



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 17, 2024 – 01:50 AM EST

PDB ID : 3VE1  
Title : The 2.9 angstrom crystal structure of Transferrin binding protein B (TbpB) from serogroup B M982 *Neisseria meningitidis* in complex with human transferrin  
Authors : Calmettes, C.; Moraes, T.F.  
Deposited on : 2012-01-06  
Resolution : 2.96 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

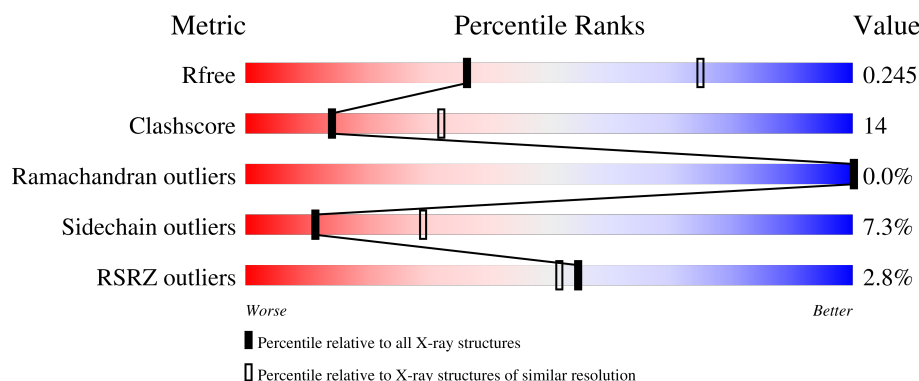
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 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))
$R_{free}$	164625	1044 (2.98-2.94)
Clashscore	180529	1097 (2.98-2.94)
Ramachandran outliers	177936	1049 (2.98-2.94)
Sidechain outliers	177891	1049 (2.98-2.94)
RSRZ outliers	164620	1044 (2.98-2.94)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	658	 4% 57% 22% 18%
1	C	658	 3% 57% 21% 19%
2	B	679	 2% 73% 24% 1%
2	D	679	 0% 72% 24% 2%

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	GOL	B	704	-	-	X	-
3	GOL	D	703	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19274 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 Transferrin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	1	0
			4240	2657	732	844	7			
1	C	536	Total	C	N	O	S	0	0	0
			4215	2640	726	842	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP Q09057
A	35	SER	-	expression tag	UNP Q09057
C	34	GLY	-	expression tag	UNP Q09057
C	35	SER	-	expression tag	UNP Q09057

- Molecule 2 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	675	Total	C	N	O	S	0	2	0
			5254	3296	910	1001	47			
2	D	677	Total	C	N	O	S	0	3	0
			5274	3310	913	1004	47			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	413	ASP	ASN	SEE REMARK 999	UNP P02787
B	429	VAL	ILE	SEE REMARK 999	UNP P02787
B	611	ASP	ASN	SEE REMARK 999	UNP P02787
D	413	ASP	ASN	SEE REMARK 999	UNP P02787
D	429	VAL	ILE	SEE REMARK 999	UNP P02787
D	611	ASP	ASN	SEE REMARK 999	UNP P02787

- Molecule 3 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
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	1	3		
4	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Fe	0	0
			1	1		
5	D	1	Total	Fe	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total	O	0	0
			37	37		
6	B	65	Total	O	0	0
			65	65		
6	C	34	Total	O	0	0
			34	34		
6	D	67	Total	O	0	0
			67	67		

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

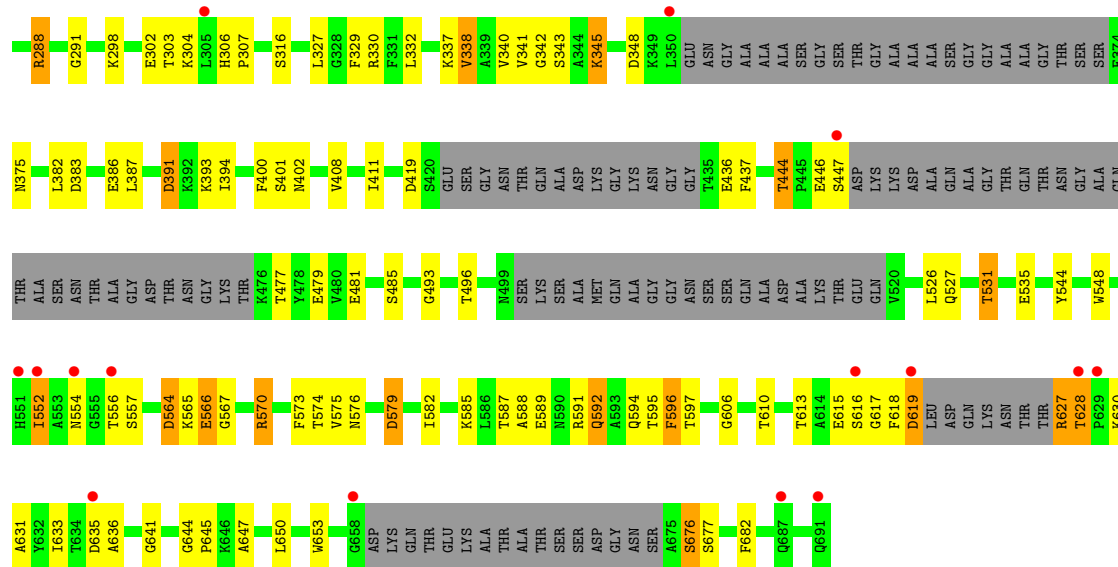
Chain A:

4% 57% 22% 18%

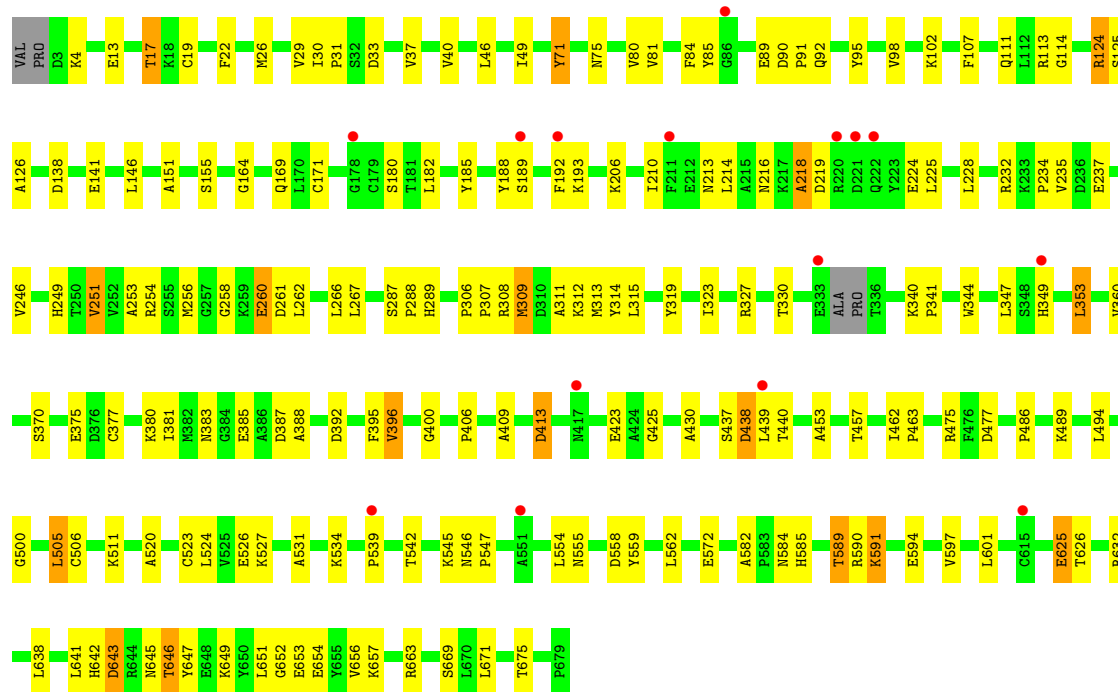
Chain C:

3% 57% 21% 19%

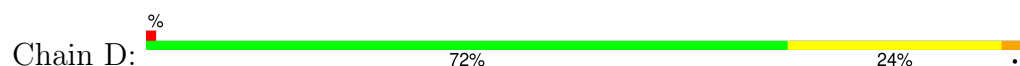
GLY SER LYS ASP Q38 R46 R49 W52 Y53 E57 S66 A70 L73 P74 L80 R83 T93 D94 S97 S108 N109 HIS GLN ASN GLY SER ALA GLY ASN G118 Y119 M120 K123 M124 H129 Q133 Y134 F140 Y141 K142 S146 E147 V148 D149 F150 K153 K154 I155 K156 Y162 I163 H166 G167 R172 K183 G184 V185 F188 D197 F198 R199 E200 I201 I202 K206 Y212 S213 G214 F215 S216 S220 E221 E222 Y223 K226 N227 L244 L253 L264 N265 N266 N267 THR ASN D271 D281 D282



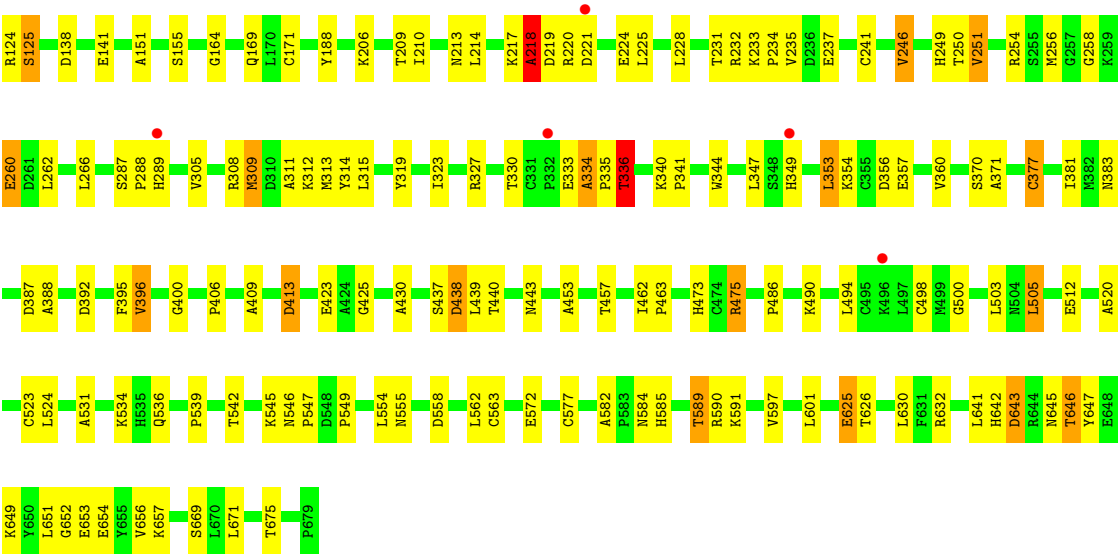
### • Molecule 2: Serotransferrin



### • Molecule 2: Serotransferrin







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.02Å 153.51Å 169.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.93 – 2.96 37.93 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.93-2.96) 99.5 (37.93-2.96)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.18 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, $R_{free}$	0.207 , 0.249 0.203 , 0.245	Depositor DCC
$R_{free}$ test set	2498 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 60.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19274	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2640e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: FE, CO3, GOL

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	0.51	0/4331	0.71	4/5826 (0.1%)
1	C	0.52	0/4300	0.72	7/5782 (0.1%)
2	B	0.56	0/5375	0.68	1/7262 (0.0%)
2	D	0.57	0/5397	0.68	3/7295 (0.0%)
All	All	0.54	0/19403	0.69	15/26165 (0.1%)

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	2
1	C	0	2
2	D	0	2
All	All	0	6

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	288	ARG	NE-CZ-NH2	-13.99	113.30	120.30
1	A	288	ARG	NE-CZ-NH1	-12.57	114.01	120.30
1	C	288	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	A	288	ARG	NE-CZ-NH2	10.76	125.68	120.30
1	C	628	THR	C-N-CD	-9.48	99.74	120.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	SER	Peptide
1	A	564	ASP	Mainchain
1	C	108	SER	Peptide
1	C	564	ASP	Mainchain
2	D	218	ALA	Peptide

## 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	4240	0	4066	133	0
1	C	4215	0	4040	127	0
2	B	5254	0	5065	136	0
2	D	5274	0	5088	139	0
3	A	12	0	16	2	0
3	B	36	0	48	8	0
3	C	6	0	8	3	0
3	D	24	0	32	5	0
4	B	4	0	0	0	0
4	D	4	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	37	0	0	3	0
6	B	65	0	0	8	0
6	C	34	0	0	4	0
6	D	67	0	0	4	0
All	All	19274	0	18363	525	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 14.

The worst 5 of 525 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)
2:B:218:ALA:O	2:B:219:ASP:HB2	1.49	1.11
2:B:124:ARG:HB3	3:B:704:GOL:H11	1.37	1.06
2:D:49:ILE:HG22	2:D:75:ASN:HD22	1.23	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:THR:HG21	1:C:592:GLN:NE2	1.80	0.96
1:C:288:ARG:HD3	3:C:701:GOL:H32	1.45	0.96

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	522/658 (79%)	501 (96%)	20 (4%)	1 (0%)	44	67
1	C	518/658 (79%)	497 (96%)	21 (4%)	0	100	100
2	B	673/679 (99%)	639 (95%)	34 (5%)	0	100	100
2	D	678/679 (100%)	650 (96%)	28 (4%)	0	100	100
All	All	2391/2674 (89%)	2287 (96%)	103 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	565	LYS

### 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	455/533 (85%)	417 (92%)	38 (8%)	9	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	452/533 (85%)	411 (91%)	41 (9%)	7	20
2	B	571/572 (100%)	536 (94%)	35 (6%)	15	36
2	D	573/572 (100%)	538 (94%)	35 (6%)	15	36
All	All	2051/2210 (93%)	1902 (93%)	149 (7%)	11	29

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	33	ASP
2	D	572	GLU
2	D	75	ASN
2	D	330	THR
2	B	235	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	227	ASN
1	C	592	GLN
2	D	289	HIS
1	A	592	GLN
2	B	75	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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	GOL	C	701	-	5,5,5	0.42	0	5,5,5	0.48	0
3	GOL	B	707	-	5,5,5	0.43	0	5,5,5	0.84	0
3	GOL	D	704	-	5,5,5	0.37	0	5,5,5	0.45	0
3	GOL	D	703	-	5,5,5	0.43	0	5,5,5	0.58	0
3	GOL	B	704	-	5,5,5	0.56	0	5,5,5	0.74	0
3	GOL	D	706	-	5,5,5	0.47	0	5,5,5	0.73	0
4	CO3	D	701	5	3,3,3	0.98	0	2,3,3	0.47	0
3	GOL	D	705	-	5,5,5	0.26	0	5,5,5	0.80	0
3	GOL	B	708	-	5,5,5	0.35	0	5,5,5	0.53	0
4	CO3	B	701	5	3,3,3	0.82	0	2,3,3	0.55	0
3	GOL	B	705	-	5,5,5	0.30	0	5,5,5	0.72	0
3	GOL	A	702	-	5,5,5	0.36	0	5,5,5	0.63	0
3	GOL	A	701	-	5,5,5	0.39	0	5,5,5	0.25	0
3	GOL	B	706	-	5,5,5	0.54	0	5,5,5	0.71	0
3	GOL	B	703	-	5,5,5	0.40	0	5,5,5	0.39	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	GOL	C	701	-	-	4/4/4/4	-
3	GOL	B	707	-	-	2/4/4/4	-
3	GOL	D	704	-	-	0/4/4/4	-
3	GOL	D	703	-	-	2/4/4/4	-
3	GOL	B	704	-	-	2/4/4/4	-
3	GOL	D	706	-	-	4/4/4/4	-
3	GOL	D	705	-	-	4/4/4/4	-
3	GOL	B	708	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	705	-	-	4/4/4/4	-
3	GOL	A	702	-	-	4/4/4/4	-
3	GOL	A	701	-	-	2/4/4/4	-
3	GOL	B	706	-	-	2/4/4/4	-
3	GOL	B	703	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	GOL	O1-C1-C2-C3
3	A	702	GOL	O1-C1-C2-O2
3	A	702	GOL	O1-C1-C2-C3
3	B	703	GOL	O1-C1-C2-C3
3	B	705	GOL	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	701	GOL	3	0
3	B	707	GOL	1	0
3	D	703	GOL	4	0
3	B	704	GOL	5	0
3	D	705	GOL	1	0
3	A	702	GOL	2	0
3	B	706	GOL	1	0
3	B	703	GOL	1	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 [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, 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	537/658 (81%)	0.14	26 (4%)	36 33	34, 66, 136, 216	14 (2%)
1	C	536/658 (81%)	0.03	21 (3%)	44 41	37, 65, 143, 191	6 (1%)
2	B	675/679 (99%)	0.11	15 (2%)	62 60	28, 59, 105, 205	9 (1%)
2	D	677/679 (99%)	0.04	5 (0%)	84 82	21, 58, 101, 179	12 (1%)
All	All	2425/2674 (90%)	0.08	67 (2%)	55 52	21, 62, 124, 216	41 (1%)

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	349[A]	HIS	7.0
1	A	268	THR	6.4
1	A	267	ASN	5.6
1	A	350	LEU	4.2
2	B	221	ASP	4.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	705	6/6	0.70	0.21	76,76,76,76	0
3	GOL	A	702	6/6	0.84	0.15	38,38,38,38	6
3	GOL	D	705	6/6	0.84	0.19	43,43,43,43	6
3	GOL	B	706	6/6	0.86	0.14	53,53,53,53	0
3	GOL	B	708	6/6	0.86	0.21	127,127,127,127	0
3	GOL	A	701	6/6	0.86	0.14	50,50,50,50	6
3	GOL	D	706	6/6	0.86	0.15	44,44,44,44	6
3	GOL	B	703	6/6	0.89	0.15	48,48,48,48	6
3	GOL	B	707	6/6	0.90	0.14	57,57,57,57	0
3	GOL	B	704	6/6	0.90	0.11	52,52,52,52	0
3	GOL	D	703	6/6	0.91	0.11	51,51,51,51	0
3	GOL	C	701	6/6	0.94	0.14	60,60,60,60	0
3	GOL	D	704	6/6	0.95	0.10	65,65,65,65	0
4	CO3	D	701	4/4	0.97	0.07	48,48,48,48	0
4	CO3	B	701	4/4	0.99	0.05	36,36,36,36	0
5	FE	B	702	1/1	0.99	0.02	43,43,43,43	0
5	FE	D	702	1/1	1.00	0.01	44,44,44,44	0

## 6.5 Other polymers

There are no such residues in this entry.