



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2017 – 10:42 PM EDT

PDB ID : 5WKG
Title : Crystal Structure of Human CD1b in Complex with PA
Authors : Shahine, A.; Gras, S.; Rossjohn, J.
Deposited on : unknown
Resolution : 2.06 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

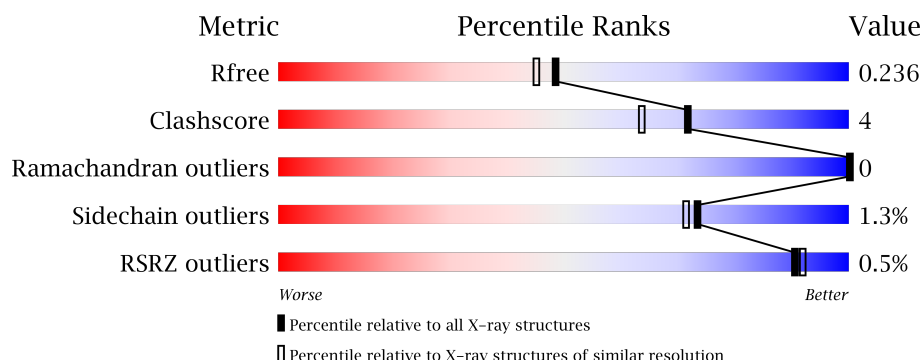
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

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X-RAY DIFFRACTION

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}	100719	2028 (2.08-2.04)
Clashscore	112137	2143 (2.08-2.04)
Ramachandran outliers	110173	2126 (2.08-2.04)
Sidechain outliers	110143	2126 (2.08-2.04)
RSRZ outliers	101464	2035 (2.08-2.04)

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	300	<div> <div></div> <div>83%</div> <div>10%</div> <div>7%</div> </div>
2	B	99	<div> <div></div> <div>92%</div> <div>6%</div> <div></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
11	EDO	A	417	-	-	-	X
7	D21	A	411	-	-	-	X
8	CUY	A	412	-	-	-	X
9	PEG	A	413	-	-	X	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 3543 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 CD1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	7	0
			2213	1419	375	408	11			

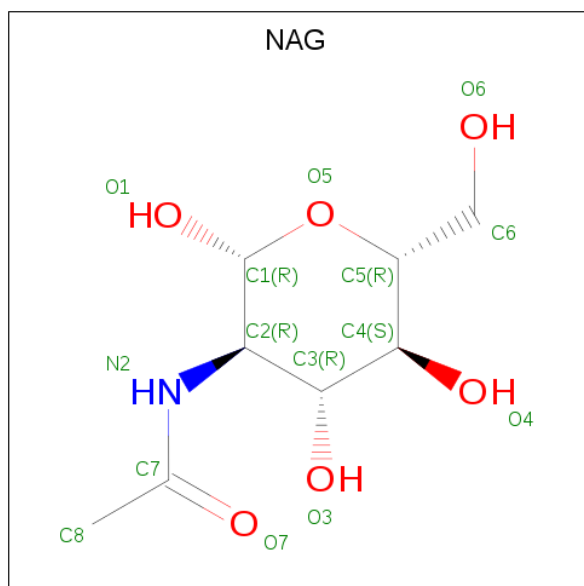
There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	GLY	-	expression tag	UNP P29016
A	280	SER	-	expression tag	UNP P29016
A	281	GLY	-	expression tag	UNP P29016
A	282	LEU	-	expression tag	UNP P29016
A	283	ASN	-	expression tag	UNP P29016
A	284	ASP	-	expression tag	UNP P29016
A	285	ILE	-	expression tag	UNP P29016
A	286	PHE	-	expression tag	UNP P29016
A	287	GLU	-	expression tag	UNP P29016
A	288	ALA	-	expression tag	UNP P29016
A	289	GLN	-	expression tag	UNP P29016
A	290	LYS	-	expression tag	UNP P29016
A	291	ILE	-	expression tag	UNP P29016
A	292	GLU	-	expression tag	UNP P29016
A	293	TRP	-	expression tag	UNP P29016
A	294	HIS	-	expression tag	UNP P29016
A	295	GLU	-	expression tag	UNP P29016
A	296	HIS	-	expression tag	UNP P29016
A	297	HIS	-	expression tag	UNP P29016
A	298	HIS	-	expression tag	UNP P29016
A	299	HIS	-	expression tag	UNP P29016
A	300	HIS	-	expression tag	UNP P29016
A	301	HIS	-	expression tag	UNP P29016

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

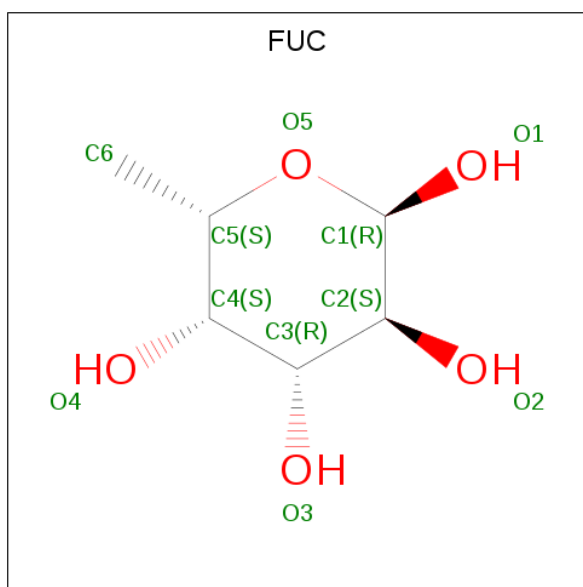
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	2	0
			818	522	138	156	2			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



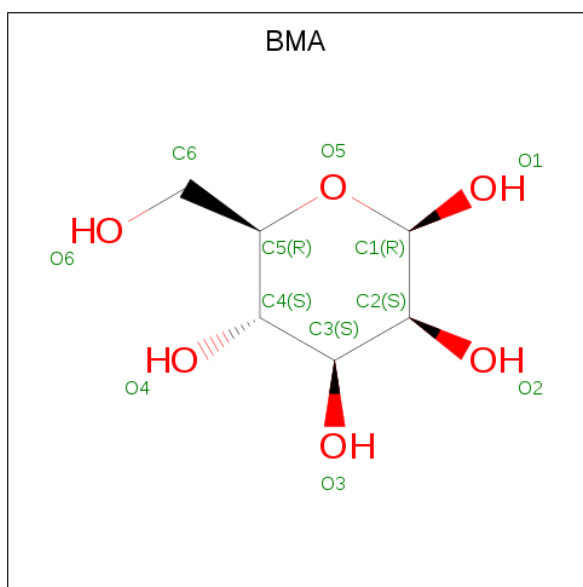
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



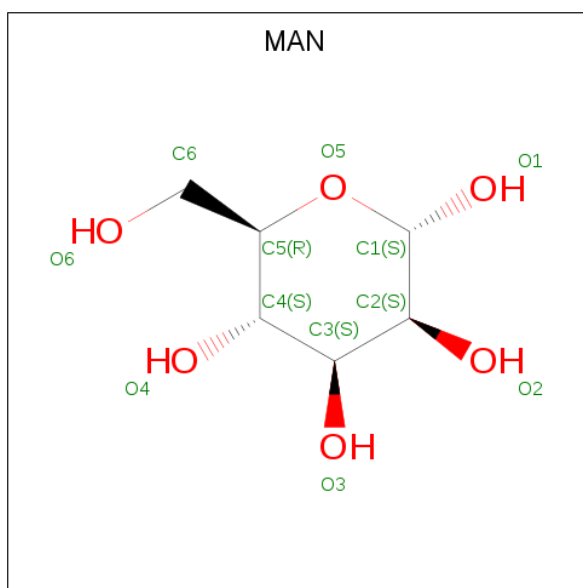
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



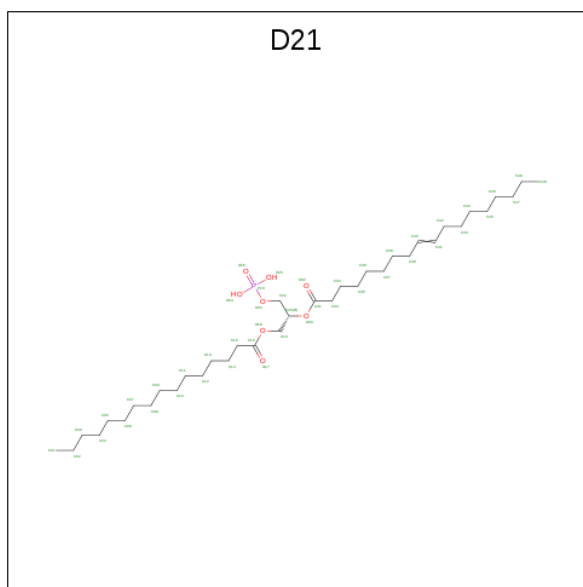
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



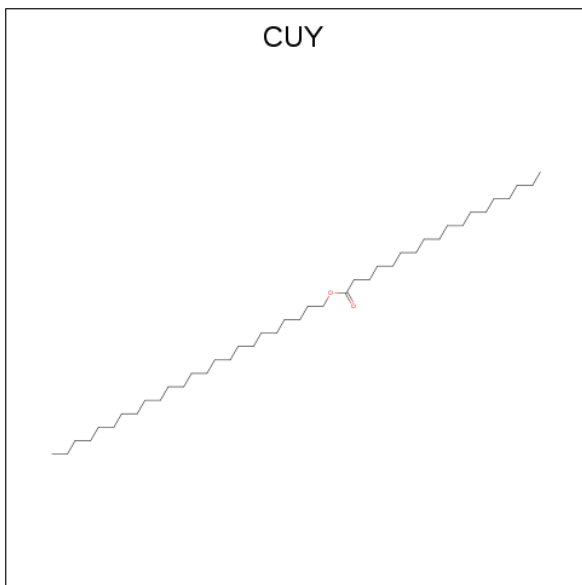
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is (2R)-1-(hexadecanoyloxy)-3-(phosphonooxy)propan-2-yl (9Z)-octadec-9-enoate (three-letter code: D21) (formula: $C_{37}H_{71}O_8P$).



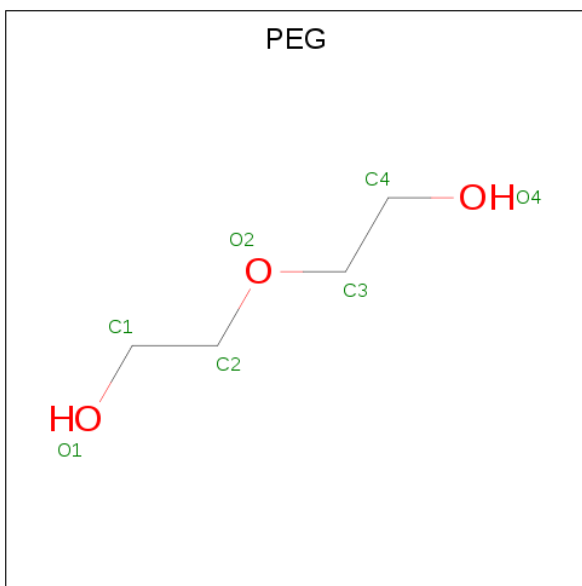
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			46	37	8	1		

- Molecule 8 is tetracosyl octadecanoate (three-letter code: CUY) (formula: $C_{42}H_{84}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			36	34	2		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

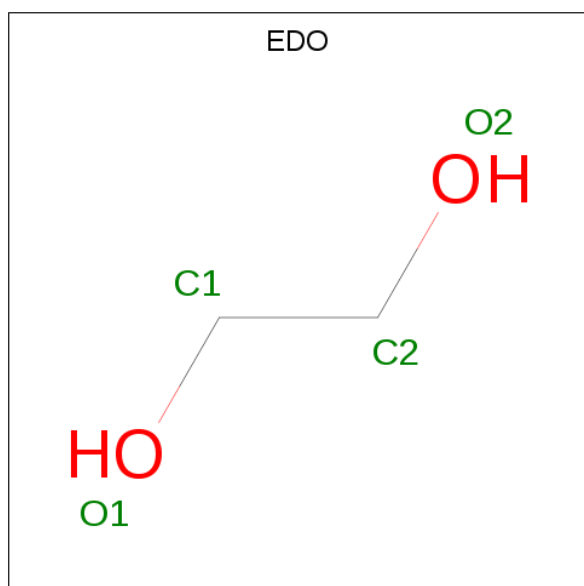


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Cl		0	0
			1	1			
10	A	3	Total	Cl		0	0
			3	3			

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 12 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	I		0	0
			1	1			
12	A	2	Total	I		0	0
			2	2			

- Molecule 13 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Na 1	0	0

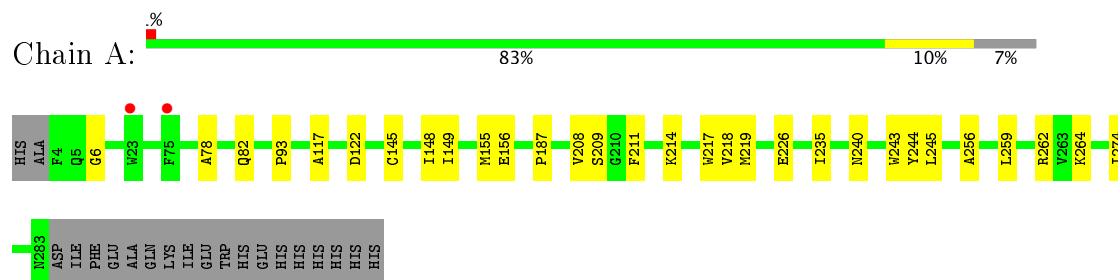
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	203	Total 203	O 203	0	0
14	B	89	Total 89	O 89	0	0

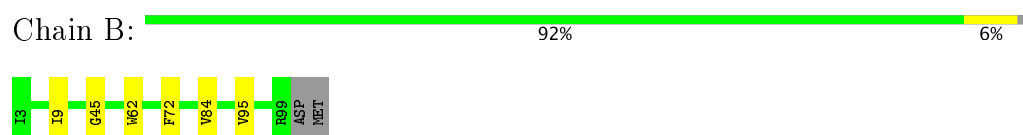
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



- Molecule 2: Beta-2-microglobulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.19Å 78.53Å 84.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.58 – 2.06 32.37 – 2.06	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.58-2.06) 100.0 (32.37-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.06Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.171 , 0.224 0.184 , 0.236	Depositor DCC
R_{free} test set	1259 reflections (5.48%)	DCC
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3543	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, BMA, NAG, CL, D21, NA, EDO, CUY, FUC, PEG, 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	0.62	0/2291	0.69	0/3107
2	B	0.63	0/844	0.70	0/1146
All	All	0.62	0/3135	0.69	0/4253

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2213	0	2136	22	0
2	B	818	0	779	4	0
3	A	56	0	47	0	0
4	A	30	0	30	0	0
5	A	11	0	8	0	0
6	A	22	0	20	0	0
7	A	46	0	0	0	0
8	A	36	0	0	0	0
9	A	7	0	10	7	0
10	A	3	0	0	0	0
10	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	4	0	6	2	0
12	A	2	0	0	0	0
12	B	1	0	0	1	0
13	B	1	0	0	0	0
14	A	203	0	0	0	0
14	B	89	0	0	0	0
All	All	3543	0	3036	25	0

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 4.

The worst 5 of 25 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:93:PRO:HB2	11:A:417:EDO:H22	1.38	1.04
1:A:243[B]:TRP:CH2	9:A:413:PEG:H22	2.18	0.79
1:A:243[B]:TRP:HH2	9:A:413:PEG:H22	1.51	0.74
1:A:93:PRO:HB2	11:A:417:EDO:C2	2.17	0.74
1:A:209:SER:HB2	1:A:244:TYR:HD1	1.66	0.61

There are no symmetry-related clashes.

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	285/300 (95%)	283 (99%)	2 (1%)	0	100	100
2	B	97/99 (98%)	97 (100%)	0	0	100	100
All	All	382/399 (96%)	380 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	234/247 (95%)	231 (99%)	3 (1%)	73	71
2	B	93/94 (99%)	92 (99%)	1 (1%)	78	76
All	All	327/341 (96%)	323 (99%)	4 (1%)	73	74

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

Mol	Chain	Res	Type
1	A	122	ASP
1	A	156	GLU
1	A	240	ASN
2	B	72	PHE

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

Mol	Chain	Res	Type
1	A	150	GLN

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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 for Mogul analysis.

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	401	1,3,4	14,14,15	1.40	3 (21%)	15,19,21	2.32	3 (20%)
4	FUC	A	402	3	9,10,11	1.23	1 (11%)	13,14,16	1.32	1 (7%)
3	NAG	A	403	3,5	14,14,15	1.47	2 (14%)	15,19,21	1.58	1 (6%)
5	BMA	A	404	3,6	11,11,12	0.31	0	13,15,17	0.58	0
6	MAN	A	405	5	11,11,12	0.29	0	13,15,17	1.04	1 (7%)
4	FUC	A	406	3	9,10,11	1.16	1 (11%)	13,14,16	1.36	2 (15%)
6	MAN	A	407	5	11,11,12	0.40	0	13,15,17	0.90	1 (7%)
3	NAG	A	408	1	14,14,15	0.56	0	15,19,21	1.52	2 (13%)
3	NAG	A	409	1,4	14,14,15	0.29	0	15,19,21	1.51	3 (20%)
4	FUC	A	410	3	9,10,11	0.45	0	13,14,16	0.78	0
7	D21	A	411	-	45,45,45	0.80	2 (4%)	49,50,50	1.05	4 (8%)
8	CUY	A	412	-	35,35,43	0.37	0	35,35,43	0.33	0
9	PEG	A	413	-	6,6,6	0.41	0	5,5,5	0.18	0
11	EDO	A	417	-	3,3,3	0.62	0	2,2,2	0.27	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	401	1,3,4	-	0/6/23/26	0/1/1/1
4	FUC	A	402	3	-	0/0/17/20	0/1/1/1
3	NAG	A	403	3,5	-	0/6/23/26	0/1/1/1
5	BMA	A	404	3,6	-	0/2/19/22	0/1/1/1
6	MAN	A	405	5	-	0/2/19/22	0/1/1/1
4	FUC	A	406	3	-	0/0/17/20	0/1/1/1
6	MAN	A	407	5	-	0/2/19/22	0/1/1/1
3	NAG	A	408	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	409	1,4	-	0/6/23/26	0/1/1/1
4	FUC	A	410	3	-	0/0/17/20	0/1/1/1
7	D21	A	411	-	-	0/47/47/47	0/0/0/0
8	CUY	A	412	-	-	0/34/34/42	0/0/0/0
9	PEG	A	413	-	-	0/4/4/4	0/0/0/0
11	EDO	A	417	-	-	0/1/1/1	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	NAG	O7-C7	-4.11	1.13	1.23
7	A	411	D21	C42-C41	-3.36	1.32	1.50
3	A	401	NAG	O7-C7	-2.83	1.16	1.23
3	A	401	NAG	O5-C1	-2.37	1.39	1.43
4	A	406	FUC	O5-C1	-2.29	1.40	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	409	NAG	O5-C1-C2	-2.88	107.47	111.47
3	A	401	NAG	C8-C7-N2	-2.43	111.71	116.11
4	A	406	FUC	O2-C2-C3	2.24	114.58	110.17
7	A	411	D21	O30-C20-C21	2.27	116.67	108.44
3	A	409	NAG	C3-C4-C5	2.28	114.24	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	413	PEG	7	0
11	A	417	EDO	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	280/300 (93%)	-0.50	2 (0%) 87 88	9, 17, 37, 55	0
2	B	97/99 (97%)	-0.59	0 100 100	10, 18, 38, 55	0
All	All	377/399 (94%)	-0.52	2 (0%) 90 92	9, 18, 38, 55	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	PHE	2.2
1	A	23	TRP	2.1

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](#)

There are no carbohydrates in this entry.

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(Å ²)	Q<0.9
11	EDO	A	417	4/4	0.92	0.19	8.79	19,22,25,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	D21	A	411	46/46	0.74	0.25	5.92	29,43,89,90	1
9	PEG	A	413	7/7	0.94	0.19	4.49	4,16,23,32	0
8	CUY	A	412	36/44	0.81	0.20	4.25	24,31,43,48	0
3	NAG	A	408	14/15	0.65	0.24	1.96	51,55,62,64	0
6	MAN	A	405	11/12	0.95	0.09	0.99	10,16,23,24	0
4	FUC	A	402	10/11	0.94	0.11	0.00	18,21,26,27	0
3	NAG	A	403	14/15	0.96	0.08	-0.19	8,14,16,19	0
5	BMA	A	404	11/12	0.94	0.08	-0.38	18,19,21,26	0
3	NAG	A	401	14/15	0.97	0.07	-0.57	10,15,17,18	0
10	CL	A	416	1/1	0.89	0.11	-0.76	85,85,85,85	0
10	CL	A	414	1/1	0.86	0.08	-0.80	42,42,42,42	0
12	IOD	A	419	1/1	0.99	0.06	-1.87	15,15,15,15	0
13	NA	B	201	1/1	0.99	0.03	-2.31	15,15,15,15	0
12	IOD	B	203	1/1	0.95	0.05	-2.31	37,37,37,37	1
12	IOD	A	418	1/1	0.98	0.05	-4.97	39,39,39,39	1
6	MAN	A	407	11/12	0.91	0.09	-	25,27,30,33	0
4	FUC	A	410	10/11	0.83	0.29	-	36,39,41,42	0
3	NAG	A	409	14/15	0.78	0.28	-	42,46,49,50	0
4	FUC	A	406	10/11	0.95	0.08	-	19,21,23,24	0
10	CL	B	202	1/1	0.96	0.13	-	42,42,42,42	0
10	CL	A	415	1/1	0.98	0.09	-	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.