



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 19, 2026 – 11:56 PM UTC

PDB ID : 4EBA / pdb_00004eba
Title : Crystal structure of the Rna14-Rna15 complex
Authors : Paulson, A.R.; Tong, L.
Deposited on : 2012-03-23
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

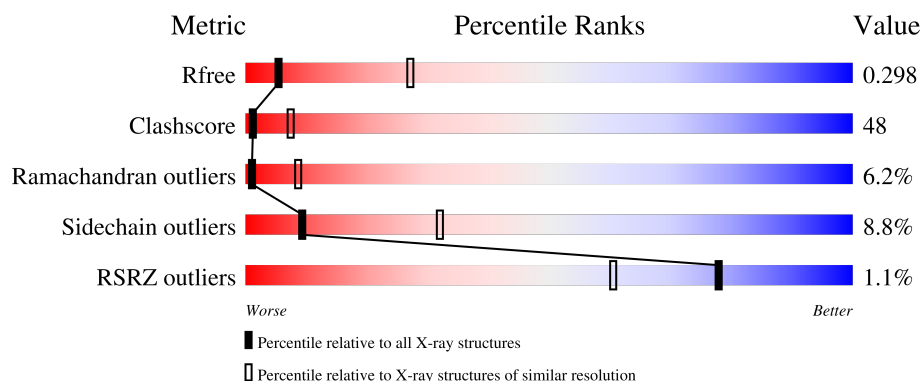
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	645	
1	B	645	
1	C	645	
1	D	645	
1	E	645	

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Mol	Chain	Length	Quality of chain
1	F	645	
2	G	174	
2	H	174	
2	I	174	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30268 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 mRNA 3'-end-processing protein Rna14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4874	3149	803	897	25			
1	B	558	Total	C	N	O	S	0	0	0
			4646	2990	772	859	25			
1	C	585	Total	C	N	O	S	0	0	0
			4874	3149	803	897	25			
1	D	551	Total	C	N	O	S	0	0	0
			4589	2957	759	848	25			
1	E	578	Total	C	N	O	S	0	0	0
			4823	3118	795	885	25			
1	F	553	Total	C	N	O	S	0	0	0
			4608	2967	764	852	25			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	expression tag	UNP Q6CII8
B	17	MET	-	expression tag	UNP Q6CII8
C	17	MET	-	expression tag	UNP Q6CII8
D	17	MET	-	expression tag	UNP Q6CII8
E	17	MET	-	expression tag	UNP Q6CII8
F	17	MET	-	expression tag	UNP Q6CII8

- Molecule 2 is a protein called Rna15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	81	Total	C	N	O	S	0	0	0
			618	395	98	119	6			
2	I	81	Total	C	N	O	S	0	0	0
			618	395	98	119	6			
2	H	81	Total	C	N	O	S	0	0	0
			618	395	98	119	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	85	MET	-	expression tag	UNP Q6CKN2
G	86	GLY	-	expression tag	UNP Q6CKN2
G	87	SER	-	expression tag	UNP Q6CKN2
G	88	SER	-	expression tag	UNP Q6CKN2
G	89	HIS	-	expression tag	UNP Q6CKN2
G	90	HIS	-	expression tag	UNP Q6CKN2
G	91	HIS	-	expression tag	UNP Q6CKN2
G	92	HIS	-	expression tag	UNP Q6CKN2
G	93	HIS	-	expression tag	UNP Q6CKN2
G	94	HIS	-	expression tag	UNP Q6CKN2
G	95	SER	-	expression tag	UNP Q6CKN2
G	96	SER	-	expression tag	UNP Q6CKN2
G	97	GLY	-	expression tag	UNP Q6CKN2
G	98	LEU	-	expression tag	UNP Q6CKN2
G	99	VAL	-	expression tag	UNP Q6CKN2
G	100	PRO	-	expression tag	UNP Q6CKN2
G	101	ARG	-	expression tag	UNP Q6CKN2
G	102	GLY	-	expression tag	UNP Q6CKN2
G	103	SER	-	expression tag	UNP Q6CKN2
G	104	HIS	-	expression tag	UNP Q6CKN2
I	85	MET	-	expression tag	UNP Q6CKN2
I	86	GLY	-	expression tag	UNP Q6CKN2
I	87	SER	-	expression tag	UNP Q6CKN2
I	88	SER	-	expression tag	UNP Q6CKN2
I	89	HIS	-	expression tag	UNP Q6CKN2
I	90	HIS	-	expression tag	UNP Q6CKN2
I	91	HIS	-	expression tag	UNP Q6CKN2
I	92	HIS	-	expression tag	UNP Q6CKN2
I	93	HIS	-	expression tag	UNP Q6CKN2
I	94	HIS	-	expression tag	UNP Q6CKN2
I	95	SER	-	expression tag	UNP Q6CKN2
I	96	SER	-	expression tag	UNP Q6CKN2
I	97	GLY	-	expression tag	UNP Q6CKN2
I	98	LEU	-	expression tag	UNP Q6CKN2
I	99	VAL	-	expression tag	UNP Q6CKN2
I	100	PRO	-	expression tag	UNP Q6CKN2
I	101	ARG	-	expression tag	UNP Q6CKN2
I	102	GLY	-	expression tag	UNP Q6CKN2
I	103	SER	-	expression tag	UNP Q6CKN2
I	104	HIS	-	expression tag	UNP Q6CKN2
H	85	MET	-	expression tag	UNP Q6CKN2
H	86	GLY	-	expression tag	UNP Q6CKN2

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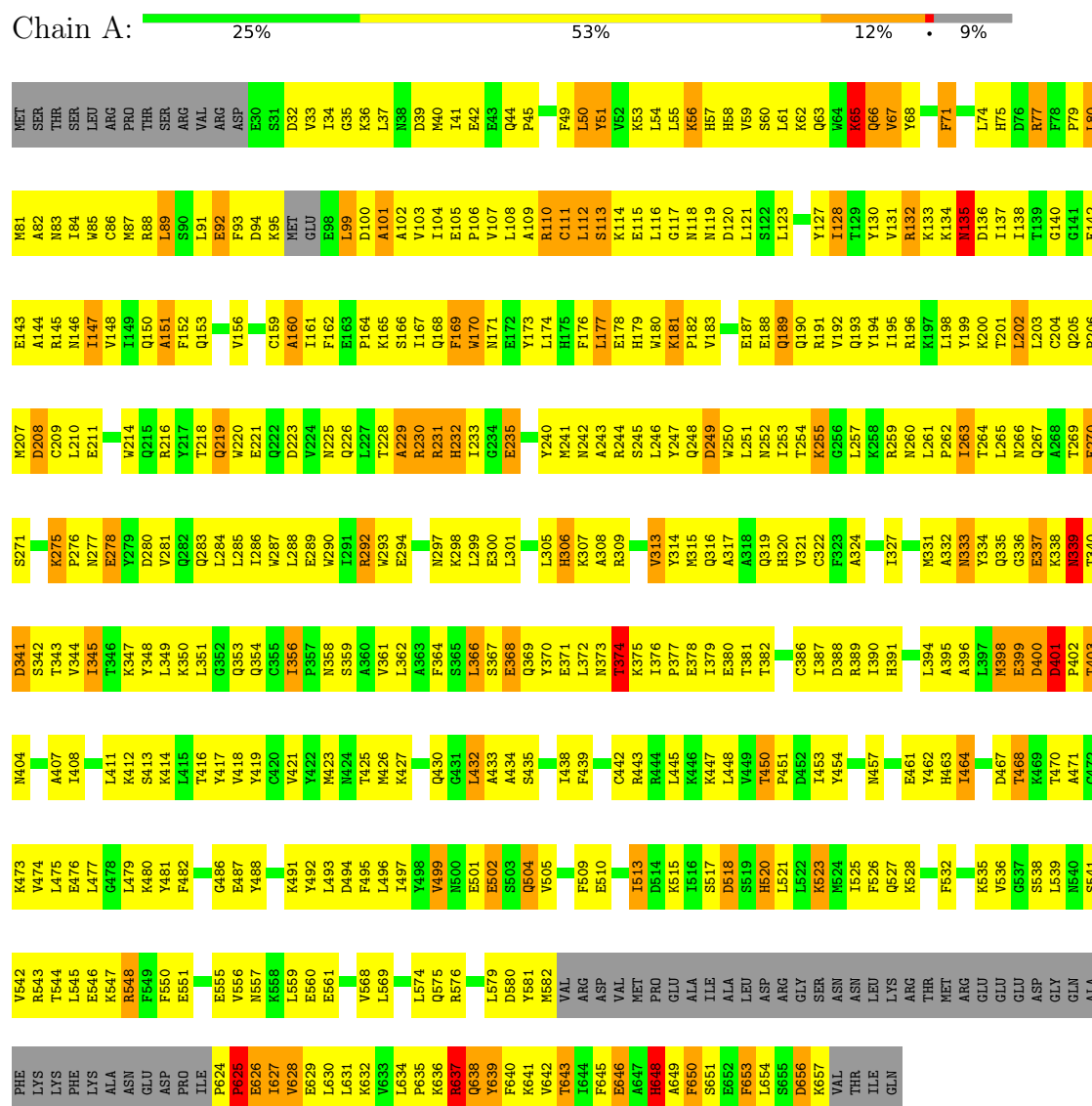
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Chain	Residue	Modelled	Actual	Comment	Reference
H	87	SER	-	expression tag	UNP Q6CKN2
H	88	SER	-	expression tag	UNP Q6CKN2
H	89	HIS	-	expression tag	UNP Q6CKN2
H	90	HIS	-	expression tag	UNP Q6CKN2
H	91	HIS	-	expression tag	UNP Q6CKN2
H	92	HIS	-	expression tag	UNP Q6CKN2
H	93	HIS	-	expression tag	UNP Q6CKN2
H	94	HIS	-	expression tag	UNP Q6CKN2
H	95	SER	-	expression tag	UNP Q6CKN2
H	96	SER	-	expression tag	UNP Q6CKN2
H	97	GLY	-	expression tag	UNP Q6CKN2
H	98	LEU	-	expression tag	UNP Q6CKN2
H	99	VAL	-	expression tag	UNP Q6CKN2
H	100	PRO	-	expression tag	UNP Q6CKN2
H	101	ARG	-	expression tag	UNP Q6CKN2
H	102	GLY	-	expression tag	UNP Q6CKN2
H	103	SER	-	expression tag	UNP Q6CKN2
H	104	HIS	-	expression tag	UNP Q6CKN2

3 Residue-property plots

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.

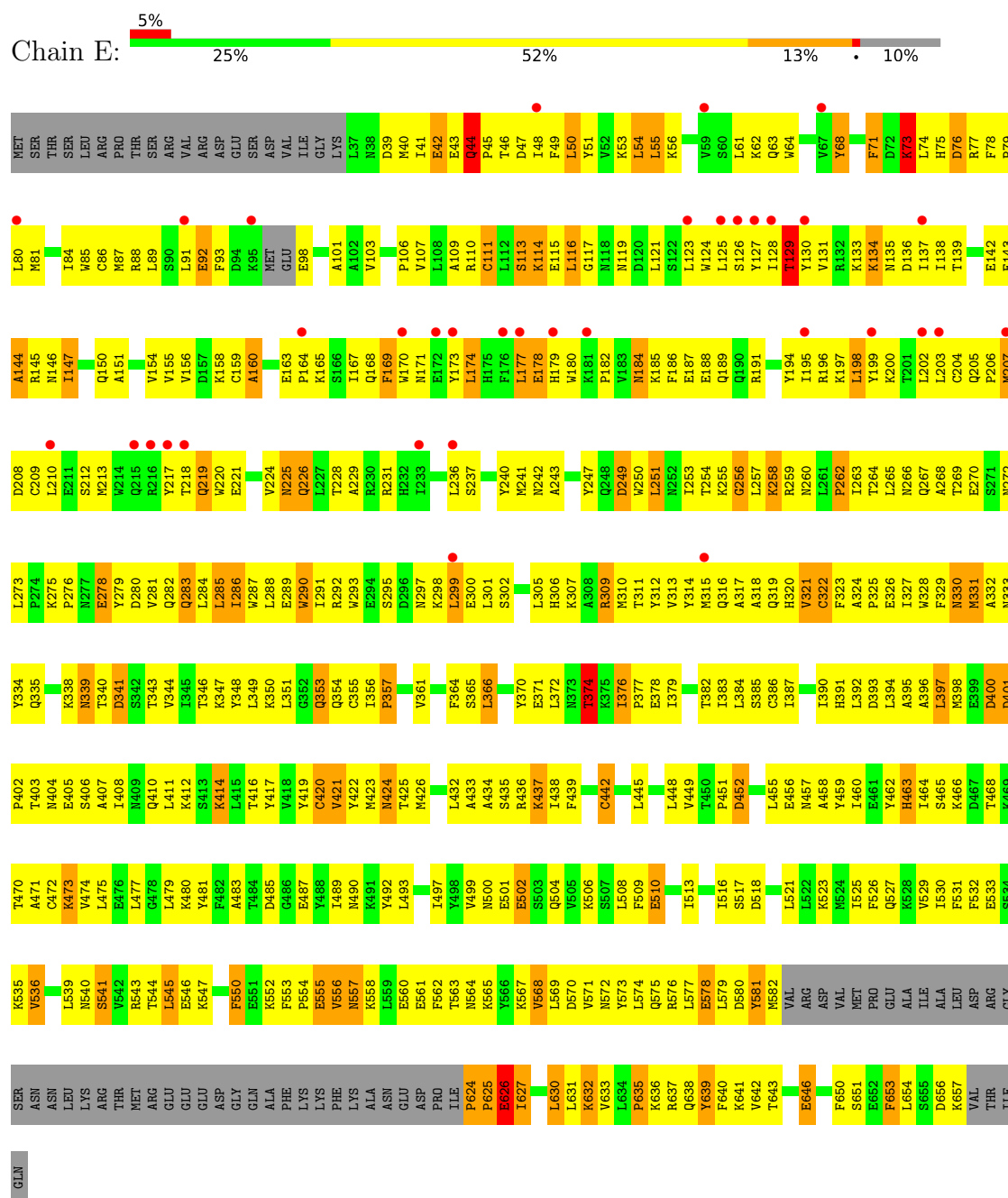
• Molecule 1: mRNA 3'-end-processing protein RNA14



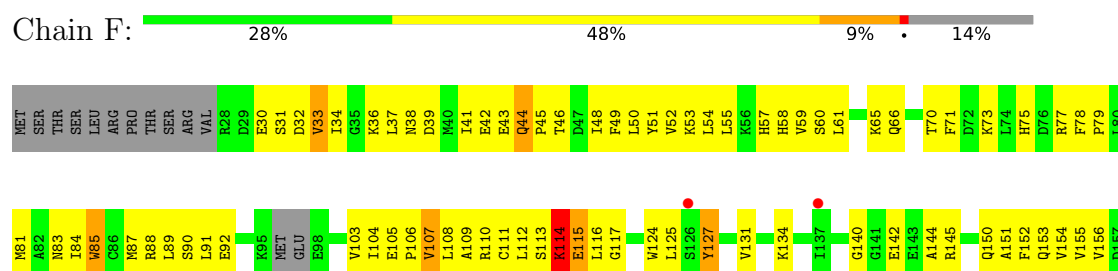
• Molecule 1: mRNA 3'-end-processing protein RNA14



• Molecule 1: mRNA 3'-end-processing protein RNA14



• Molecule 1: mRNA 3'-end-processing protein RNA14



- Molecule 2: Rna15

- Molecule 2: Rna15

- Molecule 2: Rna15

Chain H: 10% 28% 9% 53%

GLU	ASP	GLY	LEU	ASP	GLU	GLU	LYS	VAL	ASP	LEU	LEU	ARG	GLN	VAL	LEU	GLN	LEU	GLN	ASP	SER	ASP	ILE	ALA	MET	LEU	PRO	GLN	ASP	GLU	LYS	MET	ALA	VAL	TRP	GLU	LEU	LYS	GLN	ARG	ALA	MET	LYS	GLY	GLU	PHE	GLY	HIS	LEU								
L147	K148	V149	I150	Q151	H152	F153	C154	K155	D156	ASP	LYS	E159	T160	F161	V162	A163	E166	E167	A168	F169	Q170	L171	S172	Y173	A174	I175	A176	E177	L178	L179	L180	V184	C185	S186	V187	D188	Q189	L190	T191	Q192	L193	A194	MET	ALA	SER	LYS	GLN	ARG	PRO	GLU	GLN	THR	ASP	ASN	THR	VAL
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	SER	PRO	VAL	LEU	ARG	GLY	HIS	MET	VAL	GLU	ASP	VAL	LYS	PHE	P112	W113	L114	P115	V116	G117	V118	D119	V120	H121	I122	T125	T126	M129	C130	I131	S132	S133	E134	L135	G136	K137	L138	Q139	K140	D141	Q142	Q143	F144	A145	L146

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	162.04Å 162.04Å 177.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.79 – 3.30 47.79 – 3.30	Depositor EDS
% Data completeness (in resolution range)	86.4 (47.79-3.30) 86.4 (47.79-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.226 , 0.298 0.226 , 0.298	Depositor DCC
R_{free} test set	3646 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	84.8	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 76.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l 0.038 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30268	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.09% 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](#)

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	0.56	0/4982	1.00	25/6732 (0.4%)
1	B	0.56	0/4747	1.03	26/6416 (0.4%)
1	C	0.47	0/4982	0.95	17/6732 (0.3%)
1	D	0.46	0/4689	0.92	15/6338 (0.2%)
1	E	0.55	0/4931	1.04	31/6664 (0.5%)
1	F	0.51	0/4708	0.96	16/6363 (0.3%)
2	G	0.48	0/626	1.12	3/849 (0.4%)
2	H	0.44	0/626	1.13	6/849 (0.7%)
2	I	0.46	0/626	1.05	6/849 (0.7%)
All	All	0.52	0/30917	0.99	145/41792 (0.3%)

There are no bond length outliers.

The worst 5 of 145 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	SER	N-CA-C	-11.70	95.91	110.88
1	F	38	ASN	N-CA-C	-9.28	101.97	113.38
2	H	129	MET	N-CA-C	-9.27	101.97	113.38
1	C	641	LYS	N-CA-C	-9.13	101.21	111.71
1	F	85	TRP	N-CA-C	-8.85	102.05	113.12

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	4874	0	4885	541	0
1	B	4646	0	4650	429	0
1	C	4874	0	4885	422	0
1	D	4589	0	4591	404	0
1	E	4823	0	4834	536	0
1	F	4608	0	4608	424	0
2	G	618	0	632	83	0
2	H	618	0	632	95	0
2	I	618	0	632	95	0
All	All	30268	0	30349	2905	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 48.

The worst 5 of 2905 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:D:563:THR:HG22	1:D:574:LEU:HD12	1.23	1.17
1:C:557:ASN:HD22	1:C:560:GLU:HB2	1.11	1.16
1:D:468:THR:HG21	1:D:499:VAL:HG11	1.31	1.07
2:G:125:THR:HG23	2:G:129:MET:HE2	1.39	1.04
1:A:345:ILE:H	1:A:345:ILE:HD12	1.19	1.03

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	579/645 (90%)	433 (75%)	110 (19%)	36 (6%)	1	9
1	B	554/645 (86%)	414 (75%)	108 (20%)	32 (6%)	1	9
1	C	579/645 (90%)	435 (75%)	110 (19%)	34 (6%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	547/645 (85%)	398 (73%)	117 (21%)	32 (6%)	1	9
1	E	572/645 (89%)	429 (75%)	106 (18%)	37 (6%)	1	8
1	F	549/645 (85%)	422 (77%)	95 (17%)	32 (6%)	1	9
2	G	77/174 (44%)	57 (74%)	12 (16%)	8 (10%)	0	2
2	H	77/174 (44%)	56 (73%)	12 (16%)	9 (12%)	0	1
2	I	77/174 (44%)	58 (75%)	14 (18%)	5 (6%)	1	8
All	All	3611/4392 (82%)	2702 (75%)	684 (19%)	225 (6%)	1	9

5 of 225 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	A	110	ARG
1	A	135	ASN
1	A	255	LYS
1	A	337	GLU

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	544/598 (91%)	478 (88%)	66 (12%)	5	20
1	B	519/598 (87%)	470 (91%)	49 (9%)	8	30
1	C	544/598 (91%)	505 (93%)	39 (7%)	13	40
1	D	512/598 (86%)	474 (93%)	38 (7%)	13	38
1	E	538/598 (90%)	486 (90%)	52 (10%)	8	28
1	F	514/598 (86%)	476 (93%)	38 (7%)	13	38
2	G	71/154 (46%)	64 (90%)	7 (10%)	7	27
2	H	71/154 (46%)	67 (94%)	4 (6%)	19	47
2	I	71/154 (46%)	65 (92%)	6 (8%)	10	33
All	All	3384/4050 (84%)	3085 (91%)	299 (9%)	9	32

5 of 299 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	463	HIS
2	G	160	THR
1	E	541	SER
1	F	337	GLU
1	B	392	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 172 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	277	ASN
1	F	252	ASN
1	E	330	ASN
1	E	575	GLN
1	F	430	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](#)

There are no ligands in this entry.

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 [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	585/645 (90%)	-0.53	0 100 100	39, 76, 136, 149	0
1	B	558/645 (86%)	-0.55	0 100 100	36, 73, 136, 148	0
1	C	585/645 (90%)	-0.27	4 (0%) 84 70	60, 106, 149, 151	0
1	D	551/645 (85%)	-0.29	0 100 100	58, 104, 149, 151	0
1	E	578/645 (89%)	0.17	35 (6%) 27 18	57, 106, 150, 151	0
1	F	553/645 (85%)	-0.17	3 (0%) 87 76	55, 104, 148, 151	0
2	G	81/174 (46%)	-0.31	0 100 100	63, 102, 138, 151	0
2	H	81/174 (46%)	-0.20	0 100 100	90, 128, 148, 151	0
2	I	81/174 (46%)	-0.16	0 100 100	96, 125, 147, 151	0
All	All	3653/4392 (83%)	-0.27	42 (1%) 78 60	36, 99, 148, 151	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	164	PRO	3.9
1	E	137	ILE	3.9
1	E	233	ILE	3.6
1	E	173	TYR	3.5
1	E	80	LEU	3.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.