W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 01:39 PM GMT

PDB ID : 2H26
Title : human CD1b in complex with endogenous phosphatidylcholine and spacer
Authors : Garcia-Alles, L.F.; Maveyraud, L.; Vallina, A.T.; Guillet, V.; Mourey, L.
Deposited on : 2006-05-18
Resolution : 1.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
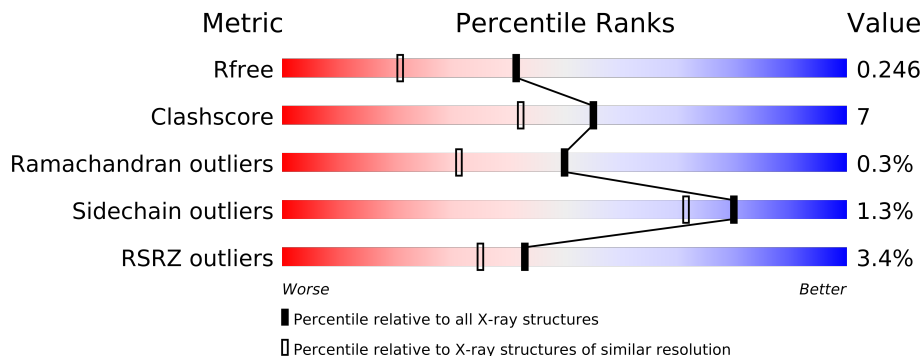
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

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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	Percentile Ranks	Value
Rfree		0.246
Clashscore		7
Ramachandran outliers		0.3%
Sidechain outliers		1.3%
RSRZ outliers		3.4%

Worse ← → Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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	286	
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
4	SO4	B	301	-	X
5	6PL	A	311	-	X
6	6UL	A	312	-	X
7	GOL	A	303	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 3423 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 CD1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total 2182	C 1400	N 368	O 404	S 10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	ILE	-	SEE REMARK 999	UNP P29016
A	901	UNK	-	SEE REMARK 999	UNP P29016
A	902	UNK	-	SEE REMARK 999	UNP P29016
A	903	UNK	-	SEE REMARK 999	UNP P29016
A	904	UNK	-	SEE REMARK 999	UNP P29016
A	905	UNK	-	SEE REMARK 999	UNP P29016

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total 818	C 520	N 137	O 158	S 3	0	2	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total 24	C 14	N 1	O 9	0	0
3	A	2	Total 24	C 14	N 1	O 9	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	ILE	-	SEE REMARK 999	UNP P29016
A	901	UNK	-	SEE REMARK 999	UNP P29016

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Chain	Residue	Modelled	Actual	Comment	Reference
A	902	UNK	-	SEE REMARK 999	UNP P29016
A	903	UNK	-	SEE REMARK 999	UNP P29016
A	904	UNK	-	SEE REMARK 999	UNP P29016
A	905	UNK	-	SEE REMARK 999	UNP P29016
A	281	ILE	-	SEE REMARK 999	UNP P29016
A	901	UNK	-	SEE REMARK 999	UNP P29016
A	902	UNK	-	SEE REMARK 999	UNP P29016
A	903	UNK	-	SEE REMARK 999	UNP P29016
A	904	UNK	-	SEE REMARK 999	UNP P29016
A	905	UNK	-	SEE REMARK 999	UNP P29016

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
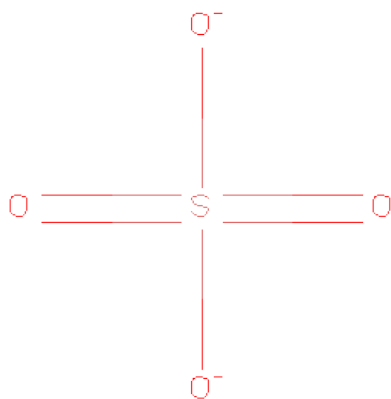
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0

- Molecule 5 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM4-OXIDE (three-letter code: 6PL) (formula: $C_{42}H_{85}NO_8P$).
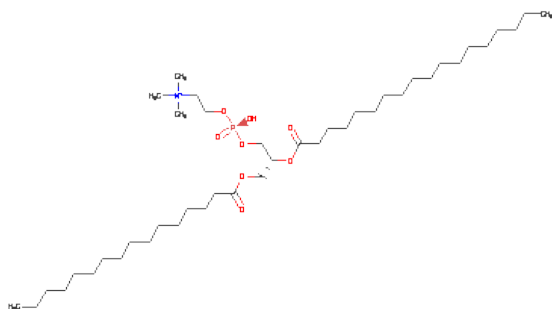
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	52	42	1	8	1	0	0

- Molecule 6 is TETRACOSYL PALMITATE (three-letter code: 6UL) (formula: $C_{40}H_{80}O_2$).
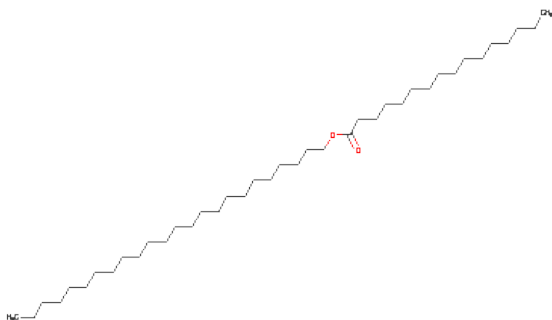
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	42	40	2	0	0

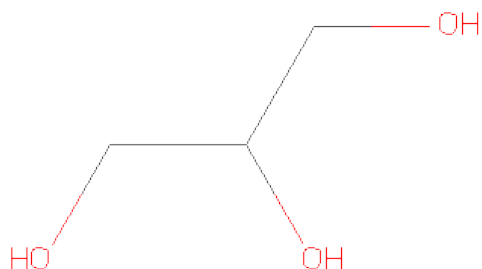- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 6	C 3	O 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	177	Total 177	O 177	0	0
8	B	88	Total 88	O 88	0	0

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.
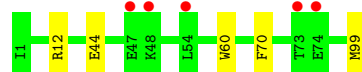
• Molecule 1: T-cell surface glycoprotein CD1b

Chain A:
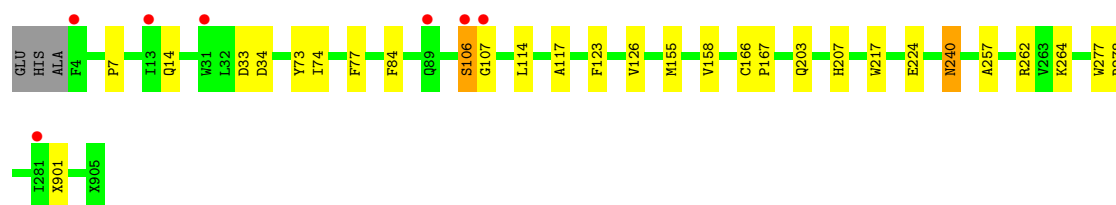
• Molecule 2: Beta-2-microglobulin

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	39.83Å 103.90Å 114.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 31.61 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-1.80) 95.9 (31.61-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.241 0.211 , 0.246	Depositor DCC
R_{free} test set	2182 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 43268 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3423	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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: GOL, NAG, 6UL, SO4, 6PL, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.76	0/2218	0.75	0/3017
2	B	0.86	0/841	0.71	0/1143
All	All	0.79	0/3059	0.74	0/4160

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	907	FUC	C1
3	A	909	FUC	C1

There are no planarity outliers.

5.2 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 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	2182	0	2050	30	0
2	B	818	0	737	7	0
3	A	48	0	44	0	0
4	B	10	0	0	0	0
5	A	52	0	84	15	0
6	A	42	0	80	13	0
7	A	6	0	8	0	0
8	A	177	0	0	2	1
8	B	88	0	0	1	0
All	All	3423	0	3003	41	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 7.

The worst 5 of 41 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:123:PHE:CD1	6:A:312:6UL:HBM1	2.23	0.73
1:A:207:HIS:HE1	2:B:99:MET:OXT	1.71	0.73
2:B:12[B]:ARG:HH11	2:B:12[B]:ARG:HG3	1.57	0.70
5:A:311:6PL:H481	6:A:312:6UL:HAA2	1.79	0.64
5:A:311:6PL:H481	6:A:312:6UL:CAA	2.28	0.62

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)
8:A:976:HOH:O	8:A:1079:HOH:O[3_545]	1.94	0.26

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	276/286 (96%)	270 (98%)	5 (2%)	1 (0%)	43	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	99/99 (100%)	98 (99%)	1 (1%)	0	100	100
All	All	375/385 (97%)	368 (98%)	6 (2%)	1 (0%)	50	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	SER

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	221/231 (96%)	219 (99%)	2 (1%)	87	83
2	B	86/94 (92%)	84 (98%)	2 (2%)	63	46
All	All	307/325 (94%)	303 (99%)	4 (1%)	80	71

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	240	ASN
2	B	44	GLU
2	B	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
2	B	89	GLN
1	A	240	ASN
1	A	152	GLN
1	A	203	GLN

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 ⓘ

4 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	NAG	A	906	1,3	12,14,15	0.72	1 (8%)	15,19,21	1.04	0
3	FUC	A	907	3	9,10,11	0.73	0	10,14,16	1.53	2 (20%)
3	NAG	A	908	1,3	12,14,15	0.52	0	15,19,21	1.15	1 (6%)
3	FUC	A	909	3	9,10,11	1.05	1 (11%)	10,14,16	1.24	1 (10%)

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	906	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	907	3	1/1/4/5	0/0/17/20	0/1/1/1
3	NAG	A	908	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	909	3	1/1/4/5	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)
3	A	909	FUC	O5-C5	-2.31	1.41	1.45
3	A	906	NAG	O5-C5	-2.05	1.41	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	907	FUC	O5-C5-C4	3.13	114.95	110.22
3	A	908	NAG	O5-C5-C4	-2.84	107.05	110.65
3	A	909	FUC	C4-C3-C2	2.67	114.09	110.50
3	A	907	FUC	C4-C3-C2	-2.16	107.60	110.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	907	FUC	C1
3	A	909	FUC	C1

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

5 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	#$|Z| > 2$
7	GOL	A	303	-	5,5,5	0.26	0	5,5,5	1.10	0
5	6PL	A	311	-	51,51,51	0.96	5 (9%)	59,59,59	0.97	3 (5%)
6	6UL	A	312	-	41,41,41	0.40	0	41,41,41	0.81	1 (2%)
4	SO4	B	301	-	4,4,4	0.32	0	6,6,6	0.35	0
4	SO4	B	302	-	4,4,4	0.19	0	6,6,6	0.32	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
7	GOL	A	303	-	-	0/4/4/4	0/0/0/0
5	6PL	A	311	-	-	0/55/55/55	0/0/0/0
6	6UL	A	312	-	-	0/40/40/40	0/0/0/0
4	SO4	B	301	-	-	0/0/0/0	0/0/0/0
4	SO4	B	302	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	311	6PL	C1-C2	2.14	1.56	1.50
5	A	311	6PL	C41-C40	-2.12	1.38	1.51
5	A	311	6PL	C39-C38	-2.05	1.38	1.51
5	A	311	6PL	C40-C39	-2.04	1.38	1.51
5	A	311	6PL	C44-C43	-2.03	1.39	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	311	6PL	O2-C31-C32	3.34	118.88	111.56
5	A	311	6PL	O3-C11-C12	2.54	119.93	111.94
6	A	312	6UL	OAQ-CAP-CAO	2.20	118.86	111.94
5	A	311	6PL	C3-O3-C11	-2.07	111.06	117.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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	278/286 (97%)	0.18	7 (2%)	54	47	20, 31, 45, 51	0
2	B	99/99 (100%)	0.27	5 (5%)	27	21	20, 32, 43, 51	0
All	All	377/385 (97%)	0.21	12 (3%)	43	37	20, 31, 44, 51	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	PHE	4.7
1	A	281	ILE	3.8
1	A	106	SER	3.2
1	A	13	ILE	3.1
2	B	74	GLU	2.8

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
3	FUC	A	909	10/11	0.34	19.85	52,58,60,60	0
3	FUC	A	907	10/11	0.28	7.25	71,73,74,74	0
3	NAG	A	906	14/15	0.22	5.13	52,58,62,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	908	14/15	0.11	1.46	34,38,43,43	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
5	6PL	A	311	52/52	0.32	5.70	51,68,90,90	0
6	6UL	A	312	42/42	0.28	3.65	43,52,59,61	0
7	GOL	A	303	6/6	0.14	3.14	23,35,41,44	0
4	SO4	B	301	5/5	0.20	2.67	40,41,43,44	0
4	SO4	B	302	5/5	0.21	1.17	69,69,70,72	0

6.5 Other polymers ⓘ

There are no such residues in this entry.