



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 04:58 pm BST

PDB ID : 6GBK
Title : Repertoires of functionally diverse enzymes through computational design at epistatic active-site positions
Authors : Khersonsky, O.; Lipsh, R.; Avizemer, Z.; Goldsmith, M.; Ashani, Y.; Leader, H.; Dym, O.; Rogotner, S.; Trudeau, D.; Tawfik, D.S.; Fleishman, S.J.
Deposited on : 2018-04-15
Resolution : 1.90 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

<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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

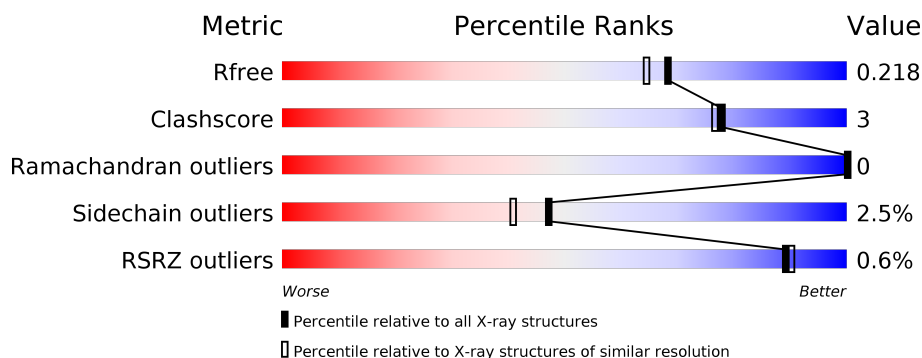
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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 $\leq 5\%$. 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	335	 90% 7% ..
1	B	335	 90% 7% ..

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
4	TRS	A	404	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5366 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 Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	2	0
			2528	1591	446	484	7			
1	B	329	Total	C	N	O	S	0	2	0
			2536	1597	445	487	7			

There are 50 discrepancies between the modelled and reference sequences:

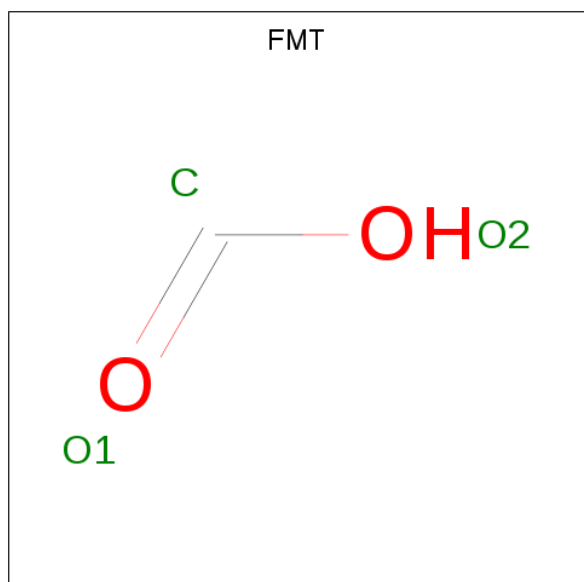
Chain	Residue	Modelled	Actual	Comment	Reference
A	31	THR	-	expression tag	UNP P0A434
A	32	ASN	-	expression tag	UNP P0A434
A	33	SER	-	expression tag	UNP P0A434
A	54	MET	THR	engineered mutation	UNP P0A434
A	77	ASP	LYS	engineered mutation	UNP P0A434
A	106	LEU	ILE	engineered mutation	UNP P0A434
A	111	GLU	SER	engineered mutation	UNP P0A434
A	118	GLU	ARG	engineered mutation	UNP P0A434
A	182	ARG	LEU	engineered mutation	UNP P0A434
A	185	ARG	LYS	engineered mutation	UNP P0A434
A	203	ASP	ALA	engineered mutation	UNP P0A434
A	214	ASP	ALA	engineered mutation	UNP P0A434
A	222	ASP	SER	engineered mutation	UNP P0A434
A	238	ASP	SER	engineered mutation	UNP P0A434
A	254	GLY	HIS	engineered mutation	UNP P0A434
A	269	ALA	SER	engineered mutation	UNP P0A434
A	274	LEU	ILE	engineered mutation	UNP P0A434
A	293	ALA	MET	engineered mutation	UNP P0A434
A	294	ASP	LYS	engineered mutation	UNP P0A434
A	317	LEU	MET	engineered mutation	UNP P0A434
A	343	ASP	GLN	engineered mutation	UNP P0A434
A	347	GLU	ALA	engineered mutation	UNP P0A434
A	348	THR	GLY	engineered mutation	UNP P0A434
A	350	MET	THR	engineered mutation	UNP P0A434
A	352	ASP	THR	engineered mutation	UNP P0A434

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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	THR	-	expression tag	UNP P0A434
B	32	ASN	-	expression tag	UNP P0A434
B	33	SER	-	expression tag	UNP P0A434
B	54	MET	THR	engineered mutation	UNP P0A434
B	77	ASP	LYS	engineered mutation	UNP P0A434
B	106	LEU	ILE	engineered mutation	UNP P0A434
B	111	GLU	SER	engineered mutation	UNP P0A434
B	118	GLU	ARG	engineered mutation	UNP P0A434
B	182	ARG	LEU	engineered mutation	UNP P0A434
B	185	ARG	LYS	engineered mutation	UNP P0A434
B	203	ASP	ALA	engineered mutation	UNP P0A434
B	214	ASP	ALA	engineered mutation	UNP P0A434
B	222	ASP	SER	engineered mutation	UNP P0A434
B	238	ASP	SER	engineered mutation	UNP P0A434
B	254	GLY	HIS	engineered mutation	UNP P0A434
B	269	ALA	SER	engineered mutation	UNP P0A434
B	274	LEU	ILE	engineered mutation	UNP P0A434
B	293	ALA	MET	engineered mutation	UNP P0A434
B	294	ASP	LYS	engineered mutation	UNP P0A434
B	317	LEU	MET	engineered mutation	UNP P0A434
B	343	ASP	GLN	engineered mutation	UNP P0A434
B	347	GLU	ALA	engineered mutation	UNP P0A434
B	348	THR	GLY	engineered mutation	UNP P0A434
B	350	MET	THR	engineered mutation	UNP P0A434
B	352	ASP	THR	engineered mutation	UNP P0A434

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).

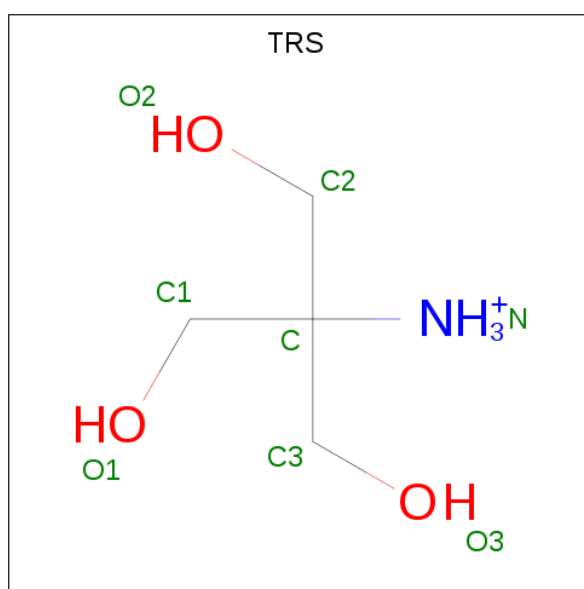


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			3	1	2		
2	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

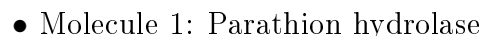


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	146	Total	O	0	0
			146	146		
5	B	138	Total	O	0	0
			138	138		

- Molecule 1: Parathion hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.75Å 53.09Å 89.23Å 90.00° 106.81° 90.00°	Depositor
Resolution (Å)	41.47 – 1.90 41.47 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.47-1.90) 99.9 (41.47-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.182 , 0.212 0.191 , 0.218	Depositor DCC
R_{free} test set	2784 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5366	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 4.97% 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: TRS, FMT, ZN

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	0.62	0/2575	0.78	1/3499 (0.0%)
1	B	0.63	0/2583	0.78	3/3512 (0.1%)
All	All	0.62	0/5158	0.78	4/7011 (0.1%)

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	7
1	B	0	2
All	All	0	9

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	225	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	B	225	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	182	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	152	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ARG	Sidechain
1	A	182	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	202	THR	Peptide
1	A	225	ARG	Sidechain
1	A	36	ARG	Sidechain
1	A	88	ARG	Sidechain
1	A	89[A]	ARG	Sidechain
1	B	189	ARG	Sidechain
1	B	202	THR	Peptide

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	2528	0	2502	17	0
1	B	2536	0	2508	12	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	8	0	12	3	0
5	A	146	0	0	1	0
5	B	138	0	0	0	0
All	All	5366	0	5022	29	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 3.

All (29) 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:89[B]:ARG:HG3	1:A:89[B]:ARG:HH21	1.23	1.04
1:A:89[B]:ARG:CG	1:A:89[B]:ARG:HH21	1.97	0.77
1:B:225:ARG:HD2	1:B:361:THR:O	1.87	0.74
1:A:89[B]:ARG:NH2	1:A:89[B]:ARG:HG3	2.01	0.73
1:A:89[B]:ARG:NH2	5:A:501:HOH:O	2.29	0.65
1:A:257:HIS:ND1	4:A:404:TRS:H21	2.12	0.64
1:A:89[B]:ARG:NH2	1:A:89[B]:ARG:CG	2.57	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLU:O	1:A:348:THR:HG23	2.05	0.57
1:A:241:THR:HG21	1:A:290:GLN:HE21	1.70	0.57
1:A:89[B]:ARG:NH1	1:A:323:ASP:OD1	2.38	0.56
1:B:89:ARG:NH2	1:B:323:ASP:OD1	2.40	0.55
1:B:344:GLU:O	1:B:348:THR:HG23	2.07	0.54
1:B:57:HIS:HB2	1:B:303:LEU:HB3	1.91	0.52
1:B:87:LEU:HD12	1:B:116:VAL:CG1	2.40	0.51
1:A:337:ARG:HD3	1:A:343:ASP:OD1	2.12	0.48
1:A:170:VAL:HG21	1:A:184:LEU:HD23	1.94	0.48
1:A:333:ILE:HG23	1:A:346:LEU:HD13	1.95	0.48
1:B:241:THR:HG21	1:B:290:GLN:HE21	1.79	0.48
1:B:353:ASN:HB2	1:B:354:PRO:HD3	1.95	0.48
1:B:302:TRP:CH2	1:B:321:ASN:HB3	2.50	0.47
1:A:302:TRP:CH2	1:A:321:ASN:HB3	2.52	0.45
1:B:57:HIS:O	1:B:303:LEU:HA	2.18	0.44
1:A:57:HIS:HB2	1:A:303:LEU:HB3	1.98	0.44
1:A:257:HIS:CE1	4:A:404:TRS:H22	2.53	0.43
1:A:262:LEU:N	1:A:262:LEU:HD13	2.34	0.43
1:B:300:ASN:OD1	1:B:328:ILE:HG12	2.20	0.42
1:A:257:HIS:CE1	4:A:404:TRS:C2	3.02	0.42
1:B:87:LEU:HD12	1:B:116:VAL:HG12	2.01	0.41
1:B:362:LEU:HD22	1:B:362:LEU:N	2.35	0.41

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	327/335 (98%)	315 (96%)	12 (4%)	0	100	100
1	B	329/335 (98%)	319 (97%)	10 (3%)	0	100	100
All	All	656/670 (98%)	634 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	266/270 (98%)	261 (98%)	5 (2%)	57	53
1	B	267/270 (99%)	259 (97%)	8 (3%)	41	33
All	All	533/540 (99%)	520 (98%)	13 (2%)	47	43

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	262	LEU
1	A	299	SER
1	A	303	LEU
1	A	306	PHE
1	A	338	GLU
1	B	89	ARG
1	B	299	SER
1	B	303	LEU
1	B	306	PHE
1	B	319	ARG
1	B	343	ASP
1	B	347	GLU
1	B	356	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	GLN
1	B	38	ASN
1	B	290	GLN

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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	FMT	A	401	1,3	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	B	401	1,3	0,2,2	0.00	-	0,1,1	0.00	-
4	TRS	A	404	-	7,7,7	0.47	0	9,9,9	4.45	6 (66%)

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	TRS	A	404	-	-	6/9/9/9	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	404	TRS	C1-C-N	-7.43	85.80	107.98
4	A	404	TRS	C3-C-N	-7.23	86.39	107.98
4	A	404	TRS	C2-C-N	-5.97	90.15	107.98
4	A	404	TRS	C3-C-C1	4.24	123.95	110.81
4	A	404	TRS	C3-C-C2	2.86	119.68	110.81
4	A	404	TRS	O1-C1-C	-2.19	104.06	111.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	TRS	C2-C-C1-O1
4	A	404	TRS	N-C-C1-O1
4	A	404	TRS	C1-C-C2-O2
4	A	404	TRS	C1-C-C3-O3
4	A	404	TRS	N-C-C2-O2
4	A	404	TRS	C2-C-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	TRS	3	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	327/335 (97%)	-0.34	0 100 100	12, 17, 27, 52	0
1	B	329/335 (98%)	-0.07	4 (1%) 79 81	12, 19, 33, 55	0
All	All	656/670 (97%)	-0.20	4 (0%) 89 90	12, 18, 31, 55	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	264	ASP	3.6
1	B	35	ASP	2.7
1	B	266	ALA	2.6
1	B	263	GLU	2.0

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
4	TRS	A	404	8/8	0.82	0.16	39,47,50,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FMT	A	401	3/3	0.97	0.09	14,14,14,14	0
2	FMT	B	401	3/3	0.98	0.07	16,16,16,17	0
3	ZN	B	402	1/1	1.00	0.04	14,14,14,14	0
3	ZN	A	403	1/1	1.00	0.03	16,16,16,16	0
3	ZN	A	402	1/1	1.00	0.03	13,13,13,13	0
3	ZN	B	403	1/1	1.00	0.04	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.