



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:48 am GMT

PDB ID : 4ZZI
Title : SIRT1/Activator/Inhibitor Complex
Authors : Dai, H.
Deposited on : 2015-05-22
Resolution : 2.73 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

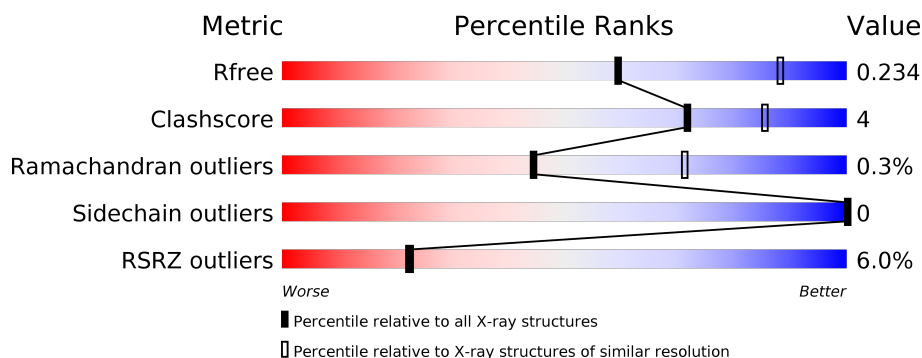
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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}	100719	3342 (2.78-2.70)
Clashscore	112137	3731 (2.78-2.70)
Ramachandran outliers	110173	3670 (2.78-2.70)
Sidechain outliers	110143	3671 (2.78-2.70)
RSRZ outliers	101464	3362 (2.78-2.70)

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	356	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2767 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-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	2679	1729	453	479	18	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

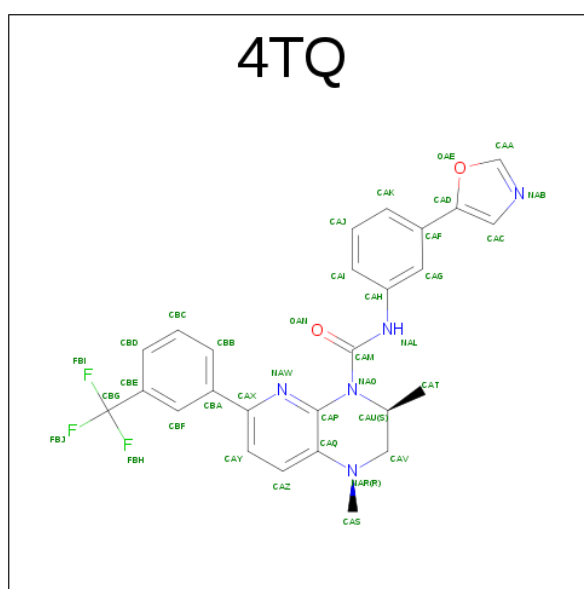
Chain	Residue	Modelled	Actual	Comment	Reference
A	633	GLY	-	expression tag	UNP Q96EB6
A	634	GLY	-	expression tag	UNP Q96EB6
A	635	GLY	-	expression tag	UNP Q96EB6
A	636	SER	-	expression tag	UNP Q96EB6
A	637	GLY	-	expression tag	UNP Q96EB6
A	638	GLY	-	expression tag	UNP Q96EB6
A	639	GLY	-	expression tag	UNP Q96EB6
A	640	SER	-	expression tag	UNP Q96EB6
A	641	GLN	-	expression tag	UNP Q96EB6
A	642	TYR	-	expression tag	UNP Q96EB6
A	643	LEU	-	expression tag	UNP Q96EB6
A	644	PHE	-	expression tag	UNP Q96EB6
A	645	LEU	-	expression tag	UNP Q96EB6
A	646	PRO	-	expression tag	UNP Q96EB6
A	647	PRO	-	expression tag	UNP Q96EB6
A	648	ASN	-	expression tag	UNP Q96EB6
A	649	ARG	-	expression tag	UNP Q96EB6
A	650	TYR	-	expression tag	UNP Q96EB6
A	651	ILE	-	expression tag	UNP Q96EB6
A	652	PHE	-	expression tag	UNP Q96EB6
A	653	HIS	-	expression tag	UNP Q96EB6
A	654	GLY	-	expression tag	UNP Q96EB6
A	655	ALA	-	expression tag	UNP Q96EB6
A	656	GLU	-	expression tag	UNP Q96EB6
A	657	VAL	-	expression tag	UNP Q96EB6
A	658	TYR	-	expression tag	UNP Q96EB6
A	659	SER	-	expression tag	UNP Q96EB6

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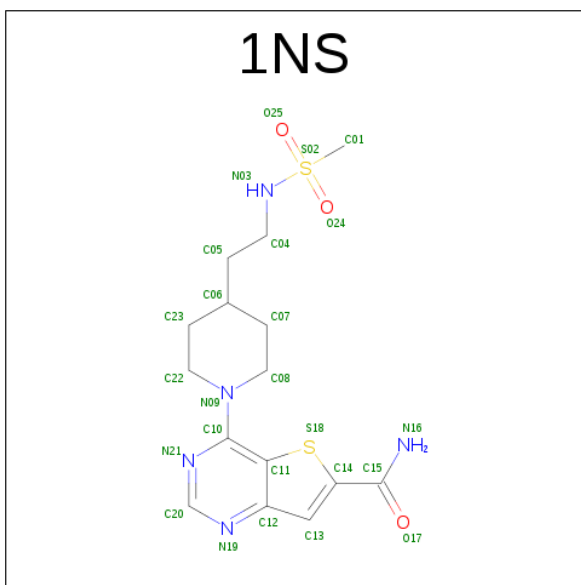
Chain	Residue	Modelled	Actual	Comment	Reference
A	660	ASP	-	expression tag	UNP Q96EB6
A	661	SER	-	expression tag	UNP Q96EB6
A	662	GLU	-	expression tag	UNP Q96EB6
A	663	ASP	-	expression tag	UNP Q96EB6
A	664	ASP	-	expression tag	UNP Q96EB6
A	665	VAL	-	expression tag	UNP Q96EB6

- Molecule 2 is (3S)-1,3-dimethyl-N-[3-(1,3-oxazol-5-yl)phenyl]-6-[3-(trifluoromethyl)phenyl]-2,3-dihydropyrido[2,3-b]pyrazine-4(1H)-carboxamide (three-letter code: 4TQ) (formula: C₂₆H₂₂F₃N₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			36	26	3	5	2		

- Molecule 3 is 4-(4-{2-[(methylsulfonyl)amino]ethyl}piperidin-1-yl)thieno[3,2-d]pyrimidine-6-carboxamide (three-letter code: 1NS) (formula: C₁₅H₂₁N₅O₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			25	15	5	3	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

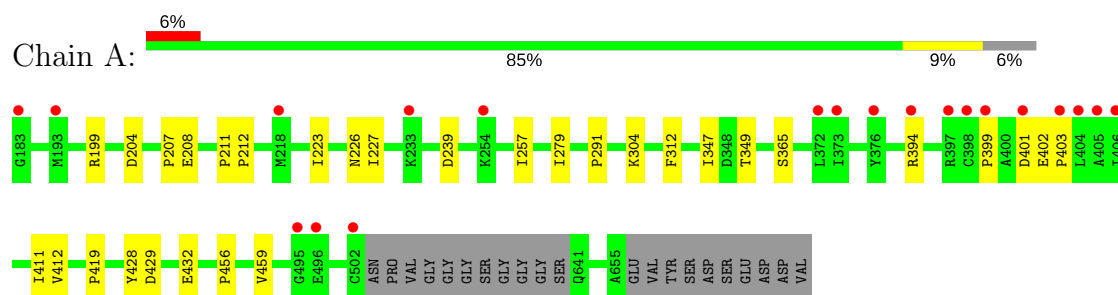
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		

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 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-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.15Å 122.15Å 104.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.98 – 2.73 39.98 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.98-2.73) 99.9 (39.98-2.73)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.191 , 0.235 0.198 , 0.234	Depositor DCC
R_{free} test set	636 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 73.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2767	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: ZN, 4TQ, 1NS

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	0.24	0/2746	0.43	0/3726

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

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	2679	0	2708	19	0
2	A	36	0	18	3	0
3	A	25	0	21	2	0
4	A	1	0	0	0	0
5	A	26	0	0	0	0
All	All	2767	0	2747	22	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 (22) 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:401:ASP:OD1	1:A:402:GLU:N	2.26	0.67
1:A:412:VAL:HG21	1:A:419:PRO:HD3	1.81	0.61
1:A:394:ARG:NH2	1:A:403:PRO:O	2.36	0.59
1:A:207:PRO:O	1:A:208:GLU:HG2	2.06	0.56
2:A:701:4TQ:NAL	2:A:701:4TQ:NAW	2.41	0.54
1:A:279:ILE:HG21	1:A:312:PHE:CE1	2.44	0.53
2:A:701:4TQ:OAN	2:A:701:4TQ:H17	2.10	0.52
1:A:239:ASP:N	1:A:239:ASP:OD1	2.42	0.51
1:A:347:ILE:HD12	1:A:411:ILE:HD13	1.93	0.51
1:A:399:PRO:HB2	1:A:401:ASP:OD1	2.10	0.51
1:A:349:THR:HG22	1:A:365:SER:HB2	1.93	0.50
1:A:204:ASP:O	1:A:207:PRO:HD3	2.13	0.48
1:A:257:ILE:HD11	1:A:429:ASP:HB3	1.96	0.48
1:A:456:PRO:HB2	1:A:459:VAL:HG23	1.96	0.47
3:A:702:1NS:S18	3:A:702:1NS:H12	2.57	0.44
1:A:226:ASN:HB3	2:A:701:4TQ:H22	2.00	0.44
1:A:428:TYR:CZ	1:A:432:GLU:HG3	2.54	0.42
1:A:412:VAL:O	3:A:702:1NS:N03	2.52	0.42
1:A:199:ARG:NH1	1:A:211:PRO:HG2	2.34	0.42
1:A:223:ILE:O	1:A:227:ILE:HG13	2.20	0.41
1:A:304:LYS:HB3	1:A:304:LYS:HE2	1.82	0.41
1:A:211:PRO:HA	1:A:212:PRO:HD3	1.90	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	331/356 (93%)	317 (96%)	13 (4%)	1 (0%)	44 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	PRO

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	301/316 (95%)	301 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 3 ligands modelled in this entry, 1 is 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
2	4TQ	A	701	-	37,40,40	2.12	7 (18%)	48,59,59	2.98	7 (14%)
3	1NS	A	702	-	22,27,27	2.59	8 (36%)	29,39,39	3.89	14 (48%)

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	4TQ	A	701	-	-	0/20/38/38	0/3/5/5
3	1NS	A	702	-	-	0/11/25/25	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	4TQ	CAF-CAD	-7.28	1.33	1.46
2	A	701	4TQ	CBA-CAX	-6.11	1.39	1.48
2	A	701	4TQ	CBG-CBE	-4.23	1.40	1.49
2	A	701	4TQ	CAM-NAO	-3.78	1.34	1.43
2	A	701	4TQ	CAH-NAL	-3.50	1.34	1.41
2	A	701	4TQ	CAQ-NAR	-3.17	1.31	1.38
2	A	701	4TQ	CAC-CAD	-2.78	1.33	1.37
3	A	702	1NS	O24-S02	-2.50	1.38	1.43
3	A	702	1NS	C07-C06	-2.00	1.46	1.52
3	A	702	1NS	C20-N21	2.35	1.38	1.33
3	A	702	1NS	C13-C12	2.81	1.54	1.42
3	A	702	1NS	C10-N09	3.73	1.48	1.36
3	A	702	1NS	O25-S02	5.28	1.53	1.43
3	A	702	1NS	S02-N03	5.37	1.68	1.61
3	A	702	1NS	C15-N16	6.41	1.45	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	4TQ	CAU-CAV-NAR	-17.32	89.42	110.87
3	A	702	1NS	O24-S02-O25	-11.91	100.75	118.78
3	A	702	1NS	N19-C20-N21	-8.55	121.41	128.86
3	A	702	1NS	C12-C11-S18	-3.66	107.49	112.00
3	A	702	1NS	C04-N03-S02	-3.25	110.09	120.78
3	A	702	1NS	C22-N09-C10	-3.17	109.48	118.81
2	A	701	4TQ	CAT-CAU-CAV	-2.27	99.90	110.68
3	A	702	1NS	O24-S02-C01	2.11	111.96	108.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	4TQ	CAC-NAB-CAA	2.39	109.50	105.78
3	A	702	1NS	C05-C04-N03	2.54	116.76	111.01
2	A	701	4TQ	CAZ-CAQ-NAR	2.91	125.33	121.94
2	A	701	4TQ	CBA-CAX-NAW	3.50	120.88	116.02
3	A	702	1NS	C01-S02-N03	3.64	110.36	107.79
3	A	702	1NS	C20-N21-C10	3.70	120.89	111.82
3	A	702	1NS	O25-S02-N03	3.78	111.23	107.17
3	A	702	1NS	O24-S02-N03	3.86	111.31	107.17
2	A	701	4TQ	NAW-CAP-NAO	5.05	123.92	117.49
3	A	702	1NS	C14-C15-N16	5.58	121.81	116.23
2	A	701	4TQ	CAS-NAR-CAQ	5.78	129.55	119.15
3	A	702	1NS	C08-N09-C10	5.78	135.79	118.81
3	A	702	1NS	C20-N19-C12	6.33	121.90	115.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	4TQ	3	0
3	A	702	1NS	2	0

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	335/356 (94%)	0.51	20 (5%)	23 22	53, 85, 148, 190	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	ILE	9.3
1	A	404	LEU	7.1
1	A	183	GLY	6.5
1	A	406	ILE	6.0
1	A	403	PRO	5.2
1	A	397	ARG	5.0
1	A	405	ALA	4.3
1	A	399	PRO	3.7
1	A	372	LEU	3.7
1	A	502	CYS	3.6
1	A	394	ARG	3.5
1	A	233	LYS	3.2
1	A	193	MET	2.7
1	A	398	CYS	2.6
1	A	401	ASP	2.4
1	A	218	MET	2.4
1	A	254	LYS	2.2
1	A	496	GLU	2.2
1	A	376	TYR	2.2
1	A	495	GLY	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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	1NS	A	702	25/25	0.98	0.21	0.62	50,63,85,103	0
2	4TQ	A	701	36/36	0.98	0.20	0.05	50,59,68,71	0
4	ZN	A	703	1/1	0.94	0.06	-1.42	159,159,159,159	0

6.5 Other polymers [i](#)

There are no such residues in this entry.