



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:04 AM UTC

PDB ID : 1LI5 / pdb_00001li5
Title : Crystal Structure of Cysteinyl-tRNA Synthetase
Authors : Newberry, K.J.; Hou, Y.-M.; Perona, J.J.
Deposited on : 2002-04-17
Resolution : 2.30 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

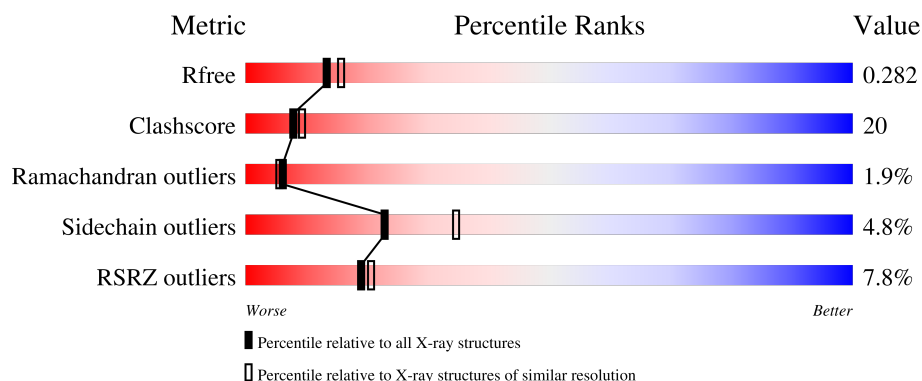
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	461	3% 55% 24% 5% 16%
1	B	461	10% 51% 25% • • 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5778 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 CYSTEINYL-TRNA SYNTHETASE.

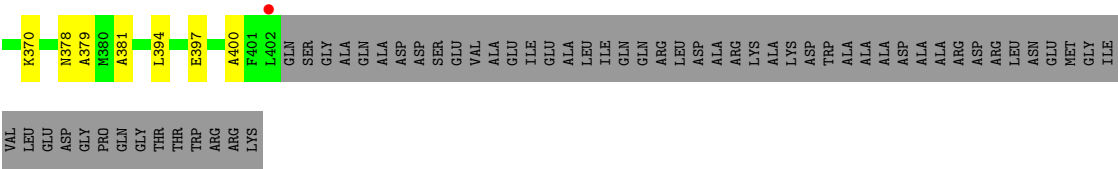
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			2949	1869	508	547	25			
1	B	369	Total	C	N	O	S	0	0	0
			2725	1727	475	502	21			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total	O	0	0
			73	73		
3	B	29	Total	O	0	0
			29	29		



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.16Å 119.16Å 144.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.30 19.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.89-2.30) 98.0 (19.89-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.283 0.244 , 0.282	Depositor DCC
R_{free} test set	5306 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5778	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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

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	0.63	6/3021 (0.2%)	1.48	34/4105 (0.8%)
1	B	0.73	10/2790 (0.4%)	1.59	32/3798 (0.8%)
All	All	0.68	16/5811 (0.3%)	1.53	66/7903 (0.8%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	GLN	N-CA	15.09	1.65	1.46
1	B	250	TYR	N-CA	12.08	1.61	1.46
1	B	249	GLN	CA-C	9.18	1.65	1.52
1	B	249	GLN	C-N	8.71	1.45	1.33
1	A	265	GLU	C-N	-8.43	1.21	1.33
1	B	247	ASP	N-CA	-8.14	1.35	1.46
1	B	157	ARG	CA-C	7.91	1.63	1.52
1	A	232	PHE	CA-C	-7.12	1.45	1.52
1	A	264	ARG	CA-C	6.61	1.61	1.52
1	A	246	HIS	C-N	-5.84	1.24	1.33
1	A	234	HIS	N-CA	-5.52	1.39	1.46
1	B	248	GLY	N-CA	-5.48	1.37	1.45
1	A	233	PRO	CA-C	-5.30	1.44	1.52
1	B	266	LYS	CA-CB	-5.23	1.45	1.53
1	B	157	ARG	N-CA	5.13	1.52	1.46
1	B	266	LYS	N-CA	-5.10	1.39	1.46

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	PHE	CA-C-N	47.90	179.71	119.84
1	B	232	PHE	C-N-CA	47.90	179.71	119.84
1	A	232	PHE	CA-C-N	36.73	165.75	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	PHE	C-N-CA	36.73	165.75	119.84
1	A	264	ARG	CA-C-N	18.12	148.00	123.00
1	A	264	ARG	C-N-CA	18.12	148.00	123.00
1	A	232	PHE	C-N-CD	-14.54	65.39	125.00
1	B	246	HIS	N-CA-C	12.99	130.60	113.72
1	A	31	THR	N-CA-C	-12.72	88.59	109.96
1	B	232	PHE	C-N-CD	-11.92	76.11	125.00
1	A	72	ASP	N-CA-C	11.18	124.86	111.33
1	A	222	ASP	N-CA-C	11.06	123.31	111.03
1	A	149	ASP	CA-C-N	10.73	130.40	119.24
1	A	149	ASP	C-N-CA	10.73	130.40	119.24
1	A	71	ASP	N-CA-C	-10.59	88.24	110.80
1	B	249	GLN	OE1-CD-NE2	-9.67	112.93	122.60
1	B	266	LYS	N-CA-C	9.54	124.54	109.65
1	A	249	GLN	OE1-CD-NE2	-9.18	113.42	122.60
1	B	196	SER	CA-C-N	7.82	129.61	119.84
1	B	196	SER	C-N-CA	7.82	129.61	119.84
1	A	265	GLU	N-CA-CB	7.58	122.48	110.57
1	B	45	VAL	N-CA-C	-7.39	103.65	110.82
1	B	133	HIS	N-CA-C	-7.18	104.14	114.12
1	A	133	HIS	N-CA-C	7.05	122.05	113.17
1	A	233	PRO	CA-N-CD	-7.04	102.14	112.00
1	B	156	SER	N-CA-C	7.04	121.87	113.28
1	B	245	ALA	CA-C-N	-6.85	111.36	122.26
1	B	245	ALA	C-N-CA	-6.85	111.36	122.26
1	A	269	LYS	N-CA-C	-6.76	103.94	111.71
1	B	249	GLN	CG-CD-NE2	6.72	126.48	116.40
1	B	222	ASP	N-CA-C	6.64	118.41	111.03
1	A	249	GLN	CG-CD-NE2	6.61	126.32	116.40
1	B	251	VAL	N-CA-C	6.57	117.34	107.75
1	A	248	GLY	O-C-N	6.51	128.28	122.88
1	B	265	GLU	N-CA-C	-6.49	100.30	110.36
1	B	247	ASP	O-C-N	6.40	131.11	122.59
1	A	223	ILE	N-CA-C	6.37	117.30	108.12
1	A	32	VAL	N-CA-CB	-6.29	100.84	111.23
1	A	246	HIS	CA-C-N	-6.22	109.57	122.07
1	A	246	HIS	C-N-CA	-6.22	109.57	122.07
1	B	60	LYS	N-CA-C	-6.20	98.42	108.41
1	A	183	LEU	N-CA-C	-6.17	105.41	113.12
1	B	182	VAL	N-CA-C	6.14	117.63	108.54
1	A	69	ASP	N-CA-C	6.08	120.86	112.90
1	B	198	TRP	N-CA-C	-6.06	105.88	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	PRO	CA-N-CD	-5.93	103.70	112.00
1	B	48	ASP	N-CA-C	-5.83	105.01	111.36
1	A	33	TYR	N-CA-C	-5.69	106.97	114.31
1	A	375	ALA	N-CA-C	-5.43	105.27	111.14
1	B	223	ILE	N-CA-C	5.34	117.56	108.86
1	B	154	VAL	N-CA-C	5.32	115.53	110.42
1	A	45	VAL	N-CA-C	-5.31	105.54	110.53
1	A	235	HIS	N-CA-C	5.29	117.05	111.28
1	A	273	ASN	CA-C-N	-5.25	115.75	123.00
1	A	273	ASN	C-N-CA	-5.25	115.75	123.00
1	A	207	ILE	N-CA-C	5.22	117.62	111.09
1	B	249	GLN	N-CA-C	5.21	121.89	110.80
1	B	246	HIS	CA-C-N	-5.17	111.66	121.54
1	B	246	HIS	C-N-CA	-5.17	111.66	121.54
1	B	129	ILE	N-CA-C	-5.14	105.69	110.53
1	A	249	GLN	N-CA-C	5.08	118.50	109.96
1	B	194	TRP	N-CA-C	-5.07	100.02	108.23
1	A	60	LYS	N-CA-C	-5.06	100.27	108.41
1	B	397	GLU	N-CA-C	-5.03	103.31	109.65
1	B	186	MET	N-CA-C	-5.03	103.15	110.24
1	A	132	GLY	N-CA-C	5.01	121.72	115.21

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	2949	0	2724	113	0
1	B	2725	0	2430	101	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	73	0	0	2	0
3	B	29	0	0	0	0
All	All	5778	0	5154	214	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 20.

All (214) 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:112:PRO:HB2	1:A:212:MET:HE2	1.32	1.09
1:A:246:HIS:HD2	3:A:1099:HOH:O	1.39	1.04
1:B:143:MET:HE1	1:B:182:VAL:HG22	1.39	1.04
1:B:148:THR:O	1:B:150:PRO:HD3	1.64	0.98
1:A:287:GLU:HG2	1:A:316:LEU:HD21	1.46	0.92
1:A:235:HIS:HD2	1:A:256:HIS:HE1	1.20	0.90
1:A:146:VAL:HG13	1:A:147:PRO:HD3	1.56	0.85
1:A:65:ARG:HG2	1:A:65:ARG:HH11	1.42	0.84
1:A:235:HIS:HD2	1:A:256:HIS:CE1	1.96	0.83
1:B:35:LEU:HD12	1:B:35:LEU:H	1.45	0.82
1:B:141:ASP:HB3	1:B:143:MET:HE3	1.60	0.81
1:B:149:ASP:HB3	1:B:152:TYR:HB2	1.64	0.79
1:A:146:VAL:HG11	1:A:179:MET:HB2	1.66	0.77
1:A:326:THR:HG21	1:A:385:ARG:HH12	1.49	0.77
1:B:235:HIS:HD2	1:B:256:HIS:NE2	1.85	0.75
1:A:335:GLY:HA2	1:A:380:MET:HE1	1.69	0.75
1:B:38:ILE:HD12	1:B:39:GLY:H	1.51	0.74
1:B:246:HIS:O	1:B:247:ASP:CB	2.28	0.74
1:B:223:ILE:HD13	1:B:255:MET:SD	2.27	0.74
1:A:362:MET:HE3	1:A:384:LEU:HD13	1.68	0.73
1:B:232:PHE:CD2	1:B:233:PRO:HD3	2.23	0.73
1:A:28:CYS:SG	1:A:235:HIS:HE1	2.13	0.72
1:A:246:HIS:CD2	3:A:1099:HOH:O	2.25	0.72
1:B:37:HIS:HA	1:B:276:THR:HA	1.71	0.72
1:B:38:ILE:HD12	1:B:39:GLY:N	2.04	0.72
1:B:220:HIS:HE1	1:B:252:ASN:OD1	1.72	0.71
1:B:65:ARG:HH11	1:B:65:ARG:HG2	1.56	0.71
1:A:362:MET:HE1	1:A:387:LEU:HD12	1.73	0.70
1:A:1:MET:HG3	1:A:14:GLU:HG3	1.72	0.70
1:A:69:ASP:HB3	1:A:115:THR:HG23	1.74	0.69
1:A:92:MET:HA	1:A:92:MET:HE2	1.74	0.69
1:B:92:MET:HE2	1:B:92:MET:HA	1.75	0.69
1:A:6:ASN:ND2	1:A:254:TRP:H	1.91	0.69
1:B:107:ARG:HH11	1:B:107:ARG:HG2	1.58	0.69
1:B:183:LEU:HD22	1:B:207:ILE:HD13	1.75	0.68
1:B:35:LEU:HD12	1:B:35:LEU:N	2.07	0.68
1:A:146:VAL:HG11	1:A:179:MET:CB	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:VAL:HB	1:B:147:PRO:HD3	1.77	0.67
1:A:37:HIS:HA	1:A:276:THR:HA	1.75	0.67
1:A:65:ARG:HG2	1:A:65:ARG:NH1	2.10	0.66
1:B:177:ASN:ND2	1:B:179:MET:H	1.94	0.66
1:A:177:ASN:ND2	1:A:179:MET:H	1.93	0.65
1:B:95:GLU:CD	1:B:278:ARG:HH22	2.05	0.65
1:B:110:MET:HA	1:B:110:MET:HE2	1.77	0.65
1:A:135:TYR:CE2	1:A:145:ASP:HB3	2.32	0.65
1:A:37:HIS:HD2	1:A:39:GLY:H	1.43	0.65
1:B:287:GLU:HG2	1:B:316:LEU:HD21	1.77	0.64
1:A:112:PRO:HB2	1:A:212:MET:CE	2.20	0.64
1:B:132:GLY:O	1:B:148:THR:HG21	1.98	0.64
1:B:366:VAL:O	1:B:370:LYS:HG2	1.98	0.63
1:B:224:HIS:HE1	1:B:238:GLU:OE1	1.82	0.63
1:A:326:THR:CG2	1:A:385:ARG:HH12	2.12	0.63
1:A:124:LEU:HD12	1:A:211:ALA:HA	1.81	0.62
1:A:328:LYS:HA	1:A:385:ARG:NH2	2.15	0.62
1:A:30:ILE:CD1	1:A:30:ILE:H	2.12	0.62
1:B:145:ASP:O	1:B:148:THR:OG1	2.15	0.62
1:A:31:THR:HA	1:A:68:THR:HB	1.83	0.61
1:A:362:MET:HE3	1:A:384:LEU:CD1	2.30	0.60
1:A:232:PHE:CD2	1:A:233:PRO:HD3	2.36	0.60
1:A:323:LEU:O	1:A:326:THR:HB	2.02	0.60
1:B:261:MET:HB3	1:B:265:GLU:O	2.02	0.60
1:A:30:ILE:H	1:A:30:ILE:HD13	1.67	0.59
1:A:224:HIS:HE1	1:A:238:GLU:OE1	1.85	0.59
1:B:137:ALA:O	1:B:140:GLY:N	2.34	0.59
1:A:32:VAL:HG21	1:A:67:ILE:HG23	1.85	0.59
1:A:334:GLY:C	1:A:380:MET:HE2	2.27	0.59
1:B:195:PRO:O	1:B:196:SER:CB	2.50	0.59
1:B:141:ASP:CB	1:B:143:MET:HE3	2.31	0.58
1:B:112:PRO:HG2	1:B:212:MET:HE3	1.86	0.58
1:A:95:GLU:HG3	1:A:278:ARG:NH2	2.18	0.58
1:B:313:ARG:O	1:B:317:GLU:HG3	2.03	0.58
1:B:112:PRO:HB2	1:B:212:MET:HE3	1.85	0.57
1:B:141:ASP:HB3	1:B:143:MET:CE	2.33	0.57
1:A:95:GLU:HG3	1:A:278:ARG:HH22	1.70	0.57
1:A:294:MET:HE3	1:A:356:TYR:OH	2.05	0.57
1:A:30:ILE:HD11	1:A:96:MET:SD	2.45	0.57
1:A:122:ILE:O	1:A:126:GLU:HG3	2.04	0.57
1:B:38:ILE:HD11	1:B:267:MET:SD	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ARG:HG3	1:B:318:ARG:HH11	1.71	0.56
1:A:235:HIS:CD2	1:A:256:HIS:HE1	2.12	0.56
1:B:298:TYR:CE1	1:B:299:ARG:HG3	2.41	0.55
1:A:32:VAL:HG12	1:A:92:MET:HB2	1.88	0.55
1:A:262:VAL:HB	1:A:273:ASN:HB2	1.88	0.55
1:B:146:VAL:HG23	1:B:180:ASP:HA	1.89	0.55
1:A:1:MET:HE3	1:A:14:GLU:OE1	2.06	0.54
1:A:117:HIS:ND1	1:A:212:MET:HE3	2.22	0.54
1:A:153:GLY:HA2	1:A:236:GLU:CD	2.33	0.54
1:B:112:PRO:CB	1:B:212:MET:HE3	2.38	0.54
1:B:135:TYR:HH	1:B:176:ARG:N	2.05	0.54
1:A:135:TYR:HE2	1:A:145:ASP:HB3	1.70	0.53
1:A:220:HIS:HE1	1:A:252:ASN:OD1	1.90	0.53
1:B:135:TYR:CD1	1:B:135:TYR:C	2.86	0.53
1:B:184:TRP:NE1	1:B:201:GLY:HA3	2.23	0.53
1:A:35:LEU:HD22	1:A:35:LEU:H	1.73	0.53
1:A:7:THR:OG1	1:A:256:HIS:HD2	1.92	0.53
1:B:117:HIS:O	1:B:121:ILE:HG13	2.09	0.53
1:A:206:HIS:CD2	1:A:237:ASN:HD22	2.27	0.52
1:B:69:ASP:OD1	1:B:115:THR:HB	2.09	0.52
1:B:326:THR:HG21	1:B:381:ALA:CB	2.40	0.51
1:A:117:HIS:HB3	1:A:120:GLU:HG2	1.93	0.51
1:A:135:TYR:HE2	1:A:145:ASP:CB	2.23	0.51
1:A:107:ARG:HG2	1:A:107:ARG:HH11	1.76	0.51
1:A:224:HIS:CE1	1:A:238:GLU:OE1	2.63	0.51
1:B:107:ARG:HG2	1:B:107:ARG:NH1	2.24	0.51
1:B:35:LEU:H	1:B:35:LEU:CD1	2.19	0.51
1:B:66:ASN:HB2	1:B:212:MET:HE1	1.91	0.51
1:B:235:HIS:CD2	1:B:256:HIS:NE2	2.72	0.51
1:A:177:ASN:HD22	1:A:179:MET:H	1.58	0.51
1:B:154:VAL:HG13	1:B:155:LEU:N	2.25	0.50
1:B:112:PRO:CG	1:B:212:MET:HE3	2.42	0.50
1:B:297:HIS:HD2	1:B:299:ARG:HB2	1.76	0.50
1:A:335:GLY:H	1:A:383:HIS:CD2	2.29	0.50
1:B:318:ARG:HG3	1:B:318:ARG:NH1	2.26	0.50
1:A:339:GLU:OE1	1:A:383:HIS:HE1	1.95	0.50
1:B:6:ASN:ND2	1:B:254:TRP:H	2.10	0.49
1:B:367:ASN:HA	1:B:370:LYS:HG3	1.95	0.49
1:A:113:ARG:C	1:A:212:MET:HE1	2.38	0.49
1:A:214:CYS:HB2	1:A:219:ASN:HD22	1.77	0.49
1:B:142:VAL:O	1:B:143:MET:HE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASP:HA	1:A:180:ASP:OD1	2.12	0.49
1:A:362:MET:HE3	1:A:384:LEU:HA	1.94	0.49
1:A:320:TYR:CZ	1:A:394:LEU:HA	2.48	0.49
1:B:145:ASP:HB3	1:B:148:THR:OG1	2.12	0.49
1:B:65:ARG:HG2	1:B:65:ARG:NH1	2.25	0.48
1:B:156:SER:HB3	1:B:231:MET:HE3	1.95	0.48
1:B:86:VAL:O	1:B:89:VAL:HG22	2.12	0.48
1:A:30:ILE:HD13	1:A:30:ILE:N	2.28	0.48
1:B:25:MET:HG3	1:B:223:ILE:HG13	1.95	0.48
1:A:101:ASP:OD1	1:A:107:ARG:NH1	2.47	0.47
1:B:262:VAL:N	1:B:265:GLU:O	2.47	0.47
1:A:112:PRO:C	1:A:212:MET:HE1	2.40	0.47
1:A:32:VAL:HG12	1:A:92:MET:CB	2.43	0.47
1:A:327:ASP:CG	1:A:329:THR:HG22	2.40	0.47
1:A:237:ASN:O	1:A:241:GLN:HG3	2.15	0.47
1:B:177:ASN:HD22	1:B:179:MET:H	1.60	0.47
1:B:297:HIS:CD2	1:B:299:ARG:HB2	2.50	0.47
1:A:235:HIS:CD2	1:A:256:HIS:CE1	2.88	0.46
1:B:97:HIS:HE1	1:B:111:GLU:OE1	1.98	0.46
1:A:335:GLY:HA2	1:A:380:MET:CE	2.43	0.46
1:B:214:CYS:HB2	1:B:219:ASN:HD22	1.80	0.46
1:B:219:ASN:O	1:B:250:TYR:HA	2.15	0.46
1:B:185:LYS:O	1:B:186:MET:C	2.58	0.46
1:A:188:LYS:O	1:A:191:GLU:HG2	2.16	0.46
1:A:220:HIS:CE1	1:A:249:GLN:HB3	2.50	0.46
1:A:70:ILE:HD12	1:A:70:ILE:N	2.31	0.46
1:B:26:TYR:HA	1:B:64:VAL:O	2.15	0.46
1:B:194:TRP:O	1:B:195:PRO:O	2.34	0.46
1:B:353:PRO:O	1:B:356:TYR:HB2	2.16	0.46
1:A:35:LEU:HD11	1:A:95:GLU:HG2	1.96	0.46
1:B:262:VAL:O	1:B:263:ASP:CB	2.64	0.46
1:B:220:HIS:CE1	1:B:252:ASN:OD1	2.60	0.45
1:B:333:ALA:HB3	1:B:379:ALA:HB1	1.97	0.45
1:B:156:SER:CB	1:B:231:MET:HE3	2.45	0.45
1:B:246:HIS:C	1:B:247:ASP:O	2.59	0.45
1:B:223:ILE:HD12	1:B:224:HIS:N	2.31	0.45
1:A:1:MET:HE2	1:A:14:GLU:HB2	1.99	0.45
1:B:29:GLY:HA3	1:B:66:ASN:O	2.17	0.45
1:B:135:TYR:HE1	1:B:137:ALA:HB2	1.82	0.45
1:A:26:TYR:HA	1:A:64:VAL:O	2.17	0.45
1:A:156:SER:CB	1:A:231:MET:HE3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:O	1:A:71:ASP:OD2	2.35	0.45
1:A:294:MET:HB2	1:A:356:TYR:OH	2.17	0.45
1:A:307:GLU:O	1:A:311:GLN:HG2	2.16	0.45
1:A:297:HIS:HE1	1:A:349:ASP:O	2.00	0.45
1:A:37:HIS:HD2	1:A:39:GLY:N	2.13	0.44
1:A:70:ILE:HD12	1:A:70:ILE:H	1.82	0.44
1:A:362:MET:CE	1:A:384:LEU:HA	2.48	0.44
1:A:71:ASP:OD2	1:A:71:ASP:C	2.60	0.44
1:B:214:CYS:HA	1:B:218:GLY:O	2.18	0.44
1:B:309:LEU:O	1:B:312:ALA:HB3	2.17	0.44
1:A:38:ILE:HG12	1:A:275:PHE:O	2.18	0.43
1:A:366:VAL:O	1:A:370:LYS:HG2	2.18	0.43
1:A:146:VAL:HG12	1:A:180:ASP:OD1	2.18	0.43
1:A:35:LEU:HD22	1:A:35:LEU:N	2.33	0.43
1:A:42:ARG:NH2	1:A:300:SER:O	2.50	0.43
1:A:262:VAL:O	1:A:263:ASP:CB	2.64	0.43
1:B:5:PHE:HA	1:B:12:LYS:HA	2.00	0.43
1:A:263:ASP:O	1:A:264:ARG:CB	2.64	0.43
1:B:326:THR:HG21	1:B:381:ALA:HB3	2.00	0.43
1:B:142:VAL:C	1:B:143:MET:HE2	2.44	0.43
1:A:72:ASP:HB2	1:A:205:TRP:CH2	2.53	0.42
1:A:274:PHE:C	1:A:274:PHE:CD2	2.97	0.42
1:B:112:PRO:HG2	1:B:212:MET:CE	2.48	0.42
1:B:72:ASP:C	1:B:74:ILE:N	2.76	0.42
1:B:214:CYS:HB2	1:B:219:ASN:ND2	2.34	0.42
1:B:196:SER:O	1:B:199:GLY:N	2.43	0.42
1:B:314:ALA:O	1:B:317:GLU:HB2	2.20	0.42
1:A:26:TYR:CD1	1:A:213:ASN:HB3	2.55	0.42
1:B:110:MET:HA	1:B:110:MET:CE	2.45	0.42
1:A:118:ILE:N	1:A:118:ILE:HD12	2.35	0.42
1:B:330:VAL:HG21	1:B:378:ASN:HB3	2.00	0.42
1:B:187:SER:N	1:B:201:GLY:HA2	2.35	0.42
1:A:232:PHE:CG	1:A:233:PRO:HD3	2.54	0.41
1:B:92:MET:HA	1:B:92:MET:CE	2.49	0.41
1:A:39:GLY:HA2	1:A:260:VAL:CG2	2.50	0.41
1:A:154:VAL:HG13	1:A:155:LEU:N	2.34	0.41
1:A:208:GLU:O	1:A:212:MET:HG3	2.20	0.41
1:A:31:THR:HG21	1:A:71:ASP:OD1	2.20	0.41
1:B:72:ASP:OD1	1:B:202:ARG:NH2	2.53	0.41
1:A:135:TYR:CD2	1:A:145:ASP:HB3	2.56	0.41
1:A:5:PHE:HA	1:A:12:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ASN:CG	1:B:178:PRO:HD2	2.45	0.41
1:B:284:TYR:CG	1:B:309:LEU:HD23	2.55	0.41
1:B:320:TYR:CZ	1:B:394:LEU:HA	2.55	0.41
1:A:1:MET:HE3	1:A:14:GLU:CD	2.46	0.41
1:A:29:GLY:HA3	1:A:66:ASN:O	2.21	0.41
1:A:75:ILE:C	1:A:75:ILE:HD12	2.46	0.41
1:A:297:HIS:CD2	1:A:299:ARG:H	2.39	0.41
1:A:30:ILE:HG12	1:A:31:THR:O	2.21	0.40
1:A:86:VAL:HG23	1:A:87:ALA:N	2.34	0.40
1:B:37:HIS:HD2	1:B:39:GLY:H	1.69	0.40
1:B:297:HIS:CD2	1:B:299:ARG:H	2.39	0.40
1:A:95:GLU:CG	1:A:278:ARG:HH22	2.33	0.40
1:B:177:ASN:OD1	1:B:178:PRO:HD2	2.21	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	382/461 (83%)	369 (97%)	9 (2%)	4 (1%)	12	15
1	B	361/461 (78%)	334 (92%)	17 (5%)	10 (3%)	4	2
All	All	743/922 (81%)	703 (95%)	26 (4%)	14 (2%)	6	5

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	PRO
1	A	266	LYS
1	B	195	PRO
1	B	233	PRO
1	B	250	TYR

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Mol	Chain	Res	Type
1	B	264	ARG
1	A	264	ARG
1	B	157	ARG
1	A	234	HIS
1	B	196	SER
1	B	249	GLN
1	B	400	ALA
1	B	275	PHE
1	B	32	VAL

5.3.2 Protein sidechains ⓘ

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	291/381 (76%)	276 (95%)	15 (5%)	21	31
1	B	250/381 (66%)	239 (96%)	11 (4%)	25	38
All	All	541/762 (71%)	515 (95%)	26 (5%)	23	35

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	30	ILE
1	A	38	ILE
1	A	42	ARG
1	A	70	ILE
1	A	120	GLU
1	A	145	ASP
1	A	146	VAL
1	A	147	PRO
1	A	187	SER
1	A	202	ARG
1	A	233	PRO
1	A	299	ARG
1	A	326	THR

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Mol	Chain	Res	Type
1	A	329	THR
1	B	1	MET
1	B	38	ILE
1	B	107	ARG
1	B	110	MET
1	B	116	HIS
1	B	148	THR
1	B	195	PRO
1	B	197	PRO
1	B	216	GLN
1	B	223	ILE
1	B	249	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	37	HIS
1	A	177	ASN
1	A	219	ASN
1	A	220	HIS
1	A	224	HIS
1	A	235	HIS
1	A	237	ASN
1	A	246	HIS
1	A	256	HIS
1	A	297	HIS
1	A	303	ASN
1	A	308	ASN
1	A	383	HIS
1	B	6	ASN
1	B	37	HIS
1	B	104	ASN
1	B	177	ASN
1	B	219	ASN
1	B	220	HIS
1	B	224	HIS
1	B	235	HIS
1	B	246	HIS
1	B	297	HIS
1	B	308	ASN
1	B	383	HIS

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Mol	Chain	Res	Type
1	B	396	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 [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	386/461 (83%)	0.28	14 (3%) 46 48	19, 32, 46, 54	0
1	B	369/461 (80%)	0.75	45 (12%) 8 9	19, 42, 62, 78	0
All	All	755/922 (81%)	0.51	59 (7%) 19 21	19, 35, 60, 78	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	GLY	8.1
1	B	263	ASP	5.6
1	B	197	PRO	4.3
1	B	402	LEU	4.2
1	B	274	PHE	4.1
1	B	265	GLU	3.5
1	B	273	ASN	3.5
1	B	158	GLN	3.3
1	B	190	GLY	3.3
1	B	275	PHE	3.3
1	B	184	TRP	3.3
1	B	176	ARG	3.2
1	A	69	ASP	3.1
1	A	247	ASP	2.9
1	B	36	CYS	2.9
1	A	32	VAL	2.9
1	B	32	VAL	2.9
1	B	89	VAL	2.9
1	A	264	ARG	2.8
1	B	283	TYR	2.8
1	B	276	THR	2.8
1	B	233	PRO	2.8
1	B	33	TYR	2.8
1	B	267	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	86	VAL	2.7
1	B	94	ALA	2.6
1	B	188	LYS	2.6
1	B	249	GLN	2.5
1	B	132	GLY	2.4
1	A	146	VAL	2.4
1	B	284	TYR	2.4
1	B	71	ASP	2.4
1	A	134	ALA	2.4
1	B	196	SER	2.4
1	B	106	LEU	2.4
1	A	158	GLN	2.4
1	B	304	TYR	2.4
1	A	263	ASP	2.4
1	B	325	GLY	2.4
1	A	249	GLN	2.3
1	A	86	VAL	2.3
1	B	277	VAL	2.3
1	B	186	MET	2.2
1	B	198	TRP	2.2
1	A	145	ASP	2.2
1	B	139	ASN	2.2
1	B	114	ALA	2.2
1	A	35	LEU	2.1
1	B	70	ILE	2.1
1	B	88	MET	2.1
1	B	200	ALA	2.1
1	A	129	ILE	2.1
1	B	323	LEU	2.1
1	B	247	ASP	2.1
1	A	84	SER	2.0
1	B	250	TYR	2.0
1	B	136	VAL	2.0
1	B	264	ARG	2.0
1	B	199	GLY	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 [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($\text{\AA}^2$)	Q<0.9
2	ZN	A	963	1/1	0.96	0.04	32,32,32,32	0
2	ZN	B	964	1/1	0.98	0.04	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.