



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:50 am GMT

PDB ID : 4GMF
Title : Apo Structure of a ThiazolinyI Imine Reductase from Yersinia enterocolitica (Irp3)
Authors : Lamb, A.L.; Meneely, K.M.
Deposited on : 2012-08-15
Resolution : 1.85 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

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 : 1.7.2 (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

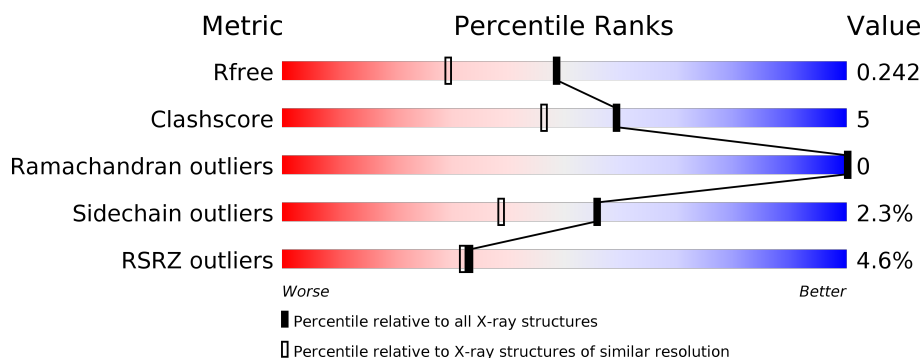
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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 ≥ 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	372	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	372	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>9%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	372	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	372	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>•</div> <div>11%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10938 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 Yersiniabactin biosynthetic protein YbtU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2628	1675	475	463	15			
1	B	329	Total	C	N	O	S	0	0	0
			2576	1643	464	454	15			
1	C	330	Total	C	N	O	S	0	0	0
			2589	1651	467	456	15			
1	D	332	Total	C	N	O	S	0	0	0
			2604	1660	469	460	15			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	GLU	-	EXPRESSION TAG	UNP A1JTG0
A	367	HIS	-	EXPRESSION TAG	UNP A1JTG0
A	368	HIS	-	EXPRESSION TAG	UNP A1JTG0
A	369	HIS	-	EXPRESSION TAG	UNP A1JTG0
A	370	HIS	-	EXPRESSION TAG	UNP A1JTG0
A	371	HIS	-	EXPRESSION TAG	UNP A1JTG0
A	372	HIS	-	EXPRESSION TAG	UNP A1JTG0
B	366	GLU	-	EXPRESSION TAG	UNP A1JTG0
B	367	HIS	-	EXPRESSION TAG	UNP A1JTG0
B	368	HIS	-	EXPRESSION TAG	UNP A1JTG0
B	369	HIS	-	EXPRESSION TAG	UNP A1JTG0
B	370	HIS	-	EXPRESSION TAG	UNP A1JTG0
B	371	HIS	-	EXPRESSION TAG	UNP A1JTG0
B	372	HIS	-	EXPRESSION TAG	UNP A1JTG0
C	366	GLU	-	EXPRESSION TAG	UNP A1JTG0
C	367	HIS	-	EXPRESSION TAG	UNP A1JTG0
C	368	HIS	-	EXPRESSION TAG	UNP A1JTG0
C	369	HIS	-	EXPRESSION TAG	UNP A1JTG0
C	370	HIS	-	EXPRESSION TAG	UNP A1JTG0
C	371	HIS	-	EXPRESSION TAG	UNP A1JTG0
C	372	HIS	-	EXPRESSION TAG	UNP A1JTG0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	366	GLU	-	EXPRESSION TAG	UNP A1JTG0
D	367	HIS	-	EXPRESSION TAG	UNP A1JTG0
D	368	HIS	-	EXPRESSION TAG	UNP A1JTG0
D	369	HIS	-	EXPRESSION TAG	UNP A1JTG0
D	370	HIS	-	EXPRESSION TAG	UNP A1JTG0
D	371	HIS	-	EXPRESSION TAG	UNP A1JTG0
D	372	HIS	-	EXPRESSION TAG	UNP A1JTG0

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



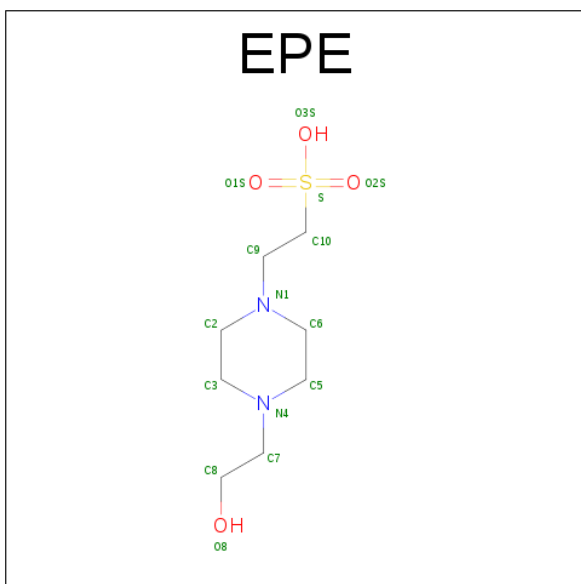
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

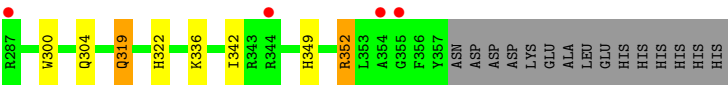
- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



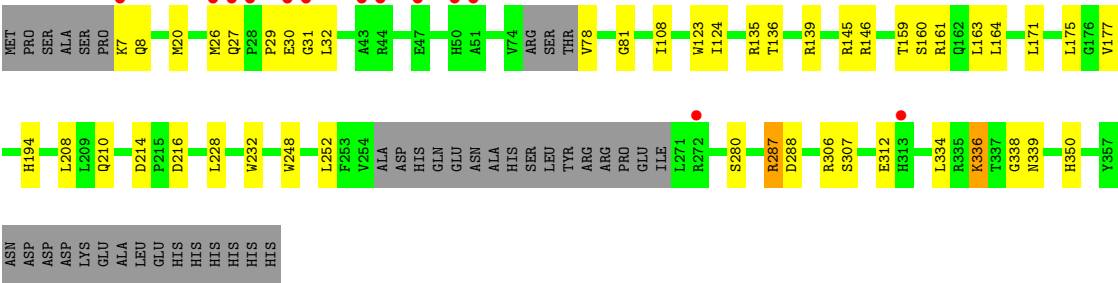
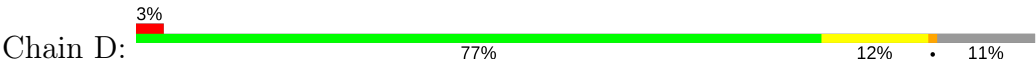
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total 105	O 105	0	0
5	B	108	Total 108	O 108	0	0
5	C	125	Total 125	O 125	0	0
5	D	160	Total 160	O 160	0	0



● Molecule 1: Yersiniabactin biosynthetic protein YbtU



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.87Å 93.90Å 181.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.97 – 1.85 40.97 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.97-1.85) 99.6 (40.97-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.40	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.196 , 0.242 0.195 , 0.242	Depositor DCC
R_{free} test set	6135 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10938	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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 39.44 % 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 3.1708e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: EPE, SO4, 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	1.05	5/2699 (0.2%)	1.03	6/3678 (0.2%)
1	B	1.12	10/2644 (0.4%)	1.00	5/3602 (0.1%)
1	C	1.07	5/2657 (0.2%)	1.02	6/3618 (0.2%)
1	D	1.14	4/2675 (0.1%)	1.02	6/3646 (0.2%)
All	All	1.10	24/10675 (0.2%)	1.02	23/14544 (0.2%)

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

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	TRP	CD2-CE2	8.56	1.51	1.41
1	B	248	TRP	CD2-CE2	6.88	1.49	1.41
1	D	123	TRP	CD2-CE2	6.52	1.49	1.41
1	A	200	TRP	CD2-CE2	6.34	1.49	1.41
1	D	232	TRP	CD2-CE2	5.91	1.48	1.41

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ARG	NE-CZ-NH2	-12.25	114.17	120.30
1	C	135	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	C	145	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	A	135	ARG	NE-CZ-NH1	9.39	124.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	ARG	NE-CZ-NH2	-6.69	116.95	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	VAL	Peptide
1	A	14	GLY	Peptide

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	2628	0	2607	37	0
1	B	2576	0	2552	22	0
1	C	2589	0	2568	30	0
1	D	2604	0	2578	29	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	B	4	0	6	0	0
3	D	4	0	6	2	0
4	D	15	0	18	3	0
5	A	105	0	0	4	0
5	B	108	0	0	2	0
5	C	125	0	0	3	0
5	D	160	0	0	5	0
All	All	10938	0	10335	112	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 5.

The worst 5 of 112 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:172:LEU:HD23	1:A:179:THR:HG23	1.36	1.01
1:A:75:ARG:N	1:A:75:ARG:HE	1.61	0.98
1:A:124:ILE:H	1:A:323:GLN:HE22	1.10	0.97
1:A:75:ARG:HE	1:A:75:ARG:H	0.95	0.89
1:D:145:ARG:HH12	3:D:403:EDO:H22	1.40	0.87

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	329/372 (88%)	323 (98%)	6 (2%)	0	100	100
1	B	321/372 (86%)	313 (98%)	8 (2%)	0	100	100
1	C	322/372 (87%)	314 (98%)	8 (2%)	0	100	100
1	D	326/372 (88%)	318 (98%)	8 (2%)	0	100	100
All	All	1298/1488 (87%)	1268 (98%)	30 (2%)	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	281/315 (89%)	273 (97%)	8 (3%)	49	31
1	B	275/315 (87%)	270 (98%)	5 (2%)	64	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	277/315 (88%)	268 (97%)	9 (3%)	44	25
1	D	279/315 (89%)	275 (99%)	4 (1%)	71	61
All	All	1112/1260 (88%)	1086 (98%)	26 (2%)	56	39

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	271	LEU
1	C	139	ARG
1	D	252	LEU
1	B	335	ARG
1	C	132	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	323	GLN
1	C	8	GLN
1	D	339	ASN
1	B	332	GLN
1	B	350	HIS

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](#)

7 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	$\# Z > 2$
2	SO4	A	401	-	4,4,4	0.39	0	6,6,6	0.73	0
2	SO4	B	401	-	4,4,4	0.36	0	6,6,6	0.33	0
3	EDO	B	402	-	3,3,3	0.29	0	2,2,2	2.03	1 (50%)
2	SO4	C	401	-	4,4,4	0.24	0	6,6,6	0.86	0
2	SO4	D	401	-	4,4,4	0.48	0	6,6,6	0.35	0
4	EPE	D	402	-	15,15,15	2.07	2 (13%)	18,20,20	3.95	9 (50%)
3	EDO	D	403	-	3,3,3	0.67	0	2,2,2	0.35	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
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
3	EDO	B	402	-	-	0/1/1/1	0/0/0/0
2	SO4	C	401	-	-	0/0/0/0	0/0/0/0
2	SO4	D	401	-	-	0/0/0/0	0/0/0/0
4	EPE	D	402	-	-	0/9/19/19	0/1/1/1
3	EDO	D	403	-	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	402	EPE	C10-S	-5.65	1.69	1.77
4	D	402	EPE	O3S-S	4.37	1.62	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	EPE	O3S-S-C10	-4.69	100.28	106.06
4	D	402	EPE	C2-C3-N4	-4.01	102.52	110.63
4	D	402	EPE	C9-N1-C2	-3.21	103.03	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	EDO	O2-C2-C1	-2.44	94.60	112.08
4	D	402	EPE	C3-C2-N1	2.63	115.96	110.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	SO4	1	0
4	D	402	EPE	3	0
3	D	403	EDO	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, 95th 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 ²)	Q<0.9
1	A	335/372 (90%)	0.13	20 (5%) 23 22	14, 27, 49, 65	0
1	B	329/372 (88%)	0.17	14 (4%) 36 34	14, 26, 46, 57	0
1	C	330/372 (88%)	0.06	14 (4%) 37 35	16, 25, 46, 76	0
1	D	332/372 (89%)	0.08	13 (3%) 40 38	12, 24, 44, 62	0
All	All	1326/1488 (89%)	0.11	61 (4%) 33 32	12, 26, 46, 76	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	43	ALA	5.3
1	A	43	ALA	4.7
1	D	30	GLU	4.6
1	C	354	ALA	4.5
1	C	270	ILE	4.3

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, 95th 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(\AA^2)	Q<0.9
3	EDO	B	402	4/4	0.88	0.12	1.91	33,35,35,39	0
4	EPE	D	402	15/15	0.95	0.16	1.21	27,41,50,53	0
2	SO4	D	401	5/5	0.97	0.14	-0.06	53,54,59,59	0
2	SO4	B	401	5/5	0.98	0.10	-0.37	49,50,58,59	0
2	SO4	A	401	5/5	0.94	0.13	-0.63	53,54,61,64	0
2	SO4	C	401	5/5	0.98	0.09	-0.84	47,47,51,56	0
3	EDO	D	403	4/4	0.87	0.08	-	37,37,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.