



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 07:52 PM GMT

PDB ID : 1FV3  
Title : THE HC FRAGMENT OF TETANUS TOXIN COMPLEXED WITH AN ANALOGUE OF ITS GANGLIOSIDE RECEPTOR GT1B  
Authors : Fotinou, C.; Emsley, P.; Black, I.; Ando, H.; Ishida, H.; Kiso, M.; Sinha, K.A.; Fairweather, N.F.; Isaacs, N.W.  
Deposited on : 2000-09-18  
Resolution : 2.30 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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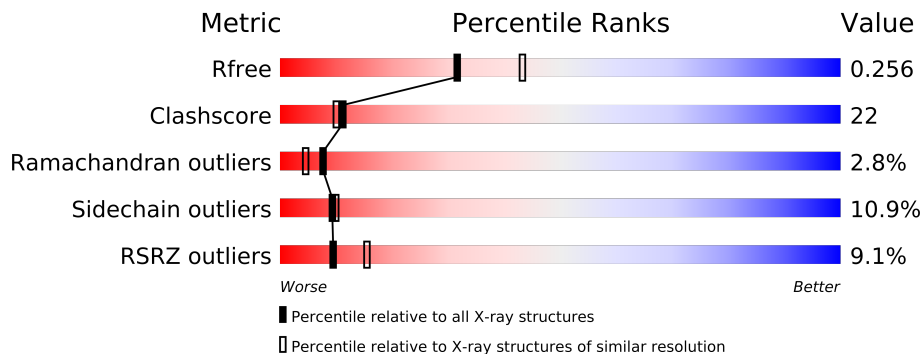
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	472	
1	B	472	

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	CEQ	A	8[A]	-	X
4	CEQ	A	8[B]	-	X
4	CEQ	B	8[A]	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7786 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 TETANUS TOXIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	1	0
			3652	2336	612	694	10			
1	B	451	Total	C	N	O	S	0	0	0
			3648	2334	611	693	10			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	844	MET	-	SEE REMARK 999	? P04958
A	845	GLY	-	SEE REMARK 999	? P04958
A	846	SER	-	SEE REMARK 999	? P04958
A	847	SER	-	SEE REMARK 999	? P04958
A	848	HIS	-	SEE REMARK 999	? P04958
A	849	HIS	-	SEE REMARK 999	? P04958
A	850	HIS	-	SEE REMARK 999	? P04958
A	851	HIS	-	SEE REMARK 999	? P04958
A	852	HIS	-	SEE REMARK 999	? P04958
A	853	HIS	-	SEE REMARK 999	? P04958
A	854	SER	-	SEE REMARK 999	? P04958
A	855	SER	-	SEE REMARK 999	? P04958
A	856	GLY	-	SEE REMARK 999	? P04958
A	857	LEU	-	SEE REMARK 999	? P04958
A	858	VAL	-	SEE REMARK 999	? P04958
A	859	PRO	-	SEE REMARK 999	? P04958
A	860	ARG	-	SEE REMARK 999	? P04958
A	861	GLY	-	SEE REMARK 999	? P04958
A	862	SER	-	SEE REMARK 999	? P04958
A	863	HIS	-	SEE REMARK 999	? P04958
A	864	MET	-	SEE REMARK 999	? P04958
B	844	MET	-	SEE REMARK 999	? P04958
B	845	GLY	-	SEE REMARK 999	? P04958
B	846	SER	-	SEE REMARK 999	? P04958
B	847	SER	-	SEE REMARK 999	? P04958

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Chain	Residue	Modelled	Actual	Comment	Reference
B	848	HIS	-	SEE REMARK 999	? P04958
B	849	HIS	-	SEE REMARK 999	? P04958
B	850	HIS	-	SEE REMARK 999	? P04958
B	851	HIS	-	SEE REMARK 999	? P04958
B	852	HIS	-	SEE REMARK 999	? P04958
B	853	HIS	-	SEE REMARK 999	? P04958
B	854	SER	-	SEE REMARK 999	? P04958
B	855	SER	-	SEE REMARK 999	? P04958
B	856	GLY	-	SEE REMARK 999	? P04958
B	857	LEU	-	SEE REMARK 999	? P04958
B	858	VAL	-	SEE REMARK 999	? P04958
B	859	PRO	-	SEE REMARK 999	? P04958
B	860	ARG	-	SEE REMARK 999	? P04958
B	861	GLY	-	SEE REMARK 999	? P04958
B	862	SER	-	SEE REMARK 999	? P04958
B	863	HIS	-	SEE REMARK 999	? P04958
B	864	MET	-	SEE REMARK 999	? P04958

- Molecule 2 is a polymer of unknown type called SUGAR (GLC-GAL-NGA-GAL-NAN-SLB-NAN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	7	Total	C	N	O	0	0
			108	59	4	45		
2	B	7	Total	C	N	O	0	0
			108	59	4	45		

There are 42 discrepancies between the modelled and reference sequences:

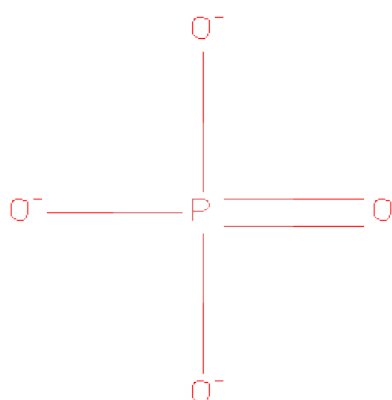
Chain	Residue	Modelled	Actual	Comment	Reference
A	844	MET	-	SEE REMARK 999	? P04958
A	845	GLY	-	SEE REMARK 999	? P04958
A	846	SER	-	SEE REMARK 999	? P04958
A	847	SER	-	SEE REMARK 999	? P04958
A	848	HIS	-	SEE REMARK 999	? P04958
A	849	HIS	-	SEE REMARK 999	? P04958
A	850	HIS	-	SEE REMARK 999	? P04958
A	851	HIS	-	SEE REMARK 999	? P04958
A	852	HIS	-	SEE REMARK 999	? P04958
A	853	HIS	-	SEE REMARK 999	? P04958
A	854	SER	-	SEE REMARK 999	? P04958
A	855	SER	-	SEE REMARK 999	? P04958

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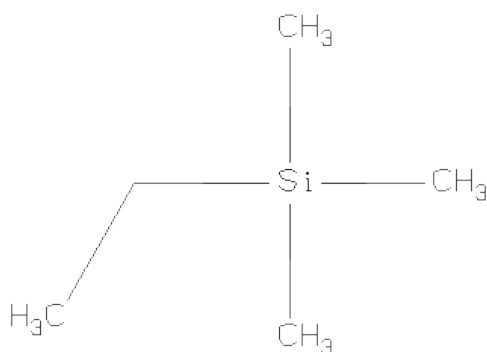
Chain	Residue	Modelled	Actual	Comment	Reference
A	856	GLY	-	SEE REMARK 999	? P04958
A	857	LEU	-	SEE REMARK 999	? P04958
A	858	VAL	-	SEE REMARK 999	? P04958
A	859	PRO	-	SEE REMARK 999	? P04958
A	860	ARG	-	SEE REMARK 999	? P04958
A	861	GLY	-	SEE REMARK 999	? P04958
A	862	SER	-	SEE REMARK 999	? P04958
A	863	HIS	-	SEE REMARK 999	? P04958
A	864	MET	-	SEE REMARK 999	? P04958
B	844	MET	-	SEE REMARK 999	? P04958
B	845	GLY	-	SEE REMARK 999	? P04958
B	846	SER	-	SEE REMARK 999	? P04958
B	847	SER	-	SEE REMARK 999	? P04958
B	848	HIS	-	SEE REMARK 999	? P04958
B	849	HIS	-	SEE REMARK 999	? P04958
B	850	HIS	-	SEE REMARK 999	? P04958
B	851	HIS	-	SEE REMARK 999	? P04958
B	852	HIS	-	SEE REMARK 999	? P04958
B	853	HIS	-	SEE REMARK 999	? P04958
B	854	SER	-	SEE REMARK 999	? P04958
B	855	SER	-	SEE REMARK 999	? P04958
B	856	GLY	-	SEE REMARK 999	? P04958
B	857	LEU	-	SEE REMARK 999	? P04958
B	858	VAL	-	SEE REMARK 999	? P04958
B	859	PRO	-	SEE REMARK 999	? P04958
B	860	ARG	-	SEE REMARK 999	? P04958
B	861	GLY	-	SEE REMARK 999	? P04958
B	862	SER	-	SEE REMARK 999	? P04958
B	863	HIS	-	SEE REMARK 999	? P04958
B	864	MET	-	SEE REMARK 999	? P04958

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ETHYL-TRIMETHYL-SILANE (three-letter code: CEQ) (formula: C<sub>5</sub>H<sub>14</sub>Si).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	Si	0	1
			12	10	2		
4	B	1	Total	C	Si	0	1
			12	10	2		

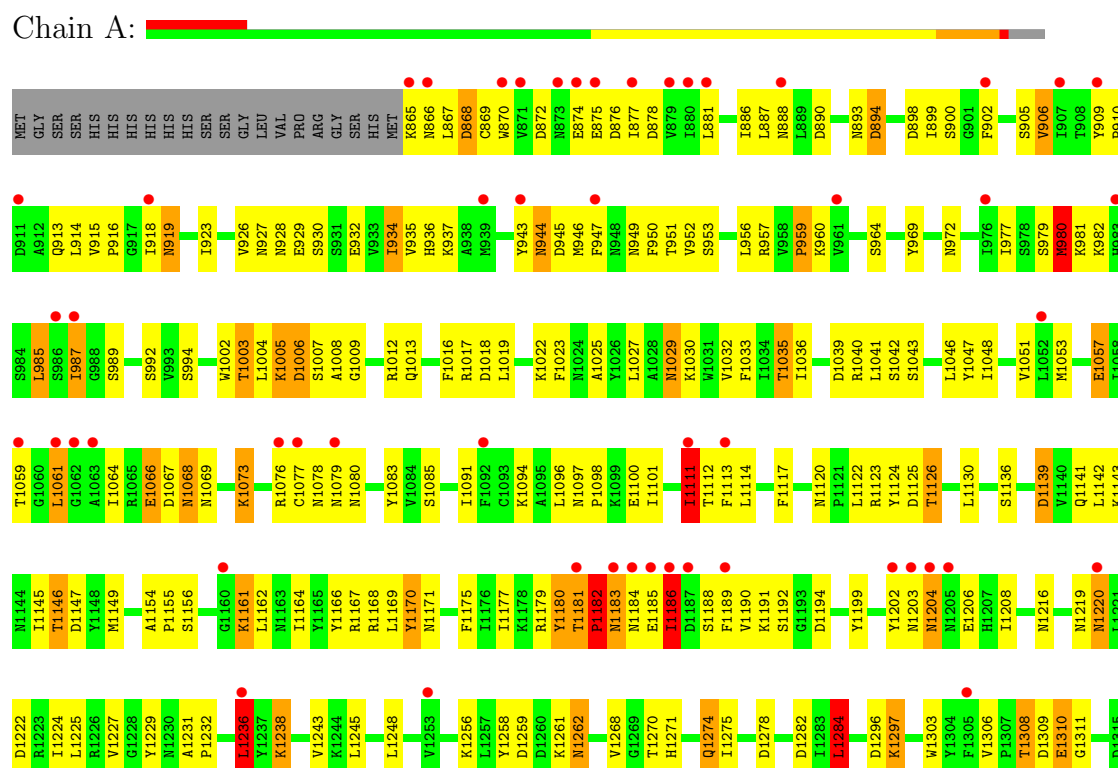
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total 87	O 87	0	0
5	B	154	Total 154	O 154	0	0

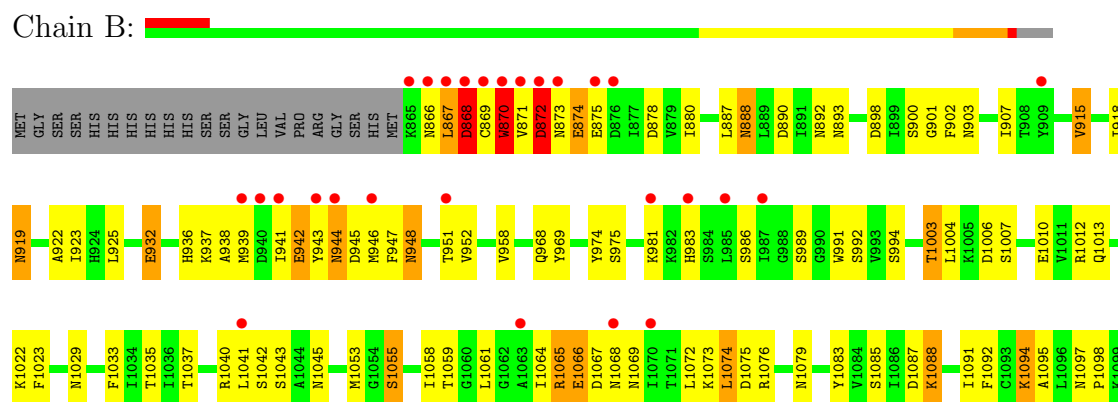
### 3 Residue-property plots

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.

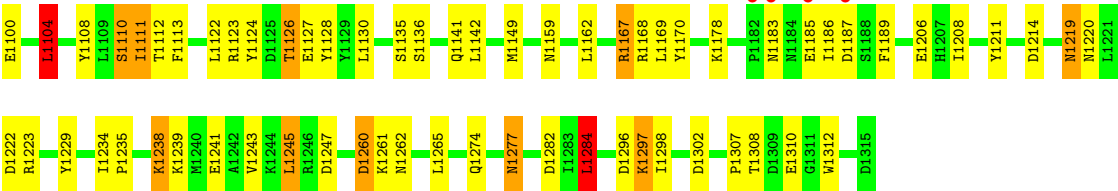
#### • Molecule 1: TETANUS TOXIN HEAVY CHAIN



#### • Molecule 1: TETANUS TOXIN HEAVY CHAIN







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.31Å 53.07Å 118.28Å 90.00° 89.78° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-2.30) 96.5 (29.93-2.30)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.237 , 0.306 0.228 , 0.256	Depositor DCC
$R_{free}$ test set	1543 reflections (3.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.7	Xtriage
Anisotropy	0.846	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 97.4	EDS
Estimated twinning fraction	0.225 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.29$ , $\langle L^2 \rangle = 0.13$	Xtriage
Outliers	0 of 49640 reflections	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	7786	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, NGA, PO4, SIA, GAL, CEQ, SLB

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	0/3740	1.07	20/5076 (0.4%)
1	B	0.94	1/3731 (0.0%)	1.13	19/5064 (0.4%)
All	All	0.85	1/7471 (0.0%)	1.10	39/10140 (0.4%)

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
1	A	0	1
2	B	1	0
All	All	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1229	TYR	CD2-CE2	-5.04	1.31	1.39

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1075	ASP	CB-CG-OD2	9.21	126.59	118.30
1	B	1222	ASP	CB-CG-OD2	8.71	126.14	118.30
1	B	1087	ASP	CB-CG-OD2	7.70	125.23	118.30
1	B	1104	LEU	CB-CG-CD1	-7.20	98.77	111.00
1	B	1282	ASP	CB-CG-OD2	6.92	124.53	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	7	SIA	C2

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1182	PRO	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3652	0	3592	170	0
1	B	3648	0	3588	150	1
2	A	108	0	87	7	0
2	B	108	0	87	10	0
3	B	5	0	0	2	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
5	A	87	0	0	4	0
5	B	154	0	0	2	0
All	All	7786	0	7354	333	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 22.

The worst 5 of 333 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1145:ILE:H	1:A:1145:ILE:HD12	1.14	1.07
1:A:985:LEU:O	1:A:985:LEU:HD22	1.54	1.06
1:B:1064:ILE:O	1:B:1064:ILE:HG22	1.68	0.93
1:B:1111:ILE:HD12	1:B:1112:THR:H	1.33	0.92
1:B:1124:TYR:O	1:B:1126:THR:HG22	1.72	0.88

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)
1:B:873:ASN:O	1:B:1127:GLU:OE1[1.565]	2.17	0.03

## 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	450/472 (95%)	399 (89%)	38 (8%)	13 (3%)	7	4
1	B	449/472 (95%)	396 (88%)	41 (9%)	12 (3%)	8	5
All	All	899/944 (95%)	795 (88%)	79 (9%)	25 (3%)	8	4

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	929	GLU
1	A	1025	ALA
1	A	1182	PRO
1	B	870	TRP
1	B	1066	GLU

### 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	408/425 (96%)	350 (86%)	58 (14%)	5	4
1	B	407/425 (96%)	375 (92%)	32 (8%)	18	21
All	All	815/850 (96%)	725 (89%)	90 (11%)	9	10

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1184	ASN
1	A	1262	ASN
1	B	1186	ILE
1	A	1185	GLU
1	A	1220	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	928	ASN
1	B	944	ASN
1	B	1216	ASN
1	B	903	ASN
1	B	1220	ASN

### 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 ⓘ

14 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	$\# Z  > 2$
2	BGC	A	1	2,4	11,11,12	1.29	1 (9%)	11,15,17	1.67	3 (27%)
2	GAL	A	2	2	10,10,12	1.32	1 (10%)	8,13,17	1.02	1 (12%)
2	NGA	A	3	2	13,14,15	0.94	1 (7%)	14,19,21	1.08	1 (7%)
2	GAL	A	4	2	11,11,12	0.69	0	10,15,17	1.11	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SIA	A	5	2	21,21,21	4.87	3 (14%)	31,31,31	4.23	12 (38%)
2	SLB	A	6	2	21,21,21	1.60	3 (14%)	31,31,31	2.27	15 (48%)
2	SIA	A	7	2	20,20,21	4.16	1 (5%)	23,28,31	1.99	2 (8%)
2	BGC	B	1	2,4	11,11,12	0.84	0	11,15,17	1.96	4 (36%)
2	GAL	B	2	2	10,10,12	1.59	2 (20%)	8,13,17	1.46	1 (12%)
2	NGA	B	3	2	13,14,15	0.74	0	14,19,21	1.52	2 (14%)
2	GAL	B	4	2	11,11,12	1.36	3 (27%)	10,15,17	0.93	1 (10%)
2	SIA	B	5	2	21,21,21	4.78	4 (19%)	31,31,31	3.60	11 (35%)
2	SLB	B	6	2	21,21,21	1.77	3 (14%)	31,31,31	3.44	18 (58%)
2	SIA	B	7	-	20,20,21	3.61	3 (15%)	23,28,31	2.35	7 (30%)

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
2	BGC	A	1	2,4	-	0/2/18/22	0/1/1/1
2	GAL	A	2	2	-	0/2/15/22	0/1/1/1
2	NGA	A	3	2	-	0/6/22/26	0/1/1/1
2	GAL	A	4	2	-	0/2/18/22	0/1/1/1
2	SIA	A	5	2	-	0/20/38/38	0/1/1/1
2	SLB	A	6	2	-	0/20/38/38	0/1/1/1
2	SIA	A	7	2	-	0/15/34/38	0/1/1/1
2	BGC	B	1	2,4	-	0/2/18/22	0/1/1/1
2	GAL	B	2	2	-	0/2/15/22	0/1/1/1
2	NGA	B	3	2	-	0/6/22/26	0/1/1/1
2	GAL	B	4	2	-	0/2/18/22	0/1/1/1
2	SIA	B	5	2	-	0/20/38/38	0/1/1/1
2	SLB	B	6	2	-	0/20/38/38	0/1/1/1
2	SIA	B	7	-	1/1/8/9	0/15/34/38	0/1/1/1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5	SIA	C2-C1	-21.21	1.31	1.53
2	B	5	SIA	C2-C1	-20.37	1.32	1.53
2	A	7	SIA	O6-C2	18.28	1.45	1.28
2	B	7	SIA	O6-C2	15.30	1.42	1.28
2	B	5	SIA	O2-C2	6.80	1.48	1.39

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5	SIA	O2-C2-O6	-14.23	85.30	109.95
2	B	6	SLB	O6-C2-C3	-10.14	104.23	110.22
2	A	5	SIA	O2-C2-C3	-9.97	95.15	109.67
2	A	5	SIA	O6-C2-C3	9.71	115.95	110.22
2	B	5	SIA	O2-C2-C1	-9.57	93.63	109.86

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	7	SIA	C2

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
4	CEQ	A	8[A]	2	5,5,5	2.40	4 (80%)	7,7,7	1.03	1 (14%)
4	CEQ	A	8[B]	2	5,5,5	2.36	4 (80%)	7,7,7	1.00	1 (14%)
3	PO4	B	301	-	4,4,4	0.38	0	6,6,6	0.30	0
4	CEQ	B	8[A]	2	5,5,5	2.35	4 (80%)	7,7,7	0.98	1 (14%)
4	CEQ	B	8[B]	2	5,5,5	2.34	4 (80%)	7,7,7	0.70	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
4	CEQ	A	8[A]	2	-	0/3/3/3	0/0/0/0
4	CEQ	A	8[B]	2	-	0/3/3/3	0/0/0/0
3	PO4	B	301	-	-	0/0/0/0	0/0/0/0
4	CEQ	B	8[A]	2	-	0/3/3/3	0/0/0/0
4	CEQ	B	8[B]	2	-	0/3/3/3	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8[A]	CEQ	SI1-C5	-3.44	1.78	1.87
4	B	8[B]	CEQ	SI1-C5	-3.33	1.79	1.87
4	A	8[B]	CEQ	SI1-C5	-3.27	1.79	1.87
4	B	8[A]	CEQ	SI1-C5	-3.22	1.79	1.87
4	A	8[A]	CEQ	SI1-C2	-2.51	1.78	1.86

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8[A]	CEQ	SI1-C5-C6	-2.32	111.18	115.73
4	A	8[A]	CEQ	SI1-C5-C6	-2.19	111.45	115.73
4	A	8[B]	CEQ	SI1-C5-C6	-2.14	111.54	115.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	451/472 (95%)	0.96	52 (11%) 5 9	27, 37, 54, 68	0
1	B	451/472 (95%)	0.71	31 (6%) 17 24	17, 29, 51, 71	0
All	All	902/944 (95%)	0.83	83 (9%) 9 15	17, 34, 54, 71	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	871	VAL	9.8
1	B	867	LEU	7.0
1	B	872	ASP	6.2
1	A	1183	ASN	5.6
1	A	870	TRP	5.4

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SIA	B	7	20/21	0.23	3.89	44,50,60,63	0
2	BGC	A	1	11/12	0.24	3.70	52,54,61,62	0
2	SIA	A	7	20/21	0.23	3.63	44,56,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SLB	A	6	21/21	0.19	2.63	47,54,60,65	0
2	SIA	B	5	21/21	0.21	2.26	46,62,68,69	0
2	SIA	A	5	21/21	0.24	2.25	53,63,66,67	0
2	GAL	A	4	11/12	0.21	1.95	46,50,51,55	0
2	SLB	B	6	21/21	0.20	1.81	42,49,54,58	0
2	NGA	A	3	14/15	0.19	1.54	50,51,53,53	0
2	NGA	B	3	14/15	0.17	1.24	36,39,42,43	0
2	BGC	B	1	11/12	0.18	1.23	45,51,57,61	0
2	GAL	A	2	10/12	0.15	-0.27	45,47,51,52	0
2	GAL	B	4	11/12	0.14	-0.61	34,37,40,40	0
2	GAL	B	2	10/12	0.14	-7.55	39,44,45,45	0

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CEQ	B	8[A]	6/6	0.66	40.96	71,75,76,76	6
4	CEQ	A	8[A]	6/6	0.40	15.13	72,76,76,76	6
4	CEQ	A	8[B]	6/6	0.40	11.74	66,68,68,68	6
3	PO4	B	301	5/5	0.11	-1.74	58,60,60,61	0
4	CEQ	B	8[B]	6/6	0.66	-	64,65,65,65	6

## 6.5 Other polymers ⓘ

There are no such residues in this entry.