



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2018 – 11:48 PM EST

PDB ID : 1FX2
Title : STRUCTURAL ANALYSIS OF ADENYLATE CYCLASES FROM TRY-
PANOSOMA BRUCEI IN THEIR MONOMERIC STATE
Authors : Bieger, B.; Essen, L.-O.
Deposited on : 2000-09-25
Resolution : 1.46 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

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 : rb-20030736
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) : rb-20030736

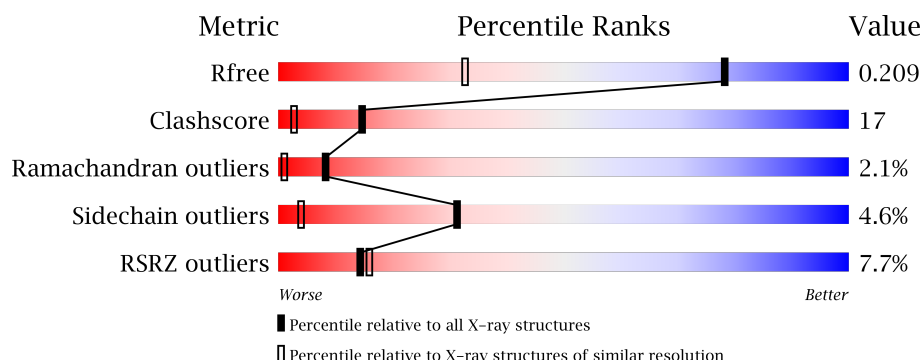
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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	1510 (1.48-1.44)
Clashscore	112137	1573 (1.48-1.44)
Ramachandran outliers	110173	1555 (1.48-1.44)
Sidechain outliers	110143	1555 (1.48-1.44)
RSRZ outliers	101464	1516 (1.48-1.44)

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	235	<div> <div>8%</div> <div>73%</div> <div>22%</div> <div>5%</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	DTT	A	1124	X	X	X	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2179 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 RECEPTOR-TYPE ADENYLATE CYCLASE GRESAG 4.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	235	1894	1181	335	364	14	21	6	0

There is a discrepancy between the modelled and reference sequences:

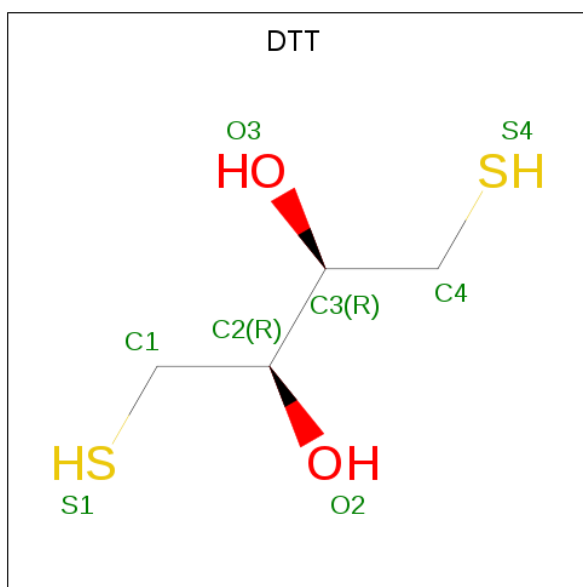
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	DELETION	UNP Q99279

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



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

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C₄H₁₀O₂S₂).

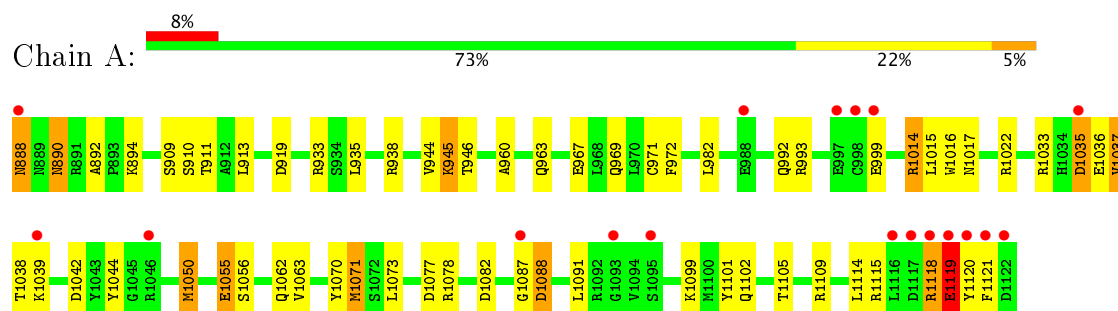


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	272	Total	O	0	0
			272	272		

- Molecule 1: RECEPTOR-TYPE ADENYLATE CYCLASE GRESAG 4.1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.60Å 60.07Å 78.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.46 10.00 – 1.46	Depositor EDS
% Data completeness (in resolution range)	95.7 (10.00-1.46) 95.9 (10.00-1.46)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 1.46Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.178 , 0.205 0.185 , 0.209	Depositor DCC
R_{free} test set	1111 reflections (2.79%)	DCC
Wilson B-factor (Å ²)	10.9	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2179	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4, DTT

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	1.24	7/1938 (0.4%)	1.25	12/2632 (0.5%)

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	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1071	MET	CG-SD	-15.73	1.40	1.81
1	A	1050	MET	CB-CG	11.44	1.88	1.51
1	A	1071	MET	CB-CG	7.24	1.74	1.51
1	A	1055	GLU	CD-OE2	-6.31	1.18	1.25
1	A	971[A]	CYS	CB-SG	-6.15	1.71	1.82
1	A	971[B]	CYS	CB-SG	-6.15	1.71	1.82
1	A	1119	GLU	CB-CG	5.44	1.62	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1050	MET	CG-SD-CE	9.30	115.08	100.20
1	A	1014	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	A	1014	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	993	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	1035	ASP	N-CA-C	7.84	132.17	111.00
1	A	1050	MET	CB-CG-SD	-7.65	89.46	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1082	ASP	CB-CG-OD1	6.84	124.46	118.30
1	A	933	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	1042	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	1119	GLU	N-CA-C	-6.19	94.29	111.00
1	A	1118	ARG	N-CA-C	5.83	126.73	111.00
1	A	1071	MET	CB-CA-C	5.26	120.93	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1101	TYR	Sidechain

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	1894	0	1806	62	0
2	A	5	0	0	0	0
3	A	8	0	6	10	0
4	A	272	0	0	23	0
All	All	2179	0	1812	63	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 17.

All (63) 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:1071:MET:CG	1:A:1071:MET:CB	1.74	1.59
1:A:1050:MET:CG	1:A:1050:MET:CB	1.87	1.50
1:A:982:LEU:HB3	4:A:1277:HOH:O	1.31	1.25
1:A:946:THR:HB	4:A:1383:HOH:O	1.61	0.99
1:A:963:GLN:HG2	4:A:1379:HOH:O	1.67	0.93
1:A:1050:MET:SD	1:A:1050:MET:CB	2.62	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:LEU:HA	1:A:1118:ARG:NH2	1.94	0.81
1:A:1071:MET:SD	1:A:1071:MET:CB	2.69	0.81
1:A:888:ASN:ND2	1:A:890:ASN:HB3	1.98	0.77
1:A:1109:ARG:NH2	3:A:1124:DTT:H42	1.99	0.76
1:A:1056:SER:HB2	1:A:1119:GLU:O	1.87	0.75
1:A:1105:THR:HG23	4:A:1386:HOH:O	1.85	0.74
1:A:992:GLN:OE1	4:A:1384:HOH:O	2.06	0.74
1:A:1016:TRP:HE3	3:A:1124:DTT:HS2	1.34	0.73
1:A:1115:ARG:HD3	4:A:1264:HOH:O	1.88	0.73
1:A:1038:THR:O	1:A:1039:LYS:HG2	1.91	0.70
1:A:1062:GLN:HE21	1:A:1102:GLN:HE21	1.41	0.69
1:A:1087:GLY:C	4:A:1387:HOH:O	2.32	0.67
1:A:1091:LEU:HA	1:A:1118:ARG:HH22	1.60	0.64
1:A:1014:ARG:NH2	4:A:1362:HOH:O	2.30	0.64
1:A:1087:GLY:O	1:A:1099:LYS:HA	1.98	0.62
1:A:888:ASN:HD21	1:A:890:ASN:HB3	1.64	0.60
1:A:1033:ARG:HD2	1:A:1044:TYR:CE1	2.37	0.59
1:A:1015:LEU:HD23	4:A:1245:HOH:O	2.03	0.59
1:A:913:LEU:HD22	1:A:982:LEU:HD23	1.85	0.59
1:A:909:SER:CA	4:A:1385:HOH:O	2.49	0.59
1:A:963:GLN:NE2	4:A:1271:HOH:O	2.36	0.58
1:A:909:SER:HA	4:A:1385:HOH:O	2.04	0.56
1:A:935:LEU:CD2	1:A:967[B]:GLU:HG2	2.35	0.56
1:A:1022:ARG:HH21	1:A:1119:GLU:CD	2.10	0.56
1:A:1109:ARG:HH22	3:A:1124:DTT:H42	1.68	0.56
1:A:1073:LEU:O	1:A:1078:ARG:NH1	2.40	0.55
1:A:1071:MET:CA	1:A:1071:MET:CG	2.82	0.54
1:A:972:PHE:HB3	3:A:1124:DTT:H11	1.89	0.53
1:A:935:LEU:HD22	1:A:967[B]:GLU:HG2	1.91	0.53
3:A:1124:DTT:O2	4:A:1158:HOH:O	2.18	0.52
1:A:999:GLU:HB3	4:A:1328:HOH:O	2.09	0.52
1:A:1022:ARG:NH2	1:A:1119:GLU:CD	2.63	0.52
1:A:1063:VAL:HB	4:A:1386:HOH:O	2.11	0.50
1:A:999:GLU:O	1:A:999:GLU:HG2	2.12	0.49
1:A:1118:ARG:HG3	1:A:1118:ARG:HH11	1.78	0.48
1:A:919:ASP:HB2	4:A:1172:HOH:O	2.13	0.48
1:A:972:PHE:HB2	3:A:1124:DTT:H12	1.94	0.48
1:A:1088:ASP:N	1:A:1088:ASP:OD1	2.47	0.47
1:A:969:GLN:OE1	3:A:1124:DTT:S1	2.70	0.47
1:A:1017:ASN:H	3:A:1124:DTT:C4	2.28	0.46
1:A:909:SER:N	4:A:1385:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:GLN:HE21	1:A:1102:GLN:NE2	2.09	0.46
1:A:1088:ASP:N	4:A:1387:HOH:O	2.49	0.46
1:A:982:LEU:CD2	4:A:1277:HOH:O	2.65	0.45
1:A:1070:TYR:CZ	1:A:1078:ARG:HD2	2.51	0.45
1:A:972:PHE:CB	3:A:1124:DTT:H11	2.49	0.43
1:A:892:ALA:O	1:A:894:LYS:HG3	2.18	0.43
1:A:935:LEU:HD21	1:A:967[B]:GLU:HG2	2.00	0.43
1:A:967[A]:GLU:HG2	4:A:1237:HOH:O	2.18	0.43
1:A:910:SER:N	4:A:1385:HOH:O	2.52	0.42
1:A:972:PHE:CB	3:A:1124:DTT:C1	2.97	0.42
1:A:982:LEU:HD22	4:A:1277:HOH:O	2.19	0.41
1:A:944:VAL:HG12	1:A:945:LYS:HD3	2.03	0.40
1:A:1077:ASP:HA	4:A:1306:HOH:O	2.21	0.40
1:A:1114:LEU:HA	1:A:1114:LEU:HD23	1.94	0.40
1:A:938:ARG:O	1:A:938:ARG:HG3	2.20	0.40
1:A:960:ALA:HA	1:A:963:GLN:HE21	1.86	0.40

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	238/235 (101%)	230 (97%)	3 (1%)	5 (2%)	8 1

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1037	VAL
1	A	1121	PHE
1	A	1119	GLU
1	A	1036	GLU
1	A	1035	ASP

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	202/198 (102%)	193 (96%)	9 (4%)	32 4

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	888	ASN
1	A	890	ASN
1	A	911	THR
1	A	945	LYS
1	A	1037	VAL
1	A	1055	GLU
1	A	1088	ASP
1	A	1119	GLU
1	A	1120	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	888	ASN
1	A	963	GLN
1	A	1102	GLN
1	A	1104	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 [i](#)

There are no carbohydrates in this entry.

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	$\# Z > 2$
2	SO4	A	1123	-	4,4,4	0.26	0	6,6,6	0.38	0
3	DTT	A	1124	-	7,7,7	19.22	6 (85%)	4,8,8	28.89	4 (100%)

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	1123	-	-	0/0/0/0	0/0/0/0
3	DTT	A	1124	-	2/2/2/2	0/8/8/8	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1124	DTT	C4-S4	-4.27	1.72	1.81
3	A	1124	DTT	C3-C2	-3.72	1.43	1.53
3	A	1124	DTT	C4-C3	-3.51	1.40	1.51
3	A	1124	DTT	C1-S1	-2.11	1.77	1.81
3	A	1124	DTT	O2-C2	35.03	2.20	1.43
3	A	1124	DTT	O3-C3	36.13	2.22	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1124	DTT	O3-C3-C2	-43.39	23.40	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1124	DTT	O2-C2-C3	-36.63	36.85	109.77
3	A	1124	DTT	C3-C4-S4	-8.29	89.06	114.43
3	A	1124	DTT	C2-C1-S1	-6.68	93.99	114.43

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1124	DTT	C2
3	A	1124	DTT	C3

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1124	DTT	10	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	233/235 (99%)	-0.04	18 (7%) 14 16	7, 13, 47, 74	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	998	CYS	10.5
1	A	1120	TYR	7.7
1	A	888	ASN	6.9
1	A	1035	ASP	5.5
1	A	1119	GLU	5.5
1	A	1118	ARG	5.1
1	A	1122	ASP	4.8
1	A	1117	ASP	4.8
1	A	1039	LYS	3.9
1	A	1121	PHE	3.5
1	A	999	GLU	3.5
1	A	1087	GLY	3.4
1	A	1093	GLY	3.3
1	A	1046	ARG	3.2
1	A	997	GLU	2.9
1	A	988[A]	GLU	2.2
1	A	1116	LEU	2.1
1	A	1095	SER	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, 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	DTT	A	1124	8/8	0.88	0.17	10.46	13,16,25,25	0
2	SO4	A	1123	5/5	0.99	0.08	-0.44	14,17,23,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.