



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 2, 2019 – 12:07 AM EDT

PDB ID : 6D9M
Title : T4-Lysozyme fusion to Geobacter GGDEF
Authors : Hallberg, Z.; Doxzen, K.; Kranzusch, P.; Hammond, M.
Deposited on : 2018-04-30
Resolution : 1.35 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

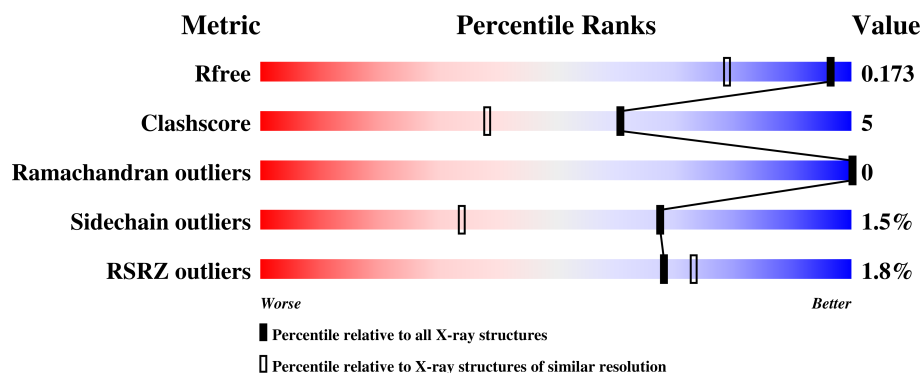
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

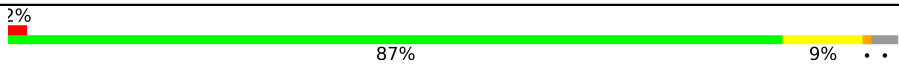
The reported resolution of this entry is 1.35 Å.

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}	111664	1197 (1.38-1.34)
Clashscore	122126	1232 (1.38-1.34)
Ramachandran outliers	120053	1215 (1.38-1.34)
Sidechain outliers	120020	1215 (1.38-1.34)
RSRZ outliers	108989	1177 (1.38-1.34)

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	337	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3306 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.

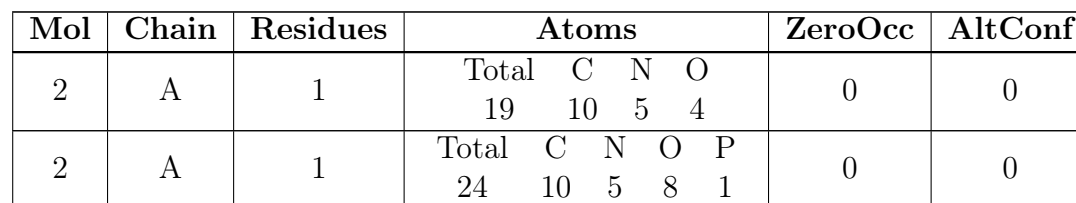
- Molecule 1 is a protein called Fusion protein of Endolysin, Response receiver sensor diguanylate cyclase, GAF domain-containing.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	24	0
			2783	1751	496	522	14			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-152	GLN	GLU	conflict	UNP D9IEF7
A	-109	THR	CYS	conflict	UNP D9IEF7
A	-66	ALA	CYS	conflict	UNP D9IEF7
A	-1	GLY	-	linker	UNP D9IEF7
A	0	SER	-	linker	UNP D9IEF7
A	167	LEU	-	expression tag	UNP Q39UD1
A	168	GLU	-	expression tag	UNP Q39UD1
A	169	HIS	-	expression tag	UNP Q39UD1
A	170	HIS	-	expression tag	UNP Q39UD1
A	171	HIS	-	expression tag	UNP Q39UD1
A	172	HIS	-	expression tag	UNP Q39UD1
A	173	HIS	-	expression tag	UNP Q39UD1
A	174	HIS	-	expression tag	UNP Q39UD1

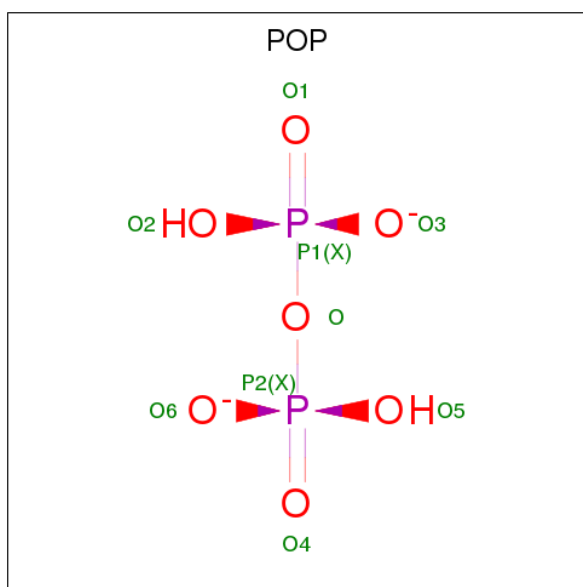
- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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- The chemical structure of Guanosine Monophosphate (GMP) is shown. It consists of a purine base (guanine) linked to a ribose sugar, which is further linked to a phosphate group. The purine base is labeled with atoms N1, N3, N7, C2, C4, C5, C6, and C8. The ribose sugar is labeled with atoms C1'(R), C2'(R), C3'(S), C4'(R), and C5'. The phosphate group is labeled with atoms O4, O5', and O3'. The structure is color-coded: nitrogen atoms are blue, carbon atoms are green, oxygen atoms are red, and hydrogen atoms are white. Stereochemistry is indicated with wedges and dashes at the sugar ring positions.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	10	5	5		

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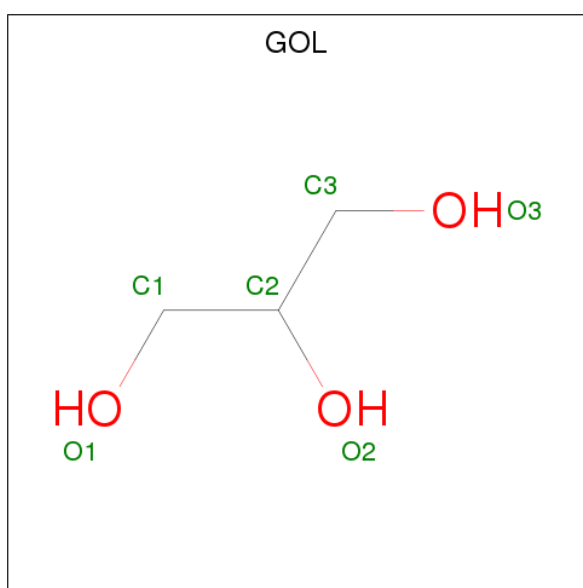


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			9	7	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

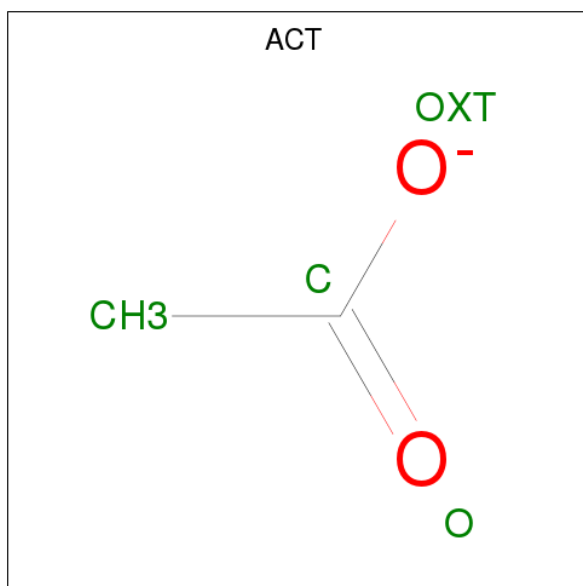
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

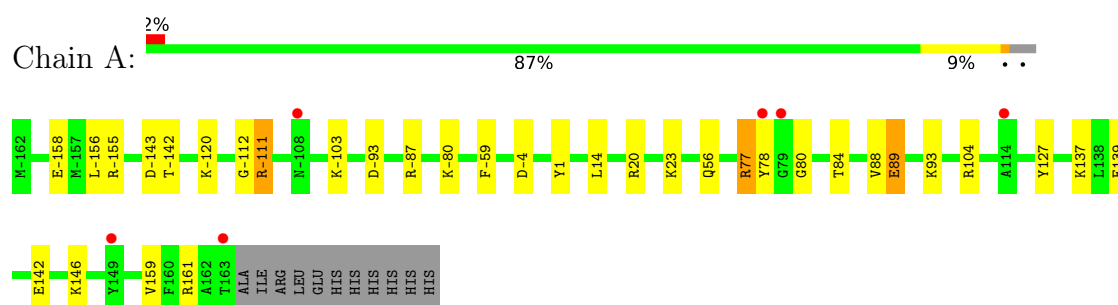
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	440	Total	O	0	0
			440	440		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Fusion protein of Endolysin, Response receiver sensor diguanylate cyclase, GAF domain-containing



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	70.68Å 111.64Å 55.34Å 90.00° 122.75° 90.00°	Depositor
Resolution (Å)	35.75 – 1.35 35.75 – 1.35	Depositor EDS
% Data completeness (in resolution range)	97.7 (35.75-1.35) 97.7 (35.75-1.35)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.35Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.154 , 0.170 0.158 , 0.173	Depositor DCC
R_{free} test set	1561 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.6	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	0.97	EDS
Total number of atoms	3306	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% 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: GOL, MG, POP, GTP, ACT, GMP

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	0.78	1/2827 (0.0%)	0.94	6/3801 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	GLU	CD-OE2	-5.34	1.19	1.25

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	A	104	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	A	104	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	A	-111	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	-93	ASP	CB-CG-OD1	5.72	123.45	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	77	ARG	Mainchain

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	2783	0	2791	26	0
2	A	43	0	22	5	0
3	A	20	0	13	1	0
4	A	9	0	0	0	0
5	A	1	0	0	0	0
6	A	6	0	8	1	0
7	A	4	0	3	0	0
8	A	440	0	0	14	2
All	All	3306	0	2837	28	2

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 28 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:-158:GLU:OE1	1:A:-155[B]:ARG:NH2	2.04	0.90
1:A:139[B]:GLU:OE1	8:A:301:HOH:O	2.02	0.76
1:A:139[B]:GLU:OE2	8:A:302:HOH:O	2.04	0.75
1:A:-142[B]:THR:OG1	2:A:202:GTP:O3A	2.13	0.67
1:A:-142[A]:THR:HG23	2:A:202:GTP:O3A	1.97	0.64

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:734:HOH:O	8:A:734:HOH:O[2_657]	1.60	0.60
8:A:338:HOH:O	8:A:592:HOH:O[2_657]	1.67	0.53

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	350/337 (104%)	344 (98%)	6 (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	294/281 (105%)	290 (99%)	4 (1%)	69	37

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-103	LYS
1	A	-80	LYS
1	A	23	LYS
1	A	93	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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$
2	GTP	A	201	-	16,21,34	1.15	2 (12%)	14,32,54	2.92	8 (57%)
2	GTP	A	202	-	21,26,34	1.23	1 (4%)	25,40,54	2.44	11 (44%)
3	GMP	A	203	-	17,22,22	0.98	2 (11%)	18,33,33	2.41	6 (33%)
4	POP	A	204	5	8,8,8	1.51	2 (25%)	9,13,13	1.15	0
6	GOL	A	206	-	5,5,5	0.93	1 (20%)	5,5,5	0.77	0
7	ACT	A	207	-	1,3,3	1.17	0	0,3,3	0.00	-

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	GTP	A	201	-	-	0/0/20/38	0/3/3/3
2	GTP	A	202	-	-	0/6/26/38	0/3/3/3
3	GMP	A	203	-	-	0/2/22/22	0/3/3/3
4	POP	A	204	5	-	0/6/6/6	0/0/0/0
6	GOL	A	206	-	-	0/4/4/4	0/0/0/0
7	ACT	A	207	-	-	0/0/0/0	0/0/0/0

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	GTP	C6-C5	-2.35	1.37	1.41
6	A	206	GOL	O2-C2	-2.02	1.37	1.43
4	A	204	POP	P2-O	2.11	1.63	1.60
2	A	201	GTP	C2-N1	2.19	1.39	1.35
3	A	203	GMP	C5-C4	2.24	1.45	1.40

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	202	GTP	N3-C2-N1	-6.18	118.89	127.25
2	A	201	GTP	N3-C2-N1	-5.82	119.38	127.25
2	A	201	GTP	C5'-C4'-C3'	-5.26	110.17	115.70
3	A	203	GMP	C6-C5-C4	-4.40	116.56	120.79
2	A	202	GTP	C5-C6-N1	-4.37	117.39	123.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	202	GTP	5	0
3	A	203	GMP	1	0
6	A	206	GOL	1	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	326/337 (96%)	0.07	6 (1%) 68 73	10, 17, 29, 45	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	THR	6.8
1	A	149	TYR	3.9
1	A	114	ALA	2.6
1	A	79[A]	GLY	2.5
1	A	78[A]	TYR	2.3

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. 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
3	GMP	A	203	20/20	0.77	0.24	20,20,20,20	0
6	GOL	A	206	6/6	0.82	0.25	33,43,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GTP	A	202	24/32	0.86	0.14	20,32,40,46	0
2	GTP	A	201	19/32	0.90	0.19	16,24,41,46	0
7	ACT	A	207	4/4	0.95	0.10	19,19,21,23	0
4	POP	A	204	9/9	0.97	0.10	20,20,20,20	0
5	MG	A	205	1/1	0.99	0.07	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.