



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:51 PM GMT

PDB ID : 3V8X  
Title : The crystal structure of transferrin binding protein A (TbpA) from Neisserial meningitidis serogroup B in complex with full length human transferrin  
Authors : Noinaj, N.; Easley, N.; Buchanan, S.K.  
Deposited on : 2011-12-23  
Resolution : 2.60 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.

---

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

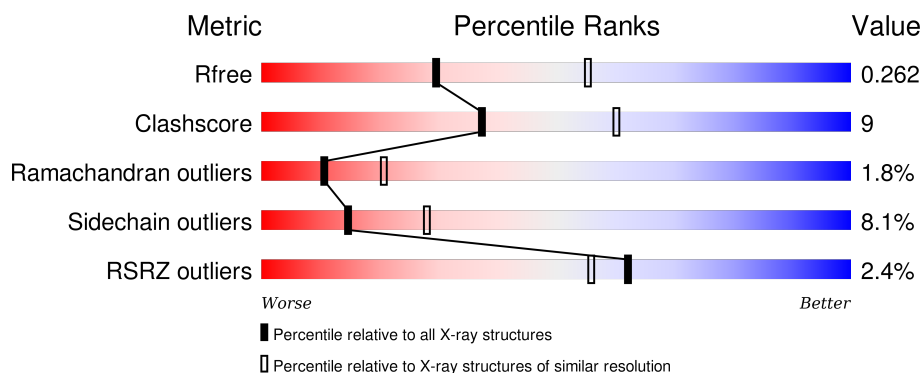
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	904	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 74%, yellow 17%, orange 2%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>74%</span> <span>17%</span> <span>• 6%</span> </div> </div>
2	B	698	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 79%, yellow 13%, orange 2%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>79%</span> <span>13%</span> <span>• • •</span> </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	C8E	A	1001	-	-	-	X
3	C8E	A	1002	-	-	-	X
5	SIA	B	717	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12233 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	853	Total	C	N	O	S	0	2	0
			6686	4176	1218	1282	10			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	EXPRESSION TAG	UNP Q9K0U9
A	13	ASP	-	EXPRESSION TAG	UNP Q9K0U9
A	14	ILE	-	EXPRESSION TAG	UNP Q9K0U9
A	15	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	16	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	17	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	18	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	19	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	20	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	21	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	22	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	23	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	24	HIS	-	EXPRESSION TAG	UNP Q9K0U9
A	435	VAL	ILE	VARIANT	UNP Q9K0U9
A	913	TYR	MET	ENGINEERED MUTATION	UNP Q9K0U9

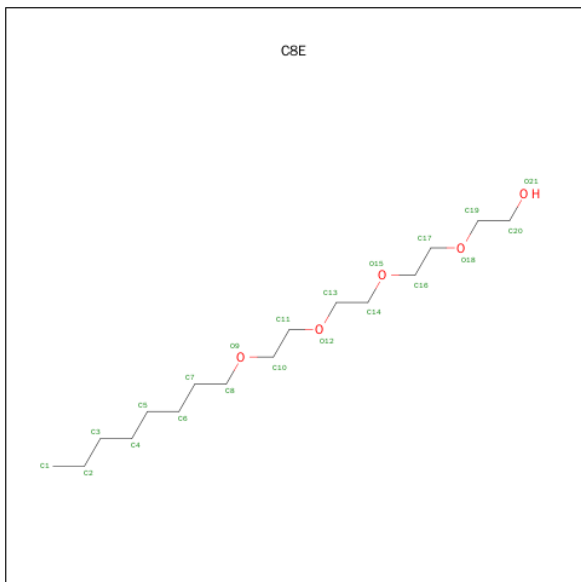
- Molecule 2 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	676	Total	C	N	O	S	0	0	0
			5050	3160	868	977	45			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	429	VAL	ILE	VARIANT	UNP P02787

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula:  $C_{16}H_{34}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	10	Total	C	N	O	0	0
			131	73	5	53		

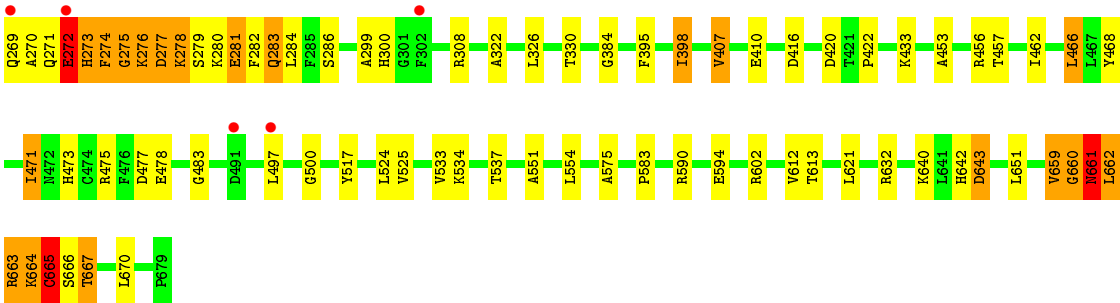
- Molecule 5 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	9	Total	C	N	O	0	0
			120	67	5	48		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	142	Total	O	0	0
			142	142		
6	B	62	Total	O	0	0
			62	62		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.01 Å   129.36 Å   198.59 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.92 – 2.60 49.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.92-2.60) 98.0 (49.47-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.61 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.208   ,   0.267 0.202   ,   0.262	Depositor DCC
$R_{free}$ test set	3604 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.3	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 71726 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, SIA, GAL, C8E, 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	0.29	0/6834	0.47	1/9244 (0.0%)
2	B	0.29	0/5166	0.44	1/7025 (0.0%)
All	All	0.29	0/12000	0.45	2/16269 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	275	GLY	N-CA-C	-5.57	99.18	113.10
1	A	448	ALA	N-CA-C	-5.07	97.30	111.00

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	6686	0	6396	91	0
2	B	5050	0	4646	120	0
3	A	42	0	68	6	0
4	B	131	0	110	7	0
5	B	120	0	101	2	0
6	A	142	0	0	2	0
6	B	62	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12233	0	11321	217	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 9.

The worst 5 of 217 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:282:PHE:O	2:B:283:GLN:HG2	1.46	1.15
2:B:275:GLY:HA2	2:B:281:GLU:O	1.48	1.12
2:B:659:VAL:HG23	2:B:660:GLY:H	0.91	1.05
2:B:269:GLN:HA	2:B:272:GLU:HG3	1.39	1.02
2:B:659:VAL:CG2	2:B:660:GLY:H	1.69	1.00

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	849/904 (94%)	807 (95%)	39 (5%)	3 (0%)	39	65
2	B	674/698 (97%)	593 (88%)	57 (8%)	24 (4%)	4	6
All	All	1523/1602 (95%)	1400 (92%)	96 (6%)	27 (2%)	11	21

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	780	SER
2	B	31	PRO
2	B	272	GLU
2	B	281	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	283	GLN

### 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	685/741 (92%)	616 (90%)	69 (10%)	9	17
2	B	520/585 (89%)	490 (94%)	30 (6%)	25	49
All	All	1205/1326 (91%)	1106 (92%)	99 (8%)	15	27

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	622	ARG
1	A	757	SER
2	B	477	ASP
1	A	650	LEU
1	A	691	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	779	GLN
2	B	283	GLN
2	B	469	ASN
2	B	661	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 ⓘ

19 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$
4	NAG	B	701	2,4	14,14,15	0.65	0	15,19,21	1.05	2 (13%)
4	NAG	B	702	4	14,14,15	0.50	0	15,19,21	1.15	2 (13%)
4	BMA	B	703	4	11,11,12	1.09	1 (9%)	14,15,17	1.76	5 (35%)
4	MAN	B	704	4	11,11,12	0.78	0	14,15,17	1.81	4 (28%)
4	NAG	B	705	4	14,14,15	0.55	0	15,19,21	1.44	1 (6%)
4	GAL	B	706	4	11,11,12	0.64	0	14,15,17	0.60	0
4	SIA	B	707	4	16,20,21	0.52	0	18,28,31	1.74	4 (22%)
4	MAN	B	708	4	11,11,12	0.62	0	14,15,17	1.49	2 (14%)
4	NAG	B	709	4	14,14,15	0.59	0	15,19,21	1.00	0
4	GAL	B	710	4	11,11,12	0.66	0	14,15,17	1.72	1 (7%)
5	NAG	B	711	2,5	14,14,15	0.67	0	15,19,21	1.15	1 (6%)
5	NAG	B	712	5	14,14,15	0.48	0	15,19,21	1.70	2 (13%)
5	BMA	B	713	5	11,11,12	1.94	3 (27%)	14,15,17	2.17	7 (50%)
5	MAN	B	714	5	11,11,12	0.56	0	14,15,17	0.80	0
5	NAG	B	715	5	14,14,15	0.48	0	15,19,21	1.05	1 (6%)
5	GAL	B	716	5	11,11,12	0.56	0	14,15,17	2.27	4 (28%)
5	SIA	B	717	5	16,20,21	0.46	0	18,28,31	1.85	3 (16%)
5	MAN	B	718	5	11,11,12	0.64	0	14,15,17	1.43	2 (14%)
5	NAG	B	719	5	14,14,15	0.51	0	15,19,21	0.57	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	NAG	B	701	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	702	4	-	0/6/23/26	0/1/1/1
4	BMA	B	703	4	-	0/2/19/22	0/1/1/1
4	MAN	B	704	4	-	0/2/19/22	0/1/1/1
4	NAG	B	705	4	-	0/6/23/26	0/1/1/1
4	GAL	B	706	4	-	0/2/19/22	0/1/1/1
4	SIA	B	707	4	-	0/14/34/38	0/1/1/1
4	MAN	B	708	4	-	0/2/19/22	1/1/1/1
4	NAG	B	709	4	-	0/6/23/26	0/1/1/1
4	GAL	B	710	4	-	0/2/19/22	0/1/1/1
5	NAG	B	711	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	712	5	-	0/6/23/26	0/1/1/1
5	BMA	B	713	5	-	0/2/19/22	0/1/1/1
5	MAN	B	714	5	-	0/2/19/22	0/1/1/1
5	NAG	B	715	5	-	0/6/23/26	0/1/1/1
5	GAL	B	716	5	-	0/2/19/22	0/1/1/1
5	SIA	B	717	5	-	0/14/34/38	0/1/1/1
5	MAN	B	718	5	-	0/2/19/22	0/1/1/1
5	NAG	B	719	5	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	713	BMA	O5-C1	2.06	1.47	1.43
4	B	703	BMA	C2-C3	2.29	1.55	1.52
5	B	713	BMA	C2-C3	2.50	1.56	1.52
5	B	713	BMA	C1-C2	4.84	1.63	1.52

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	717	SIA	C7-C6-C5	-4.53	107.47	114.32
5	B	713	BMA	C3-C4-C5	-3.27	104.50	110.20
4	B	704	MAN	C6-C5-C4	-3.19	105.14	113.02
5	B	716	GAL	O6-C6-C5	-2.93	101.66	111.33
5	B	718	MAN	O5-C1-C2	-2.91	106.13	110.86

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	708	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	703	BMA	1	0
4	B	704	MAN	4	0
4	B	705	NAG	1	0
4	B	707	SIA	2	0
5	B	713	BMA	1	0
5	B	714	MAN	2	0
5	B	715	NAG	1	0

## 5.6 Ligand geometry [i](#)

2 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	$\# Z  > 2$
3	C8E	A	1001	-	20,20,20	0.40	0	19,19,19	0.34	0
3	C8E	A	1002	-	20,20,20	0.43	0	19,19,19	0.67	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	C8E	A	1001	-	-	0/18/18/18	0/0/0/0
3	C8E	A	1002	-	-	0/18/18/18	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	C8E	1	0
3	A	1002	C8E	5	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	853/904 (94%)	-0.10	12 (1%) 78 74	37, 69, 111, 155	0
2	B	676/698 (96%)	-0.04	24 (3%) 46 38	43, 82, 152, 212	0
All	All	1529/1602 (95%)	-0.07	36 (2%) 62 56	37, 74, 136, 212	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	267	LEU	5.0
2	B	256	MET	4.5
2	B	37	VAL	4.3
2	B	24	ASP	4.2
2	B	302	PHE	4.1

### 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](#)

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(Å <sup>2</sup> )	Q<0.9
5	SIA	B	717	20/21	0.88	0.32	3.80	73,91,144,146	0
4	NAG	B	701	14/15	0.95	0.14	-0.32	54,67,82,86	0
5	NAG	B	711	14/15	0.90	0.18	-0.64	67,113,122,131	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	702	14/15	0.97	0.10	-2.56	55,66,71,80	0
5	NAG	B	719	14/15	0.62	0.36	-	157,178,187,187	0
5	NAG	B	715	14/15	0.86	0.23	-	113,135,143,144	0
5	MAN	B	718	11/12	0.60	0.22	-	167,175,185,187	0
5	BMA	B	713	11/12	0.63	0.19	-	150,169,201,202	0
4	MAN	B	708	11/12	0.79	0.25	-	85,118,141,153	0
4	NAG	B	709	14/15	0.90	0.15	-	118,125,145,150	0
4	SIA	B	707	20/21	0.62	0.43	-	149,166,174,174	0
4	NAG	B	705	14/15	0.91	0.25	-	81,103,113,123	0
4	MAN	B	704	11/12	0.83	0.28	-	79,95,116,128	0
4	GAL	B	706	11/12	0.60	0.28	-	30,142,156,165	0
4	BMA	B	703	11/12	0.95	0.14	-	54,64,85,108	0
4	GAL	B	710	11/12	0.77	0.16	-	139,154,157,160	0
5	GAL	B	716	11/12	0.51	0.40	-	30,133,150,153	0
5	NAG	B	712	14/15	0.85	0.21	-	111,144,158,162	0
5	MAN	B	714	11/12	0.83	0.18	-	137,153,155,157	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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	C8E	A	1001	21/21	0.79	0.24	4.07	70,101,117,118	0
3	C8E	A	1002	21/21	0.83	0.25	3.97	48,77,98,106	0

## 6.5 Other polymers

There are no such residues in this entry.