



Full wwPDB X-ray Structure Validation Report ⓘ

May 10, 2021 – 10:01 am BST

PDB ID : 7NDK
Title : Crystal structure of ZC3H12C PIN catalytic mutant
Authors : Garg, A.; Heinemann, U.
Deposited on : 2021-02-01
Resolution : 2.34 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
Xtriage (Phenix) : 1.13
EDS : 2.18
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) : 2.18

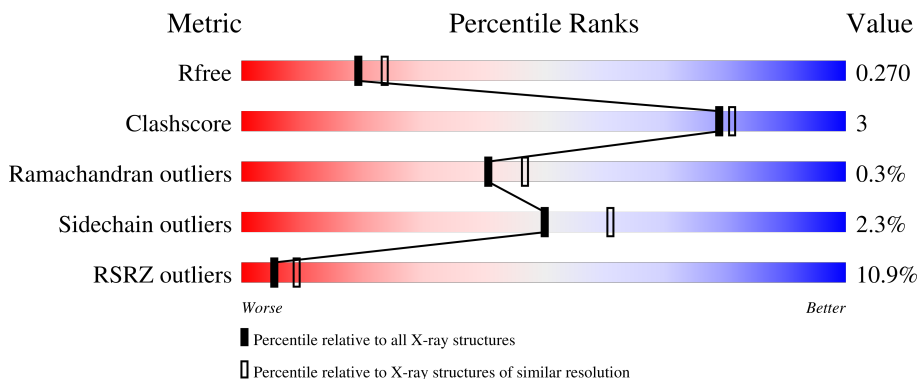
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	164	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5% 86% 9% 5%</p>
1	B	164	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 88% 5% 7%</p>
1	C	164	<div style="display: flex; align-items: center;"> <div style="width: 16%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">16% 85% 10% 5%</p>
1	D	164	<div style="display: flex; align-items: center;"> <div style="width: 16%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">16% 84% 13% .</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5226 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 Probable ribonuclease ZC3H12C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	155	1278	818	226	229	5	0	0	0
1	B	153	1268	812	225	226	5	0	0	0
1	C	156	1284	822	229	228	5	0	0	0
1	D	159	1300	832	229	234	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	ASN	ASP	conflict	UNP Q5DTV4
B	271	ASN	ASP	conflict	UNP Q5DTV4
C	271	ASN	ASP	conflict	UNP Q5DTV4
D	271	ASN	ASP	conflict	UNP Q5DTV4

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	30	Total	O	0	0
			30	30		

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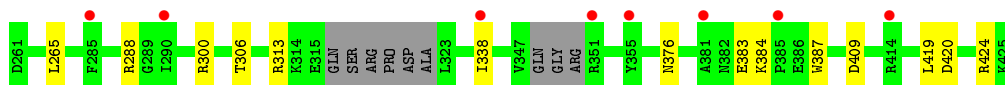
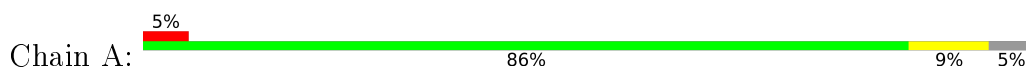
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	21	Total O 21 21	0	0
3	D	19	Total O 19 19	0	0

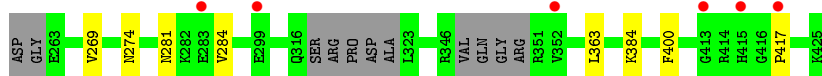
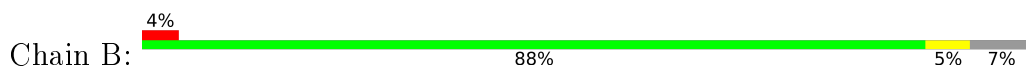
3 Residue-property plots [i](#)

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.

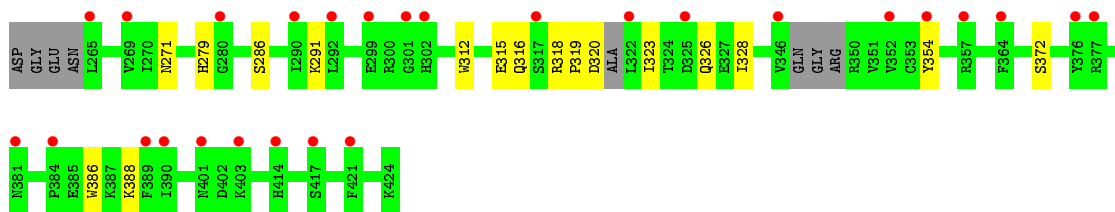
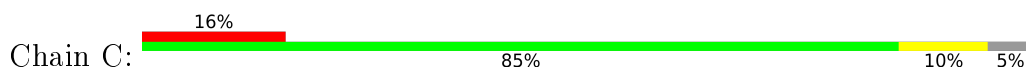
- Molecule 1: Probable ribonuclease ZC3H12C



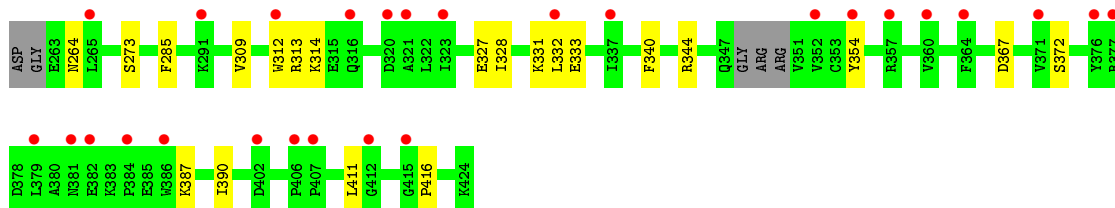
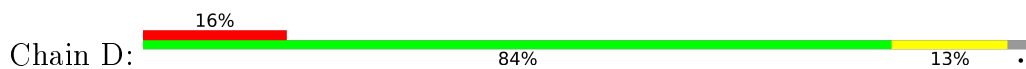
- Molecule 1: Probable ribonuclease ZC3H12C



- Molecule 1: Probable ribonuclease ZC3H12C



- Molecule 1: Probable ribonuclease ZC3H12C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.75Å 61.48Å 111.62Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	38.75 – 2.34 38.75 – 2.34	Depositor EDS
% Data completeness (in resolution range)	96.9 (38.75-2.34) 96.9 (38.75-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.229 , 0.275 0.226 , 0.270	Depositor DCC
R_{free} test set	1087 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
Reported twinning fraction	0.521 for H, K, L 0.479 for -h,-k,l	Depositor
Outliers	2 of 21739 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5226	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.48% 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: NA

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	0/1305	0.63	0/1756
1	B	0.43	0/1295	0.68	0/1742
1	C	0.41	0/1312	0.68	0/1766
1	D	0.43	0/1329	0.66	0/1793
All	All	0.42	0/5241	0.66	0/7057

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	1278	0	1280	9	0
1	B	1268	0	1272	6	0
1	C	1284	0	1285	8	0
1	D	1300	0	1296	7	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	0	0	2	0
3	B	30	0	0	2	0
3	C	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	19	0	0	1	0
All	All	5226	0	5133	29	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 3.

All (29) 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:288:ARG:NH2	3:A:501:HOH:O	2.27	0.67
1:D:344:ARG:NH2	3:D:601:HOH:O	2.27	0.66
1:B:274:ASN:ND2	3:B:601:HOH:O	2.33	0.60
1:D:309:VAL:O	1:D:340:PHE:HA	2.05	0.57
1:C:291:LYS:HG3	1:C:328:ILE:HG12	1.92	0.52
1:D:328:ILE:HG22	1:D:332:LEU:HD12	1.92	0.52
1:C:291:LYS:CG	1:C:328:ILE:HG12	2.41	0.51
1:C:320:ASP:OD2	1:C:320:ASP:N	2.44	0.51
1:C:323:ILE:HG12	1:C:326:GLN:NE2	2.26	0.51
1:A:265:LEU:HD23	1:A:424:ARG:HG2	1.94	0.49
1:C:271:ASN:HD22	1:C:372:SER:HG	1.61	0.49
1:B:269:VAL:HG23	3:B:620:HOH:O	2.13	0.49
1:A:384:LYS:HD2	1:A:387:TRP:CD2	2.49	0.47
1:A:306:THR:HA	1:A:338:ILE:O	2.15	0.47
1:A:383:GLU:HA	1:B:417:PRO:HB3	1.97	0.47
1:B:281:ASN:HB2	1:B:284:VAL:HG22	1.96	0.47
1:D:411:LEU:HD23	1:D:416:PRO:HD2	1.98	0.46
1:A:376:ASN:N	3:A:505:HOH:O	2.47	0.45
1:B:269:VAL:HG22	1:B:363:LEU:HD22	1.99	0.45
1:A:300:ARG:NH2	1:A:420:ASP:OD1	2.50	0.45
1:D:387:LYS:HA	1:D:390:ILE:HB	2.00	0.44
1:B:281:ASN:CB	1:B:284:VAL:HG22	2.49	0.43
1:D:273:SER:HA	1:D:285:PHE:CE2	2.54	0.42
1:D:331:LYS:O	1:D:333:GLU:N	2.51	0.42
1:C:318:ARG:N	1:C:319:PRO:HD2	2.35	0.41
1:C:312:TRP:HA	1:C:315:GLU:HB3	2.02	0.41
1:A:409:ASP:HA	1:A:419:LEU:HB2	2.03	0.41
1:A:384:LYS:HD2	1:A:387:TRP:CE2	2.56	0.40
1:C:279:HIS:CE1	1:C:286:SER:HG	2.39	0.40

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	149/164 (91%)	137 (92%)	12 (8%)	0	100	100
1	B	147/164 (90%)	138 (94%)	9 (6%)	0	100	100
1	C	150/164 (92%)	135 (90%)	15 (10%)	0	100	100
1	D	155/164 (94%)	140 (90%)	13 (8%)	2 (1%)	12	9
All	All	601/656 (92%)	550 (92%)	49 (8%)	2 (0%)	41	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	327	GLU
1	D	354	TYR

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	142/149 (95%)	141 (99%)	1 (1%)	84	90
1	B	141/149 (95%)	139 (99%)	2 (1%)	67	78
1	C	142/149 (95%)	138 (97%)	4 (3%)	43	53
1	D	144/149 (97%)	138 (96%)	6 (4%)	30	37
All	All	569/596 (96%)	556 (98%)	13 (2%)	50	61

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	313	ARG
1	B	384	LYS
1	B	400	PHE
1	C	316	GLN
1	C	354	TYR
1	C	386	TRP
1	C	388	LYS
1	D	264	ASN
1	D	312	TRP
1	D	313	ARG
1	D	314	LYS
1	D	367	ASP
1	D	372	SER

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

Mol	Chain	Res	Type
1	C	271	ASN
1	D	326	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 monosaccharides 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 [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

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	155/164 (94%)	0.37	8 (5%) 27 38	37, 59, 72, 85	0
1	B	153/164 (93%)	0.38	6 (3%) 39 50	32, 57, 74, 93	0
1	C	156/164 (95%)	1.09	27 (17%) 1 2	42, 68, 89, 97	0
1	D	159/164 (96%)	0.96	27 (16%) 1 2	34, 66, 96, 125	0
All	All	623/656 (94%)	0.70	68 (10%) 5 9	32, 62, 86, 125	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	384	PRO	7.6
1	C	390	ILE	6.5
1	C	346	VAL	5.8
1	D	381	ASN	5.7
1	D	320	ASP	5.2
1	D	360	VAL	5.1
1	D	379	LEU	5.0
1	D	332	LEU	4.6
1	A	414	ARG	4.4
1	C	265	LEU	4.1
1	C	381	ASN	4.0
1	C	301	GLY	3.9
1	D	291	LYS	3.8
1	D	412	GLY	3.7
1	D	323	ILE	3.7
1	D	321	ALA	3.5
1	B	415	HIS	3.5
1	C	322	LEU	3.5
1	C	292	LEU	3.5
1	C	403	LYS	3.4
1	A	351	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	364	PHE	3.3
1	C	384	PRO	3.3
1	B	413	GLY	3.2
1	B	417	PRO	3.2
1	D	386	TRP	3.1
1	C	401	ASN	3.0
1	A	381	ALA	2.9
1	D	316	GLN	2.8
1	B	352	VAL	2.8
1	D	354	TYR	2.8
1	D	377	ARG	2.8
1	D	376	TYR	2.8
1	D	265	LEU	2.8
1	D	407	PRO	2.8
1	D	382	GLU	2.8
1	C	269	VAL	2.7
1	D	402	ASP	2.7
1	C	352	VAL	2.7
1	A	338	ILE	2.6
1	D	357	ARG	2.6
1	B	299	GLU	2.6
1	C	354	TYR	2.6
1	C	325	ASP	2.5
1	A	285	PHE	2.5
1	A	355	TYR	2.5
1	D	364	PHE	2.5
1	A	385	PRO	2.5
1	C	280	GLY	2.5
1	B	283	GLU	2.4
1	D	415	GLY	2.4
1	C	302	HIS	2.3
1	C	290	ILE	2.3
1	D	406	PRO	2.3
1	C	377	ARG	2.3
1	C	421	PHE	2.2
1	D	312	TRP	2.2
1	C	414	HIS	2.2
1	D	337	ILE	2.2
1	C	376	TYR	2.2
1	A	290	ILE	2.1
1	D	371	VAL	2.1
1	D	352	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	299	GLU	2.1
1	C	389	PHE	2.1
1	C	417	SER	2.1
1	C	357	ARG	2.1
1	C	317	SER	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
2	NA	B	501	1/1	0.93	0.17	43,43,43,43	0
2	NA	D	501	1/1	0.94	0.20	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.