



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 06:25 AM EDT

PDB ID : 3C9F
Title : Crystal structure of 5'-nucleotidase from *Candida albicans* SC5314
Authors : Patskovsky, Y.; Romero, R.; Gilmore, M.; Eberle, M.; Bain, K.; Smith, D.; Wasserman, S.R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-02-15
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 : 2.23.2
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) : 2.23.2

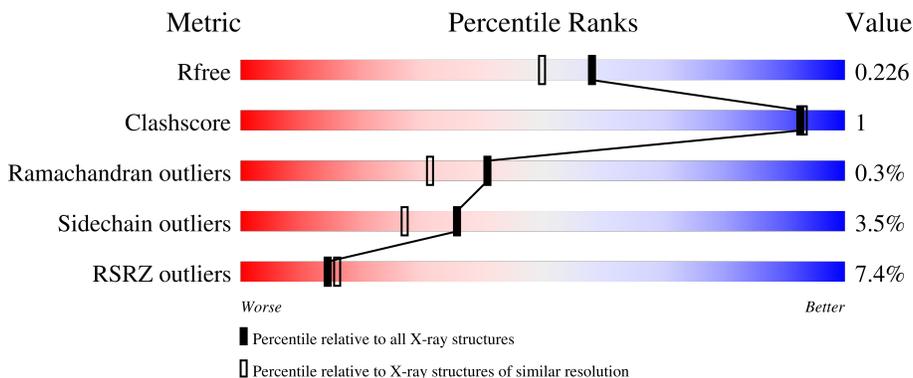
1 Overall quality at a glance

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 of 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	557	 8% 89% 6% 5%
1	B	557	 6% 91% 6% ...

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9842 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 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	531	4457	2886	748	817	6	0	18	0
1	B	540	4538	2932	767	832	7	0	19	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	expression tag	UNP Q5A5Q7
A	13	SER	-	expression tag	UNP Q5A5Q7
A	14	LEU	-	expression tag	UNP Q5A5Q7
A	62	MET	LEU	engineered mutation	UNP Q5A5Q7
A	151	LEU	SER	engineered mutation	UNP Q5A5Q7
A	157	LEU	SER	engineered mutation	UNP Q5A5Q7
A	172	MET	LEU	engineered mutation	UNP Q5A5Q7
A	323	LEU	SER	engineered mutation	UNP Q5A5Q7
A	367	LEU	SER	engineered mutation	UNP Q5A5Q7
A	561	GLU	-	expression tag	UNP Q5A5Q7
A	562	GLY	-	expression tag	UNP Q5A5Q7
A	563	HIS	-	expression tag	UNP Q5A5Q7
A	564	HIS	-	expression tag	UNP Q5A5Q7
A	565	HIS	-	expression tag	UNP Q5A5Q7
A	566	HIS	-	expression tag	UNP Q5A5Q7
A	567	HIS	-	expression tag	UNP Q5A5Q7
A	568	HIS	-	expression tag	UNP Q5A5Q7
B	12	MET	-	expression tag	UNP Q5A5Q7
B	13	SER	-	expression tag	UNP Q5A5Q7
B	14	LEU	-	expression tag	UNP Q5A5Q7
B	62	MET	LEU	engineered mutation	UNP Q5A5Q7
B	151	LEU	SER	engineered mutation	UNP Q5A5Q7
B	157	LEU	SER	engineered mutation	UNP Q5A5Q7
B	172	MET	LEU	engineered mutation	UNP Q5A5Q7
B	323	LEU	SER	engineered mutation	UNP Q5A5Q7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	367	LEU	SER	engineered mutation	UNP Q5A5Q7
B	561	GLU	-	expression tag	UNP Q5A5Q7
B	562	GLY	-	expression tag	UNP Q5A5Q7
B	563	HIS	-	expression tag	UNP Q5A5Q7
B	564	HIS	-	expression tag	UNP Q5A5Q7
B	565	HIS	-	expression tag	UNP Q5A5Q7
B	566	HIS	-	expression tag	UNP Q5A5Q7
B	567	HIS	-	expression tag	UNP Q5A5Q7
B	568	HIS	-	expression tag	UNP Q5A5Q7

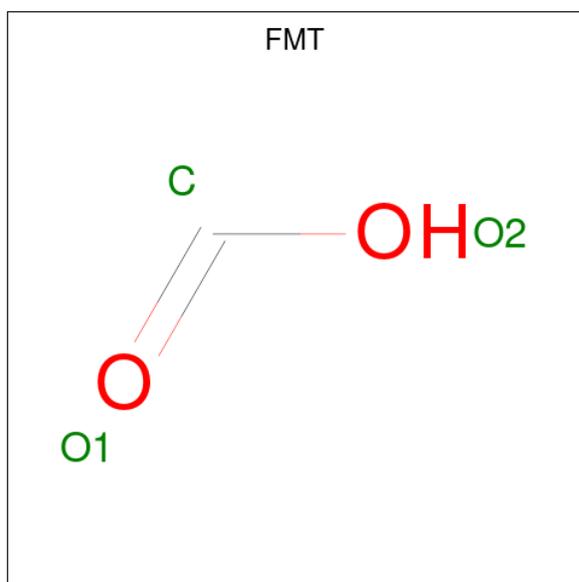
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	3	Total	Na	0	0
			3	3		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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

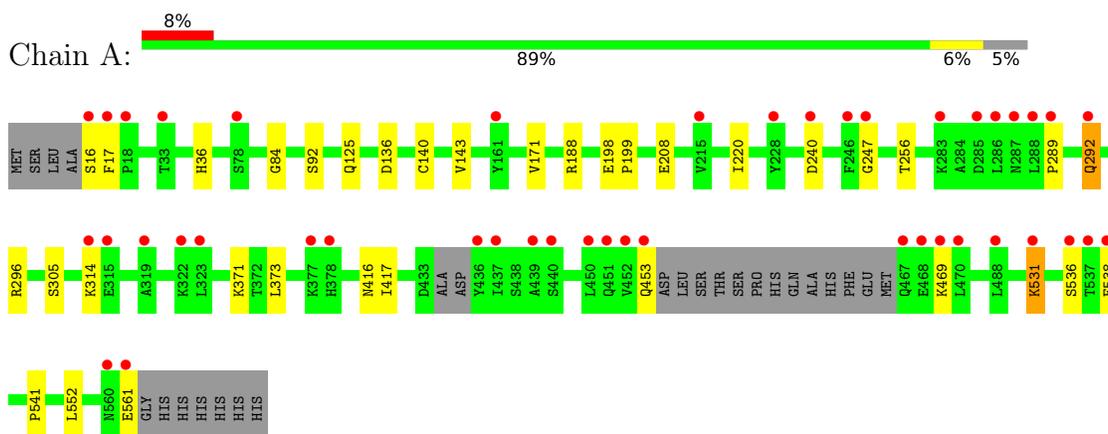
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	380	Total O 381 381	0	1
5	B	453	Total O 454 454	0	1

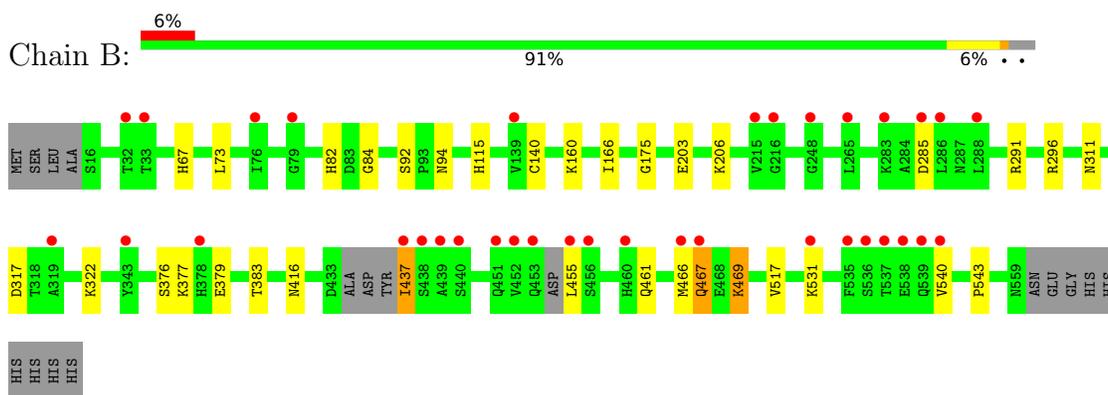
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 5'-nucleotidase



- Molecule 1: 5'-nucleotidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.95Å 106.74Å 150.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 36.15 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-1.90) 99.0 (36.15-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.85Å)	Xtrriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.186 , 0.225 0.188 , 0.226	Depositor DCC
R_{free} test set	4265 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtrriage
Anisotropy	0.138	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.009 for k,h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9842	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: FMT, NA, 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	0.53	0/4629	0.64	0/6294
1	B	0.55	1/4718 (0.0%)	0.66	2/6414 (0.0%)
All	All	0.54	1/9347 (0.0%)	0.65	2/12708 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	CYS	CB-SG	-5.94	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466[A]	MET	CA-C-O	5.15	130.92	120.10
1	B	466[B]	MET	CA-C-O	5.15	130.92	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4457	0	4399	14	0
1	B	4538	0	4459	17	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
4	A	3	0	1	0	0
4	B	3	0	1	0	0
5	A	381	0	0	2	0
5	B	454	0	0	2	0
All	All	9842	0	8860	26	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 1.

All (26) 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:188[A]:ARG:HH11	1:B:467:GLN:HB2	1.37	0.85
1:A:188[B]:ARG:HH22	1:B:467:GLN:HA	1.42	0.84
1:A:140[B]:CYS:SG	1:A:143:VAL:HB	2.42	0.59
1:A:188[A]:ARG:NH1	1:B:467:GLN:HB2	2.15	0.57
1:B:82[A]:HIS:CD2	1:B:94:ASN:HD22	2.24	0.55
1:B:203:GLU:OE1	1:B:206:LYS:HE2	2.10	0.51
1:B:376:SER:HB2	1:B:379:GLU:HB2	1.92	0.50
1:A:373:LEU:HD13	1:A:552:LEU:HD11	1.94	0.50
1:B:437:ILE:O	1:B:437:ILE:HG13	2.08	0.50
1:A:188[B]:ARG:HH12	1:B:467:GLN:HB2	1.75	0.50
1:A:289:PRO:HD2	1:A:292:GLN:HE21	1.78	0.48
1:B:160:LYS:HE2	5:B:668:HOH:O	2.13	0.48
1:B:317:ASP:HB3	1:B:322:LYS:HD2	1.96	0.48
1:B:291:ARG:NH1	5:B:789:HOH:O	2.46	0.47
1:A:36:HIS:NE2	5:A:975[B]:HOH:O	2.36	0.46
1:A:371:LYS:HG3	5:A:659:HOH:O	2.16	0.46
1:B:82[A]:HIS:NE2	1:B:115:HIS:O	2.49	0.45
1:A:531:LYS:HA	1:A:531:LYS:HD3	1.81	0.45
1:B:67:HIS:CD2	1:B:166:ILE:HG13	2.53	0.44
1:A:220:ILE:HG23	1:A:247:GLY:HA3	1.99	0.43
1:A:188[A]:ARG:HH11	1:B:467:GLN:CB	2.19	0.42
1:A:198:GLU:HA	1:A:199:PRO:HD2	1.84	0.42
1:A:417[B]:ILE:HD11	1:A:541:PRO:HG3	2.01	0.42
1:B:383:THR:HA	1:B:517:VAL:O	2.21	0.41
1:B:469:LYS:H	1:B:469:LYS:HG2	1.57	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	543/557 (98%)	523 (96%)	19 (4%)	1 (0%)	47	38
1	B	553/557 (99%)	531 (96%)	20 (4%)	2 (0%)	34	24
All	All	1096/1114 (98%)	1054 (96%)	39 (4%)	3 (0%)	41	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	543	PRO
1	A	84	GLY
1	B	84	GLY

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	505/509 (99%)	483 (96%)	22 (4%)	28	19
1	B	514/509 (101%)	500 (97%)	14 (3%)	44	38
All	All	1019/1018 (100%)	983 (96%)	36 (4%)	36	27

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	17	PHE
1	A	92	SER
1	A	125	GLN
1	A	136	ASP
1	A	171	VAL
1	A	208[A]	GLU
1	A	208[B]	GLU
1	A	240	ASP
1	A	256[A]	THR
1	A	256[B]	THR
1	A	292	GLN
1	A	296	ARG
1	A	305	SER
1	A	314	LYS
1	A	416	ASN
1	A	453	GLN
1	A	469	LYS
1	A	531	LYS
1	A	536	SER
1	A	538	GLU
1	A	561	GLU
1	B	73	LEU
1	B	92	SER
1	B	285	ASP
1	B	296	ARG
1	B	311	ASN
1	B	377	LYS
1	B	416	ASN
1	B	437	ILE
1	B	455	LEU
1	B	461	GLN
1	B	467	GLN
1	B	469	LYS
1	B	531	LYS
1	B	540	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	292	GLN
1	A	451	GLN

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Mol	Chain	Res	Type
1	A	525	ASN
1	A	554	ASN
1	B	21	ASN
1	B	67	HIS
1	B	244	GLN
1	B	461	GLN
1	B	525	ASN
1	B	559	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	FMT	B	607	2	0,2,2	-	-	0,1,1	-	-
4	FMT	A	607	2	0,2,2	-	-	0,1,1	-	-

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	531/557 (95%)	0.27	44 (8%) 11 13	19, 36, 69, 115	0
1	B	540/557 (96%)	0.15	35 (6%) 18 21	18, 33, 64, 121	0
All	All	1071/1114 (96%)	0.21	79 (7%) 14 16	18, 34, 68, 121	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	PHE	8.2
1	A	16	SER	6.0
1	B	538	GLU	5.9
1	B	455	LEU	5.7
1	A	561	GLU	5.3
1	B	453	GLN	5.2
1	B	456	SER	4.9
1	A	469	LYS	4.9
1	A	467	GLN	4.8
1	A	468	GLU	4.6
1	A	437	ILE	4.6
1	A	18	PRO	4.5
1	A	286	LEU	4.4
1	B	378	HIS	4.4
1	A	285	ASP	4.3
1	A	538	GLU	4.0
1	A	215[A]	VAL	4.0
1	A	314	LYS	4.0
1	A	436	TYR	3.9
1	A	452	VAL	3.9
1	A	560	ASN	3.9
1	B	460	HIS	3.8
1	B	531	LYS	3.6
1	B	440[A]	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	343	TYR	3.6
1	A	488	LEU	3.6
1	B	536	SER	3.5
1	A	323	LEU	3.5
1	B	215[A]	VAL	3.5
1	B	467	GLN	3.4
1	A	319	ALA	3.4
1	B	452	VAL	3.4
1	B	437	ILE	3.3
1	B	537	THR	3.3
1	B	439	ALA	3.2
1	A	378	HIS	3.2
1	A	240	ASP	3.2
1	A	470	LEU	3.1
1	A	377	LYS	3.1
1	B	539	GLN	3.1
1	A	289	PRO	3.0
1	A	536	SER	3.0
1	A	439	ALA	3.0
1	A	440[A]	SER	3.0
1	A	537	THR	3.0
1	A	246	PHE	2.9
1	B	535	PHE	2.9
1	B	466[A]	MET	2.9
1	B	285	ASP	2.9
1	B	76	ILE	2.8
1	B	33	THR	2.8
1	A	531	LYS	2.7
1	A	228	TYR	2.7
1	A	315	GLU	2.7
1	A	453	GLN	2.7
1	A	288	LEU	2.6
1	B	540	VAL	2.6
1	B	283	LYS	2.5
1	B	286	LEU	2.5
1	A	292	GLN	2.5
1	A	283	LYS	2.5
1	B	216	GLY	2.4
1	B	32	THR	2.4
1	B	319	ALA	2.4
1	A	33	THR	2.4
1	A	451	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	248	GLY	2.3
1	B	288	LEU	2.2
1	A	78	SER	2.2
1	B	265	LEU	2.2
1	A	287	ASN	2.2
1	A	161	TYR	2.2
1	B	79	GLY	2.1
1	B	139	VAL	2.1
1	B	438[A]	SER	2.1
1	B	451	GLN	2.1
1	A	322	LYS	2.1
1	A	247	GLY	2.0
1	A	450	LEU	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 monosaccharides 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	NA	B	603	1/1	0.84	0.10	59,59,59,59	0
3	NA	B	606	1/1	0.87	0.24	54,54,54,54	0
3	NA	B	604	1/1	0.94	0.05	44,44,44,44	0
3	NA	A	605	1/1	0.96	0.08	44,44,44,44	0
4	FMT	A	607	3/3	0.97	0.16	26,26,27,36	0
4	FMT	B	607	3/3	0.97	0.20	33,33,37,38	0
2	ZN	A	601	1/1	1.00	0.07	32,32,32,32	0
2	ZN	B	601	1/1	1.00	0.06	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.