



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:36 AM GMT

PDB ID : 2NYR
Title : Crystal Structure of Human Sirtuin Homolog 5 in Complex with Suramin
Authors : Min, J.R.; Antoshenko, T.; Allali-Hassani, A.; Dong, A.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)
Deposited on : 2006-11-21
Resolution : 2.06 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

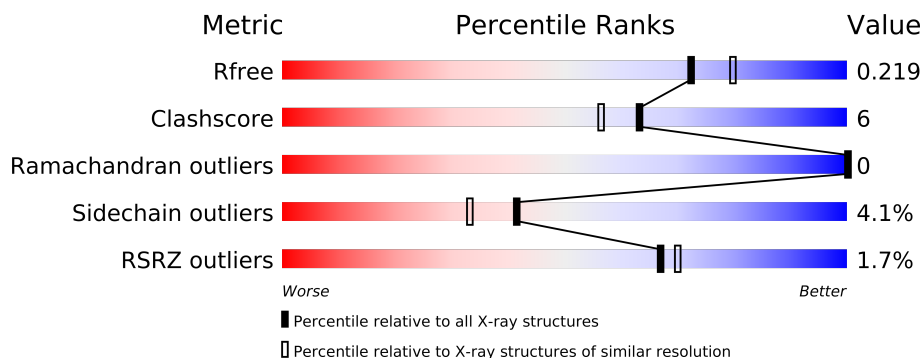
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.06 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}	66092	1224 (2.08-2.04)
Clashscore	79885	1390 (2.08-2.04)
Ramachandran outliers	78287	1381 (2.08-2.04)
Sidechain outliers	78261	1381 (2.08-2.04)
RSRZ outliers	66119	1225 (2.08-2.04)

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	271	
1	B	271	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4288 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.

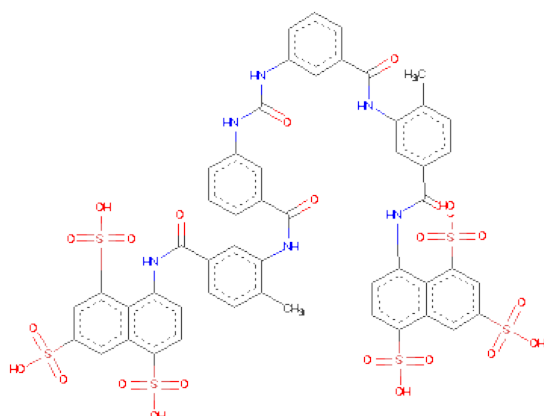
- Molecule 1 is a protein called NAD-dependent deacetylase sirtuin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1978	1249	358	359	12			
1	B	258	Total	C	N	O	S	0	0	0
			1969	1244	357	356	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLY	-	EXPRESSION TAG	UNP Q9NXA8
A	33	SER	-	EXPRESSION TAG	UNP Q9NXA8
B	32	GLY	-	EXPRESSION TAG	UNP Q9NXA8
B	33	SER	-	EXPRESSION TAG	UNP Q9NXA8

- Molecule 2 is 8,8'-[CARBONYLBIS[IMINO-3,1-PHENYLENECARBONYLIMINO(4-METHYL-3,1-PHENYLENE)CARBONYLIMINO]]BIS-1,3,5-NAPHTHALENETRISULFONIC ACID (three-letter code: SVR) (formula: C₅₁H₄₀N₆O₂₃S₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			86	51	6	23	6		

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

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

- Molecule 4 is water.

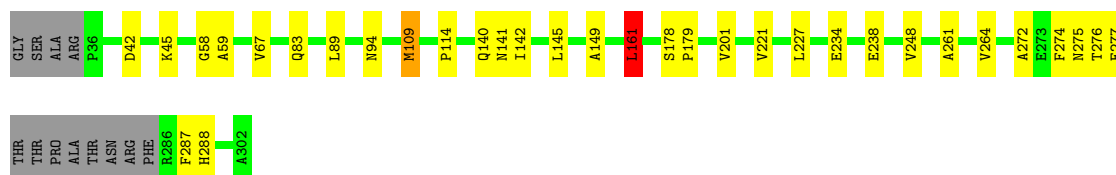
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	142	Total	O	0	0
			142	142		
4	B	111	Total	O	0	0
			111	111		

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.

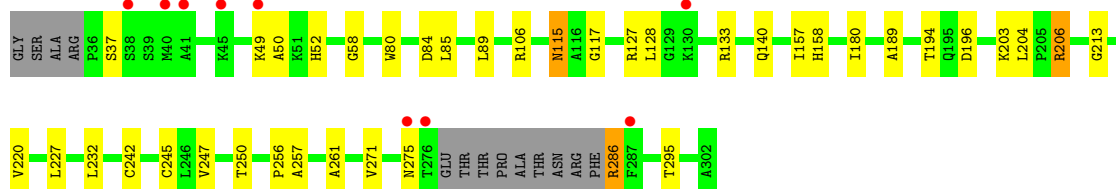
- Molecule 1: NAD-dependent deacetylase sirtuin-5

Chain A: 



- Molecule 1: NAD-dependent deacetylase sirtuin-5

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.20Å 116.20Å 55.99Å 90.00° 90.46° 90.00°	Depositor
Resolution (Å)	58.12 – 2.06 40.32 – 2.06	Depositor EDS
% Data completeness (in resolution range)	86.2 (58.12-2.06) 84.5 (40.32-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.269 0.180 , 0.219	Depositor DCC
R_{free} test set	1402 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.0	EDS
Estimated twinning fraction	0.188 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 28070 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4288	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: ZN, SVR

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	0/2028	0.52	1/2749 (0.0%)
1	B	0.48	2/2019 (0.1%)	0.68	2/2737 (0.1%)
All	All	0.44	2/4047 (0.0%)	0.61	3/5486 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	286	ARG	CZ-NH2	8.35	1.44	1.33
1	B	286	ARG	NE-CZ	6.44	1.41	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	ARG	NE-CZ-NH1	-16.25	112.17	120.30
1	B	286	ARG	NE-CZ-NH2	12.58	126.59	120.30
1	A	161	LEU	CA-CB-CG	5.34	127.59	115.30

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	1978	0	1945	18	0
1	B	1969	0	1939	26	0
2	B	86	0	37	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	142	0	0	0	0
4	B	111	0	0	2	0
All	All	4288	0	3921	44	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 6.

All (44) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:206:ARG:HG3	1:B:206:ARG:HH11	1.37	0.86
1:B:206:ARG:HG3	1:B:206:ARG:NH1	1.92	0.84
1:A:42:ASP:O	1:A:45:LYS:HG2	1.78	0.83
1:A:142:ILE:HD11	2:B:401:SVR:O85	1.83	0.79
1:B:206:ARG:CG	1:B:206:ARG:HH11	2.04	0.70
1:B:115:ASN:HD22	1:B:117:GLY:H	1.43	0.67
1:A:142:ILE:O	1:A:161:LEU:HD22	1.96	0.66
1:A:109:MET:CE	1:A:109:MET:HA	2.30	0.61
1:B:106:ARG:NH1	1:B:180:ILE:HB	2.15	0.60
1:B:128:LEU:HB3	1:B:133:ARG:HB2	1.85	0.59
1:B:50:ALA:HB1	4:B:550:HOH:O	2.02	0.58
1:A:109:MET:HE2	1:A:109:MET:HA	1.88	0.56
1:B:247:VAL:HG21	1:B:261:ALA:HB2	1.87	0.56
1:B:140:GLN:NE2	1:B:256:PRO:HD2	2.22	0.55
1:B:206:ARG:NH1	1:B:213:GLY:O	2.40	0.54
1:A:261:ALA:O	1:A:264:VAL:HG22	2.08	0.54
1:A:275:ASN:OD1	1:A:288:HIS:HE1	1.91	0.53
1:A:248:VAL:HG12	1:A:274:PHE:HB2	1.92	0.51
1:A:59:ALA:HA	1:A:141:ASN:HD21	1.76	0.50
1:B:115:ASN:HD22	1:B:117:GLY:N	2.07	0.49
1:A:276:THR:O	1:A:277:GLU:HB3	2.12	0.49
1:A:234:GLU:O	1:A:238:GLU:HG2	2.12	0.49
1:A:58:GLY:HA2	1:A:140:GLN:HE21	1.77	0.48
1:A:221:VAL:HG11	1:A:227:LEU:HD23	1.96	0.47
1:A:272:ALA:HA	1:A:287:PHE:HB2	1.94	0.47
1:B:157:ILE:HD12	1:B:227:LEU:HD21	1.96	0.47
1:B:189:ALA:HB3	1:B:194:THR:HG21	1.96	0.47
1:A:67:VAL:HG22	1:A:109:MET:HE2	1.98	0.45
1:B:140:GLN:NE2	1:B:257:ALA:H	2.15	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:37:SER:HB3	1:B:286:ARG:O	2.17	0.44
1:A:67:VAL:HA	1:A:109:MET:HE1	1.99	0.44
1:B:58:GLY:HA3	1:B:250:THR:HG22	1.99	0.44
1:B:203:LYS:HB3	1:B:203:LYS:HE2	1.68	0.44
1:B:227:LEU:HD22	1:B:232:LEU:HD13	2.00	0.43
1:B:52:HIS:HB3	1:B:242:CYS:HA	1.99	0.43
1:B:247:VAL:HG21	1:B:261:ALA:CB	2.49	0.43
1:A:114:PRO:HB3	1:A:149:ALA:HB2	2.01	0.42
1:B:80:TRP:HB3	1:B:84:ASP:HB2	2.01	0.41
1:B:220:VAL:HG13	4:B:513:HOH:O	2.19	0.41
1:B:204:LEU:O	1:B:206:ARG:CD	2.68	0.41
1:A:178:SER:HA	1:A:179:PRO:HA	1.88	0.41
1:B:115:ASN:ND2	1:B:117:GLY:H	2.14	0.41
1:B:245:CYS:HB3	1:B:271:VAL:HG22	2.02	0.40
1:B:227:LEU:CD2	1:B:232:LEU:HD13	2.50	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	255/271 (94%)	253 (99%)	2 (1%)	0	100	100
1	B	254/271 (94%)	248 (98%)	6 (2%)	0	100	100
All	All	509/542 (94%)	501 (98%)	8 (2%)	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	206/215 (96%)	199 (97%)	7 (3%)	49	42
1	B	205/215 (95%)	195 (95%)	10 (5%)	35	24
All	All	411/430 (96%)	394 (96%)	17 (4%)	41	33

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	89	LEU
1	A	94	ASN
1	A	109	MET
1	A	145	LEU
1	A	161	LEU
1	A	201	VAL
1	B	49	LYS
1	B	85	LEU
1	B	89	LEU
1	B	115	ASN
1	B	127	ARG
1	B	158	HIS
1	B	196	ASP
1	B	206	ARG
1	B	275	ASN
1	B	295	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	140	GLN
1	A	141	ASN
1	A	288	HIS
1	A	290	GLN
1	B	115	ASN
1	B	140	GLN
1	B	263	GLN

5.3.3 RNA ⓘ

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 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	$\# Z > 2$
2	SVR	B	401	-	93,93,93	2.01	10 (10%)	145,145,145	2.00	31 (21%)

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	SVR	B	401	-	-	0/76/76/76	0/4/8/8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	SVR	C22-S31	-8.33	1.60	1.76
2	B	401	SVR	C76-S83	-7.87	1.61	1.76
2	B	401	SVR	C11-S17	-7.31	1.61	1.78
2	B	401	SVR	C71-S75	-6.85	1.62	1.78
2	B	401	SVR	C15-S21	-6.64	1.63	1.78
2	B	401	SVR	C69-S73	-6.46	1.63	1.78
2	B	401	SVR	C18-C11	2.17	1.40	1.37
2	B	401	SVR	C43-N44	-2.15	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	SVR	C74-C69	2.09	1.40	1.37
2	B	401	SVR	C43-N41	-2.05	1.33	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	SVR	C6-C11-S17	6.97	129.25	121.05
2	B	401	SVR	C66-C69-S73	6.84	129.10	121.05
2	B	401	SVR	C18-C11-S17	-6.26	110.86	117.67
2	B	401	SVR	C15-C10-C6	5.47	122.68	118.03
2	B	401	SVR	C74-C69-S73	-5.39	111.81	117.67
2	B	401	SVR	C16-C10-C15	-5.15	117.12	123.20
2	B	401	SVR	C71-C68-C66	4.54	121.89	118.03
2	B	401	SVR	C6-C3-N1	4.53	128.04	120.62
2	B	401	SVR	C72-C68-C71	-4.52	117.86	123.20
2	B	401	SVR	C55-N53-C51	-4.41	114.34	126.83
2	B	401	SVR	C68-C71-S75	4.17	125.96	121.05
2	B	401	SVR	O23-S17-C11	3.95	110.68	106.20
2	B	401	SVR	C7-C3-N1	-3.90	111.84	123.07
2	B	401	SVR	C49-C51-N53	3.69	122.88	115.86
2	B	401	SVR	O78-S73-C69	3.52	110.19	106.20
2	B	401	SVR	C60-C57-C55	3.31	120.18	117.42
2	B	401	SVR	O82-S75-C71	3.27	110.07	106.09
2	B	401	SVR	C67-C65-N63	-3.17	113.94	123.07
2	B	401	SVR	O29-S21-C15	3.10	109.71	106.20
2	B	401	SVR	C10-C15-S21	3.08	124.67	121.05
2	B	401	SVR	C66-C65-N63	2.91	125.38	120.62
2	B	401	SVR	C20-C13-N19	2.74	123.15	118.63
2	B	401	SVR	C12-C15-C10	-2.68	118.54	121.00
2	B	401	SVR	C14-C20-C13	2.55	119.55	117.42
2	B	401	SVR	C70-C71-C68	-2.31	118.88	121.00
2	B	401	SVR	C76-C74-C69	2.22	122.53	120.10
2	B	401	SVR	C47-C46-N44	-2.20	113.01	120.12
2	B	401	SVR	C69-C66-C68	2.19	118.12	116.09
2	B	401	SVR	C48-C46-N44	2.08	127.37	120.39
2	B	401	SVR	O81-S75-C71	2.03	108.50	106.20
2	B	401	SVR	O54-C51-C49	-2.02	117.46	121.01

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	259/271 (95%)	-0.22	0 100 100	11, 18, 25, 32	0
1	B	258/271 (95%)	0.12	9 (3%) 42 42	13, 22, 43, 51	0
All	All	517/542 (95%)	-0.05	9 (1%) 67 70	11, 19, 36, 51	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	LYS	2.8
1	B	41	ALA	2.6
1	B	38	SER	2.6
1	B	130	LYS	2.5
1	B	276	THR	2.4
1	B	40	MET	2.2
1	B	49	LYS	2.1
1	B	275	ASN	2.1
1	B	287	PHE	2.0

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(\AA^2)	Q<0.9
2	SVR	B	401	86/86	0.12	0.27	19,23,29,31	0
3	ZN	A	501	1/1	0.08	-0.94	24,24,24,24	0
3	ZN	B	501	1/1	0.06	-2.98	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.