



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:14 pm BST

PDB ID : 3NET
Title : Crystal structure of histidyl-tRNA synthetase from Nostoc sp. PCC 7120
Authors : Chang, C.; Bigelow, L.; Carroll, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2010-06-09
Resolution : 2.70 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

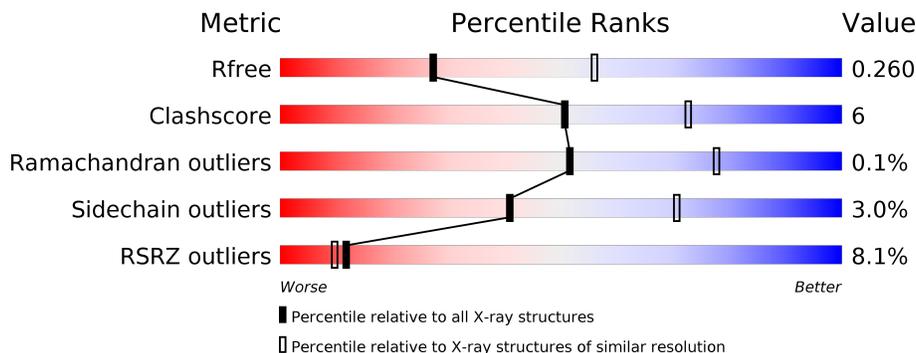
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	465	 7% (red), 76% (green), 16% (yellow), 7% (grey)
1	B	465	 8% (red), 78% (green), 11% (yellow), 11% (grey)

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6572 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.

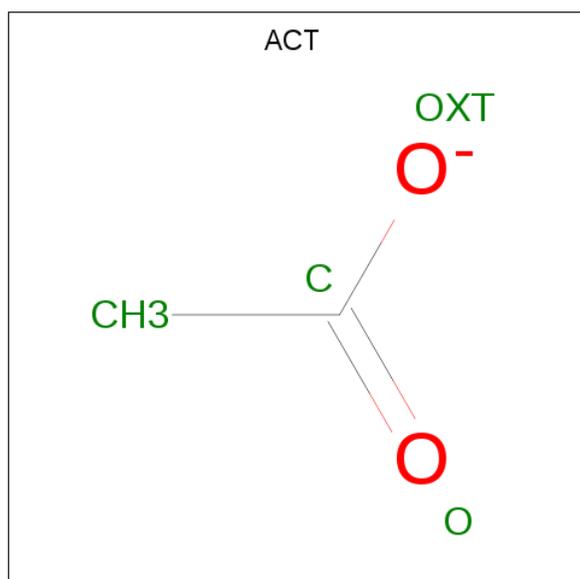
- Molecule 1 is a protein called Histidyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
1	A	431	3276	2091	558	617	5	5	0	0	0
1	B	415	3181	2032	540	599	5	5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8YMC2
A	-1	ASN	-	expression tag	UNP Q8YMC2
A	0	ALA	-	expression tag	UNP Q8YMC2
B	-2	SER	-	expression tag	UNP Q8YMC2
B	-1	ASN	-	expression tag	UNP Q8YMC2
B	0	ALA	-	expression tag	UNP Q8YMC2

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

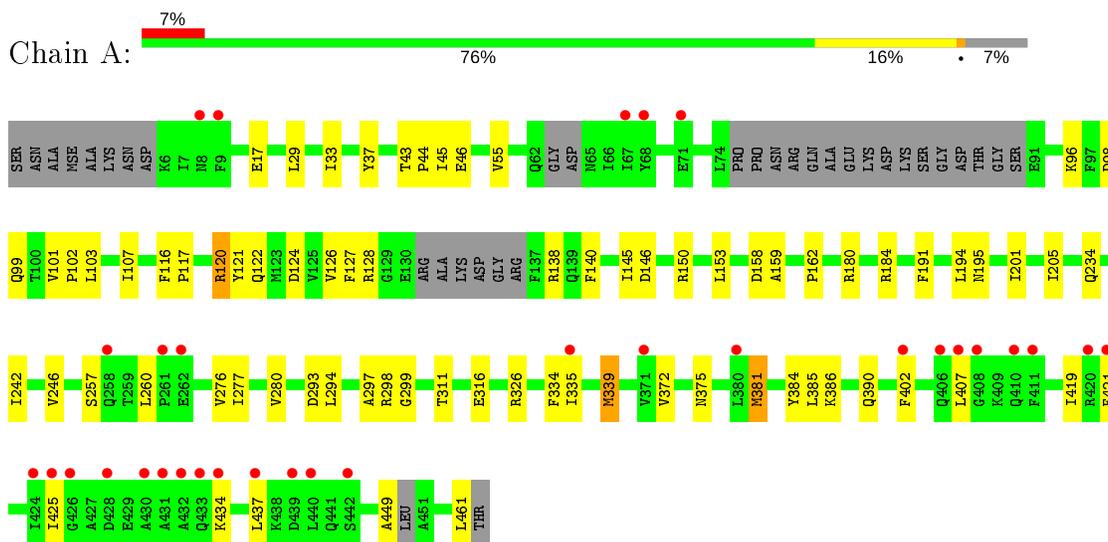
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total	O	0	0
			73	73		
3	B	38	Total	O	0	0
			38	38		

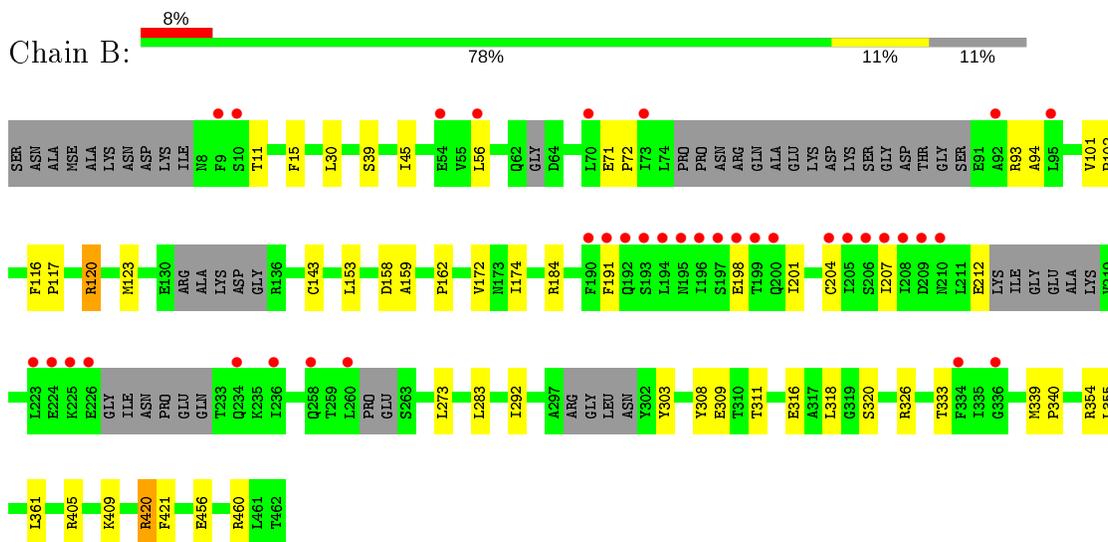
3 Residue-property plots [i](#)

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: Histidyl-tRNA synthetase



- Molecule 1: Histidyl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	73.66Å 73.66Å 521.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.89 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.1 (50.00-2.70) 93.1 (49.89-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.217 , 0.265 0.215 , 0.260	Depositor DCC
R_{free} test set	1925 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtrriage
Anisotropy	0.389	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6572	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: ACT

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	0.49	0/3318	0.60	0/4483
1	B	0.45	0/3218	0.58	0/4343
All	All	0.47	0/6536	0.59	0/8826

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	3276	0	3249	43	0
1	B	3181	0	3162	32	0
2	A	4	0	3	0	0
3	A	73	0	0	2	0
3	B	38	0	0	1	0
All	All	6572	0	6414	73	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 6.

All (73) 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:107:ILE:HG21	1:A:339:MSE:HE1	1.35	1.04
1:A:180:ARG:HD2	3:A:532:HOH:O	1.58	1.02
1:A:45:ILE:HG12	1:A:120:ARG:HG3	1.56	0.87
1:B:309:GLU:HG2	1:B:320:SER:HB2	1.69	0.74
1:A:191:PHE:HB3	1:A:201:ILE:HG12	1.72	0.69
1:B:11:THR:HG21	1:B:15:PHE:O	1.93	0.69
1:A:29:LEU:O	1:A:33:ILE:HG12	1.96	0.66
1:A:107:ILE:HG21	1:A:339:MSE:CE	2.22	0.64
1:A:128:ARG:HD2	1:A:140:PHE:HZ	1.62	0.64
1:B:45:ILE:HG12	1:B:120:ARG:HD3	1.80	0.62
1:A:120:ARG:NH2	1:A:146:ASP:OD1	2.33	0.62
1:B:405:ARG:HH21	1:B:409:LYS:HD3	1.65	0.62
1:A:421:PHE:HE1	1:A:461:LEU:HD13	1.65	0.60
1:A:372:VAL:HG23	1:A:419:ILE:HG21	1.84	0.59
1:A:120:ARG:HG2	1:A:121:TYR:N	2.18	0.58
1:B:101:VAL:HB	1:B:102:PRO:HD3	1.86	0.58
1:A:44:PRO:HB3	1:A:121:TYR:CZ	2.39	0.57
1:B:198:GLU:HA	1:B:201:ILE:HG22	1.88	0.55
1:A:103:LEU:HD13	1:A:120:ARG:HD3	1.90	0.54
1:A:138:ARG:NH1	1:B:93:ARG:HH12	2.05	0.54
1:A:46:GLU:HG3	1:A:124:ASP:OD1	2.09	0.53
1:B:123:MSE:HG2	1:B:143:CYS:SG	2.49	0.52
1:A:116:PHE:HA	1:A:117:PRO:C	2.30	0.52
1:A:335:ILE:HG13	1:A:339:MSE:HE2	1.92	0.52
1:A:434:LYS:HA	1:A:449:ALA:HA	1.91	0.51
1:B:30:LEU:CD2	1:B:123:MSE:HE2	2.41	0.51
1:A:184:ARG:NH1	1:A:299:GLY:O	2.42	0.51
1:A:276:VAL:O	1:A:280:VAL:HG23	2.11	0.50
1:A:375:ASN:ND2	1:A:402:PHE:O	2.41	0.49
1:B:273:LEU:HD21	1:B:292:ILE:CD1	2.42	0.49
1:B:311:THR:HG21	1:B:316:GLU:HG3	1.93	0.49
1:B:153:LEU:O	1:B:326:ARG:NH2	2.39	0.49
1:B:191:PHE:HB3	1:B:201:ILE:HD11	1.95	0.49
1:B:56:LEU:HD12	1:B:94:ALA:HB3	1.95	0.49
1:B:420:ARG:HD3	1:B:421:PHE:CE1	2.49	0.48
1:A:381:MSE:HE2	1:A:384:TYR:HD2	1.79	0.48
1:B:355:LEU:HD13	1:B:361:LEU:HD22	1.96	0.48
1:A:45:ILE:HG12	1:A:120:ARG:CG	2.37	0.47
1:B:184:ARG:HG2	1:B:303:TYR:O	2.15	0.47
1:A:246:VAL:HG11	1:A:277:ILE:HG21	1.97	0.46
1:B:116:PHE:HA	1:B:117:PRO:C	2.33	0.46
1:A:101:VAL:HB	1:A:102:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:O	1:A:195:ASN:HB2	2.16	0.46
1:B:30:LEU:HD23	1:B:123:MSE:HE2	1.97	0.46
1:B:172:VAL:HG12	1:B:174:ILE:HG23	1.98	0.45
1:A:384:TYR:HE1	1:A:425:ILE:HB	1.82	0.45
1:B:456:GLU:OE1	1:B:460:ARG:NH1	2.50	0.45
1:A:55:VAL:HA	1:A:334:PHE:HZ	1.81	0.44
1:A:242:ILE:HB	1:A:294:LEU:HD12	2.00	0.44
1:B:71:GLU:HA	1:B:72:PRO:HD3	1.88	0.44
1:A:121:TYR:HB3	1:A:145:ILE:HG22	1.99	0.44
1:B:204:CYS:HA	1:B:207:ILE:HG12	1.99	0.43
1:B:309:GLU:HG2	1:B:320:SER:CB	2.43	0.43
1:B:326:ARG:HD3	3:B:483:HOH:O	2.16	0.43
1:B:318:LEU:O	1:B:354:ARG:NH2	2.52	0.42
1:B:303:TYR:HA	1:B:326:ARG:O	2.20	0.42
1:B:339:MSE:HA	1:B:340:PRO:HD3	1.93	0.42
1:A:311:THR:CG2	1:A:316:GLU:HG3	2.49	0.42
1:A:99:GLN:OE1	1:A:122:GLN:HG2	2.19	0.42
1:A:159:ALA:O	1:A:162:PRO:HD2	2.20	0.41
1:A:205:ILE:HG23	1:A:297:ALA:HB1	2.02	0.41
1:A:386:LYS:HE2	1:A:390:GLN:NE2	2.35	0.41
1:A:128:ARG:O	1:A:138:ARG:HA	2.21	0.41
1:A:96:LYS:HD3	1:A:126:VAL:HG12	2.03	0.41
1:A:153:LEU:HB3	1:A:326:ARG:NH2	2.36	0.41
1:A:326:ARG:HD3	3:A:516:HOH:O	2.21	0.41
1:B:159:ALA:O	1:B:162:PRO:HD2	2.20	0.41
1:B:273:LEU:HD21	1:B:292:ILE:HD13	2.03	0.40
1:A:180:ARG:HD3	1:A:293:ASP:OD2	2.21	0.40
1:B:355:LEU:HB3	1:B:361:LEU:HB2	2.03	0.40
1:A:127:PHE:HA	1:A:138:ARG:O	2.21	0.40
1:A:33:ILE:HG22	1:A:37:TYR:CE2	2.57	0.40
1:A:385:LEU:HD22	1:B:283:LEU:HD21	2.04	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	421/465 (90%)	399 (95%)	21 (5%)	1 (0%)	47	73
1	B	399/465 (86%)	380 (95%)	19 (5%)	0	100	100
All	All	820/930 (88%)	779 (95%)	40 (5%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	ARG

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	341/393 (87%)	328 (96%)	13 (4%)	33	62
1	B	334/393 (85%)	327 (98%)	7 (2%)	53	80
All	All	675/786 (86%)	655 (97%)	20 (3%)	41	70

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	43	THR
1	A	98	ASP
1	A	120	ARG
1	A	150	ARG
1	A	158	ASP
1	A	234	GLN
1	A	257	SER
1	A	260	LEU
1	A	339	MSE
1	A	381	MSE
1	A	407	LEU

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Mol	Chain	Res	Type
1	A	437	LEU
1	B	39	SER
1	B	120	ARG
1	B	158	ASP
1	B	212	GLU
1	B	308	TYR
1	B	333	THR
1	B	420	ARG

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](#)

1 ligand is modelled in this entry.

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	ACT	A	501	-	1,3,3	1.39	0	0,3,3	0.00	-

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	426/465 (91%)	0.33	32 (7%) 14 12	35, 56, 123, 152	0
1	B	410/465 (88%)	0.37	36 (8%) 10 8	37, 74, 159, 189	0
All	All	836/930 (89%)	0.35	68 (8%) 12 10	35, 67, 137, 189	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	LYS	7.9
1	A	425	ILE	7.0
1	B	196	ILE	6.6
1	B	207	ILE	6.0
1	A	432	ALA	5.9
1	B	209	ASP	5.8
1	B	224	GLU	5.2
1	A	431	ALA	5.1
1	A	440	LEU	4.7
1	A	434	LYS	4.7
1	A	439	ASP	4.6
1	B	194	LEU	4.5
1	B	226	GLU	4.3
1	B	197	SER	4.3
1	B	70	LEU	4.3
1	A	407	LEU	4.2
1	B	236	ILE	4.1
1	B	192	GLN	4.0
1	A	426	GLY	4.0
1	A	408	GLY	4.0
1	B	199	THR	4.0
1	B	193	SER	3.8
1	B	204	CYS	3.8
1	B	190	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	191	PHE	3.7
1	A	433	GLN	3.6
1	B	210	ASN	3.5
1	A	68	TYR	3.4
1	B	334	PHE	3.4
1	B	73	ILE	3.3
1	A	261	PRO	3.2
1	A	402	PHE	3.2
1	A	421	PHE	3.1
1	B	9	PHE	3.0
1	B	54	GLU	3.0
1	B	208	ILE	3.0
1	A	420	ARG	3.0
1	B	206	SER	3.0
1	A	406	GLN	2.8
1	A	410	GLN	2.8
1	A	437	LEU	2.8
1	B	56	LEU	2.8
1	A	430	ALA	2.8
1	B	200	GLN	2.7
1	A	335	ILE	2.7
1	B	234	GLN	2.7
1	B	336	GLY	2.5
1	A	371	VAL	2.5
1	B	223	LEU	2.5
1	B	10	SER	2.5
1	B	92	ALA	2.4
1	A	71	GLU	2.4
1	A	380	LEU	2.3
1	A	428	ASP	2.3
1	B	260	LEU	2.3
1	A	9	PHE	2.3
1	A	67	ILE	2.3
1	A	8	ASN	2.2
1	B	95	LEU	2.2
1	B	198	GLU	2.2
1	A	442	SER	2.1
1	B	258	GLN	2.1
1	A	411	PHE	2.1
1	A	424	ILE	2.1
1	B	205	ILE	2.1
1	B	195	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	262	GLU	2.0
1	A	258	GLN	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 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. 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	ACT	A	501	4/4	0.86	0.22	110,110,111,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.