Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:30 PM GMT

PDB ID : 2H2U
Title : Crystal structure of the E130Y mutant of human soluble calcium-activated nucleotidase (SCAN) with calcium ion
Authors : Yang, M.; Horii, K.; Herr, A.B.; Kirley, T.L.
Deposited on : 2006-05-19
Resolution : 2.40 Å(reported)

1 Overall quality at a glance (i)

The reported resolution of this entry is 2.40 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	Percentile Ranks	Value
Rfree		0.286
Clashscore		10
Ramachandran outliers		0.3%
Sidechain outliers		10.9%
RSRZ outliers		2.1%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
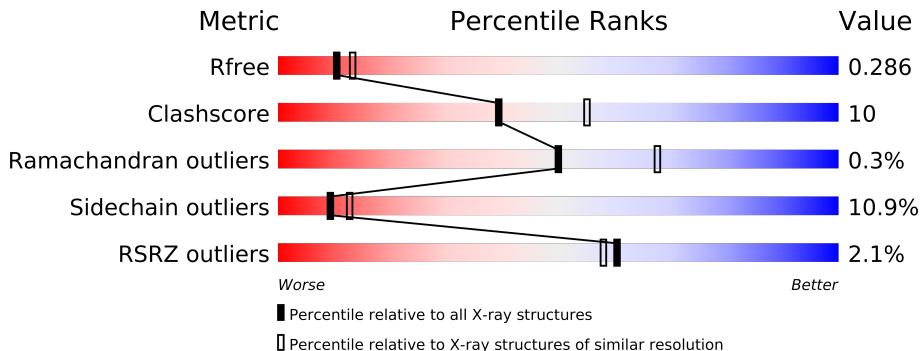
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	339	
1	B	339	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5035 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Soluble calcium-activated nucleotidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2491	1588	417	483	3			
1	B	317	Total	C	N	O	S	0	0	0
			2513	1603	421	486	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	CLONING ARTIFACT	UNP Q8WVQ1
A	-6	SER	-	CLONING ARTIFACT	UNP Q8WVQ1
A	-5	HIS	-	CLONING ARTIFACT	UNP Q8WVQ1
A	-4	MET	-	CLONING ARTIFACT	UNP Q8WVQ1
A	-3	ALA	-	CLONING ARTIFACT	UNP Q8WVQ1
A	-2	SER	-	CLONING ARTIFACT	UNP Q8WVQ1
A	90	TYR	GLU	ENGINEERED	UNP Q8WVQ1
B	-7	GLY	-	CLONING ARTIFACT	UNP Q8WVQ1
B	-6	SER	-	CLONING ARTIFACT	UNP Q8WVQ1
B	-5	HIS	-	CLONING ARTIFACT	UNP Q8WVQ1
B	-4	MET	-	CLONING ARTIFACT	UNP Q8WVQ1
B	-3	ALA	-	CLONING ARTIFACT	UNP Q8WVQ1
B	-2	SER	-	CLONING ARTIFACT	UNP Q8WVQ1
B	90	TYR	GLU	ENGINEERED	UNP Q8WVQ1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total O 18 18		0	0
3	B	11	Total O 11 11		0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Soluble calcium-activated nucleotidase 1

Chain A:
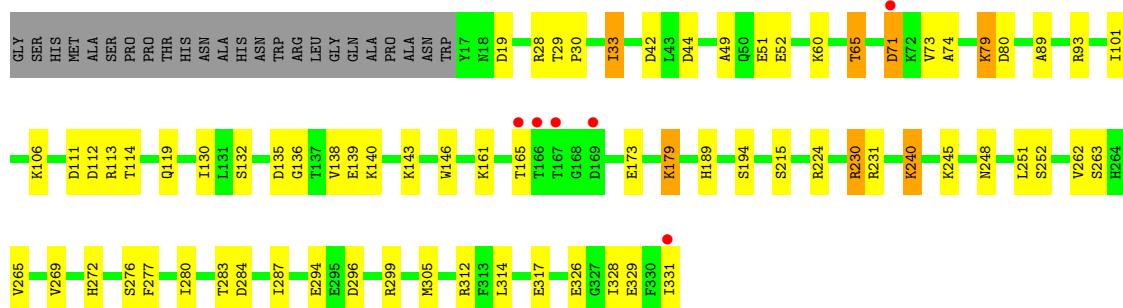
- Molecule 1: Soluble calcium-activated nucleotidase 1

Chain B:
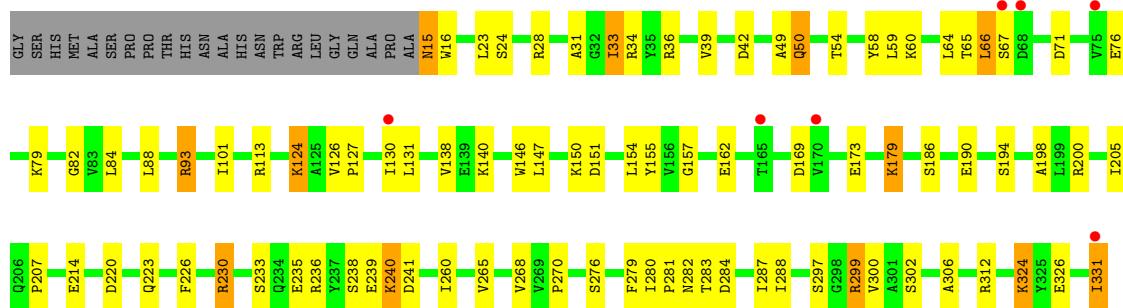
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	42.89Å 52.41Å 77.81Å 100.94° 106.51° 99.32°	Depositor
Resolution (Å)	47.04 – 2.40 47.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.5 (47.04-2.40) 86.5 (47.01-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.285 0.217 , 0.286	Depositor DCC
R_{free} test set	1075 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 20960 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5035	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5　Model quality ⓘ

5.1　Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.61	0/2554	0.72	0/3468
1	B	0.56	0/2578	0.71	1/3502 (0.0%)
All	All	0.59	0/5132	0.71	1/6970 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	42	ASP	CB-CG-OD1	5.15	122.93	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2　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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2491	0	2405	40	0
1	B	2513	0	2421	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	18	0	0	0	0
3	B	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5035	0	4826	94	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (94) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:93:ARG:HH21	1:B:93:ARG:HG2	1.10	1.11
1:B:230:ARG:HH11	1:B:230:ARG:HG3	1.17	1.10
1:A:230:ARG:HH11	1:A:230:ARG:HG3	0.95	1.10
1:B:28:ARG:HD2	1:B:33:ILE:HD13	1.46	0.96
1:A:230:ARG:HG3	1:A:230:ARG:NH1	1.76	0.95
1:B:34:ARG:HG2	1:B:65:THR:HG22	1.48	0.94
1:A:230:ARG:HH11	1:A:230:ARG:CG	1.79	0.94
1:B:34:ARG:CG	1:B:65:THR:HG22	2.00	0.91
1:B:230:ARG:HH11	1:B:230:ARG:CG	1.86	0.88
1:A:240:LYS:HE2	1:A:240:LYS:H	1.40	0.87
1:B:93:ARG:NH2	1:B:93:ARG:HG2	1.90	0.76
1:B:36:ARG:HG3	1:B:331:ILE:HG13	1.68	0.75
1:B:93:ARG:CG	1:B:93:ARG:HH21	1.99	0.70
1:A:138:VAL:HG12	1:A:140:LYS:H	1.57	0.69
1:A:111:ASP:OD2	1:A:114:THR:OG1	2.05	0.68
1:A:42:ASP:HB2	1:A:326:GLU:HG3	1.76	0.68
1:B:230:ARG:HG3	1:B:230:ARG:NH1	1.93	0.67
1:B:23:LEU:HB2	1:B:331:ILE:HG22	1.77	0.67
1:B:34:ARG:HG3	1:B:65:THR:HG22	1.79	0.65
1:B:58:TYR:HB2	1:B:82:GLY:O	1.96	0.64
1:A:139:GLU:OE1	1:B:124:LYS:HB3	1.97	0.64
1:A:71:ASP:HA	1:A:312:ARG:HH22	1.63	0.63
1:A:93:ARG:HB3	1:A:113:ARG:HG3	1.78	0.63
1:B:200:ARG:HD2	1:B:205:ILE:O	1.99	0.63
1:A:248:ASN:HB2	1:A:265:VAL:O	1.99	0.62
1:A:179:LYS:NZ	1:A:189:HIS:ND1	2.48	0.60
1:B:24:SER:N	1:B:331:ILE:OXT	2.34	0.60
1:A:42:ASP:CB	1:A:326:GLU:HG3	2.31	0.59
1:B:220:ASP:O	1:B:223:GLN:OE1	2.22	0.57
1:B:131:LEU:HD22	1:B:179:LYS:HG2	1.87	0.57
1:A:283:THR:O	1:A:284:ASP:HB2	2.06	0.56
1:B:138:VAL:HG12	1:B:140:LYS:H	1.71	0.56
1:B:240:LYS:HE2	1:B:240:LYS:H	1.70	0.56
1:B:300:VAL:HG21	1:B:324:LYS:HD3	1.89	0.54
1:B:93:ARG:CG	1:B:93:ARG:NH2	2.66	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:240:LYS:N	1:A:240:LYS:HE2	2.18	0.54
1:A:79:LYS:HE3	1:A:80:ASP:H	1.72	0.54
1:A:329:GLU:OE1	1:A:329:GLU:HA	2.08	0.53
1:B:226:PHE:CD2	1:B:279:PHE:HZ	2.26	0.53
1:A:33:ILE:HD12	1:A:33:ILE:N	2.24	0.53
1:B:230:ARG:CG	1:B:230:ARG:NH1	2.57	0.53
1:A:251:LEU:HD23	1:A:262:VAL:HG22	1.91	0.52
1:B:240:LYS:CE	1:B:240:LYS:H	2.23	0.51
1:A:73:VAL:HG23	1:A:314:LEU:HD12	1.93	0.51
1:B:28:ARG:CD	1:B:33:ILE:HD13	2.30	0.51
1:A:106:LYS:HG2	1:A:119:GLN:NE2	2.25	0.51
1:B:283:THR:O	1:B:284:ASP:HB2	2.10	0.51
1:B:268:VAL:HG12	1:B:270:PRO:HD3	1.93	0.51
1:A:139:GLU:OE1	1:B:124:LYS:CB	2.58	0.50
1:A:106:LYS:HG2	1:A:119:GLN:HE22	1.77	0.50
1:A:231:ARG:HA	1:A:245:LYS:O	2.13	0.49
1:A:224:ARG:HD3	1:A:252:SER:HB2	1.93	0.49
1:B:198:ALA:O	1:B:260:ILE:HD13	2.13	0.49
1:B:58:TYR:CB	1:B:82:GLY:O	2.59	0.49
1:A:287:ILE:HD13	1:A:314:LEU:HD11	1.94	0.49
1:A:269:VAL:HG11	1:A:272:HIS:ND1	2.29	0.48
1:A:276:SER:HB3	1:A:328:ILE:HG22	1.94	0.48
1:B:39:VAL:HG23	1:B:60:LYS:HB3	1.97	0.46
1:A:280:ILE:HD12	1:A:287:ILE:CG2	2.45	0.46
1:B:31:ALA:O	1:B:67:SER:HA	2.16	0.46
1:A:65:THR:HG23	1:A:74:ALA:HB3	1.98	0.46
1:B:15:ASN:HB3	1:B:16:TRP:H	1.60	0.46
1:B:130:ILE:O	1:B:130:ILE:HG23	2.15	0.46
1:A:215:SER:HG	1:A:277:PHE:HD2	1.62	0.46
1:B:162:GLU:HG2	1:B:173:GLU:HG2	1.97	0.46
1:B:300:VAL:CG2	1:B:324:LYS:HD3	2.46	0.45
1:B:66:LEU:HD22	1:B:280:ILE:HG21	1.99	0.45
1:A:29:THR:HB	1:A:30:PRO:HD2	1.98	0.44
1:B:49:ALA:HB3	1:B:54:THR:HB	1.98	0.44
1:A:130:ILE:HG23	1:A:130:ILE:O	2.18	0.44
1:A:89:ALA:O	1:B:88:LEU:HD12	2.18	0.44
1:B:299:ARG:O	1:B:299:ARG:HG3	2.18	0.44
1:B:147:LEU:HD22	1:B:154:LEU:HD11	2.01	0.43
1:A:280:ILE:HD12	1:A:287:ILE:HG22	2.00	0.43
1:B:126:VAL:HA	1:B:127:PRO:HD2	1.89	0.43
1:A:230:ARG:NH1	1:A:230:ARG:CG	2.48	0.43
1:B:50:GLN:HE21	1:B:50:GLN:HB2	1.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:214:GLU:CD	1:B:230:ARG:HD2	2.39	0.42
1:A:136:GLY:HA3	1:A:189:HIS:CE1	2.54	0.42
1:B:280:ILE:HA	1:B:281:PRO:HD3	1.95	0.42
1:A:146:TRP:HB3	1:A:215:SER:HA	2.01	0.42
1:B:238:SER:OG	1:B:241:ASP:OD1	2.22	0.42
1:B:280:ILE:HD12	1:B:287:ILE:HG22	2.01	0.42
1:B:324:LYS:HE3	1:B:324:LYS:HB2	1.69	0.42
1:B:288:ILE:O	1:B:306:ALA:HA	2.20	0.42
1:B:150:LYS:HB3	1:B:155:TYR:CE2	2.55	0.41
1:A:112:ASP:HB2	1:A:143:LYS:HG2	2.01	0.41
1:B:93:ARG:NH1	1:B:113:ARG:NH1	2.69	0.41
1:B:64:LEU:C	1:B:64:LEU:HD23	2.40	0.41
1:B:146:TRP:CE2	1:B:157:GLY:HA3	2.55	0.41
1:B:238:SER:HB2	1:B:240:LYS:HE3	2.02	0.41
1:A:49:ALA:HB3	1:A:51:GLU:HB2	2.03	0.41
1:B:200:ARG:CZ	1:B:207:PRO:HG3	2.52	0.40
1:B:331:ILE:HG12	1:B:331:ILE:H	1.60	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	313/339 (92%)	299 (96%)	13 (4%)	1 (0%)	50	68
1	B	315/339 (93%)	295 (94%)	19 (6%)	1 (0%)	50	68
All	All	628/678 (93%)	594 (95%)	32 (5%)	2 (0%)	50	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	297	SER
1	A	296	ASP

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	265/283 (94%)	240 (91%)	25 (9%)	13	18
1	B	267/283 (94%)	234 (88%)	33 (12%)	7	8
All	All	532/566 (94%)	474 (89%)	58 (11%)	9	13

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	28	ARG
1	A	33	ILE
1	A	44	ASP
1	A	52	GLU
1	A	60	LYS
1	A	65	THR
1	A	71	ASP
1	A	79	LYS
1	A	101	ILE
1	A	132	SER
1	A	135	ASP
1	A	161	LYS
1	A	165	THR
1	A	173	GLU
1	A	179	LYS
1	A	194	SER
1	A	230	ARG
1	A	240	LYS
1	A	263	SER
1	A	294	GLU
1	A	299	ARG
1	A	305	MET
1	A	317	GLU
1	A	331	ILE
1	B	15	ASN
1	B	33	ILE
1	B	50	GLN
1	B	59	LEU

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Mol	Chain	Res	Type
1	B	66	LEU
1	B	71	ASP
1	B	76	GLU
1	B	79	LYS
1	B	84	LEU
1	B	93	ARG
1	B	101	ILE
1	B	124	LYS
1	B	151	ASP
1	B	169	ASP
1	B	179	LYS
1	B	186	SER
1	B	190	GLU
1	B	194	SER
1	B	230	ARG
1	B	233	SER
1	B	235	GLU
1	B	236	ARG
1	B	239	GLU
1	B	240	LYS
1	B	265	VAL
1	B	276	SER
1	B	282	ASN
1	B	299	ARG
1	B	302	SER
1	B	312	ARG
1	B	324	LYS
1	B	326	GLU
1	B	331	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	B	50	GLN
1	B	104	ASN
1	B	264	HIS

5.3.3 RNA (i)

There are no RNA chains 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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	315/339 (92%)	0.07	6 (1%)	64	61	27, 44, 59, 73	0
1	B	317/339 (93%)	0.20	7 (2%)	59	57	31, 47, 62, 70	0
All	All	632/678 (93%)	0.14	13 (2%)	60	58	27, 46, 61, 73	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	VAL	3.6
1	A	166	THR	3.3
1	A	71	ASP	3.1
1	A	167	THR	2.8
1	B	331	ILE	2.5
1	B	67	SER	2.5
1	B	75	VAL	2.5
1	A	331	ILE	2.4
1	A	165	THR	2.3
1	B	165	THR	2.3
1	B	68	ASP	2.2
1	A	169	ASP	2.1
1	B	130	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	CA	B	1001	1/1	0.15	-0.26	57,57,57,57	0
2	CA	A	1000	1/1	0.09	-1.74	47,47,47,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.