



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 17, 2018 – 12:01 AM EDT

PDB ID : 6DDK
Title : Crystal structure of the double mutant (D52N/R367Q) of the full-length NT5C2 in the basal state
Authors : Forouhar, F.; Dieck, C.L.; Tzoneva, G.; Carpenter, Z.; Ambesi-Impiombato, A.; Sanchez-Martin, M.; Kirschner-Schwabe, R.; Lew, S.; Seetharaman, J.; Ferrando, A.A.; Tong, L.
Deposited on : 2018-05-10
Resolution : 2.50 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031172
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-20031172

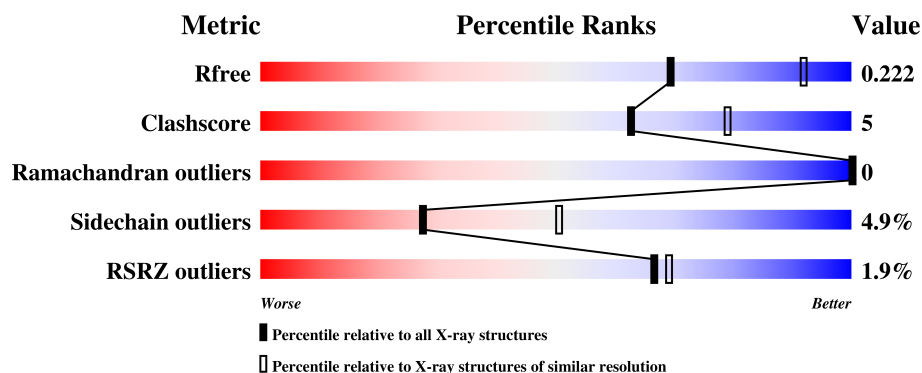
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	579	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>10%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	579	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>10%</div> <div>•</div> <div>17%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8526 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 Cytosolic purine 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	0	0
			4071	2627	679	744	21			
1	B	482	Total	C	N	O	S	0	0	0
			3931	2539	655	717	20			

There are 40 discrepancies between the modelled and reference sequences:

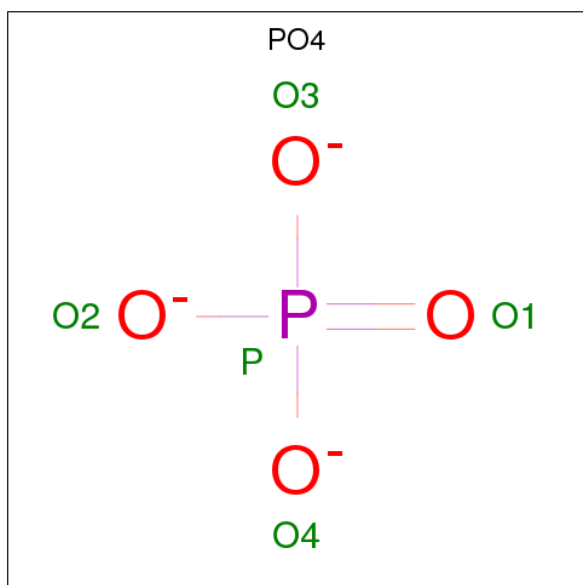
Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	GLY	-	expression tag	UNP P49902
A	-16	SER	-	expression tag	UNP P49902
A	-15	SER	-	expression tag	UNP P49902
A	-14	HIS	-	expression tag	UNP P49902
A	-13	HIS	-	expression tag	UNP P49902
A	-12	HIS	-	expression tag	UNP P49902
A	-11	HIS	-	expression tag	UNP P49902
A	-10	HIS	-	expression tag	UNP P49902
A	-9	HIS	-	expression tag	UNP P49902
A	-8	SER	-	expression tag	UNP P49902
A	-7	SER	-	expression tag	UNP P49902
A	-6	GLY	-	expression tag	UNP P49902
A	-5	LEU	-	expression tag	UNP P49902
A	-4	VAL	-	expression tag	UNP P49902
A	-3	PRO	-	expression tag	UNP P49902
A	-2	ARG	-	expression tag	UNP P49902
A	-1	GLY	-	expression tag	UNP P49902
A	0	SER	-	expression tag	UNP P49902
A	52	ASN	ASP	engineered mutation	UNP P49902
A	367	GLN	ARG	engineered mutation	UNP P49902
B	-17	GLY	-	expression tag	UNP P49902
B	-16	SER	-	expression tag	UNP P49902
B	-15	SER	-	expression tag	UNP P49902
B	-14	HIS	-	expression tag	UNP P49902
B	-13	HIS	-	expression tag	UNP P49902

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP P49902
B	-11	HIS	-	expression tag	UNP P49902
B	-10	HIS	-	expression tag	UNP P49902
B	-9	HIS	-	expression tag	UNP P49902
B	-8	SER	-	expression tag	UNP P49902
B	-7	SER	-	expression tag	UNP P49902
B	-6	GLY	-	expression tag	UNP P49902
B	-5	LEU	-	expression tag	UNP P49902
B	-4	VAL	-	expression tag	UNP P49902
B	-3	PRO	-	expression tag	UNP P49902
B	-2	ARG	-	expression tag	UNP P49902
B	-1	GLY	-	expression tag	UNP P49902
B	0	SER	-	expression tag	UNP P49902
B	52	ASN	ASP	engineered mutation	UNP P49902
B	367	GLN	ARG	engineered mutation	UNP P49902

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	290	Total 290	O 290	0	0
3	B	224	Total 224	O 224	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	121.85Å 171.40Å 122.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.50 49.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.81-2.50) 100.0 (49.81-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.162 , 0.223 0.162 , 0.222	Depositor DCC
R_{free} test set	4459 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.9	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	0.94	EDS
Total number of atoms	8526	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: PO4

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	0.40	0/4177	0.57	1/5645 (0.0%)
1	B	0.38	0/4032	0.54	1/5445 (0.0%)
All	All	0.39	0/8209	0.56	2/11090 (0.0%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	LEU	CA-CB-CG	-5.96	101.60	115.30
1	A	113	ASP	CB-CG-OD1	5.03	122.82	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	PHE	Peptide
1	B	51	PHE	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	4071	0	3997	37	0
1	B	3931	0	3876	39	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	290	0	0	5	0
3	B	224	0	0	1	0
All	All	8526	0	7873	74	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 5.

All (74) 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:B:506:THR:HG22	1:B:509:ARG:H	1.52	0.74
1:A:100:LEU:HD11	1:A:437:MET:HG2	1.75	0.68
1:A:302:LEU:HD23	1:B:190:LEU:HD11	1.76	0.67
1:B:399:LEU:HD13	1:B:419:ILE:HD13	1.79	0.64
1:B:148:GLU:OE2	1:B:195:ARG:NH1	2.31	0.63
1:A:399:LEU:HD13	1:A:419:ILE:HD12	1.83	0.60
1:A:295:PHE:HZ	1:A:335:ILE:HD12	1.69	0.58
1:A:287:LEU:HD13	1:A:335:ILE:HD11	1.86	0.57
1:B:76:ARG:O	1:B:80:ILE:HG13	2.04	0.57
1:A:306:ASP:O	1:A:310:GLY:N	2.28	0.55
1:A:76:ARG:NE	1:A:80:ILE:HD11	2.23	0.54
1:B:232:LEU:HB3	1:B:233:PRO:HD3	1.90	0.54
1:B:375:LEU:HB3	1:B:463:ALA:HB2	1.90	0.52
1:A:195:ARG:NH2	1:A:199:GLN:OE1	2.43	0.52
1:A:190:LEU:HD21	1:B:302:LEU:HD23	1.91	0.52
1:A:25:LYS:HE2	1:A:25:LYS:H	1.75	0.52
1:A:303:ARG:HG3	1:A:312:LEU:HD22	1.92	0.51
1:B:359:LYS:NZ	3:B:716:HOH:O	2.41	0.51
1:A:429:ASP:OD2	3:A:701:HOH:O	2.20	0.50
1:B:296:PHE:HB3	1:B:358:LEU:HD13	1.93	0.50
1:B:290:ALA:O	1:B:295:PHE:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LEU:HD22	1:A:419:ILE:HG12	1.95	0.49
1:A:422:ARG:NH1	1:A:425:LYS:HZ2	2.11	0.49
1:A:311:LYS:HD2	1:A:317:TYR:OH	2.13	0.48
1:B:288:VAL:O	1:B:328:SER:HA	2.13	0.48
1:A:500:MET:HE2	3:A:810:HOH:O	2.14	0.47
1:A:157:PHE:O	1:A:160:PRO:HD2	2.14	0.47
1:A:288:VAL:O	1:A:328:SER:HA	2.14	0.46
1:A:466:ILE:HA	1:A:466:ILE:HD12	1.83	0.46
1:B:466:ILE:HA	1:B:466:ILE:HD12	1.81	0.46
1:B:51:PHE:O	1:B:247:LEU:HD12	2.16	0.46
1:B:309:THR:HB	1:B:311:LYS:HG2	1.98	0.46
1:A:303:ARG:HB3	1:A:314:ILE:HA	1.97	0.45
1:B:157:PHE:O	1:B:160:PRO:HD2	2.17	0.45
1:B:423:ILE:O	1:B:427:THR:HG23	2.17	0.44
1:A:232:LEU:HB3	1:A:233:PRO:HD3	1.98	0.44
1:A:61:LYS:HG2	1:A:227:VAL:HG23	2.00	0.44
1:A:76:ARG:O	1:A:80:ILE:HG13	2.17	0.44
1:A:130:GLY:O	1:A:133:THR:HB	2.19	0.43
1:A:268:HIS:HB3	3:A:848:HOH:O	2.17	0.43
1:A:161:GLU:OE2	1:A:202:ARG:NH1	2.52	0.43
1:B:338:LEU:HA	1:B:338:LEU:HD23	1.86	0.43
1:B:308:LYS:HG3	1:B:308:LYS:H	1.58	0.43
1:B:304:GLN:NE2	1:B:316:THR:HG23	2.34	0.43
1:A:86:LEU:HG	1:A:89:PHE:CE2	2.54	0.42
1:B:86:LEU:HD21	1:B:168:LEU:HD21	2.02	0.42
1:B:219:VAL:HG13	1:B:258:LYS:HG2	2.01	0.42
1:A:132:GLU:H	1:A:132:GLU:HG3	1.71	0.42
1:B:313:LYS:HD3	1:B:317:TYR:HA	2.00	0.42
1:B:486:HIS:O	1:B:490:VAL:HG13	2.20	0.42
1:A:230:GLY:O	1:A:233:PRO:HD2	2.20	0.42
1:B:207:TRP:O	1:B:211:LYS:HB2	2.20	0.42
1:B:175:CYS:HB3	1:B:178:TYR:HD2	1.85	0.41
1:B:76:ARG:HD3	1:B:207:TRP:CE3	2.55	0.41
1:A:161:GLU:OE1	1:A:202:ARG:NH1	2.53	0.41
1:B:295:PHE:CZ	1:B:335:ILE:HD12	2.56	0.41
1:A:359:LYS:HE3	1:A:359:LYS:HB3	1.84	0.41
1:B:80:ILE:HG21	1:B:80:ILE:HD13	1.89	0.41
1:B:207:TRP:CD1	1:B:211:LYS:HE3	2.55	0.41
1:B:130:GLY:O	1:B:133:THR:HB	2.20	0.41
1:A:175:CYS:SG	1:A:177:ARG:HG3	2.61	0.41
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:HH11	1:B:202:ARG:HG3	1.86	0.41
1:A:302:LEU:HD21	1:A:338:LEU:HD11	2.02	0.41
1:B:211:LYS:HA	1:B:211:LYS:HD3	1.87	0.41
1:B:76:ARG:NE	1:B:80:ILE:HD11	2.36	0.41
1:B:145:ASP:O	1:B:147:THR:N	2.54	0.40
1:A:235:LEU:HB2	1:A:469:LEU:HD13	2.04	0.40
1:B:294:LEU:HA	1:B:294:LEU:HD13	1.89	0.40
1:B:372:ILE:O	1:B:463:ALA:HA	2.21	0.40
1:B:76:ARG:HD3	1:B:207:TRP:CD2	2.57	0.40
1:A:39:ARG:HD3	3:A:775:HOH:O	2.21	0.40
1:A:425:LYS:HD2	3:A:701:HOH:O	2.22	0.40
1:B:222:LEU:HD13	1:B:262:TYR:HB2	2.04	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	496/579 (86%)	485 (98%)	11 (2%)	0	100	100
1	B	478/579 (83%)	466 (98%)	12 (2%)	0	100	100
All	All	974/1158 (84%)	951 (98%)	23 (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	445/520 (86%)	424 (95%)	21 (5%)	29	52
1	B	430/520 (83%)	408 (95%)	22 (5%)	26	48
All	All	875/1040 (84%)	832 (95%)	43 (5%)	27	50

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	144	ARG
1	A	147	THR
1	A	195	ARG
1	A	202	ARG
1	A	213	SER
1	A	271	LYS
1	A	287	LEU
1	A	294	LEU
1	A	303	ARG
1	A	311	LYS
1	A	357	ILE
1	A	358	LEU
1	A	363	ARG
1	A	377	GLN
1	A	417	SER
1	A	419	ILE
1	A	422	ARG
1	A	425	LYS
1	A	455	MET
1	A	544	ILE
1	B	32	TYR
1	B	79	SER
1	B	147	THR
1	B	161	GLU
1	B	195	ARG
1	B	211	LYS
1	B	213	SER
1	B	254	LYS
1	B	258	LYS
1	B	294	LEU
1	B	303	ARG
1	B	308	LYS
1	B	311	LYS

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Mol	Chain	Res	Type
1	B	322	GLN
1	B	342	LYS
1	B	377	GLN
1	B	387	SER
1	B	406	LEU
1	B	419	ILE
1	B	446	ARG
1	B	455	MET
1	B	466	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	548	HIS

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](#)

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	PO4	A	601	-	4,4,4	0.77	0	6,6,6	0.59	0
2	PO4	B	601	-	4,4,4	0.83	0	6,6,6	0.76	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	PO4	A	601	-	-	0/0/0/0	0/0/0/0
2	PO4	B	601	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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	500/579 (86%)	-0.36	8 (1%) 72 74	10, 28, 69, 99	2 (0%)
1	B	482/579 (83%)	-0.36	11 (2%) 60 63	19, 35, 68, 124	3 (0%)
All	All	982/1158 (84%)	-0.36	19 (1%) 66 69	10, 32, 69, 124	5 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	LEU	5.4
1	B	320	PRO	5.4
1	B	24	LEU	4.8
1	A	537	PHE	4.3
1	B	318	THR	3.8
1	A	24	LEU	3.6
1	B	495	VAL	3.6
1	B	317	TYR	3.3
1	A	539	LEU	3.2
1	B	185	PHE	3.2
1	B	494	HIS	3.2
1	A	542	GLN	3.1
1	A	318	THR	3.0
1	B	186	LYS	2.9
1	A	358	LEU	2.8
1	A	540	ALA	2.7
1	A	320	PRO	2.6
1	B	380	HIS	2.2
1	B	323	HIS	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. 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(\AA^2)	Q<0.9
2	PO4	B	601	5/5	0.99	0.09	21,25,30,30	0
2	PO4	A	601	5/5	1.00	0.09	10,11,16,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.