



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:13 PM GMT

PDB ID : 3T8X  
Title : Crystal structure of human CD1b in complex with synthetic antigenic diacyl  
ulfglycolipid SGL12 and endogenous spacer  
Authors : Garcia-Alles, L.F.; Maveyraud, L.; Mourey, L.; Julien, S.  
Deposited on : 2011-08-02  
Resolution : 1.90 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](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

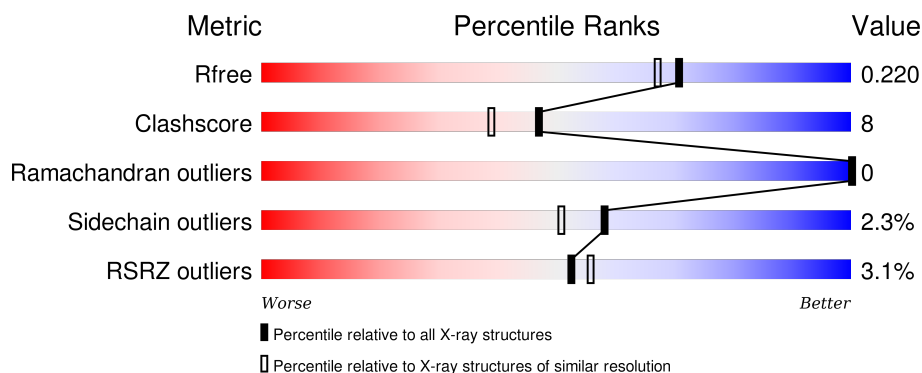
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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. 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	301	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>9%</div> </div> </div>
1	C	301	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>8%</div> </div> </div>
2	B	99	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
2	D	99	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>8%</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
3	FUC	A	1002	X	-	-	-
3	FUC	C	2022	X	-	-	-
5	SO4	C	303	-	-	-	X
6	ACT	A	303	-	-	-	X
7	T8X	A	304	-	-	X	X
7	T8X	C	304	-	-	-	X
8	ULI	A	305	-	-	-	X
8	ULI	C	305	-	-	-	X
9	GOL	B	100	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6803 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	275	Total	C	N	O	S	0	1	0
			2147	1379	365	393	10			
1	C	277	Total	C	N	O	S	0	3	0
			2138	1376	357	395	10			

There are 42 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	285	GLY	-	EXPRESSION TAG	UNP P29016
C	286	GLY	-	EXPRESSION TAG	UNP P29016
C	287	GLY	-	EXPRESSION TAG	UNP P29016
C	288	LEU	-	EXPRESSION TAG	UNP P29016
C	289	ASN	-	EXPRESSION TAG	UNP P29016
C	290	ASP	-	EXPRESSION TAG	UNP P29016
C	291	ILE	-	EXPRESSION TAG	UNP P29016
C	292	PHE	-	EXPRESSION TAG	UNP P29016
C	293	GLU	-	EXPRESSION TAG	UNP P29016
C	294	ALA	-	EXPRESSION TAG	UNP P29016
C	295	GLN	-	EXPRESSION TAG	UNP P29016
C	296	LYS	-	EXPRESSION TAG	UNP P29016
C	297	ILE	-	EXPRESSION TAG	UNP P29016
C	298	GLU	-	EXPRESSION TAG	UNP P29016
C	299	TRP	-	EXPRESSION TAG	UNP P29016
C	300	HIS	-	EXPRESSION TAG	UNP P29016
C	301	GLU	-	EXPRESSION TAG	UNP P29016

- 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	0	0
			810	518	135	154	3			
2	D	99	Total	C	N	O	S	0	0	0
			807	515	137	152	3			

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

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

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

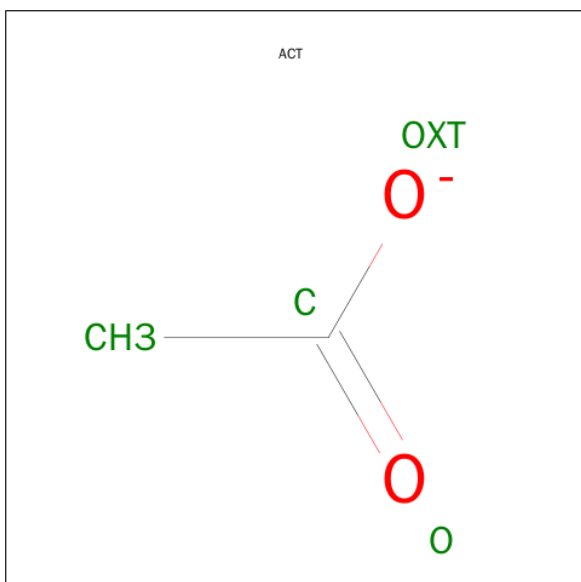
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



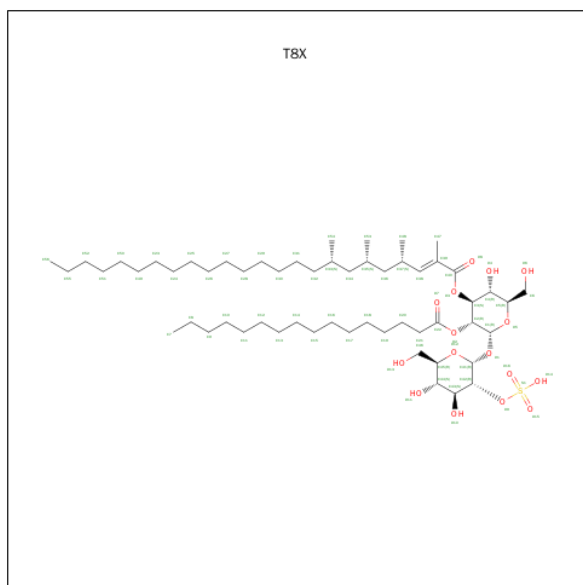
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



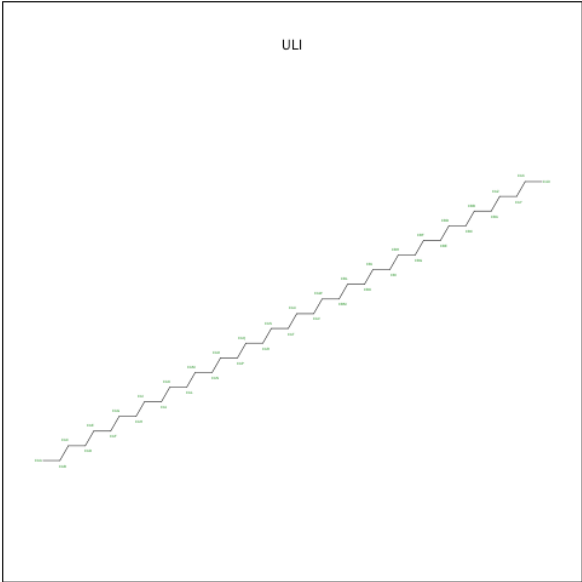
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is 2-O-SULFO-ALPHA-D-GLUCOPYRANOSYL 2-O-HEXADECANOYL-3-O-[(2E,4S,6S,8S)-2,4,6,8-TETRAMETHYLTETRACOS-2-ENOYL]-ALPHA-D-GLUCOPYRANOSIDE (three-letter code: T8X) (formula: C<sub>56</sub>H<sub>104</sub>O<sub>16</sub>S).



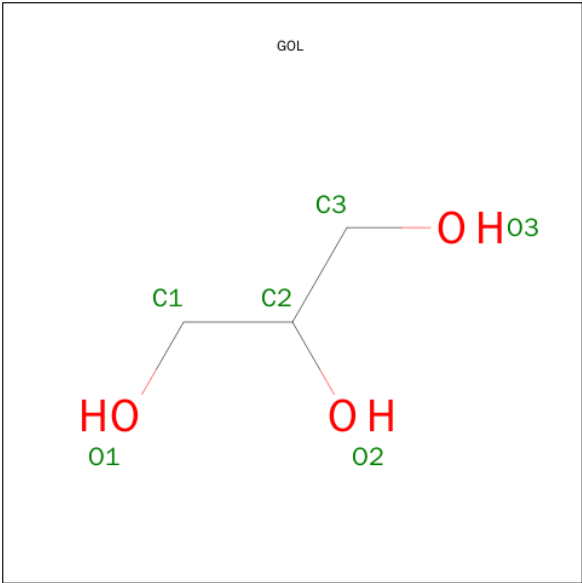
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			73	56	16	1		
7	C	1	Total	C				0
			31	31				0

- Molecule 8 is TETRACONTANE (three-letter code: ULI) (formula: C<sub>40</sub>H<sub>82</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	C	0	0
			40	40		
8	C	1	Total	C	0	0
			39	39		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	3	Total	C	N	O	0	0
			38	22	2	14		

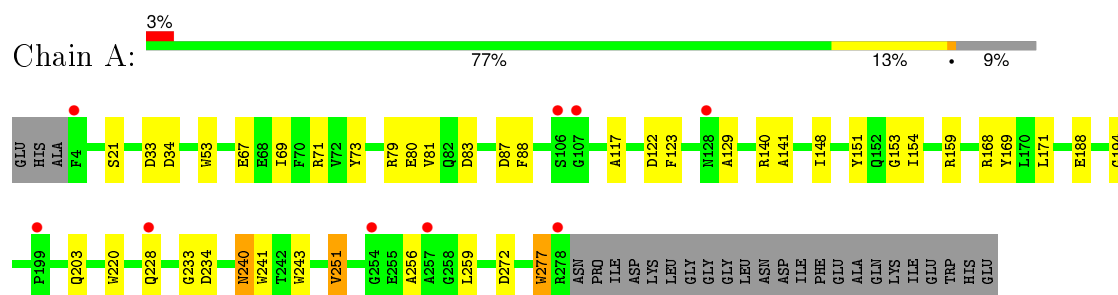
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	194	Total	O	0	0
			194	194		
11	B	97	Total	O	0	0
			97	97		
11	C	162	Total	O	0	0
			162	162		
11	D	72	Total	O	0	0
			72	72		

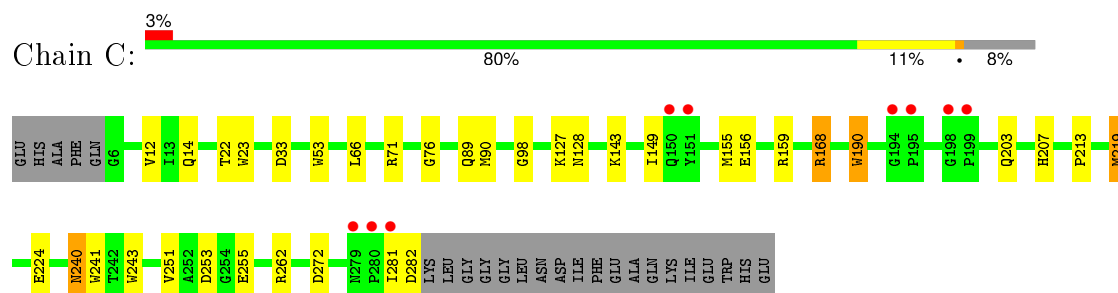
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

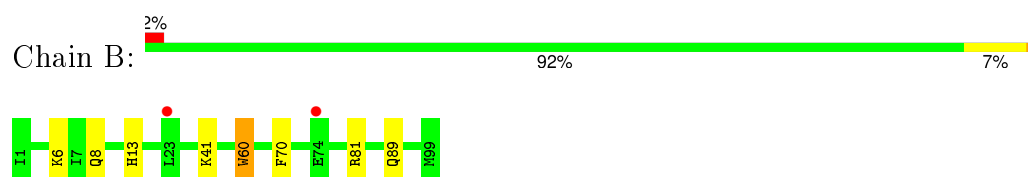
- Molecule 1: T-cell surface glycoprotein CD1b



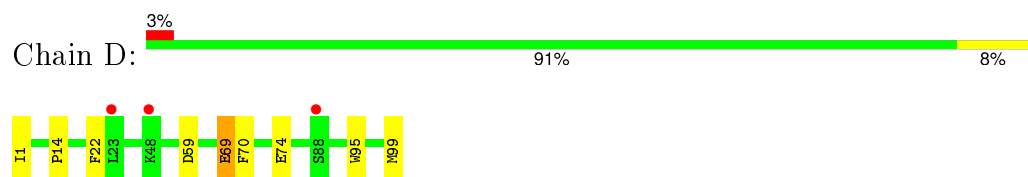
- Molecule 1: T-cell surface glycoprotein CD1b



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.25Å 67.58Å 88.19Å 90.00° 112.26° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.5 (20.00-1.90) 92.6 (20.00-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.165 , 0.211 0.173 , 0.220	Depositor DCC
$R_{free}$ test set	4044 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 60.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 80867 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6803	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: GOL, BMA, NAG, ACT, ULI, SO4, T8X, MAN, 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	1.27	6/2207 (0.3%)	1.06	11/2998 (0.4%)
1	C	1.17	6/2198 (0.3%)	1.01	7/2992 (0.2%)
2	B	1.22	1/833 (0.1%)	1.00	1/1131 (0.1%)
2	D	1.03	1/830 (0.1%)	0.93	1/1127 (0.1%)
All	All	1.20	14/6068 (0.2%)	1.02	20/8248 (0.2%)

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	1	0
3	C	1	0
All	All	2	0

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	TRP	CD2-CE2	6.79	1.49	1.41
2	B	60	TRP	CD2-CE2	6.06	1.48	1.41
1	A	53	TRP	CD2-CE2	6.00	1.48	1.41
1	C	241	TRP	CD2-CE2	5.93	1.48	1.41
2	D	95	TRP	CD2-CE2	5.86	1.48	1.41

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	NE-CZ-NH2	-8.02	116.29	120.30
2	D	59	ASP	CB-CG-OD1	7.55	125.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	A	83	ASP	CB-CG-OD2	7.49	125.05	118.30
1	A	272	ASP	CB-CG-OD2	6.73	124.36	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1002	FUC	C1
3	C	2022	FUC	C1

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	2147	0	2051	27	0
1	C	2138	0	2014	22	0
2	B	810	0	749	5	0
2	D	807	0	753	7	0
3	A	24	0	22	0	0
3	C	24	0	22	0	0
4	A	60	0	52	2	0
5	A	5	0	0	0	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
6	A	4	0	3	0	0
7	A	73	0	103	33	0
7	C	31	0	61	4	0
8	A	40	0	82	16	0
8	C	39	0	77	8	0
9	B	12	0	16	4	0
9	D	6	0	8	0	0
10	C	38	0	34	0	0
11	A	194	0	0	1	1
11	B	97	0	0	1	0
11	C	162	0	0	10	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	72	0	0	3	0
All	All	6803	0	6047	91	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 91 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)
7:A:304:T8X:C56	8:A:305:ULI:HAA	1.47	1.41
7:A:304:T8X:C56	8:A:305:ULI:CAA	2.11	1.28
1:C:22[A]:THR:HG22	11:C:311:HOH:O	1.03	1.21
1:C:219:MET:HE1	11:C:472:HOH:O	1.04	1.20
7:A:304:T8X:HCTA	8:A:305:ULI:HAA	1.31	1.12

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:490:HOH:O	11:C:479:HOH:O[4_546]	2.19	0.01

## 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	274/301 (91%)	272 (99%)	2 (1%)	0	100	100
1	C	278/301 (92%)	274 (99%)	4 (1%)	0	100	100
2	B	97/99 (98%)	97 (100%)	0	0	100	100
2	D	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
All	All	746/800 (93%)	738 (99%)	8 (1%)	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	221/247 (90%)	217 (98%)	4 (2%)	66	61
1	C	216/247 (87%)	210 (97%)	6 (3%)	51	41
2	B	87/94 (93%)	85 (98%)	2 (2%)	58	51
2	D	88/94 (94%)	86 (98%)	2 (2%)	58	51
All	All	612/682 (90%)	598 (98%)	14 (2%)	58	51

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	143	LYS
1	C	155	MET
1	C	281	ILE
2	B	89	GLN
1	C	240	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	51	HIS
2	B	89	GLN
1	C	225	GLN
1	A	228	GLN
1	A	240	ASN

### 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 ⓘ

12 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	1001	1,3	14,14,15	1.13	1 (7%)	15,19,21	1.80	5 (33%)
3	FUC	A	1002	3	10,10,11	1.46	1 (10%)	14,14,16	2.71	8 (57%)
4	NAG	A	1011	1,4	14,14,15	0.74	0	15,19,21	2.02	4 (26%)
4	FUC	A	1012	4	10,10,11	1.84	1 (10%)	14,14,16	2.58	4 (28%)
4	NAG	A	1013	4	14,14,15	0.76	0	15,19,21	1.36	3 (20%)
4	BMA	A	1014	4	11,11,12	0.81	0	14,15,17	1.87	3 (21%)
4	MAN	A	1016	4	11,11,12	0.85	1 (9%)	14,15,17	2.42	5 (35%)
3	NAG	C	2021	1,3	14,14,15	0.73	0	15,19,21	2.22	5 (33%)
3	FUC	C	2022	3	10,10,11	1.24	1 (10%)	14,14,16	3.36	6 (42%)
10	NAG	C	2031	1,10	14,14,15	0.97	1 (7%)	15,19,21	1.65	4 (26%)
10	FUC	C	2032	10	10,10,11	1.59	1 (10%)	14,14,16	3.48	8 (57%)
10	NAG	C	2033	10	14,14,15	0.90	0	15,19,21	1.74	5 (33%)

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	1001	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	1002	3	1/1/4/5	0/0/17/20	0/1/1/1
4	NAG	A	1011	1,4	-	0/6/23/26	0/1/1/1
4	FUC	A	1012	4	-	0/0/17/20	0/1/1/1
4	NAG	A	1013	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	A	1014	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1016	4	-	0/2/19/22	0/1/1/1
3	NAG	C	2021	1,3	-	0/6/23/26	0/1/1/1
3	FUC	C	2022	3	1/1/4/5	0/0/17/20	0/1/1/1
10	NAG	C	2031	1,10	-	0/6/23/26	0/1/1/1
10	FUC	C	2032	10	-	0/0/17/20	0/1/1/1
10	NAG	C	2033	10	-	0/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1012	FUC	O5-C1	-5.04	1.35	1.43
10	C	2032	FUC	O5-C1	-4.00	1.37	1.43
3	A	1002	FUC	O5-C1	-3.53	1.37	1.43
3	C	2022	FUC	O5-C1	-3.11	1.38	1.43
10	C	2031	NAG	O3-C3	-2.50	1.37	1.43

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	2032	FUC	C1-C2-C3	-8.24	99.80	109.54
3	C	2022	FUC	C1-C2-C3	-8.14	99.92	109.54
4	A	1012	FUC	C1-C2-C3	-7.22	101.00	109.54
10	C	2032	FUC	C1-O5-C5	-5.95	103.19	112.38
3	C	2022	FUC	C1-O5-C5	-5.69	103.59	112.38

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	2022	FUC	C1
3	A	1002	FUC	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1013	NAG	1	0
4	A	1016	MAN	1	0

## 5.6 Ligand geometry

13 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	SO4	A	302	-	4,4,4	0.66	0	6,6,6	0.93	1 (16%)
6	ACT	A	303	-	1,3,3	2.92	1 (100%)	0,3,3	0.00	-
7	T8X	A	304	-	74,74,74	1.65	10 (13%)	89,94,94	1.84	15 (16%)
8	ULI	A	305	-	39,39,39	0.59	1 (2%)	38,38,38	1.14	2 (5%)
9	GOL	B	100	-	5,5,5	0.41	0	5,5,5	0.79	0
9	GOL	B	101	-	5,5,5	0.89	0	5,5,5	1.52	1 (20%)
5	SO4	C	302	-	4,4,4	0.33	0	6,6,6	0.58	0
5	SO4	C	303	-	4,4,4	0.78	0	6,6,6	0.15	0
7	T8X	C	304	-	29,29,74	0.55	0	27,27,94	0.55	0
8	ULI	C	305	-	38,38,39	0.53	0	37,37,38	1.07	3 (8%)
5	SO4	D	100	-	4,4,4	1.30	0	6,6,6	0.38	0
5	SO4	D	101	-	4,4,4	0.56	0	6,6,6	0.77	0
9	GOL	D	102	-	5,5,5	0.66	0	5,5,5	1.58	1 (20%)

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	SO4	A	302	-	-	0/0/0/0	0/0/0/0
6	ACT	A	303	-	-	0/0/0/0	0/0/0/0
7	T8X	A	304	-	-	1/68/108/108	0/2/2/2
8	ULI	A	305	-	-	0/37/37/37	0/0/0/0
9	GOL	B	100	-	-	0/4/4/4	0/0/0/0
9	GOL	B	101	-	-	0/4/4/4	0/0/0/0
5	SO4	C	302	-	-	0/0/0/0	0/0/0/0
5	SO4	C	303	-	-	0/0/0/0	0/0/0/0
7	T8X	C	304	-	-	0/25/25/108	0/0/0/2
8	ULI	C	305	-	-	0/36/36/37	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	D	100	-	-	0/0/0/0	0/0/0/0
5	SO4	D	101	-	-	0/0/0/0	0/0/0/0
9	GOL	D	102	-	-	0/4/4/4	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	304	T8X	O3-C3	-3.60	1.39	1.44
7	A	304	T8X	O9-S1	-3.37	1.46	1.57
7	A	304	T8X	C40-C39	-3.31	1.38	1.50
8	A	305	ULI	CAZ-CAY	-2.08	1.39	1.51
7	A	304	T8X	O16-S1	2.19	1.53	1.45

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	304	T8X	C1-C2-C3	-6.11	97.90	110.75
7	A	304	T8X	O5-C1-C2	-3.90	101.62	109.47
7	A	304	T8X	C42-O9-S1	-3.80	111.54	118.77
7	A	304	T8X	C3-O3-C40	-2.83	111.84	117.61
9	B	101	GOL	O3-C3-C2	-2.76	96.79	110.18

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	304	T8X	C39-C38-C37-C36

There are no ring outliers.

6 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	304	T8X	33	0
8	A	305	ULI	16	0
9	B	100	GOL	3	0
9	B	101	GOL	1	0
7	C	304	T8X	4	0
8	C	305	ULI	8	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	275/301 (91%)	-0.16	9 (3%) 50 53	19, 32, 56, 77	0
1	C	277/301 (92%)	-0.15	9 (3%) 51 54	25, 36, 56, 74	0
2	B	99/99 (100%)	-0.24	2 (2%) 68 71	19, 32, 53, 62	0
2	D	99/99 (100%)	-0.05	3 (3%) 54 57	26, 41, 61, 72	0
All	All	750/800 (93%)	-0.15	23 (3%) 52 56	19, 35, 57, 77	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	SER	4.5
1	C	195	PRO	4.3
1	C	198	GLY	3.9
1	C	281	ILE	3.4
1	A	257	ALA	3.3

### 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	1013	14/15	0.86	0.16	1.22	40,45,52,56	0
10	NAG	C	2031	14/15	0.98	0.11	0.59	39,44,50,53	0
4	NAG	A	1011	14/15	0.98	0.05	-0.82	30,36,42,45	0
3	NAG	C	2021	14/15	0.87	0.24	-	57,69,75,84	0
4	BMA	A	1014	11/12	0.82	0.34	-	62,75,95,97	0
4	FUC	A	1012	10/11	0.93	0.18	-	46,49,52,59	0
4	MAN	A	1016	11/12	0.78	0.36	-	73,90,95,96	0
3	FUC	C	2022	10/11	0.94	0.28	-	68,72,76,83	0
10	NAG	C	2033	14/15	0.89	0.25	-	44,54,67,75	0
10	FUC	C	2032	10/11	0.88	0.24	-	45,56,61,74	0
3	NAG	A	1001	14/15	0.90	0.16	-	58,64,74,77	0
3	FUC	A	1002	10/11	0.90	0.30	-	60,69,74,75	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
9	GOL	B	100	6/6	0.72	0.22	8.67	49,63,65,65	0
6	ACT	A	303	4/4	0.41	0.29	4.82	68,71,76,76	0
8	ULI	A	305	40/40	0.93	0.21	4.70	31,47,62,78	0
8	ULI	C	305	39/40	0.85	0.27	4.66	45,57,68,78	0
7	T8X	C	304	31/73	0.80	0.21	4.19	41,58,66,68	0
5	SO4	C	303	5/5	0.89	0.20	3.62	77,78,104,104	0
7	T8X	A	304	73/73	0.74	0.22	2.09	40,72,112,116	0
9	GOL	D	102	6/6	0.88	0.14	0.49	52,57,70,77	0
5	SO4	C	302	5/5	0.99	0.07	-0.45	43,52,57,62	0
5	SO4	D	100	5/5	0.99	0.06	-2.31	42,46,48,50	0
5	SO4	A	302	5/5	0.73	0.27	-	84,88,106,107	0
9	GOL	B	101	6/6	0.90	0.18	-	45,53,63,69	0
5	SO4	D	101	5/5	0.95	0.10	-	66,76,84,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.