	A	18	0	31	3	0
7	A	20	0	30	0	0
8	B	13	0	18	14	0
9	A	205	0	0	11	0
9	B	103	0	0	6	0
All	All	3613	0	3208	89	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 14.

All (89) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:295:MAN:H2	4:A:296:MAN:H5	1.12	1.09
4:A:295:MAN:H2	4:A:296:MAN:C5	1.93	0.98
2:B:11:SER:OG	8:B:100:PG4:H72	1.67	0.94
1:A:196:VAL:HG11	2:B:99:MET:HG3	1.50	0.93
4:A:295:MAN:C2	4:A:296:MAN:H5	1.99	0.91
1:A:192:TRP:HE1	8:B:100:PG4:H81	1.39	0.88
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.57	0.86
1:A:195:SER:OG	1:A:204[B]:ARG:NH1	2.10	0.84
1:A:89:SER:HB2	1:A:90:PRO:O	1.76	0.84
4:A:297:FUC:C6	9:A:389:HOH:O	2.29	0.80
1:A:192:TRP:HE1	8:B:100:PG4:C8	1.96	0.78
1:A:130:GLY:H	4:A:297:FUC:H61	1.49	0.76
1:A:192:TRP:NE1	8:B:100:PG4:H81	1.99	0.76
4:A:296:MAN:O4	9:A:463:HOH:O	2.05	0.75
1:A:89:SER:HA	1:A:90:PRO:C	2.07	0.74
1:A:130:GLY:H	4:A:297:FUC:C6	2.02	0.73
1:A:130:GLY:N	4:A:297:FUC:H61	2.04	0.72
1:A:201:HIS:CD2	1:A:202:GLY:N	2.59	0.71
1:A:107:TYR:CB	1:A:108:PRO:HD2	2.24	0.67
4:A:297:FUC:H5	9:A:389:HOH:O	1.94	0.66
2:B:8:GLN:HB3	8:B:100:PG4:H11	1.76	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:196:VAL:HG11	2:B:99:MET:CG	2.24	0.65
4:A:297:FUC:C5	9:A:389:HOH:O	2.44	0.65
1:A:158:ALA:O	1:A:162:MET:HG3	1.96	0.64
4:A:297:FUC:H62	9:A:389:HOH:O	1.95	0.63
1:A:105:GLU:HG2	1:A:107:TYR:CE1	2.34	0.62
2:B:99:MET:OXT	8:B:100:PG4:H42	1.98	0.62
8:B:100:PG4:C5	8:B:100:PG4:H82	2.25	0.61
1:A:89:SER:CA	1:A:90:PRO:C	2.69	0.61
1:A:234[B]:ARG:HD2	9:A:383:HOH:O	2.02	0.60
1:A:107:TYR:HB3	1:A:108:PRO:CD	2.31	0.59
2:B:69:GLU:HG3	9:B:140:HOH:O	2.01	0.59
1:A:88:MET:O	1:A:91:LYS:HB2	2.03	0.59
1:A:107:TYR:CB	1:A:108:PRO:CD	2.81	0.58
2:B:1:ILE:CG1	2:B:2:GLN:H	2.17	0.58
1:A:201:HIS:CD2	1:A:202:GLY:H	2.24	0.54
2:B:32:PRO:HB2	2:B:33:PRO:HD2	1.89	0.54
1:A:234[A]:ARG:HB2	9:A:383:HOH:O	2.08	0.53
2:B:1:ILE:HG12	2:B:2:GLN:H	1.74	0.52
1:A:57:LYS:HD2	1:A:177:GLU:OE1	2.09	0.52
2:B:77:THR:HG22	9:B:198:HOH:O	2.10	0.52
1:A:192:TRP:CE2	8:B:100:PG4:H81	2.45	0.51
1:A:195:SER:OG	1:A:204[B]:ARG:CZ	2.59	0.51
1:A:85:VAL:HG11	1:A:94:TYR:CZ	2.45	0.51
1:A:88:MET:CE	1:A:92:GLU:HG2	2.41	0.51
8:B:100:PG4:H22	9:B:104:HOH:O	2.11	0.51
1:A:148:LYS:HG3	9:A:376:HOH:O	2.11	0.51
1:A:196:VAL:HG23	1:A:205:GLN:HB3	1.93	0.51
1:A:209:HIS:HE1	2:B:99:MET:OXT	1.95	0.50
1:A:21:ARG:HH11	1:A:21:ARG:HG3	1.77	0.50
1:A:254:GLU:HG2	1:A:255:ALA:N	2.26	0.49
1:A:86:LYS:HG3	9:A:388:HOH:O	2.13	0.48
8:B:100:PG4:C5	8:B:100:PG4:C8	2.90	0.48
1:A:118:VAL:HG11	5:A:298:C8P:H6	1.94	0.48
1:A:209:HIS:CE1	8:B:100:PG4:H51	2.49	0.47
1:A:234[A]:ARG:HG2	1:A:247:LEU:HD11	1.96	0.47
1:A:53:TRP:CG	1:A:179:GLY:HA2	2.49	0.47
2:B:1:ILE:CG1	2:B:2:GLN:N	2.76	0.47
1:A:21:ARG:NH1	1:A:21:ARG:HG3	2.30	0.47
1:A:182:ASP:O	1:A:185:LYS:HG2	2.14	0.47
1:A:154:GLN:OE1	9:A:379:HOH:O	2.21	0.47
1:A:29[A]:VAL:HG21	2:B:55:SER:OG	2.15	0.47
1:A:195:SER:O	2:B:98:ASP:HB3	2.15	0.46

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:97:ARG:O	8:B:100:PG4:O5	2.32	0.46
1:A:192:TRP:CZ2	8:B:100:PG4:H81	2.51	0.46
1:A:89:SER:HB2	1:A:90:PRO:C	2.35	0.45
1:A:88:MET:HE3	1:A:92:GLU:HG2	1.98	0.45
8:B:100:PG4:C8	8:B:100:PG4:H52	2.47	0.45
2:B:6[A]:GLN:HG2	9:B:101:HOH:O	2.16	0.45
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.53	0.44
1:A:17:SER:O	1:A:24:SER:HA	2.16	0.44
1:A:89:SER:HA	1:A:91:LYS:N	2.32	0.44
5:A:298:C8P:H31A	6:A:299:PLM:HG3	2.00	0.44
1:A:89:SER:CB	1:A:90:PRO:O	2.59	0.43
1:A:35:LEU:HD12	1:A:183:LEU:HD23	2.01	0.43
2:B:1:ILE:HG12	2:B:2:GLN:N	2.34	0.43
2:B:19:LYS:HD3	9:B:237:HOH:O	2.18	0.43
1:A:201:HIS:HD2	1:A:202:GLY:H	1.66	0.43
6:A:299:PLM:HC2	6:A:299:PLM:HF2	1.76	0.43
6:A:299:PLM:HD1	6:A:299:PLM:HA1	1.80	0.42
1:A:191:ALA:HA	1:A:209:HIS:O	2.19	0.42
4:A:295:MAN:H2	4:A:296:MAN:O5	2.17	0.42
1:A:129:TRP:CD1	4:A:296:MAN:H2	2.54	0.42
1:A:214:TYR:CG	1:A:215:PRO:HA	2.55	0.42
2:B:7:ILE:HD12	2:B:91:LYS:HD3	2.01	0.41
1:A:123:LYS:HD3	9:A:408:HOH:O	2.20	0.41
1:A:53:TRP:CD1	1:A:179:GLY:HA2	2.55	0.41
2:B:83:LYS:HG3	9:B:201:HOH:O	2.21	0.41
1:A:69:MET:SD	1:A:163:LEU:HD11	2.62	0.40

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	279/287 (97%)	272 (98%)	4 (1%)	3 (1%)	21	7
2	B	98/99 (99%)	96 (98%)	2 (2%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	377/386 (98%)	368 (98%)	6 (2%)	3 (1%)	27	12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	91	LYS
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	246/250 (98%)	240 (98%)	6 (2%)	61	53
2	B	94/93 (101%)	93 (99%)	1 (1%)	84	82
All	All	340/343 (99%)	333 (98%)	7 (2%)	71	59

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

Mol	Chain	Res	Type
1	A	24	SER
1	A	88	MET
1	A	107	TYR
1	A	196	VAL
1	A	226[A]	ASP
1	A	226[B]	ASP
2	B	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	201	HIS
2	B	31	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 ⓘ

10 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$
3	NAG	A	288	1,3	12,14,15	0.72	0	15,19,21	1.79	3 (20%)
3	NAG	A	289	3	12,14,15	0.42	0	15,19,21	1.42	1 (6%)
3	NAG	A	290	1,3	12,14,15	0.90	1 (8%)	15,19,21	1.84	1 (6%)
3	NAG	A	291	3	12,14,15	0.65	0	15,19,21	1.50	1 (6%)
4	NAG	A	292	1,4	12,14,15	1.25	1 (8%)	15,19,21	1.61	2 (13%)
4	NAG	A	293	4	12,14,15	0.76	0	15,19,21	1.16	1 (6%)
4	BMA	A	294	4	10,11,12	0.77	0	11,15,17	1.62	1 (9%)
4	MAN	A	295	4	10,11,12	0.76	0	11,15,17	2.32	5 (45%)
4	MAN	A	296	4	10,11,12	0.64	0	11,15,17	2.68	5 (45%)
4	FUC	A	297	4	9,10,11	0.99	0	10,14,16	2.57	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
3	NAG	A	288	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	289	3	-	0/6/23/26	0/1/1/1
3	NAG	A	290	1,3	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	291	3	-	0/6/23/26	0/1/1/1
4	NAG	A	292	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	293	4	-	0/6/23/26	0/1/1/1
4	BMA	A	294	4	-	0/2/19/22	0/1/1/1
4	MAN	A	295	4	-	0/2/19/22	0/1/1/1
4	MAN	A	296	4	-	0/2/19/22	0/1/1/1
4	FUC	A	297	4	-	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	292	NAG	O5-C5	-3.79	1.38	1.45
3	A	290	NAG	O5-C5	-2.19	1.41	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	296	MAN	O5-C5-C6	6.33	113.62	106.98
3	A	290	NAG	O5-C5-C6	5.90	113.17	106.98
3	A	291	NAG	O5-C5-C6	5.06	112.29	106.98
3	A	288	NAG	O5-C5-C6	4.76	111.98	106.98
4	A	295	MAN	O5-C5-C6	4.72	111.93	106.98
4	A	297	FUC	O4-C4-C5	-4.21	100.04	109.78
4	A	292	NAG	O5-C5-C6	4.17	111.36	106.98
4	A	296	MAN	O5-C5-C4	3.87	115.57	110.65
4	A	297	FUC	C6-C5-C4	-3.61	107.19	113.06
3	A	289	NAG	O5-C5-C4	3.61	115.24	110.65
4	A	295	MAN	O5-C5-C4	-3.50	106.21	110.65
3	A	288	NAG	O5-C5-C4	-3.48	106.23	110.65
4	A	294	BMA	O5-C5-C6	3.40	110.55	106.98
4	A	295	MAN	C4-C3-C2	3.36	115.02	110.50
4	A	297	FUC	O2-C2-C3	3.25	117.18	110.18
4	A	297	FUC	O3-C3-C2	3.12	115.64	109.94
4	A	297	FUC	O4-C4-C3	2.84	116.72	110.35
4	A	296	MAN	C3-C4-C5	2.48	114.64	110.20
3	A	288	NAG	O3-C3-C4	-2.36	105.05	110.35
4	A	293	NAG	O3-C3-C4	-2.32	105.16	110.35
4	A	292	NAG	C8-C7-N2	2.26	120.53	116.11
4	A	296	MAN	C6-C5-C4	-2.17	107.75	113.00
4	A	295	MAN	O4-C4-C3	-2.07	105.70	110.35
4	A	295	MAN	O2-C2-C3	2.06	114.61	110.18
4	A	296	MAN	O3-C3-C2	2.03	113.66	109.94

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	$\# Z  > 2$
5	C8P	A	298	-	49,49,49	0.77	1 (2%)	60,60,60	1.24	5 (8%)
6	PLM	A	299	-	17,17,17	0.63	0	17,17,17	1.23	2 (11%)
7	EDO	A	300	-	3,3,3	0.41	0	2,2,2	0.69	0
7	EDO	A	301	-	3,3,3	0.85	0	2,2,2	0.57	0
7	EDO	A	302[A]	-	3,3,3	0.63	0	2,2,2	1.66	0
7	EDO	A	302[B]	-	3,3,3	0.47	0	2,2,2	1.08	0
7	EDO	A	303	-	3,3,3	0.38	0	2,2,2	0.56	0
8	PG4	B	100	-	12,12,12	1.04	0	11,11,11	1.29	2 (18%)

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	C8P	A	298	-	-	0/43/63/63	0/2/2/2
6	PLM	A	299	-	-	0/15/15/15	0/0/0/0
7	EDO	A	300	-	-	0/1/1/1	0/0/0/0
7	EDO	A	301	-	-	0/1/1/1	0/0/0/0
7	EDO	A	302[A]	-	-	0/1/1/1	0/0/0/0
7	EDO	A	302[B]	-	-	0/1/1/1	0/0/0/0
7	EDO	A	303	-	-	0/1/1/1	0/0/0/0
8	PG4	B	100	-	-	0/10/10/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	298	C8P	O18-C19	2.74	1.45	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	A	298	C8P	C26-C25-N	3.67	122.81	115.83
6	A	299	PLM	O1-C1-C2	3.31	125.93	114.22
5	A	298	C8P	O25-C25-N	-3.19	117.53	123.08
6	A	299	PLM	O1-C1-O2	-3.05	115.53	123.30
5	A	298	C8P	C18-C17-C16	-2.92	106.24	112.53
8	B	100	PG4	O4-C6-C5	-2.92	97.23	110.47
5	A	298	C8P	C16-C17-N	-2.27	106.30	110.91
5	A	298	C8P	O18-C19-C20	2.17	110.95	108.18
8	B	100	PG4	O3-C5-C6	2.01	119.59	110.47

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	273/287 (95%)	0.29	20 (7%) 15 14	3, 12, 32, 48	0
2	B	99/99 (100%)	0.12	2 (2%) 62 63	5, 12, 26, 36	0
All	All	372/386 (96%)	0.24	22 (5%) 20 22	3, 12, 30, 48	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	PRO	7.3
1	A	109	GLY	5.6
1	A	108	PRO	5.3
1	A	110	ASN	5.1
1	A	107	TYR	4.9
1	A	200	ALA	4.5
1	A	89	SER	4.4
1	A	201	HIS	4.3
1	A	111	ALA	3.7
1	A	87	MET	3.6
1	A	21	ARG	3.4
1	A	92	GLU	3.3
1	A	197	PRO	3.1
1	A	93	ASP	3.0
1	A	91	LYS	2.8
1	A	86	LYS	2.5
1	A	199	SER	2.4
2	B	1	ILE	2.3
2	B	48	LYS	2.2
1	A	8	TYR	2.2
1	A	196	VAL	2.1
1	A	202	GLY	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	MAN	A	296	11/12	0.44	25.35	44,48,51,53	0
4	FUC	A	297	10/11	0.49	9.49	45,51,52,53	0
3	NAG	A	288	14/15	0.32	7.94	45,56,62,63	0
4	BMA	A	294	11/12	0.36	4.44	53,56,58,58	0
4	MAN	A	295	11/12	0.26	3.27	51,56,60,62	0
4	NAG	A	293	14/15	0.24	2.34	39,45,51,55	0
4	NAG	A	292	14/15	0.11	0.37	21,26,36,44	0
3	NAG	A	290	14/15	0.11	0.23	28,35,42,51	0
3	NAG	A	289	14/15	0.31	-	61,65,68,68	0
3	NAG	A	291	14/15	0.39	-	56,59,63,66	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	EDO	A	302[B]	4/4	0.19	5.43	20,27,28,33	4
7	EDO	A	302[A]	4/4	0.19	5.43	20,22,22,23	4
7	EDO	A	301	4/4	0.15	5.31	20,23,25,27	0
6	PLM	A	299	18/18	0.20	5.27	31,36,40,43	0
8	PG4	B	100	13/13	0.19	2.38	18,32,38,38	0
7	EDO	A	303	4/4	0.16	1.88	26,34,36,38	0
7	EDO	A	300	4/4	0.12	1.63	16,19,26,30	0
5	C8P	A	298	48/48	0.13	0.34	18,28,39,43	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.