



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:47 am GMT

PDB ID : 5L7E  
Title : MCR IN COMPLEX WITH ligand  
Authors : Edman, K.; Aagaard, A.; Backstrom, S.; Xue, Y.  
Deposited on : 2016-06-03  
Resolution : 1.86 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

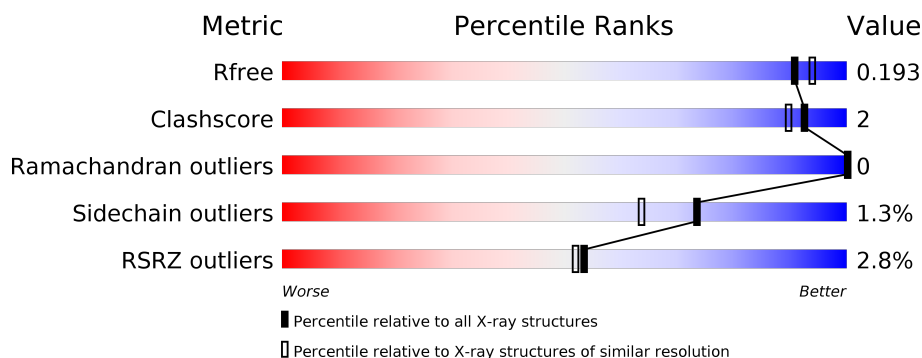
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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))
$R_{free}$	100719	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (1.86-1.86)

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	305	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>•</div> <div>20%</div> </div> </div>
2	B	10	<div> <div>90%</div> <div>10%</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	NHE	A	1101	-	-	-	X
4	MPD	A	1102	-	-	-	X
5	SO4	A	1103	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 2358 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 Mineralocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	7	0
			2060	1332	336	378	14			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	713	MET	-	initiating methionine	UNP P08235
A	714	HIS	-	expression tag	UNP P08235
A	715	ASN	-	expression tag	UNP P08235
A	716	HIS	-	expression tag	UNP P08235
A	717	ASN	-	expression tag	UNP P08235
A	718	HIS	-	expression tag	UNP P08235
A	719	ASN	-	expression tag	UNP P08235
A	720	HIS	-	expression tag	UNP P08235
A	721	ASN	-	expression tag	UNP P08235
A	722	HIS	-	expression tag	UNP P08235
A	723	ASN	-	expression tag	UNP P08235
A	724	HIS	-	expression tag	UNP P08235
A	725	ASN	-	expression tag	UNP P08235
A	726	GLY	-	expression tag	UNP P08235
A	727	GLY	-	expression tag	UNP P08235
A	728	GLU	-	expression tag	UNP P08235
A	729	ASN	-	expression tag	UNP P08235
A	730	LEU	-	expression tag	UNP P08235
A	731	TYR	-	expression tag	UNP P08235
A	732	PHE	-	expression tag	UNP P08235
A	733	GLN	-	expression tag	UNP P08235
A	734	GLY	-	expression tag	UNP P08235
A	808	SER	CYS	conflict	UNP P08235
A	810	LEU	SER	conflict	UNP P08235
A	910	SER	CYS	conflict	UNP P08235
A	985	GLY	-	expression tag	UNP P08235
A	986	GLY	-	expression tag	UNP P08235

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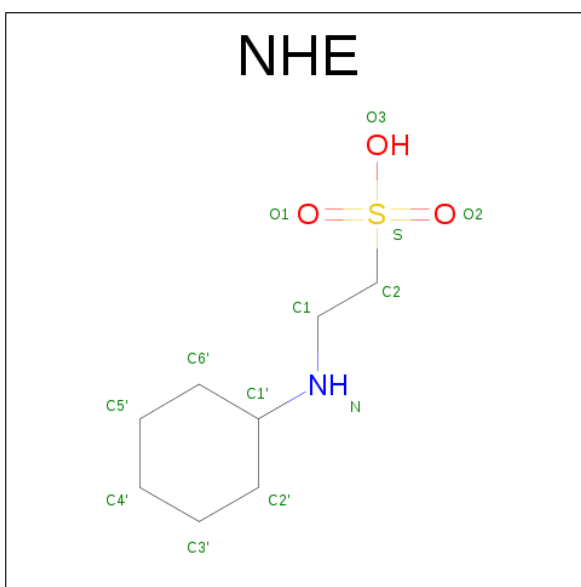
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Chain	Residue	Modelled	Actual	Comment	Reference
A	987	SER	-	expression tag	UNP P08235
A	988	LEU	-	expression tag	UNP P08235
A	989	VAL	-	expression tag	UNP P08235
A	990	PRO	-	expression tag	UNP P08235
A	991	ARG	-	expression tag	UNP P08235
A	992	GLY	-	expression tag	UNP P08235
A	993	SER	-	expression tag	UNP P08235
A	994	GLY	-	expression tag	UNP P08235
A	995	GLY	-	expression tag	UNP P08235
A	996	GLY	-	expression tag	UNP P08235
A	997	SER	-	expression tag	UNP P08235
A	998	GLY	-	expression tag	UNP P08235
A	999	GLY	-	expression tag	UNP P08235
A	1000	SER	-	expression tag	UNP P08235
A	1001	GLY	-	expression tag	UNP P08235
A	1002	GLY	-	expression tag	UNP P08235
A	1003	PRO	-	expression tag	UNP P08235
A	1004	GLN	-	expression tag	UNP P08235
A	1005	ALA	-	expression tag	UNP P08235
A	1006	GLN	-	expression tag	UNP P08235
A	1007	GLN	-	expression tag	UNP P08235
A	1008	LYS	-	expression tag	UNP P08235
A	1009	SER	-	expression tag	UNP P08235
A	1010	LEU	-	expression tag	UNP P08235
A	1011	LEU	-	expression tag	UNP P08235
A	1012	GLN	-	expression tag	UNP P08235
A	1013	GLN	-	expression tag	UNP P08235
A	1014	LEU	-	expression tag	UNP P08235
A	1015	LEU	-	expression tag	UNP P08235
A	1016	THR	-	expression tag	UNP P08235
A	1017	GLU	-	expression tag	UNP P08235

- Molecule 2 is a protein called NCOA1 peptide.

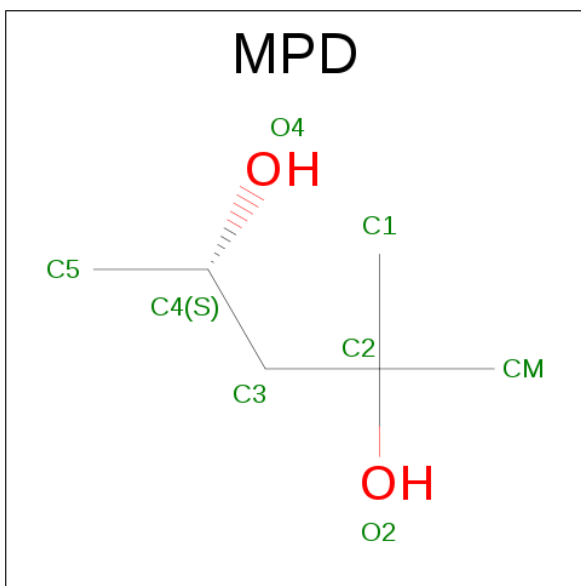
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	0
			82	52	13	17			

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C<sub>8</sub>H<sub>17</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



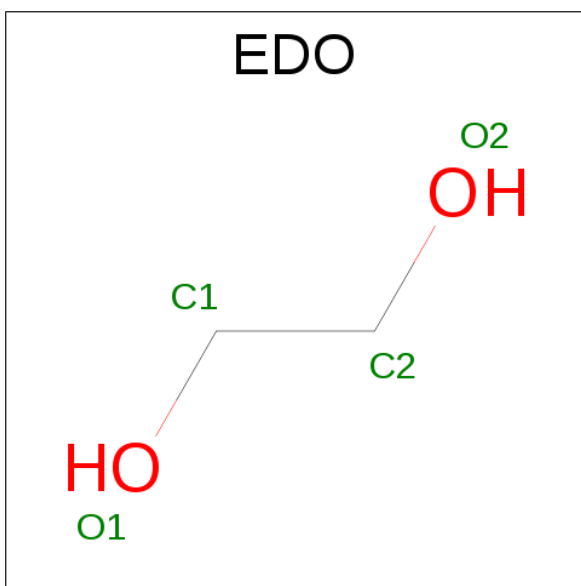
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		

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



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

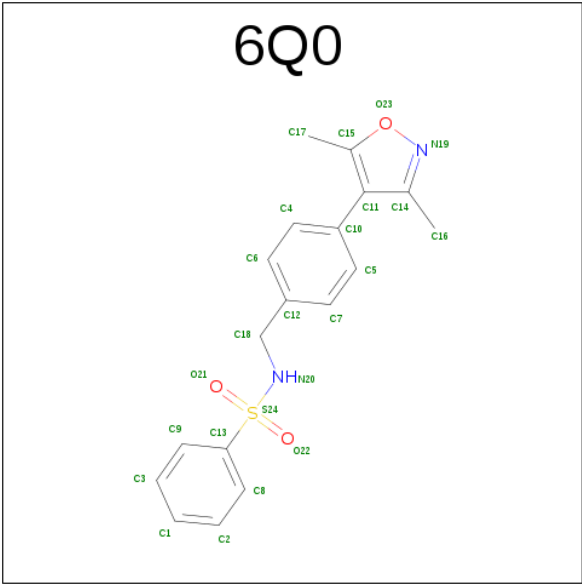
- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 7 is {N}-[[4-(3,5-dimethyl-1,2-oxazol-4-yl)phenyl]methyl]benzenesulfonamide

(three-letter code: 6Q0) (formula: C<sub>18</sub>H<sub>18</sub>N<sub>2</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			24	18	2	3	1		

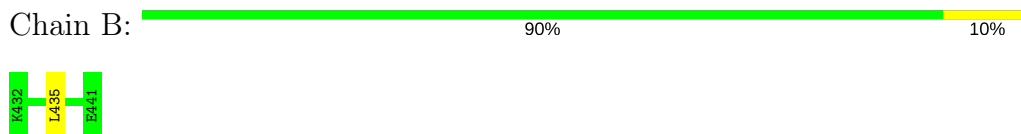
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	153	Total	O	0	0
			153	153		
8	B	5	Total	O	0	0
			5	5		



i

- Molecule 1: Mineralocorticoid receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.62Å 77.83Å 78.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.35 – 1.86 41.24 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.9 (41.35-1.86) 98.9 (41.24-1.86)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 1.86Å)	Xtriage
Refinement program	BUSTER	Depositor
R, $R_{free}$	0.180 , 0.197 0.179 , 0.193	Depositor DCC
$R_{free}$ test set	1287 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2358	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NHE, SO4, MPD, 6Q0, EDO

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	0/2107	0.56	0/2843
2	B	0.39	0/81	0.54	0/106
All	All	0.50	0/2188	0.56	0/2949

There are no bond length outliers.

There are no bond angle outliers.

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	2060	0	2062	8	0
2	B	82	0	90	0	0
3	A	13	0	17	2	0
4	A	8	0	14	2	0
5	A	5	0	0	0	0
6	A	8	0	12	0	0
7	A	24	0	0	0	0
8	A	153	0	0	0	0
8	B	5	0	0	0	0
All	All	2358	0	2195	8	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 2.

All (8) 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:A:749:ILE:HG23	3:A:1101:NHE:H2'2	1.85	0.57
1:A:919:GLN:H	1:A:919:GLN:HE21	1.54	0.54
1:A:873:LYS:HD2	4:A:1102:MPD:H53	1.93	0.51
1:A:780:VAL:HG22	4:A:1102:MPD:H52	1.97	0.45
1:A:749:ILE:HD11	1:A:828:TYR:HE1	1.82	0.45
1:A:916:GLN:HB3	1:A:919:GLN:HE22	1.80	0.45
1:A:751:TYR:CZ	3:A:1101:NHE:H2'1	2.55	0.41
1:A:816:TRP:HB2	1:A:869:TYR:CE1	2.55	0.41

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	247/305 (81%)	245 (99%)	2 (1%)	0	100	100
2	B	8/10 (80%)	8 (100%)	0	0	100	100
All	All	255/315 (81%)	253 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	233/272 (86%)	231 (99%)	2 (1%)	82	77
2	B	10/10 (100%)	9 (90%)	1 (10%)	9	1
All	All	243/282 (86%)	240 (99%)	3 (1%)	73	67

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	919	GLN
1	A	950	HIS
2	B	435	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	919	GLN
1	A	923	GLN

### 5.3.3 RNA [i](#)

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](#)

6 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	NHE	A	1101	-	13,13,13	3.44	4 (30%)	15,17,17	4.18	9 (60%)
4	MPD	A	1102	-	7,7,7	0.31	0	9,10,10	0.77	0
5	SO4	A	1103	-	4,4,4	0.17	0	6,6,6	0.09	0
6	EDO	A	1104	-	3,3,3	0.42	0	2,2,2	0.41	0
6	EDO	A	1105	-	3,3,3	0.40	0	2,2,2	0.17	0
7	6Q0	A	1106	-	21,26,26	2.25	3 (14%)	30,37,37	0.88	1 (3%)

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	NHE	A	1101	-	-	0/7/15/15	0/1/1/1
4	MPD	A	1102	-	-	0/5/5/5	0/0/0/0
5	SO4	A	1103	-	-	0/0/0/0	0/0/0/0
6	EDO	A	1104	-	-	0/1/1/1	0/0/0/0
6	EDO	A	1105	-	-	0/1/1/1	0/0/0/0
7	6Q0	A	1106	-	-	0/16/16/16	0/2/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	NHE	C2-S	-8.14	1.65	1.77
7	A	1106	6Q0	C11-C10	-2.67	1.45	1.50
7	A	1106	6Q0	O22-S24	2.01	1.45	1.43
3	A	1101	NHE	C5'-C6'	2.46	1.59	1.53
3	A	1101	NHE	O3-S	3.51	1.59	1.47
3	A	1101	NHE	O2-S	7.82	1.68	1.45
7	A	1106	6Q0	S24-N20	9.18	1.73	1.61

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	NHE	O1-S-C2	-6.89	100.87	106.79
3	A	1101	NHE	O2-S-C2	-4.71	102.74	106.79
3	A	1101	NHE	O3-S-O2	-4.00	102.19	111.37
7	A	1106	6Q0	O21-S24-C13	-2.34	105.06	107.95
3	A	1101	NHE	C5'-C6'-C1'	3.14	115.72	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	NHE	C3'-C2'-C1'	3.17	115.77	111.11
3	A	1101	NHE	O3-S-O1	3.24	118.79	111.37
3	A	1101	NHE	C4'-C3'-C2'	3.45	118.54	111.42
3	A	1101	NHE	C4'-C5'-C6'	3.52	118.69	111.42
3	A	1101	NHE	O3-S-C2	10.82	119.36	106.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	NHE	2	0
4	A	1102	MPD	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	243/305 (79%)	-0.09	7 (2%) 52 50	13, 23, 47, 66	0
2	B	10/10 (100%)	-0.12	0 100 100	27, 33, 56, 57	0
All	All	253/315 (80%)	-0.09	7 (2%) 53 52	13, 23, 48, 66	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	950	HIS	4.9
1	A	952	LEU	4.4
1	A	951	ALA	3.8
1	A	916	GLN	3.6
1	A	908	THR	2.6
1	A	884	ASP	2.2
1	A	759	PRO	2.1

### 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](#)

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
4	MPD	A	1102	8/8	0.88	0.31	9.27	51,52,54,54	0
3	NHE	A	1101	13/13	0.88	0.21	3.12	36,49,53,54	0
5	SO4	A	1103	5/5	0.93	0.13	2.89	109,113,114,115	0
6	EDO	A	1104	4/4	0.94	0.14	1.23	35,38,39,40	0
6	EDO	A	1105	4/4	0.85	0.20	0.37	46,48,50,52	0
7	6Q0	A	1106	24/24	0.96	0.10	0.34	14,20,26,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.