



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:19 PM UTC

PDB ID : 8CCZ / pdb_00008ccz
Title : Crystal structure of human Sirt3 in complex with an inhibiting HIV1 Tat-37-59 peptide
Authors : Adolph, R.S.; Steegborn, C.
Deposited on : 2023-01-28
Resolution : 1.95 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

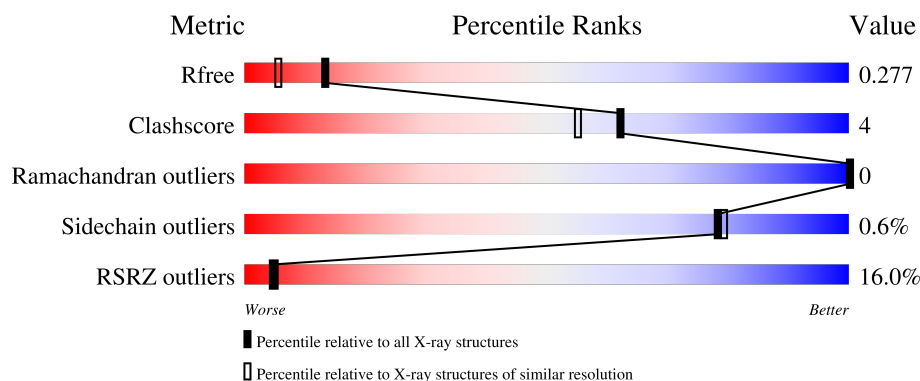
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	282	
1	B	282	
2	C	23	
2	D	23	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5037 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 NAD-dependent protein deacetylase sirtuin-3, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	1	0
			2155	1388	370	388	9			
1	B	274	Total	C	N	O	S	0	1	0
			2154	1387	371	387	9			

- Molecule 2 is a protein called Protein Tat.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	14	Total	C	N	O	0	0	0
			127	75	35	17			
2	D	14	Total	C	N	O	0	0	0
			127	75	35	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	37	ALA	CYS	engineered mutation	UNP P12506
D	37	ALA	CYS	engineered mutation	UNP P12506

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	231	Total	O	0	0
			231	231		

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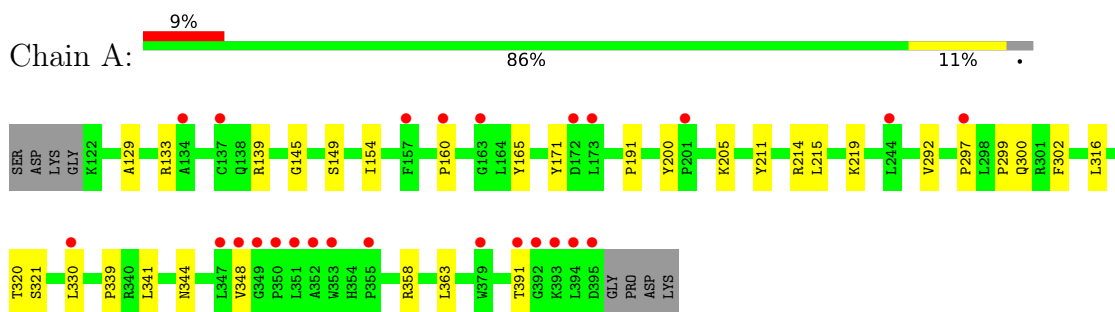
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	209	Total 209	O 209	0	0
4	C	16	Total 16	O 16	0	0
4	D	16	Total 16	O 16	0	0

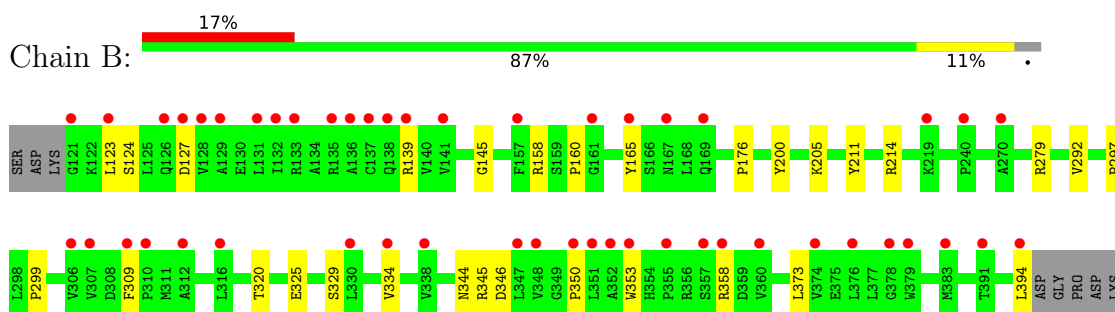
3 Residue-property plots [i](#)

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.

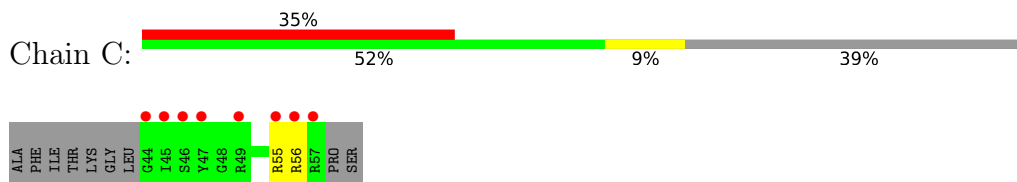
- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



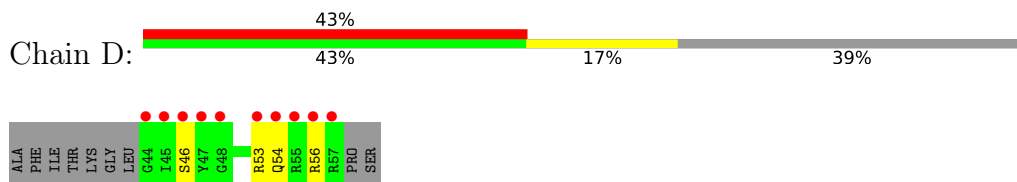
- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



- Molecule 2: Protein Tat



- Molecule 2: Protein Tat



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.55Å 78.12Å 76.58Å 90.00° 96.09° 90.00°	Depositor
Resolution (Å)	54.24 – 1.95 54.24 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (54.24-1.95) 90.4 (54.24-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.227 , 0.276 0.228 , 0.277	Depositor DCC
R_{free} test set	2335 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5037	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.56% 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: 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	0.10	0/2213	0.29	0/3015
1	B	0.10	0/2209	0.29	0/3009
2	C	0.16	0/127	0.55	0/162
2	D	0.16	0/127	0.52	0/162
All	All	0.10	0/4676	0.31	0/6348

There are no bond length outliers.

There are no bond angle outliers.

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	2155	0	2169	17	0
1	B	2154	0	2167	18	0
2	C	127	0	142	2	0
2	D	127	0	142	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	231	0	0	1	0
4	B	209	0	0	3	0
4	C	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	16	0	0	1	0
All	All	5037	0	4620	38	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 4.

All (38) 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:300:GLN:HE22	2:D:46:SER:HA	1.57	0.69
2:D:56:ARG:NH1	4:D:101:HOH:O	2.32	0.62
1:B:158:ARG:HD3	1:B:176:PRO:HG3	1.83	0.61
1:A:149:SER:HB3	1:A:154:ILE:HD12	1.85	0.59
1:B:345:ARG:NH2	4:B:509:HOH:O	2.38	0.56
1:A:292:VAL:HG21	1:A:299:PRO:HD3	1.87	0.56
1:B:139:ARG:NH2	4:B:510:HOH:O	2.38	0.55
1:B:205:LYS:HD2	1:B:394:LEU:HD23	1.88	0.55
1:A:339:PRO:HG3	1:A:358:ARG:HH11	1.71	0.54
1:A:321:SER:HA	1:A:348:VAL:HG21	1.88	0.54
1:B:279:ARG:NH2	4:B:503:HOH:O	2.32	0.53
1:B:292:VAL:HG21	1:B:299:PRO:HD3	1.91	0.52
1:B:325:GLU:HG2	2:D:53:ARG:HB2	1.91	0.52
1:A:139:ARG:NH2	4:A:516:HOH:O	2.44	0.50
1:B:145:GLY:HA3	1:B:320:THR:HB	1.93	0.50
1:A:297:PRO:HG2	1:B:297:PRO:HG2	1.94	0.50
1:A:211:TYR:HA	1:A:214:ARG:HB3	1.96	0.47
1:B:211:TYR:HA	1:B:214:ARG:HB3	1.95	0.47
1:A:215:LEU:HD22	1:A:219:LYS:HE2	1.96	0.47
1:B:344:ASN:ND2	1:B:346:ASP:H	2.13	0.47
2:C:55:ARG:NH2	4:C:103:HOH:O	2.49	0.46
1:A:171:TYR:CG	1:A:191:PRO:HG3	2.51	0.45
1:B:325:GLU:OE2	1:B:329[B]:SER:OG	2.25	0.45
1:B:344:ASN:HD22	1:B:346:ASP:H	1.64	0.45
2:C:56:ARG:HD3	2:C:56:ARG:HA	1.59	0.44
1:B:124:SER:H	1:B:127:ASP:HB2	1.83	0.43
1:A:145:GLY:HA3	1:A:320:THR:HB	2.00	0.42
1:A:344:ASN:O	1:A:363:LEU:HA	2.19	0.42
1:A:129:ALA:O	1:A:133:ARG:HG3	2.20	0.42
1:A:316:LEU:HD22	1:A:341:LEU:HD23	2.00	0.42
1:B:309:PHE:HD2	1:B:334:VAL:HG13	1.83	0.41
2:D:53:ARG:C	2:D:54:GLN:HG2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:PRO:HA	1:B:353:TRP:CD1	2.56	0.41
1:A:302:PHE:CE1	1:A:330:LEU:HD11	2.55	0.41
1:A:160:PRO:HA	1:A:165:TYR:CD2	2.55	0.41
1:B:160:PRO:HA	1:B:165:TYR:CG	2.55	0.41
1:A:205:LYS:HE3	1:A:391:THR:HG23	2.02	0.41
1:B:123:LEU:HD21	1:B:358:ARG:HH21	1.85	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	273/282 (97%)	267 (98%)	6 (2%)	0	100	100
1	B	273/282 (97%)	267 (98%)	6 (2%)	0	100	100
2	C	12/23 (52%)	9 (75%)	3 (25%)	0	100	100
2	D	12/23 (52%)	11 (92%)	1 (8%)	0	100	100
All	All	570/610 (93%)	554 (97%)	16 (3%)	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	239/244 (98%)	238 (100%)	1 (0%)	84	85
1	B	238/244 (98%)	236 (99%)	2 (1%)	73	74
2	C	12/19 (63%)	12 (100%)	0	100	100
2	D	12/19 (63%)	12 (100%)	0	100	100
All	All	501/526 (95%)	498 (99%)	3 (1%)	78	79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	TYR
1	B	200	TYR
1	B	373	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	HIS
1	B	300	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

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

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	274/282 (97%)	0.87	25 (9%) 15 17	17, 32, 55, 75	1 (0%)
1	B	274/282 (97%)	1.13	49 (17%) 3 3	21, 36, 64, 75	1 (0%)
2	C	14/23 (60%)	2.29	8 (57%) 0 0	27, 69, 86, 89	0
2	D	14/23 (60%)	2.45	10 (71%) 0 0	30, 71, 75, 79	0
All	All	576/610 (94%)	1.07	92 (15%) 5 5	17, 35, 66, 89	2 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	45	ILE	5.8
1	A	353	TRP	5.5
2	D	45	ILE	5.4
2	D	47	TYR	5.2
1	B	353	TRP	4.6
1	A	352	ALA	4.2
2	C	47	TYR	4.0
1	B	136	ALA	3.7
1	B	350	PRO	3.7
1	A	244	LEU	3.6
1	A	394	LEU	3.5
1	A	350	PRO	3.4
1	B	391	THR	3.4
1	B	137	CYS	3.3
2	C	44	GLY	3.3
2	C	46	SER	3.1
2	D	57	ARG	3.1
1	A	172	ASP	3.1
1	B	355	PRO	3.1
1	B	123	LEU	3.0
1	A	347	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	139	ARG	2.9
2	C	55	ARG	2.9
1	B	360	VAL	2.9
1	B	351	LEU	2.9
2	D	53	ARG	2.8
1	A	137	CYS	2.8
1	B	131	LEU	2.8
1	A	392	GLY	2.8
1	B	316	LEU	2.8
2	D	46	SER	2.8
1	B	129	ALA	2.8
1	A	348	VAL	2.7
1	B	167	ASN	2.7
1	A	173	LEU	2.7
1	A	351	LEU	2.7
1	B	135	ARG	2.6
2	D	56	ARG	2.6
1	A	391	THR	2.6
1	A	201	PRO	2.6
2	C	56	ARG	2.6
2	D	44	GLY	2.6
2	D	48	GLY	2.6
1	B	270	ALA	2.6
1	B	357	SER	2.6
1	B	240	PRO	2.5
2	C	49	ARG	2.5
1	B	169	GLN	2.5
1	B	347	LEU	2.5
1	A	379	TRP	2.5
1	B	379	TRP	2.5
1	B	348	VAL	2.5
1	A	163	GLY	2.4
1	A	349	GLY	2.4
1	B	378	GLY	2.4
1	B	165	TYR	2.4
1	B	157	PHE	2.4
2	D	55	ARG	2.4
1	A	157	PHE	2.4
1	B	309	PHE	2.4
1	A	395	ASP	2.4
1	A	134	ALA	2.4
1	A	393	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	394	LEU	2.3
1	A	355	PRO	2.3
1	B	161	GLY	2.3
2	C	57	ARG	2.3
1	B	376	LEU	2.3
1	B	310	PRO	2.3
1	B	334	VAL	2.3
1	A	330	LEU	2.3
1	B	352	ALA	2.2
1	B	138	GLN	2.2
1	A	160	PRO	2.2
2	D	54	GLN	2.2
1	B	312	ALA	2.2
1	B	128	VAL	2.2
1	B	126	GLN	2.2
1	B	141	VAL	2.2
1	B	121	GLY	2.2
1	B	330	LEU	2.2
1	A	297	PRO	2.2
1	B	132	ILE	2.1
1	B	383	MET	2.1
1	B	133	ARG	2.1
1	B	307	VAL	2.1
1	B	338	VAL	2.1
1	B	374	VAL	2.1
1	B	219	LYS	2.1
1	B	127	ASP	2.0
1	B	306	VAL	2.0
1	B	358	ARG	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	ZN	A	401	1/1	0.99	0.02	26,26,26,26	0
3	ZN	B	401	1/1	0.99	0.02	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.