



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:57 AM GMT

PDB ID : 3GMP  
Title : Structure of mouse CD1d in complex with PBS-25  
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](mailto: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.

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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

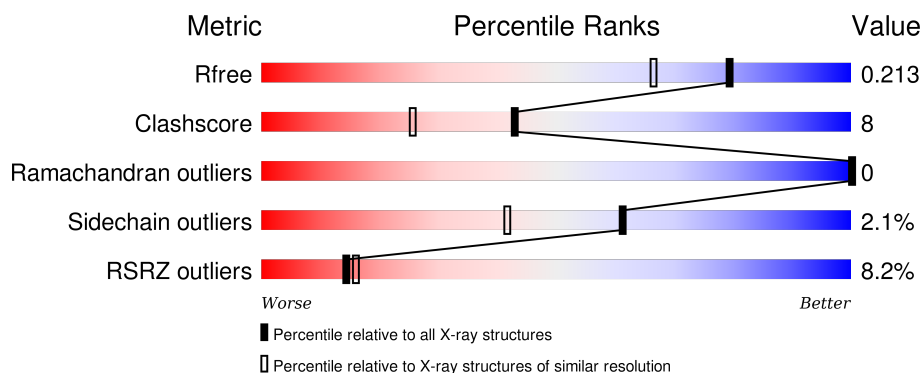
# 1 Overall quality at a glance

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  $\geq 3$ , 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	<div> <div>9%</div> <div>77%</div> <div>15%</div> <div>7%</div> </div>
2	B	99	<div> <div>3%</div> <div>89%</div> <div>11%</div> </div>

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
5	FUC	A	299	-	-	-	X
7	PLM	A	301	-	-	-	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 3591 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	7	0
			2219	1410	385	411	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: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

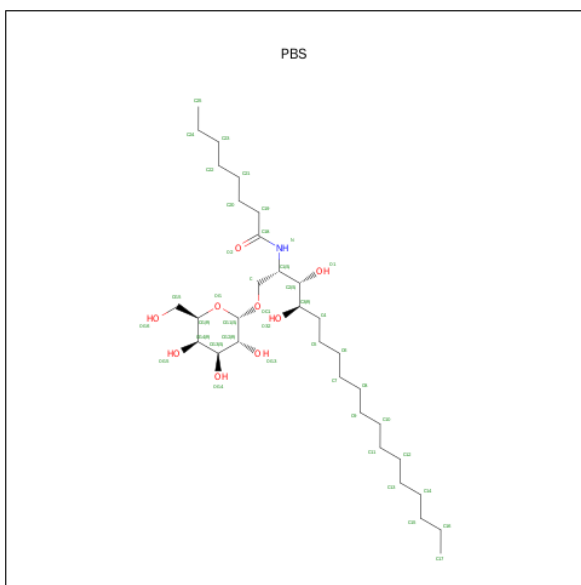
- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

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).

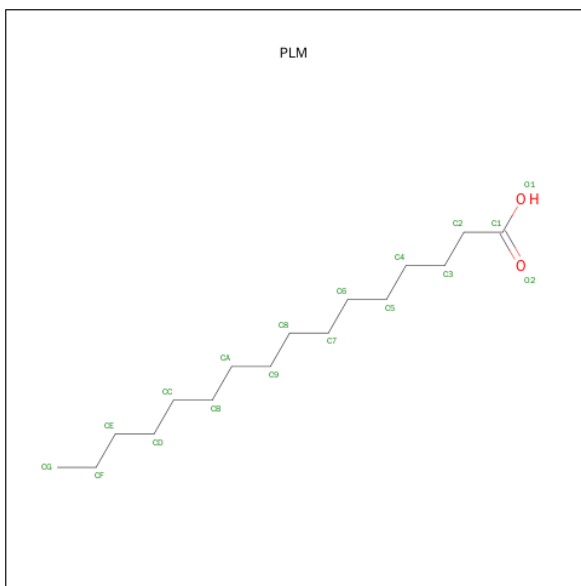
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 6 is (2S,3S,4R)-N-OCTANOYL-1-[(ALPHA-D-GALACTOPYRANOSYL)OXY]-2-AMINO-OCTADECANE-3,4-DIOL (three-letter code: PBS) (formula: C<sub>32</sub>H<sub>63</sub>NO<sub>9</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			42	32	1	9		

- Molecule 7 is PALMITIC ACID (three-letter code: PLM) (formula:  $\text{C}_{16}\text{H}_{32}\text{O}_2$ ).



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:  $\text{C}_2\text{H}_6\text{O}_2$ ).



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		

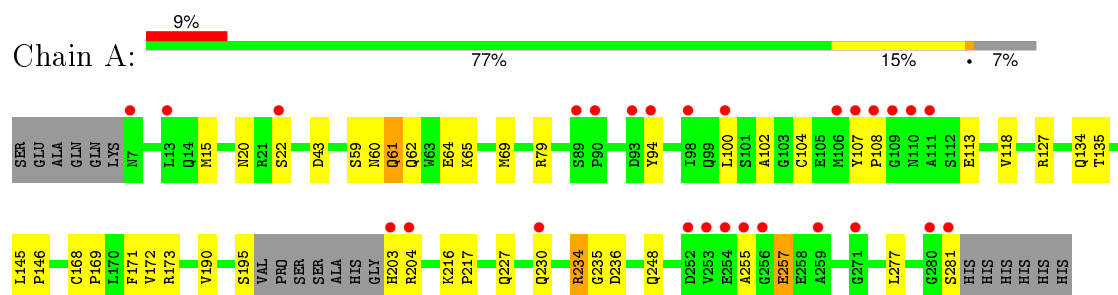
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	218	Total	O	0	5
			223	223		
9	B	89	Total	O	0	1
			90	90		

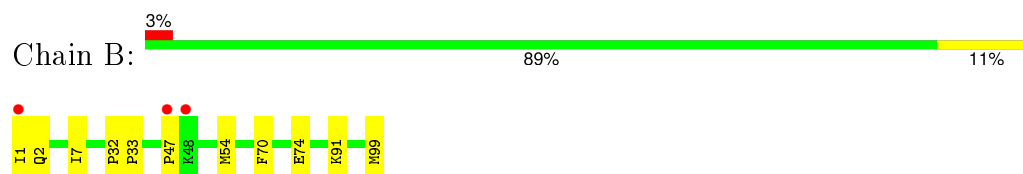
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	41.71Å 97.73Å 55.49Å 90.00° 106.52° 90.00°	Depositor
Resolution (Å)	27.78 – 1.70 27.78 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.78-1.70) 99.6 (27.78-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.176 , 0.216 0.179 , 0.213	Depositor DCC
$R_{free}$ test set	2361 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 46664 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3591	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, PBS, 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	1.04	2/2282 (0.1%)	0.95	0/3098
2	B	1.14	2/859 (0.2%)	1.01	0/1164
All	All	1.07	4/3141 (0.1%)	0.97	0/4262

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	MET	CG-SD	-8.15	1.59	1.81
2	B	54	MET	CB-CG	6.02	1.70	1.51
1	A	104	CYS	CB-SG	5.92	1.92	1.82
1	A	171	PHE	CD1-CE1	5.04	1.49	1.39

There are no bond angle outliers.

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	2219	0	2111	44	3
2	B	833	0	806	10	1
3	A	14	0	13	3	0
4	A	61	0	52	0	1
5	A	71	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	42	0	63	1	0
7	A	18	0	31	0	0
8	A	16	0	24	2	0
8	B	4	0	6	0	0
9	A	223	0	0	3	2
9	B	90	0	0	4	1
All	All	3591	0	3167	53	5

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 8.

All (53) 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)
1:A:203:HIS:N	1:A:255:ALA:HB2	1.60	1.16
1:A:257:GLU:O	1:A:257:GLU:HG2	1.41	1.11
1:A:59:SER:OG	1:A:62:GLN:HG3	1.48	1.10
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.18	1.09
1:A:234:ARG:HH11	1:A:234:ARG:HG2	1.10	1.08
1:A:60:ASN:O	1:A:64:GLU:HG2	1.66	0.95
1:A:107:TYR:CB	1:A:108:PRO:HD2	2.00	0.89
1:A:22:SER:CB	3:A:288:NAG:H82	2.02	0.89
1:A:257:GLU:O	1:A:257:GLU:CG	2.23	0.85
1:A:61:GLN:HE22	1:A:65:LYS:HE3	1.44	0.82
1:A:234:ARG:NH1	1:A:234:ARG:HG2	1.90	0.79
1:A:248:GLN:OE1	2:B:99:MET:HG2	1.84	0.78
1:A:22:SER:HB2	3:A:288:NAG:H82	1.68	0.76
1:A:118:VAL:HG11	6:A:300:PBS:H132	1.69	0.75
1:A:203:HIS:N	1:A:255:ALA:CB	2.47	0.74
1:A:248:GLN:HG3	8:A:303:EDO:H21	1.70	0.74
1:A:107:TYR:HB3	1:A:108:PRO:CD	2.09	0.74
1:A:236:ASP:OD2	9:A:519:HOH:O	2.06	0.73
1:A:234:ARG:CG	1:A:234:ARG:HH11	1.98	0.71
1:A:61:GLN:HE22	1:A:65:LYS:CE	2.05	0.68
1:A:22:SER:HB3	3:A:288:NAG:H82	1.76	0.66
1:A:61:GLN:NE2	1:A:65:LYS:HE3	2.11	0.66
2:B:1:ILE:HG13	2:B:2:GLN:N	2.13	0.64
2:B:2:GLN:HG2	9:B:268:HOH:O	2.02	0.59
2:B:2:GLN:NE2	9:B:268:HOH:O	1.97	0.59
2:B:7:ILE:HD12	2:B:91:LYS:HD3	1.84	0.59
1:A:107:TYR:CB	1:A:108:PRO:CD	2.75	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:CG	1:A:234:ARG:NH1	2.65	0.55
1:A:195:SER:OG	1:A:204:ARG:NH1	2.41	0.53
1:A:100[A]:LEU:HD21	1:A:102:ALA:HB2	1.90	0.53
1:A:234:ARG:HD2	9:A:451:HOH:O	2.09	0.52
1:A:248:GLN:HG3	8:A:303:EDO:C2	2.39	0.51
2:B:7:ILE:CD1	2:B:91:LYS:HD3	2.40	0.51
1:A:173:ARG:HH11	1:A:173:ARG:HG2	1.76	0.51
1:A:61:GLN:NE2	1:A:65:LYS:CE	2.73	0.50
1:A:134[B]:GLN:HG2	1:A:135:THR:O	2.14	0.48
2:B:74:GLU:OE1	2:B:74:GLU:HA	2.14	0.48
1:A:100[A]:LEU:C	1:A:100[A]:LEU:HD23	2.35	0.47
1:A:168:CYS:HB3	1:A:169:PRO:CD	2.45	0.47
1:A:20:ASN:HA	1:A:94:TYR:CD1	2.51	0.46
1:A:69:MET:HE2	1:A:69:MET:HB2	1.60	0.46
1:A:59:SER:HG	1:A:62:GLN:HG3	1.72	0.46
2:B:47:PRO:O	9:B:261:HOH:O	2.21	0.45
1:A:230:GLN:HA	1:A:230:GLN:OE1	2.17	0.45
1:A:127:ARG:HE	1:A:134[B]:GLN:CD	2.22	0.43
1:A:168:CYS:O	1:A:172:VAL:HG23	2.19	0.43
2:B:32:PRO:HB2	2:B:33:PRO:HD2	2.00	0.43
2:B:2:GLN:CG	9:B:268:HOH:O	2.64	0.42
1:A:234:ARG:NH1	1:A:235:GLY:O	2.53	0.41
1:A:145:LEU:HB3	1:A:146:PRO:HD3	2.02	0.41
1:A:43:ASP:OD2	9:A:445:HOH:O	2.21	0.40
1:A:277:LEU:HA	1:A:277:LEU:HD23	1.80	0.40
1:A:216:LYS:N	1:A:217:PRO:CD	2.85	0.40

All (5) 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)
2:B:1:ILE:CD1	9:B:392:HOH:O[1_655]	1.51	0.69
1:A:79:ARG:NH1	1:A:230:GLN:NE2[2_555]	2.07	0.13
9:A:433:HOH:O	9:A:448:HOH:O[1_655]	2.10	0.10
1:A:190:VAL:CG2	4:A:292:MAN:O3[2_445]	2.10	0.10
1:A:227[A]:GLN:OE1	9:A:337:HOH:O[2_545]	2.13	0.07

## 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	271/287 (94%)	266 (98%)	5 (2%)	0	100	100
2	B	99/99 (100%)	97 (98%)	2 (2%)	0	100	100
All	All	370/386 (96%)	363 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	241/250 (96%)	235 (98%)	6 (2%)	55	34
2	B	95/93 (102%)	94 (99%)	1 (1%)	80	69
All	All	336/343 (98%)	329 (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	61	GLN
1	A	113	GLU
1	A	234	ARG
1	A	257	GLU
1	A	281	SER
2	B	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	229	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	14,14,15	0.68	0	15,19,21	1.80	6 (40%)
4	NAG	A	290	4	14,14,15	0.75	0	15,19,21	1.33	1 (6%)
4	BMA	A	291	4	11,11,12	0.50	0	14,15,17	1.94	3 (21%)
4	MAN	A	292	4	11,11,12	0.53	0	14,15,17	1.45	1 (7%)
4	MAN	A	293	4	11,11,12	0.54	0	14,15,17	1.74	3 (21%)
5	NAG	A	294	1,5	14,14,15	0.93	0	15,19,21	1.02	0
5	NAG	A	295	5	14,14,15	0.59	0	15,19,21	1.62	2 (13%)
5	BMA	A	296	5	11,11,12	0.85	0	14,15,17	1.96	6 (42%)
5	MAN	A	297	5	11,11,12	0.69	0	14,15,17	1.63	4 (28%)
5	MAN	A	298	5	11,11,12	0.62	0	14,15,17	1.93	4 (28%)
5	FUC	A	299	5	10,10,11	0.71	0	14,14,16	1.92	2 (14%)

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

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	291	BMA	C3-C4-C5	-5.08	101.34	110.20
5	A	295	NAG	C2-N2-C7	-4.80	116.87	123.04
5	A	299	FUC	O5-C1-C2	-4.59	103.41	110.86
5	A	298	MAN	O2-C2-C1	-4.16	100.87	109.21
4	A	293	MAN	C2-C3-C4	-4.05	104.15	111.04
5	A	297	MAN	O3-C3-C4	-3.38	102.72	110.34
4	A	290	NAG	C3-C4-C5	-3.20	104.61	110.20
4	A	289	NAG	C3-C4-C5	-3.16	104.69	110.20
5	A	298	MAN	C3-C4-C5	-3.01	104.94	110.20
4	A	292	MAN	C6-C5-C4	-2.96	105.72	113.02
5	A	298	MAN	C1-C2-C3	-2.91	106.10	109.54
5	A	296	BMA	O2-C2-C3	-2.79	104.51	110.12
5	A	296	BMA	O6-C6-C5	-2.57	102.85	111.33
4	A	289	NAG	O7-C7-C8	-2.54	117.41	122.06
5	A	296	BMA	O2-C2-C1	-2.51	104.18	109.21
5	A	296	BMA	O3-C3-C4	-2.33	105.10	110.34
4	A	293	MAN	C3-C4-C5	-2.30	106.18	110.20
5	A	297	MAN	O5-C1-C2	-2.12	107.42	110.86
5	A	297	MAN	O3-C3-C2	-2.12	106.17	110.00
4	A	289	NAG	C1-O5-C5	-2.03	109.67	112.25
4	A	291	BMA	O5-C5-C6	2.03	111.75	107.35
5	A	298	MAN	O3-C3-C2	2.08	113.75	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	295	NAG	C8-C7-N2	2.11	120.15	116.11
4	A	289	NAG	C8-C7-N2	2.21	120.33	116.11
5	A	296	BMA	C1-C2-C3	2.30	112.26	109.54
5	A	297	MAN	C1-O5-C5	2.44	115.34	112.25
4	A	289	NAG	O5-C5-C6	2.56	112.89	107.35
5	A	299	FUC	C1-O5-C5	3.11	117.19	112.38
4	A	289	NAG	C4-C3-C2	3.28	116.33	111.23
4	A	293	MAN	O5-C5-C6	3.51	114.95	107.35
5	A	296	BMA	C1-O5-C5	3.82	117.10	112.25
4	A	291	BMA	C1-C2-C3	3.87	114.12	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	292	MAN	0	1

## 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	0.88	0	15,19,21	1.32	2 (13%)
6	PBS	A	300	-	41,42,42	0.82	2 (4%)	47,51,51	1.55	10 (21%)
7	PLM	A	301	-	14,17,17	0.48	0	14,17,17	0.56	0
8	EDO	A	302	-	3,3,3	0.47	0	2,2,2	0.70	0
8	EDO	A	303	-	3,3,3	0.60	0	2,2,2	0.67	0
8	EDO	A	304[A]	-	3,3,3	0.39	0	2,2,2	0.84	0
8	EDO	A	304[B]	-	3,3,3	0.47	0	2,2,2	0.06	0
8	EDO	B	100	-	3,3,3	0.85	0	2,2,2	0.45	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	PBS	A	300	-	-	0/40/60/60	0/1/1/1
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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	300	PBS	OC1-CG1	2.68	1.45	1.40
6	A	300	PBS	C-C1	2.85	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	300	PBS	C7-C8-C9	-2.83	99.90	114.53
6	A	300	PBS	C1-N-C18	-2.79	118.43	123.61
6	A	300	PBS	C21-C20-C19	-2.71	103.36	113.29
6	A	300	PBS	C19-C18-N	-2.50	111.76	115.83
6	A	300	PBS	C8-C9-C10	-2.34	102.43	114.53
6	A	300	PBS	CG3-CG4-CG	-2.18	106.40	110.20
3	A	288	NAG	C1-O5-C5	-2.18	109.49	112.25
6	A	300	PBS	CG1-CG2-CG3	2.38	114.66	109.97
3	A	288	NAG	C4-C3-C2	2.74	115.49	111.23
6	A	300	PBS	O2-C18-C19	2.79	126.80	121.98
6	A	300	PBS	OG-CG-CG4	3.32	115.91	109.68
6	A	300	PBS	C-OC1-CG1	3.56	121.31	113.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	288	NAG	3	0
6	A	300	PBS	1	0
8	A	303	EDO	2	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, 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	268/287 (93%)	0.53	27 (10%) 9 9	14, 20, 39, 53	0
2	B	99/99 (100%)	0.05	3 (3%) 54 58	13, 19, 29, 36	0
All	All	367/386 (95%)	0.40	30 (8%) 14 16	13, 19, 36, 53	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	PRO	7.6
1	A	255	ALA	7.3
1	A	281	SER	6.8
1	A	109	GLY	6.7
1	A	203	HIS	6.0
1	A	280	GLY	6.0
1	A	110	ASN	5.6
1	A	256	GLY	4.4
1	A	93	ASP	4.3
1	A	111	ALA	4.2
1	A	107	TYR	4.2
2	B	1	ILE	4.0
1	A	7	ASN	4.0
2	B	48	LYS	3.2
1	A	100[A]	LEU	3.0
1	A	22	SER	3.0
1	A	90	PRO	2.8
1	A	204	ARG	2.7
1	A	254	GLU	2.7
1	A	259	ALA	2.6
1	A	253	VAL	2.4
1	A	252	ASP	2.4
2	B	47	PRO	2.3
1	A	89	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	230	GLN	2.2
1	A	98	ILE	2.2
1	A	94	TYR	2.2
1	A	13	LEU	2.1
1	A	271	GLY	2.0
1	A	106	MET	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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MAN	A	292	11/12	0.82	0.20	4.41	33,40,47,49	0
5	MAN	A	297	11/12	0.91	0.22	2.77	29,32,38,43	0
5	FUC	A	299	10/11	0.80	0.23	2.51	33,36,39,41	0
5	NAG	A	294	14/15	0.92	0.09	0.44	24,26,28,29	0
4	NAG	A	289	14/15	0.95	0.11	-0.12	28,36,41,42	0
4	BMA	A	291	11/12	0.74	0.40	-	52,57,61,63	0
4	NAG	A	290	14/15	0.81	0.32	-	49,52,54,57	0
5	NAG	A	295	14/15	0.91	0.13	-	30,33,36,38	0
5	BMA	A	296	11/12	0.86	0.21	-	32,34,41,46	0
5	MAN	A	298	11/12	0.84	0.27	-	52,55,56,58	0
4	MAN	A	293	11/12	0.54	0.38	-	60,63,65,67	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, 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	PLM	A	301	18/18	0.84	0.29	4.43	36,43,47,48	0
8	EDO	A	304[A]	4/4	0.94	0.17	2.71	27,29,29,31	4
8	EDO	A	304[B]	4/4	0.94	0.17	2.64	25,26,26,27	4
8	EDO	B	100	4/4	0.96	0.13	2.32	20,22,26,30	0
8	EDO	A	303	4/4	0.89	0.15	1.88	25,31,34,41	0
6	PBS	A	300	42/42	0.90	0.13	0.68	23,30,39,45	0
8	EDO	A	302	4/4	0.96	0.13	0.29	21,22,25,30	0
3	NAG	A	288	14/15	0.69	0.37	-	52,59,67,69	0

## 6.5 Other polymers

There are no such residues in this entry.