



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:19 PM UTC

PDB ID : 3NET / pdb_00003net
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 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

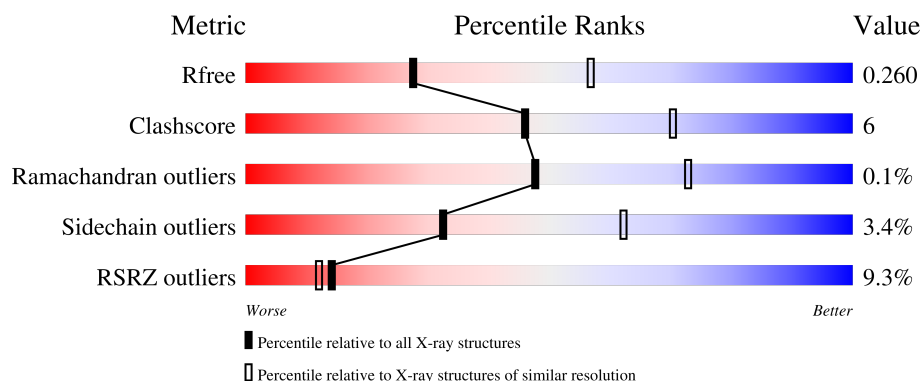
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	465	7% 75% 16% • 7%
1	B	465	10% 77% 11% • 11%

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.

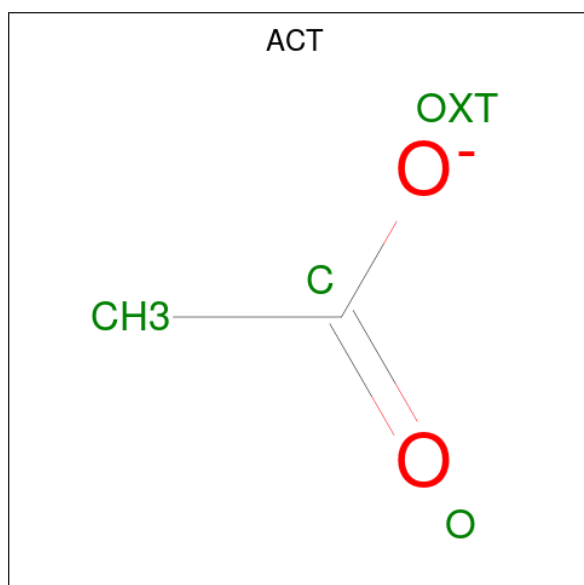
- Molecule 1 is a protein called Histidyl-tRNA synthetase.

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

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 (CCD ID: ACT) (formula: C₂H₃O₂).



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

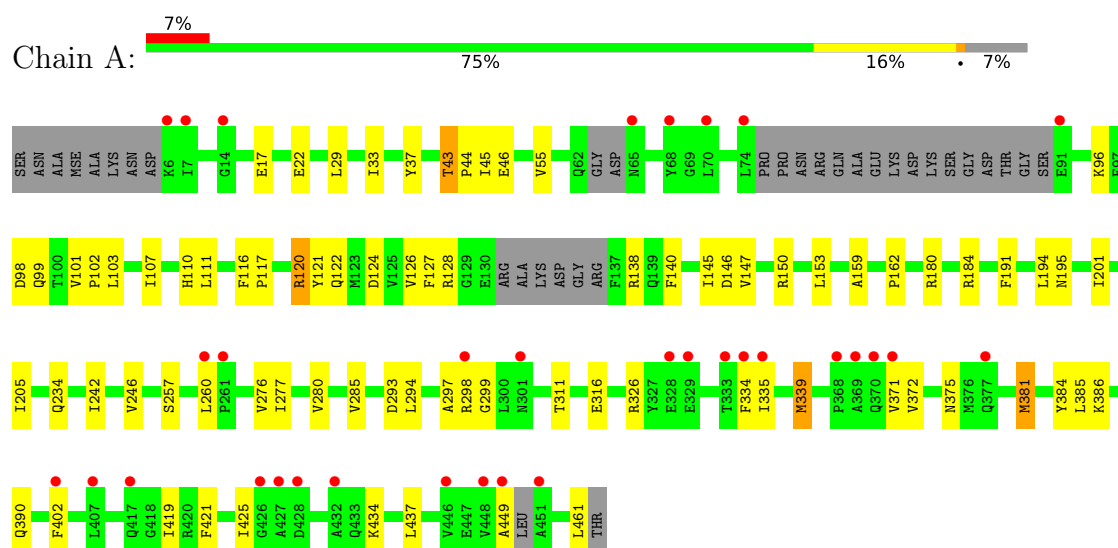
- Molecule 3 is water.

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

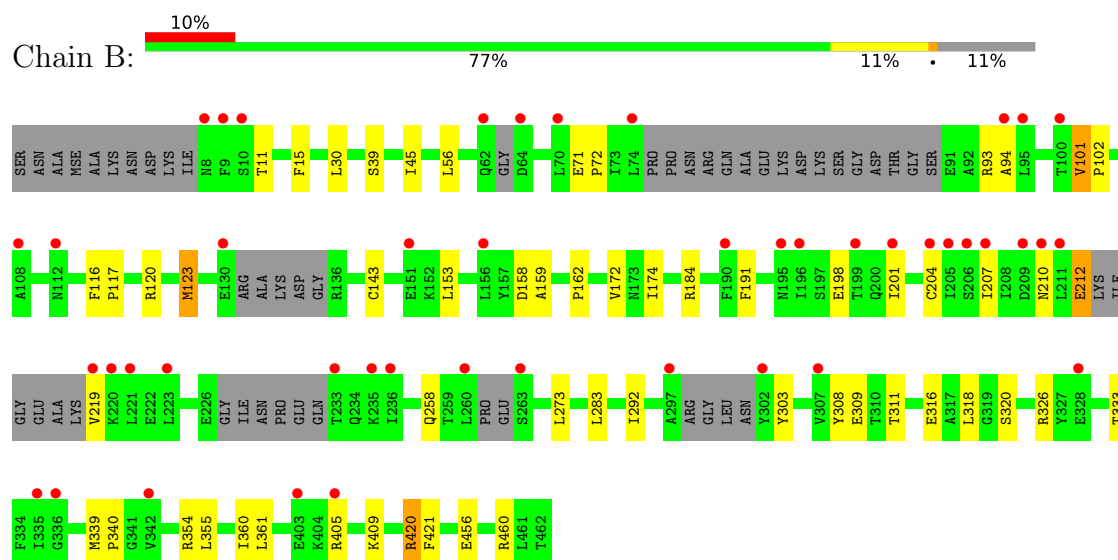
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: 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 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.1 (50.00-2.70) 93.1 (50.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.69Å)	Xtriage
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	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 69.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6572	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

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	0.61	0/3318	0.86	4/4483 (0.1%)
1	B	0.57	1/3218 (0.0%)	0.87	1/4343 (0.0%)
All	All	0.59	1/6536 (0.0%)	0.86	5/8826 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	VAL	CA-CB	5.10	1.57	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	VAL	CA-C-N	-5.79	114.30	120.03
1	A	285	VAL	C-N-CA	-5.79	114.30	120.03
1	B	360	ILE	CB-CA-C	-5.69	104.36	112.22
1	A	43	THR	CA-C-N	-5.38	113.72	120.51
1	A	43	THR	C-N-CA	-5.38	113.72	120.51

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	3276	0	3249	44	0
1	B	3181	0	3162	33	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	75	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 (75) 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:A:116:PHE:HA	1:A:117:PRO:C	2.30	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: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:B:116:PHE:HA	1:B:117:PRO:C	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:101:VAL:HB	1:A:102:PRO:HD3	1.97	0.46
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:210:ASN:C	1:B:212:GLU:H	2.26	0.42
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:99:GLN:OE1	1:A:122:GLN:HG2	2.19	0.42
1:A:311:THR:CG2	1:A:316:GLU:HG3	2.49	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:110:HIS:O	1:A:111:LEU:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:33:ILE:HG22	1:A:37:TYR:CE2	2.57	0.40
1:A:127:PHE:HA	1:A:138:ARG:O	2.21	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%)	43	68
1	B	399/465 (86%)	380 (95%)	19 (5%)	0	100	100
All	All	820/930 (88%)	779 (95%)	40 (5%)	1 (0%)	48	73

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	341/393 (87%)	327 (96%)	14 (4%)	27	56
1	B	334/393 (85%)	325 (97%)	9 (3%)	39	69
All	All	675/786 (86%)	652 (97%)	23 (3%)	32	62

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	22	GLU
1	A	43	THR
1	A	98	ASP
1	A	120	ARG
1	A	147	VAL
1	A	150	ARG
1	A	234	GLN
1	A	257	SER
1	A	260	LEU
1	A	339	MSE
1	A	371	VAL
1	A	381	MSE
1	A	437	LEU
1	B	39	SER
1	B	123	MSE
1	B	158	ASP
1	B	212	GLU
1	B	219	VAL
1	B	258	GLN
1	B	308	TYR
1	B	333	THR
1	B	420	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	HIS
1	A	390	GLN
1	B	142	GLN
1	B	258	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](#)

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	-	3,3,3	0.78	0	3,3,3	1.30	0

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 ⓘ

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%)	0.28	33 (7%) 19 17	35, 56, 123, 152	0
1	B	410/465 (88%)	0.59	45 (10%) 10 9	37, 74, 159, 189	0
All	All	836/930 (89%)	0.43	78 (9%) 14 12	35, 67, 137, 189	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	219	VAL	7.3
1	B	74	LEU	6.4
1	B	62	GLN	5.3
1	B	10	SER	4.8
1	B	9	PHE	4.8
1	B	205	ILE	4.5
1	B	263	SER	4.3
1	B	95	LEU	4.2
1	B	221	LEU	4.2
1	B	130	GLU	4.0
1	B	297	ALA	4.0
1	B	8	ASN	3.8
1	A	7	ILE	3.8
1	B	236	ILE	3.8
1	A	333	THR	3.8
1	A	329	GLU	3.7
1	A	451	ALA	3.7
1	A	68	TYR	3.7
1	A	407	LEU	3.6
1	A	369	ALA	3.6
1	A	74	LEU	3.6
1	B	220	LYS	3.6
1	B	336	GLY	3.6
1	B	209	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	211	LEU	3.5
1	A	70	LEU	3.5
1	A	377	GLN	3.5
1	B	70	LEU	3.4
1	B	233	THR	3.4
1	B	151	GLU	3.4
1	A	402	PHE	3.4
1	A	65	ASN	3.3
1	A	449	ALA	3.3
1	B	195	ASN	3.2
1	B	403	GLU	3.2
1	A	370	GLN	3.1
1	B	207	ILE	3.1
1	A	428	ASP	3.0
1	A	260	LEU	3.0
1	A	427	ALA	3.0
1	B	235	LYS	3.0
1	A	368	PRO	2.8
1	A	328	GLU	2.8
1	B	223	LEU	2.8
1	B	342	VAL	2.8
1	B	260	LEU	2.7
1	B	199	THR	2.7
1	A	417	GLN	2.6
1	B	335	ILE	2.6
1	A	432	ALA	2.6
1	B	190	PHE	2.6
1	A	426	GLY	2.6
1	A	261	PRO	2.5
1	B	302	TYR	2.5
1	A	371	VAL	2.4
1	B	100	THR	2.3
1	B	204	CYS	2.3
1	B	201	ILE	2.3
1	A	334	PHE	2.2
1	B	108	ALA	2.2
1	A	298	ARG	2.2
1	A	335	ILE	2.2
1	B	328	GLU	2.2
1	A	301	ASN	2.1
1	B	112	ASN	2.1
1	B	156	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	448	VAL	2.1
1	B	94	ALA	2.1
1	B	405	ARG	2.1
1	A	446	VAL	2.1
1	B	196	ILE	2.1
1	B	210	ASN	2.1
1	A	14	GLY	2.1
1	B	307	VAL	2.1
1	A	91	GLU	2.0
1	B	64	ASP	2.0
1	A	6	LYS	2.0
1	B	206	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 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(Å ²)	Q<0.9
2	ACT	A	501	4/4	0.68	0.26	110,110,111,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.