



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 07:15 PM GMT

PDB ID : 4RDT  
Title : Structure of the bacterial Zn-transporter ZnuD from *Neisseria meningitidis*  
(flexible conformation bound to a zinc ion)  
Authors : Calmettes, C.; El Bakkouri, M.; Moraes, T.F.  
Deposited on : 2014-09-19  
Resolution : 3.20 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

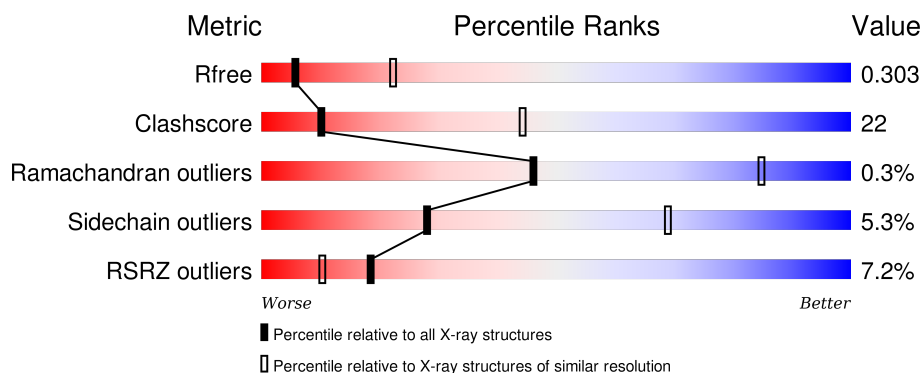
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	748	<div> <div>5%</div> <div>53%</div> <div>29%</div> <div>•</div> <div>15%</div> </div>
1	B	748	<div> <div>7%</div> <div>54%</div> <div>28%</div> <div>••</div> <div>15%</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
2	ZN	A	801	-	-	-	X
3	GOL	A	802	-	-	-	X
3	GOL	A	804	-	-	-	X
4	C8E	A	806	-	-	X	X
5	SO4	A	807	-	-	X	-
5	SO4	B	802	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10159 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 ZnuD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	635	Total	C	N	O	S	0	1	0
			5044	3158	932	945	9			
1	B	635	Total	C	N	O	S	0	0	0
			5032	3150	927	946	9			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q9JZN9
A	-12	ALA	-	EXPRESSION TAG	UNP Q9JZN9
A	-11	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-10	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-9	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-8	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-7	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-6	HIS	-	EXPRESSION TAG	UNP Q9JZN9
A	-5	LEU	-	EXPRESSION TAG	UNP Q9JZN9
A	-4	VAL	-	EXPRESSION TAG	UNP Q9JZN9
A	-3	PRO	-	EXPRESSION TAG	UNP Q9JZN9
A	-2	ARG	-	EXPRESSION TAG	UNP Q9JZN9
A	-1	GLY	-	EXPRESSION TAG	UNP Q9JZN9
A	0	SER	-	EXPRESSION TAG	UNP Q9JZN9
B	-13	MET	-	EXPRESSION TAG	UNP Q9JZN9
B	-12	ALA	-	EXPRESSION TAG	UNP Q9JZN9
B	-11	HIS	-	EXPRESSION TAG	UNP Q9JZN9
B	-10	HIS	-	EXPRESSION TAG	UNP Q9JZN9
B	-9	HIS	-	EXPRESSION TAG	UNP Q9JZN9
B	-8	HIS	-	EXPRESSION TAG	UNP Q9JZN9
B	-7	HIS	-	EXPRESSION TAG	UNP Q9JZN9
B	-6	HIS	-	EXPRESSION TAG	UNP Q9JZN9
B	-5	LEU	-	EXPRESSION TAG	UNP Q9JZN9
B	-4	VAL	-	EXPRESSION TAG	UNP Q9JZN9
B	-3	PRO	-	EXPRESSION TAG	UNP Q9JZN9

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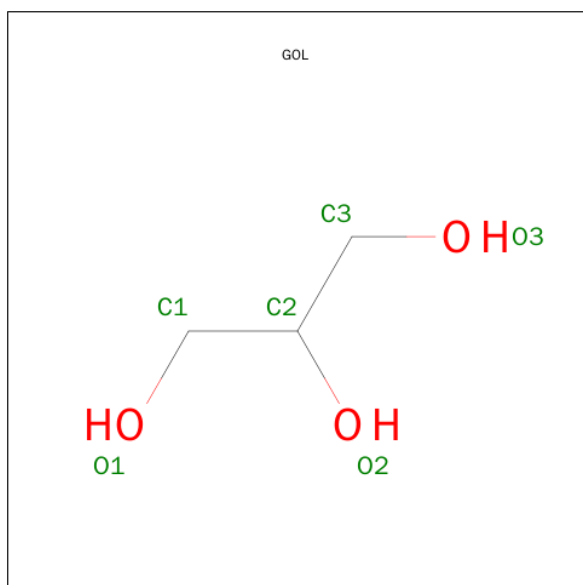
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ARG	-	EXPRESSION TAG	UNP Q9JZN9
B	-1	GLY	-	EXPRESSION TAG	UNP Q9JZN9
B	0	SER	-	EXPRESSION TAG	UNP Q9JZN9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

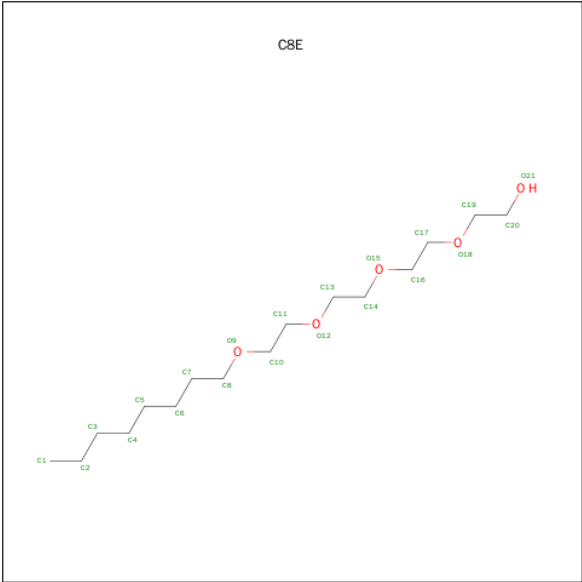
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

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



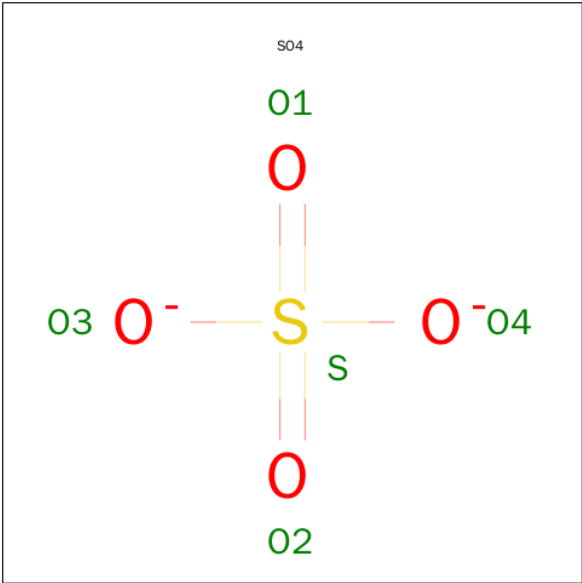
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



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

- 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	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	2	Total	O	0	0
			2	2		

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 ( $\text{RSRZ} > 2$ ). 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.

[illegible]

Chain B:

7% 54% 28% 2% 15%

MET ALA HIS HIS HIS HIS HIS LEU VAL LEU VAL PRO ARG ARG GLY SER SER GLU GLU THR THR GLU GLN SER SER VAL ASP ASP LEU LEU THR VAL SER VAL VAL VAL GLY LYS LYS SER SER ARG P20 R21 A22 T23 S24 G25 L26 L27 H28 T29 S30 K35 I36 I37 D40 T41 L42 R43 Q44 R45 A46 V47 L48

L652	D653	Y659	Q664	K665	K666	L667	E671	T674	P675	L682	Y686	R687	R688	R689	T690	R691	Y692	E693	E694	W697	K700	L704	Q707	H712	R724	S725	F726	T727	V730	N731	V732	K733	F734																						
F578	Y579	E584	I585	Y586	F587	K588	P589	T590	P591	R592	Y593	R594	I595	G596	V597	S598	R603	G604	R605	L609	P610	SER	PRQ	GLY	ARG	GLU	ASP	ALA	ASN	ARG	PHE	ILE	ALA	GLN	D628	P636	R639	L640	G641	F642	H643	L644	K645	A646	S647	L648	T649	D650	R651						
H496	V500	F505	N509	K510	H511	N512	N513	K514	E515	R516	S517	N518	N519	I520	E521	L522	Y526	Q532	Y533	Y538	R539	N540	R541	N544	Y545	I546	L551	N552	D553	GLY	ARG	GLY	PRQ	LYS	SER	ILE	ASP	GLU	ASP	S564	E565	M566	K567	L568	Y571	S574	G575								
L398	D399	N401	K402	V402	Q403	Q409	W415	R425	Q429	R430	A431	S432	I433	GLN	TYR	ASP	LYS	ALA	ALA	LEU	ILE	Q532	ARG	GLU	ASN	TYR	ASN	ASN	TYR	Q552	Q555	D573	E274	D275	I276	A357	R358	L361	R362	R363	Q364	L369	K370	G371	S372	K373	L378	Q379	L385	L388	S389	E390	K393	Q394	P395
R307	R308	K309	A315	E316	R317	K318	F321	P322	G323	F324	L327	R328	V329	R330	D335	T336	R337	R338	V346	E347	R348	R349	N352	Q355	N356	A357	R358	L361	R362	R363	Q364	L369	K370	G371	S372	K373	L378	Q379	L385	L388	S389	E390	K393	Q394	P395										
HIS	GLU	TYR	ASP	D248	C249	R250	A251	D252	I253	I254	W255	Q256	K257	S258	L259	ILE	ASN	LYS	ARG	TYR	LEU	GLN	LEU	TYR	PRQ	HIS	LEU	T272	E273	E274	D275	I276	D277	Y278	D279	N280	L283	F287	HIS	ASP	ASP	ASN	ALA	HIS	ALA	THR	HIS	S299	G300	W303	I304	D305	L306		
G159	M160	L161	E162	K163	L164	T165	S166	G167	G168	L173	F177	V178	H180	T181	G182	G183	L184	Y185	R186	G187	S188	G189	D190	R201	L202	Q210	T211	G212	S213	I214	G215	L216	S217	W218	V219	Q220	E221	K222	G223	F224	I225	Y229	S230	E231	R232	D233	S299	G235	Y236	A240	HIS	SER			
H60	G67	R74	R80	L81	L84	N85	H86	H87	G88	E89	T90	G91	N92	N93	A94	H100	M103	V104	D105	V112	E113	I114	L115	R116	V119	T120	L121	L122	Y123	G126	V127	V128	A129	D136	G137	K138	I139	P140	E141	K142	M143	E151	L152	R155	L156	S157	S158								

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.34Å 156.23Å 158.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 3.20 49.93 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.93-3.20) 93.4 (49.93-3.20)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.270 , 0.305 0.267 , 0.303	Depositor DCC
$R_{free}$ test set	1544 reflections (3.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.1	Xtriage
Anisotropy	0.874	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 68.6	EDS
Estimated twinning fraction	0.046 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	7 of 42104 reflections (0.017%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10159	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	122.0	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 81.23 % 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 3.7266e-07. 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, 0.375 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, ZN, C8E, SO4

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	0.41	0/5160	0.76	11/6969 (0.2%)
1	B	0.36	0/5144	0.74	11/6948 (0.2%)
All	All	0.39	0/10304	0.75	22/13917 (0.2%)

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	LEU	CA-CB-CG	8.03	133.76	115.30
1	B	369	LEU	CA-CB-CG	7.98	133.66	115.30
1	B	648	LEU	CA-CB-CG	7.76	133.16	115.30
1	A	216	LEU	CB-CG-CD2	7.67	124.04	111.00
1	A	173	LEU	CA-CB-CG	7.23	131.94	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	5044	0	4883	220	0
1	B	5032	0	4868	209	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	18	0	24	2	0
4	A	42	0	68	24	0
5	A	5	0	0	3	0
5	B	5	0	0	2	0
6	A	9	0	0	0	0
6	B	2	0	0	1	0
All	All	10159	0	9843	436	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 22.

The worst 5 of 436 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:MET:CG	1:B:219:VAL:HG21	1.65	1.26
1:B:283:LEU:HG	1:B:287:PHE:CE2	1.71	1.25
1:B:283:LEU:CG	1:B:287:PHE:HE2	1.54	1.20
1:A:465:LEU:HD12	4:A:806:C8E:C17	1.72	1.19
1:A:465:LEU:HD12	4:A:806:C8E:H171	1.26	1.12

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	622/748 (83%)	569 (92%)	51 (8%)	2 (0%)	46 85
1	B	621/748 (83%)	569 (92%)	50 (8%)	2 (0%)	46 85
All	All	1243/1496 (83%)	1138 (92%)	101 (8%)	4 (0%)	46 85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	ALA
1	B	251	ALA
1	A	636	PRO
1	B	636	PRO

### 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	527/625 (84%)	500 (95%)	27 (5%)	29	70
1	B	526/625 (84%)	497 (94%)	29 (6%)	27	68
All	All	1053/1250 (84%)	997 (95%)	56 (5%)	28	69

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	692	TYR
1	B	218	TRP
1	B	666	LYS
1	A	707	GLN
1	B	152	LEU

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

Mol	Chain	Res	Type
1	A	685	ASN
1	A	712	HIS
1	B	412	GLN
1	A	552	ASN
1	A	630	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	A	802	-	5,5,5	0.35	0	5,5,5	0.23	0
3	GOL	A	803	-	5,5,5	0.40	0	5,5,5	0.17	0
3	GOL	A	804	-	5,5,5	0.38	0	5,5,5	0.31	0
4	C8E	A	805	-	20,20,20	0.33	0	19,19,19	0.51	0
4	C8E	A	806	-	20,20,20	0.34	0	19,19,19	0.49	0
5	SO4	A	807	-	4,4,4	0.31	0	6,6,6	0.06	0
5	SO4	B	802	-	4,4,4	0.31	0	6,6,6	0.06	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	A	802	-	-	0/4/4/4	0/0/0/0
3	GOL	A	803	-	-	0/4/4/4	0/0/0/0
3	GOL	A	804	-	-	0/4/4/4	0/0/0/0
4	C8E	A	805	-	-	0/18/18/18	0/0/0/0
4	C8E	A	806	-	-	0/18/18/18	0/0/0/0
5	SO4	A	807	-	-	0/0/0/0	0/0/0/0
5	SO4	B	802	-	-	0/0/0/0	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.

6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	GOL	1	0
3	A	804	GOL	1	0
4	A	805	C8E	1	0
4	A	806	C8E	23	0
5	A	807	SO4	3	0
5	B	802	SO4	2	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	635/748 (84%)	0.16	35 (5%) 29 16	43, 87, 164, 259	0
1	B	635/748 (84%)	0.49	56 (8%) 12 7	94, 137, 213, 273	0
All	All	1270/1496 (84%)	0.32	91 (7%) 18 10	43, 119, 195, 273	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	647	SER	7.4
1	B	28	HIS	6.5
1	B	29	THR	6.3
1	A	591	PRO	6.0
1	B	646	ALA	5.6

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	GOL	A	804	6/6	0.70	0.81	10.09	97,104,112,113	0
3	GOL	A	802	6/6	0.67	0.66	7.30	118,132,135,137	0
4	C8E	A	806	21/21	0.86	0.52	3.67	80,98,130,132	0
2	ZN	A	801	1/1	0.93	0.34	2.28	127,127,127,127	0
4	C8E	A	805	21/21	0.89	0.32	0.90	39,92,137,142	0
2	ZN	B	801	1/1	0.95	0.20	-0.12	82,82,82,82	0
5	SO4	A	807	5/5	0.74	0.26	-	157,158,162,169	0
5	SO4	B	802	5/5	0.61	0.23	-	173,176,176,177	0
3	GOL	A	803	6/6	0.62	0.74	-	92,113,117,123	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.