



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 08:16 AM EDT

PDB ID : 2O8H
Title : Crystal structure of the catalytic domain of rat phosphodiesterase 10A
Authors : Pandit, J.; Marr, E.S.
Deposited on : unknown
Resolution : 1.80 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-20030345
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-20030345

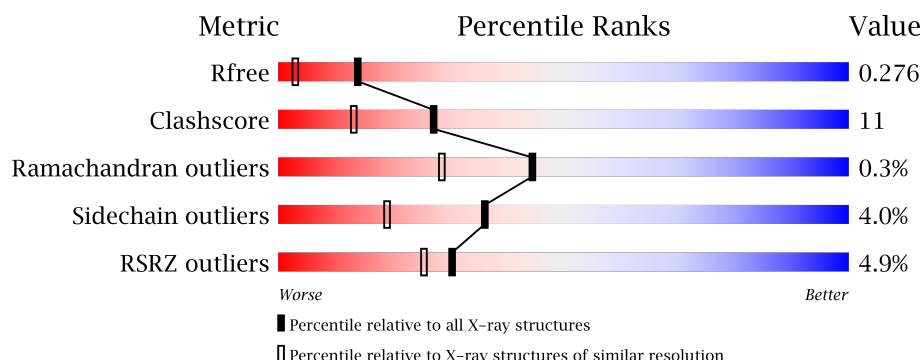
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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	362	<div> <div>4%</div> <div>65%</div> <div>18%</div> <div>•</div> <div>15%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2839 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 Phosphodiesterase-10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2491	1588	430	451	22			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	MET	-	INITIATING METHIONINE	UNP Q9QYJ6
A	424	HIS	-	EXPRESSION TAG	UNP Q9QYJ6
A	425	HIS	-	EXPRESSION TAG	UNP Q9QYJ6
A	426	HIS	-	EXPRESSION TAG	UNP Q9QYJ6
A	427	HIS	-	EXPRESSION TAG	UNP Q9QYJ6
A	428	HIS	-	EXPRESSION TAG	UNP Q9QYJ6
A	429	HIS	-	EXPRESSION TAG	UNP Q9QYJ6
A	430	SER	-	CLONING ARTIFACT	UNP Q9QYJ6
A	431	SER	-	CLONING ARTIFACT	UNP Q9QYJ6
A	432	GLY	-	CLONING ARTIFACT	UNP Q9QYJ6
A	433	LEU	-	CLONING ARTIFACT	UNP Q9QYJ6
A	434	VAL	-	CLONING ARTIFACT	UNP Q9QYJ6
A	435	PRO	-	CLONING ARTIFACT	UNP Q9QYJ6
A	436	ARG	-	CLONING ARTIFACT	UNP Q9QYJ6
A	437	GLY	-	CLONING ARTIFACT	UNP Q9QYJ6
A	438	SER	-	CLONING ARTIFACT	UNP Q9QYJ6
A	439	ALA	-	CLONING ARTIFACT	UNP Q9QYJ6
A	440	MET	-	CLONING ARTIFACT	UNP Q9QYJ6
A	441	GLY	-	CLONING ARTIFACT	UNP Q9QYJ6

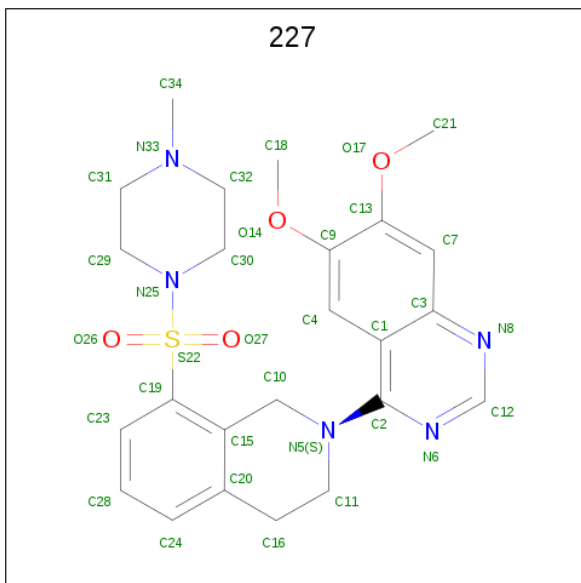
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is 6,7-DIMETHOXY-4-{8-[(4-METHYLPIPERAZIN-1-YL)SULFONYL]-3,4-DIHYDROISOQUINOLIN-2(1H)-YL}QUINAZOLINE (three-letter code: 227) (formula: C₂₄H₂₉N₅O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			34	24	5	4	1		

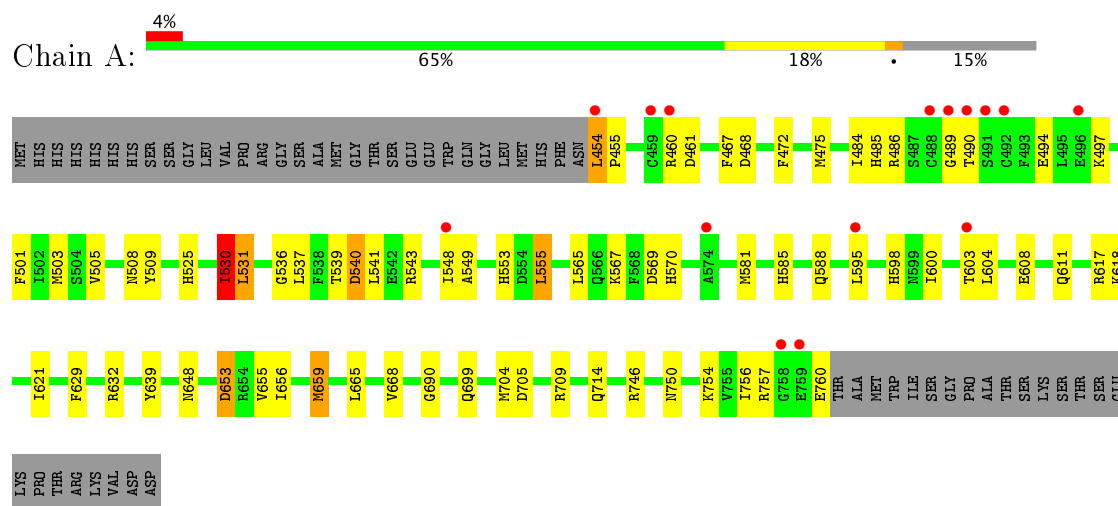
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	312	Total	O	0	0
			312	312		

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: Phosphodiesterase-10A



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	120.62Å 120.62Å 82.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.80 23.67 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (30.00-1.80) 91.6 (23.67-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.273 0.228 , 0.276	Depositor DCC
R_{free} test set	2905 reflections (8.32%)	DCC
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2839	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 227, ZN, MG

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	0.70	1/2552 (0.0%)	0.82	7/3455 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	659	MET	SD-CE	-5.84	1.45	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	653	ASP	CB-CG-OD2	6.53	124.18	118.30
1	A	468	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	461	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	530	ILE	CB-CA-C	-5.86	99.88	111.60
1	A	705	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	569	ASP	CB-CG-OD2	5.09	122.88	118.30

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	2491	0	2455	57	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	34	0	29	0	0
5	A	312	0	0	23	0
All	All	2839	0	2484	57	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 11.

All (57) 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:656:ILE:HA	1:A:659:MET:HE3	1.22	1.12
1:A:530:ILE:O	1:A:530:ILE:HG22	1.69	0.90
1:A:656:ILE:CA	1:A:659:MET:HE3	2.01	0.89
1:A:655:VAL:HG12	1:A:659:MET:HE2	1.56	0.86
1:A:539:THR:HB	5:A:17:HOH:O	1.79	0.82
1:A:497:LYS:HB3	5:A:151:HOH:O	1.80	0.81
1:A:508:ASN:HB3	5:A:306:HOH:O	1.86	0.75
1:A:588:GLN:OE1	5:A:306:HOH:O	2.03	0.75
1:A:655:VAL:HG12	1:A:659:MET:CE	2.23	0.69
1:A:530:ILE:C	5:A:292:HOH:O	2.33	0.66
1:A:714:GLN:NE2	1:A:756:ILE:HG12	2.13	0.64
1:A:467:PHE:HB3	1:A:525:HIS:CE1	2.33	0.63
1:A:746:ARG:NE	5:A:310:HOH:O	2.30	0.63
1:A:595:LEU:HD13	5:A:282:HOH:O	2.00	0.60
1:A:494:GLU:HB2	5:A:234:HOH:O	2.02	0.58
1:A:531:LEU:N	5:A:292:HOH:O	2.35	0.57
1:A:699:GLN:HG2	5:A:133:HOH:O	2.03	0.57
1:A:760:GLU:C	5:A:131:HOH:O	2.42	0.57
1:A:595:LEU:HB3	1:A:598:HIS:ND1	2.20	0.56
1:A:655:VAL:O	1:A:659:MET:HE2	2.06	0.55
1:A:750:ASN:ND2	1:A:754:LYS:HE3	2.21	0.55
1:A:608:GLU:HG2	5:A:213:HOH:O	2.07	0.54
1:A:655:VAL:C	1:A:659:MET:HE2	2.29	0.53
1:A:490:THR:HG22	5:A:117:HOH:O	2.09	0.53
1:A:750:ASN:HD21	1:A:754:LYS:HE3	1.75	0.52
1:A:617:ARG:O	1:A:621:ILE:HG12	2.10	0.51
1:A:565:LEU:HD22	1:A:570:HIS:CG	2.44	0.51
1:A:509:TYR:CE1	1:A:555:LEU:HD13	2.47	0.50
1:A:555:LEU:O	1:A:585:HIS:ND1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:HIS:HA	1:A:489:GLY:O	2.12	0.49
1:A:497:LYS:CD	5:A:151:HOH:O	2.60	0.49
1:A:604:LEU:HG	1:A:608:GLU:HB3	1.94	0.49
1:A:540:ASP:OD1	1:A:543:ARG:NH2	2.45	0.48
1:A:699:GLN:CG	5:A:133:HOH:O	2.59	0.48
1:A:454:LEU:O	1:A:455:PRO:C	2.52	0.48
1:A:536:GLY:HA2	5:A:184:HOH:O	2.14	0.47
1:A:665:LEU:O	1:A:668:VAL:HG22	2.15	0.46
1:A:690:GLY:HA3	1:A:704:MET:O	2.15	0.46
1:A:567:LYS:NZ	5:A:284:HOH:O	2.49	0.45
1:A:639:TYR:HB2	5:A:171:HOH:O	2.16	0.45
1:A:548:ILE:HD13	1:A:600:ILE:CD1	2.47	0.45
1:A:617:ARG:HD3	5:A:98:HOH:O	2.17	0.45
1:A:537:LEU:HD11	5:A:254:HOH:O	2.17	0.44
1:A:548:ILE:HD13	1:A:600:ILE:HD11	1.99	0.44
1:A:604:LEU:HG	1:A:608:GLU:CB	2.48	0.43
1:A:618:LYS:HE2	1:A:653:ASP:OD2	2.18	0.43
1:A:746:ARG:NH2	5:A:310:HOH:O	2.51	0.43
1:A:484:ILE:HG22	1:A:485:HIS:N	2.33	0.43
1:A:655:VAL:C	1:A:659:MET:CE	2.87	0.43
1:A:501:PHE:O	1:A:505:VAL:HG23	2.19	0.42
1:A:549:ALA:O	1:A:553:HIS:HB3	2.20	0.42
1:A:629:PHE:HB3	5:A:281:HOH:O	2.19	0.42
1:A:530:ILE:CG2	1:A:530:ILE:O	2.39	0.41
1:A:565:LEU:HD11	1:A:581:MET:SD	2.60	0.41
1:A:497:LYS:HD2	5:A:151:HOH:O	2.21	0.41
1:A:472:PHE:HB2	1:A:475:MET:HG3	2.03	0.41
1:A:541:LEU:HD12	1:A:611:GLN:NE2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	305/362 (84%)	296 (97%)	8 (3%)	1 (0%)	44 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	530	ILE

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	275/322 (85%)	264 (96%)	11 (4%)	36 19

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	454	LEU
1	A	460	ARG
1	A	486	ARG
1	A	503	MET
1	A	531	LEU
1	A	555	LEU
1	A	603	THR
1	A	632	ARG
1	A	648	ASN
1	A	709	ARG
1	A	757	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	566	GLN
1	A	588	GLN
1	A	611	GLN
1	A	634	GLN

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Mol	Chain	Res	Type
1	A	648	ASN
1	A	733	GLN
1	A	750	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
4	227	A	999	-	37,38,38	1.89	7 (18%)	53,56,56	2.74	21 (39%)

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
4	227	A	999	-	-	0/20/39/39	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	227	O27-S22	-3.54	1.39	1.43
4	A	999	227	C3-N8	-2.57	1.32	1.37
4	A	999	227	C15-C19	-2.14	1.39	1.41
4	A	999	227	C7-C13	2.32	1.40	1.36
4	A	999	227	C2-N5	2.45	1.44	1.36
4	A	999	227	C19-S22	5.69	1.85	1.78
4	A	999	227	S22-N25	6.69	1.73	1.63

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	227	N8-C12-N6	-7.55	122.28	128.86
4	A	999	227	O27-S22-O26	-5.73	109.82	119.46
4	A	999	227	O14-C9-C4	-4.43	119.84	125.25
4	A	999	227	C32-C30-N25	-4.21	105.64	108.94
4	A	999	227	C1-C3-N8	-3.66	118.98	122.89
4	A	999	227	C30-N25-S22	-3.24	110.95	117.06
4	A	999	227	C29-N25-S22	-2.99	111.41	117.06
4	A	999	227	O27-S22-C19	-2.65	102.29	107.36
4	A	999	227	C23-C19-S22	-2.18	114.35	117.48
4	A	999	227	C1-C2-N6	-2.16	117.39	122.72
4	A	999	227	O17-C13-C7	-2.08	122.72	125.25
4	A	999	227	C7-C3-C1	2.29	122.29	119.63
4	A	999	227	C15-C10-N5	2.65	116.46	111.72
4	A	999	227	O14-C9-C13	2.93	119.42	115.41
4	A	999	227	C12-N6-C2	3.32	119.98	111.82
4	A	999	227	C21-O17-C13	3.41	122.44	117.54
4	A	999	227	C18-O14-C9	3.74	122.92	117.54
4	A	999	227	C31-N33-C32	4.13	114.97	109.47
4	A	999	227	C12-N8-C3	4.28	119.75	115.27
4	A	999	227	O26-S22-C19	5.09	117.08	107.36
4	A	999	227	O27-S22-N25	7.99	114.23	106.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	307/362 (84%)	0.17	15 (4%) 30 25	28, 38, 55, 69	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	758	GLY	4.1
1	A	491	SER	3.9
1	A	460	ARG	3.2
1	A	492	CYS	3.1
1	A	759	GLU	3.0
1	A	454	LEU	2.8
1	A	488	CYS	2.7
1	A	490	THR	2.6
1	A	496	GLU	2.6
1	A	595	LEU	2.4
1	A	574	ALA	2.3
1	A	548	ILE	2.1
1	A	459	CYS	2.1
1	A	489	GLY	2.1
1	A	603	THR	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
4	227	A	999	34/34	0.96	0.11	0.02	28,35,37,39	0
2	ZN	A	1001	1/1	1.00	0.05	-4.06	34,34,34,34	0
3	MG	A	1002	1/1	0.98	0.03	-7.06	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.