wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 06:36 am GMT

PDB ID	:	5AOU
Title	:	Structure of the engineered retro-aldolase RA95.5-8F apo
Authors	:	Obexer, R.; Mittl, P.; Hilvert, D.
Deposited on	:	2015-09-11
Resolution	:	1.10 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

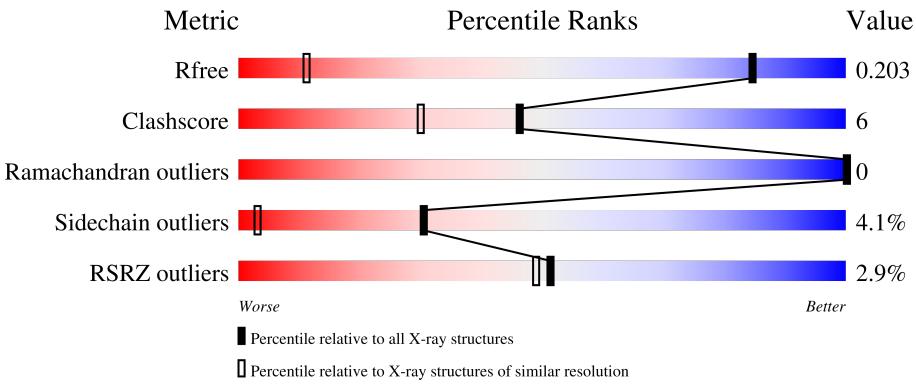
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.10 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}	130704	1619 (1.14-1.06)
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

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 >=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 <=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	258	3% 74% 18% • • 6%

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	PO4	A	5006	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2304 atoms, of which 9 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 INDOLE-3-GLYCEROL PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	242	2079	1324	9	348	390	8	0	13	1

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2246	LEU	-	expression tag	UNP Q06121
A	2247	ILE	-	expression tag	UNP Q06121
A	2248	GLU	-	expression tag	UNP Q06121
A	2249	GLY	-	expression tag	UNP Q06121
A	2250	SER	-	expression tag	UNP Q06121
A	2251	LEU	-	expression tag	UNP Q06121
A	2252	GLU	-	expression tag	UNP Q06121
A	2253	HIS	-	expression tag	UNP Q06121
A	2254	HIS	-	expression tag	UNP Q06121
A	2255	HIS	-	expression tag	UNP Q06121
A	2256	HIS	-	expression tag	UNP Q06121
A	2257	HIS	-	expression tag	UNP Q06121
A	2258	HIS	-	expression tag	UNP Q06121
A	1010	GLU	LYS	engineered mutation	UNP Q06121
A	1022	VAL	PHE	engineered mutation	UNP Q06121
A	1023	HIS	ARG	engineered mutation	UNP Q06121
A	1051	TYR	GLU	engineered mutation	UNP Q06121
A	1053	LEU	LYS	engineered mutation	UNP Q06121
A	2070	ALA	SER	engineered mutation	UNP Q06121
A	2072	TYR	PHE	engineered mutation	UNP Q06121
A	2075	PRO	ARG	engineered mutation	UNP Q06121
A	2083	LYS	LEU	engineered mutation	UNP Q06121
A	2090	ASP	ASN	engineered mutation	UNP Q06121
A	2095	MET	THR	engineered mutation	UNP Q06121
A	2110	ASN	LYS	engineered mutation	UNP Q06121
A	2135	GLU	LYS	engineered mutation	UNP Q06121
A	2151	GLY	SER	engineered mutation	UNP Q06121

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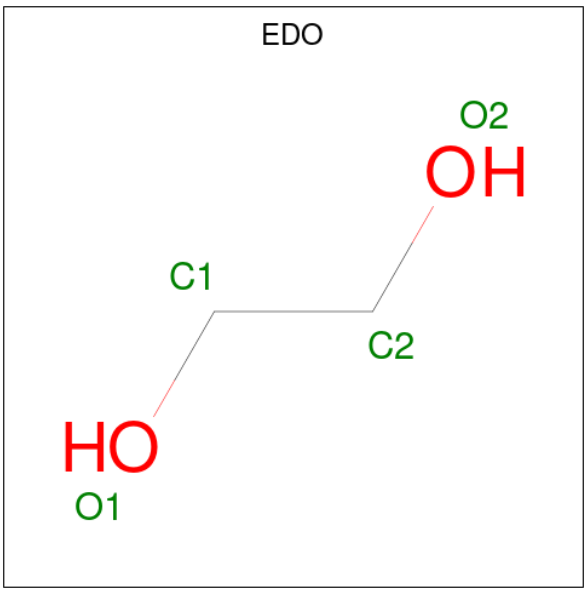
Chain	Residue	Modelled	Actual	Comment	Reference
A	2159	LEU	GLU	engineered mutation	UNP Q06121
A	2178	THR	GLY	engineered mutation	UNP Q06121
A	2180	TYR	ASN	engineered mutation	UNP Q06121
A	2182	MET	ARG	engineered mutation	UNP Q06121
A	2183	ASN	ASP	engineered mutation	UNP Q06121
A	2184	PHE	LEU	engineered mutation	UNP Q06121
A	2187	GLY	LEU	engineered mutation	UNP Q06121
A	2209	PRO	ALA	engineered mutation	UNP Q06121
A	2210	LEU	GLU	engineered mutation	UNP Q06121
A	2211	LEU	SER	engineered mutation	UNP Q06121
A	2212	ASP	GLY	engineered mutation	UNP Q06121
A	2213	PHE	ILE	engineered mutation	UNP Q06121
A	2214	PHE	SER	engineered mutation	UNP Q06121
A	2216	PRO	ARG	engineered mutation	UNP Q06121
A	2231	MET	LEU	engineered mutation	UNP Q06121
A	2233	SER	GLY	engineered mutation	UNP Q06121

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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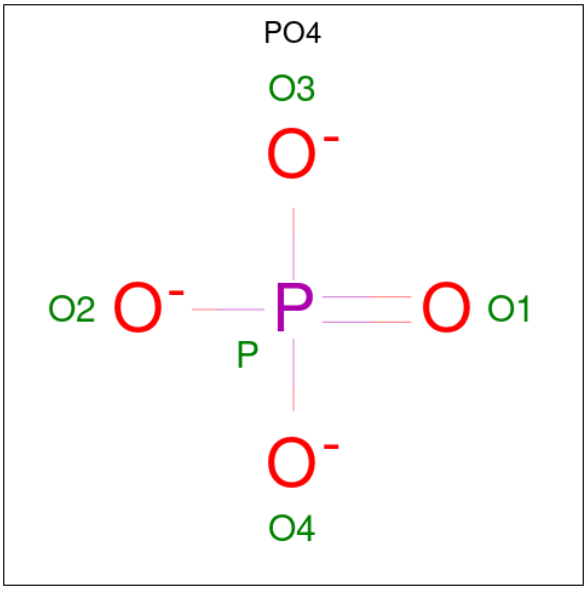
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
			Total	C	O		
2	A	1	4	2	2	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is water.

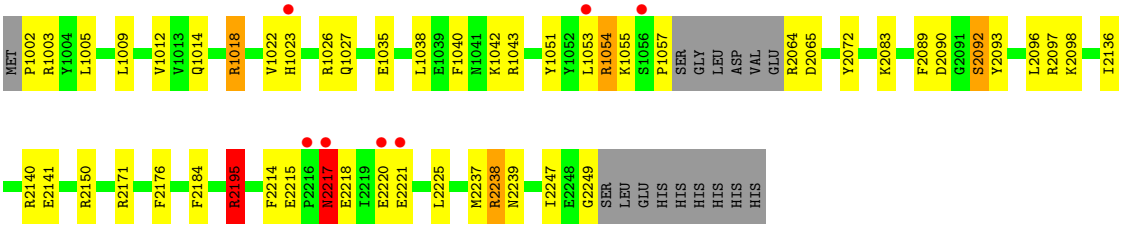
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	190	190	190	0	0

3 Residue-property plots (i)

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.

• Molecule 1: INDOLE-3-GLYCEROL PHOSPHATE SYNTHASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	75.09Å 84.76Å 37.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.20 – 1.10 42.38 – 1.10	Depositor EDS
% Data completeness (in resolution range)	88.8 (56.20-1.10) 90.3 (42.38-1.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 1.10Å)	Xtriage
Refinement program	SHELXL	Depositor
R, R_{free}	0.169 , 0.219 0.164 , 0.203	Depositor DCC
R_{free} test set	4272 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	11.3	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 81.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	2304	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, MHO, 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	0.74	0/2093	1.59	39/2822 (1.4%)

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1054	ARG	NE-CZ-NH1	-15.91	112.34	120.30
1	A	1054	ARG	NE-CZ-NH2	15.29	127.94	120.30
1	A	2150	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	A	1026	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	A	2072	TYR	CB-CG-CD1	9.71	126.83	121.00

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	2070	9	2114	27	0
2	A	20	0	30	2	0
3	A	15	0	0	0	0
4	A	190	0	0	7	0
All	All	2295	9	2144	27	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 6.

The worst 5 of 27 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:2171:ARG:HH12	2:A:3009:EDO:H22	1.30	0.95
1:A:1054:ARG:HD2	4:A:4079:HOH:O	1.81	0.80
1:A:2215[B]:GLU:HB2	1:A:2217:ASN:OD1	1.83	0.77
1:A:2215[A]:GLU:HA	1:A:2215[A]:GLU:OE1	1.88	0.72
1:A:2092[B]:SER:HB3	4:A:4103:HOH:O	1.98	0.64

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	250/258 (97%)	248 (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	231/234 (99%)	221 (96%)	10 (4%)	29 3

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2217	ASN
1	A	2220	GLU
1	A	2247	ILE
1	A	2083	LYS
1	A	2092[A]	SER

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

Mol	Chain	Res	Type
1	A	1041	ASN
1	A	2228	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	MHO	A	2237	1	7,8,9	1.61	1 (14%)	4,9,11	1.87	1 (25%)

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
1	MHO	A	2237	1	-	2/6/7/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2237	MHO	OD1-SD	4.20	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2237	MHO	CE-SD-CG	3.30	105.22	97.71

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2237	MHO	CB-CG-SD-OD1
1	A	2237	MHO	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	EDO	A	3007	-	3,3,3	0.58	0	2,2,2	0.46	0
3	PO4	A	5005	-	4,4,4	1.60	1 (25%)	6,6,6	0.89	0
3	PO4	A	5006	-	4,4,4	1.69	1 (25%)	6,6,6	2.35	3 (50%)
2	EDO	A	3003	-	3,3,3	0.96	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EDO	A	3009	-	3,3,3	0.53	0	2,2,2	0.11	0
3	PO4	A	5001	-	4,4,4	0.32	0	6,6,6	0.65	0
2	EDO	A	3005	-	3,3,3	0.54	0	2,2,2	0.64	0
2	EDO	A	3004	-	3,3,3	0.43	0	2,2,2	1.38	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	EDO	A	3007	-	-	0/1/1/1	-
2	EDO	A	3003	-	-	0/1/1/1	-
2	EDO	A	3009	-	-	1/1/1/1	-
2	EDO	A	3005	-	-	0/1/1/1	-
2	EDO	A	3004	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5006	PO4	P-O3	2.74	1.62	1.54
3	A	5005	PO4	P-O3	2.36	1.61	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	5006	PO4	O4-P-O2	3.91	120.51	107.97
3	A	5006	PO4	O4-P-O3	-3.19	97.73	107.97
3	A	5006	PO4	O3-P-O2	-2.67	99.39	107.97

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3004	EDO	O1-C1-C2-O2
2	A	3009	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3009	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	241/258 (93%)	-0.11	7 (2%) 51 49	8, 14, 43, 68	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2216	PRO	5.4
1	A	1023	HIS	3.6
1	A	1056	SER	3.5
1	A	1053	LEU	3.1
1	A	2217	ASN	2.3

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	B-factors(Å^2)	Q<0.9
1	MHO	A	2237	9/10	0.95	0.13	14,35,44,47	1

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, 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	B-factors(Å^2)	Q<0.9
2	EDO	A	3009	4/4	0.70	0.20	72,74,77,78	0
2	EDO	A	3004	4/4	0.87	0.15	22,32,34,45	4
2	EDO	A	3003	4/4	0.92	0.08	14,20,20,25	0
2	EDO	A	3005	4/4	0.96	0.09	14,16,22,24	0
2	EDO	A	3007	4/4	0.97	0.07	14,23,28,33	4
3	PO4	A	5005	5/5	0.97	0.07	15,21,33,38	5
3	PO4	A	5006	5/5	0.97	0.10	20,23,45,48	0
3	PO4	A	5001	5/5	0.99	0.07	15,19,28,29	5

6.5 Other polymers (i)

There are no such residues in this entry.