



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:31 PM UTC

PDB ID : 6C6K / pdb_00006c6k
Title : Structural basis for preferential recognition of cap 0 RNA by a human IFIT1-IFIT3 protein complex
Authors : Amarasinghe, G.K.; Leung, D.W.; Johnson, B.; Xu, W.
Deposited on : 2018-01-18
Resolution : 2.54 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

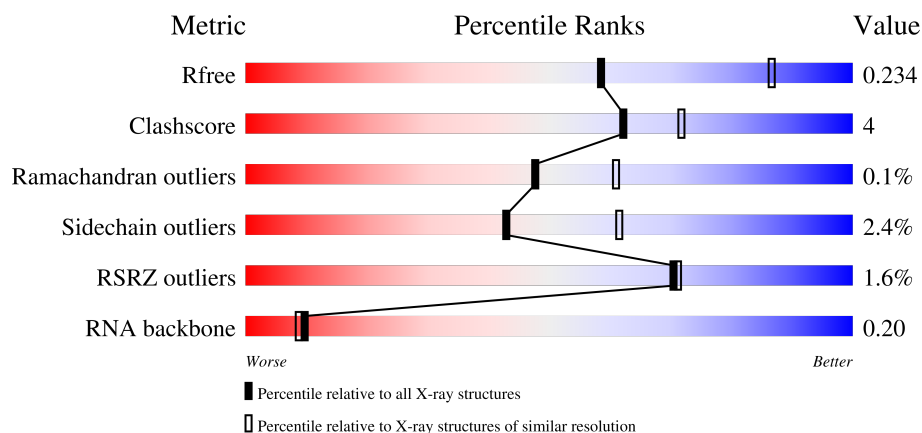
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

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	465	2% 87% 11% .
1	B	465	% 87% 11% .
2	C	44	2% 93% 7%
2	D	44	2% 91% 9%

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Mol	Chain	Length	Quality of chain
3	E	11	9% 36% 36% 27%
3	F	11	9% 45% 45% 9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8993 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 Interferon-induced protein with tetratricopeptide repeats 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	5	0
			3745	2386	648	690	21			
1	B	454	Total	C	N	O	S	0	2	0
			3717	2362	649	685	21			

- Molecule 2 is a protein called Interferon-induced protein with tetratricopeptide repeats 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	44	Total	C	N	O	S	0	0	0
			351	226	61	63	1			
2	D	44	Total	C	N	O	S	0	1	0
			357	230	62	64	1			

- Molecule 3 is a RNA chain called RNA (5'-R((M7G)*P*AP*UP*AP*GP*GP*CP*GP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	11	Total	C	N	O	P	0	0	0
			248	108	48	80	12			
3	F	11	Total	C	N	O	P	0	0	0
			248	108	48	80	12			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	E	3	Total	Mg	0	0
			3	3		

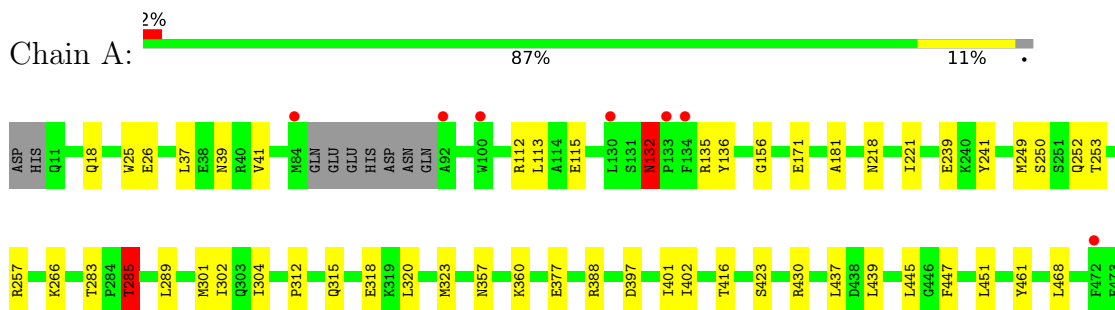
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	141	Total 141	O 141	0	0
5	B	139	Total 139	O 139	0	0
5	C	8	Total 8	O 8	0	0
5	D	6	Total 6	O 6	0	0
5	E	14	Total 14	O 14	0	0
5	F	15	Total 15	O 15	0	0

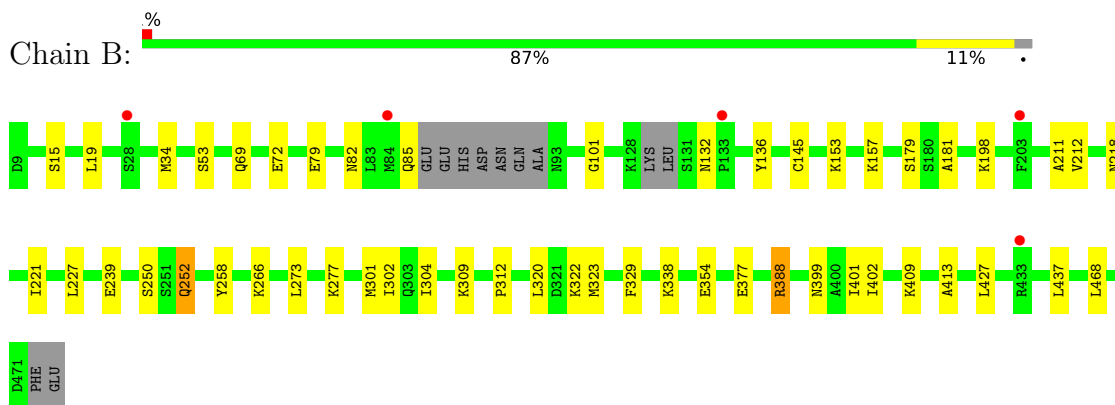
3 Residue-property plots

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.

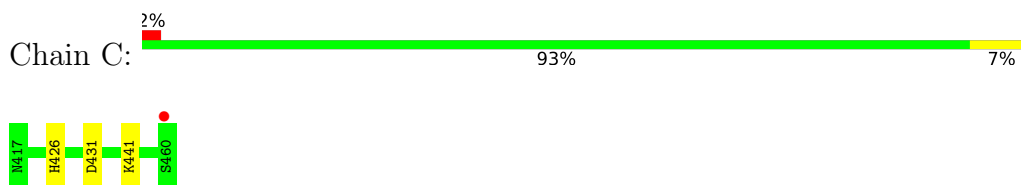
- Molecule 1: Interferon-induced protein with tetratricopeptide repeats 1



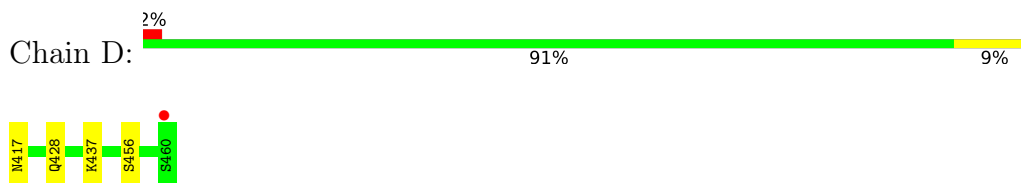
- Molecule 1: Interferon-induced protein with tetratricopeptide repeats 1



- Molecule 2: Interferon-induced protein with tetratricopeptide repeats 3

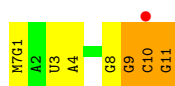


- Molecule 2: Interferon-induced protein with tetratricopeptide repeats 3



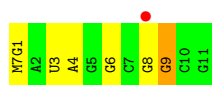
- Molecule 3: RNA (5'-R((M7G)*P*AP*UP*AP*GP*GP*CP*GP*GP*CP*G)-3')

Chain E:  9% 36% 36% 27%



- Molecule 3: RNA (5'-R((M7G)*P*AP*UP*AP*GP*GP*CP*GP*GP*CP*G)-3')

Chain F:  9% 45% 45% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.96Å 80.48Å 88.05Å 79.82° 78.81° 90.04°	Depositor
Resolution (Å)	84.96 – 2.54 84.96 – 2.54	Depositor EDS
% Data completeness (in resolution range)	85.6 (84.96-2.54) 85.7 (84.96-2.54)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.54Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.169 , 0.237 0.175 , 0.234	Depositor DCC
R_{free} test set	1947 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.7	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	0.95	EDS
Total number of atoms	8993	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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: MG, M7G

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	0.93	0/3830	1.05	4/5145 (0.1%)
1	B	0.93	0/3792	1.04	0/5091
2	C	0.83	0/358	0.96	0/481
2	D	0.83	0/367	0.99	0/493
3	E	0.51	0/245	1.04	1/381 (0.3%)
3	F	0.52	0/245	1.09	0/381
All	All	0.90	0/8837	1.04	5/11972 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	U	C4'-C3'-O3'	-6.13	103.80	113.00
1	A	285	THR	N-CA-CB	-5.98	101.62	110.53
1	A	156	GLY	N-CA-C	5.61	119.68	112.83
1	A	132	ASN	CA-C-N	-5.26	113.26	119.84
1	A	132	ASN	C-N-CA	-5.26	113.26	119.84

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	3745	0	3781	39	1
1	B	3717	0	3736	29	1
2	C	351	0	351	1	0
2	D	357	0	359	2	0
3	E	248	0	126	6	0
3	F	248	0	126	4	0
4	B	1	0	0	0	0
4	E	3	0	0	0	0
5	A	141	0	0	4	0
5	B	139	0	0	3	0
5	C	8	0	0	0	0
5	D	6	0	0	1	0
5	E	14	0	0	0	0
5	F	15	0	0	0	0
All	All	8993	0	8479	70	1

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 4.

All (70) 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:B:252:GLN:NE2	5:B:601:HOH:O	1.99	0.95
1:A:252[B]:GLN:HE21	1:A:252[B]:GLN:HA	1.28	0.95
1:A:252[B]:GLN:HA	1:A:252[B]:GLN:NE2	1.90	0.85
1:A:218:ASN:HD21	3:E:1:M7G:HM73	1.45	0.82
1:A:218:ASN:HD21	3:E:1:M7G:CM7	1.96	0.77
1:A:252[B]:GLN:HE21	1:A:252[B]:GLN:CA	1.96	0.74
1:A:388:ARG:NH2	3:E:9:G:N7	2.38	0.71
1:A:241:TYR:OH	5:A:501:HOH:O	2.16	0.62
1:A:257:ARG:NH2	1:A:283[B]:THR:HG21	2.15	0.62
1:B:145:CYS:SG	1:B:179:SER:OG	2.57	0.62
1:B:181:ALA:HB1	1:B:221:ILE:HD11	1.83	0.61
1:A:357:ASN:ND2	1:A:360:LYS:HG3	2.17	0.60
1:A:447:PHE:CE2	1:A:451:LEU:HD11	2.36	0.60
1:A:304:ILE:HD12	1:A:323:MET:HE1	1.88	0.56
1:A:397:ASP:OD2	1:A:430:ARG:NH2	2.37	0.56
1:B:212:VAL:HG23	1:B:221:ILE:HG22	1.87	0.56
1:A:257:ARG:HH21	1:A:283[B]:THR:HG21	1.71	0.55
1:A:304:ILE:HD12	1:A:323:MET:CE	2.37	0.55
1:A:257:ARG:HH21	1:A:283[A]:THR:HG21	1.72	0.54
1:B:69:GLN:HE21	1:B:72:GLU:HG3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LEU:HD13	1:B:101:GLY:HA2	1.89	0.53
1:B:239:GLU:OE1	1:B:266:LYS:HE3	2.09	0.53
1:A:181:ALA:HB1	1:A:221:ILE:HD11	1.91	0.52
1:A:252[A]:GLN:HE21	1:B:329:PHE:HE1	1.57	0.52
1:B:198:LYS:HD2	1:B:413:ALA:HB1	1.90	0.52
1:A:239:GLU:OE1	1:A:266:LYS:HE3	2.11	0.51
1:B:399:ASN:HA	1:B:402:ILE:HD12	1.93	0.50
1:B:211:ALA:HB1	1:B:221:ILE:HD13	1.94	0.50
1:A:283[A]:THR:HG21	5:A:563:HOH:O	2.12	0.50
1:B:401:ILE:HG13	1:B:427:LEU:HD23	1.93	0.50
1:B:212:VAL:CG2	1:B:221:ILE:HG22	2.43	0.49
1:B:377:GLU:HB2	5:B:681:HOH:O	2.12	0.49
1:A:132:ASN:HD22	1:A:132:ASN:N	2.10	0.49
1:A:39:ASN:HB3	1:A:285:THR:CG2	2.43	0.48
1:B:338:LYS:NZ	3:F:3:U:O4	2.47	0.48
1:B:82:ASN:ND2	5:B:612:HOH:O	2.45	0.47
1:B:301:MET:HE2	1:B:302:ILE:HG13	1.97	0.47
1:A:112:ARG:NE	1:A:115:GLU:OE1	2.44	0.47
1:B:227:LEU:HD11	1:B:258:TYR:HB3	1.96	0.47
1:B:15:SER:HB3	1:B:136:TYR:CE2	2.51	0.47
1:A:388:ARG:HD3	5:A:548:HOH:O	2.15	0.46
1:B:218:ASN:HD21	3:F:1:M7G:HM73	1.81	0.46
1:A:285:THR:HB	5:A:565:HOH:O	2.15	0.46
1:B:304:ILE:HD12	1:B:323:MET:HE1	1.99	0.45
1:A:18:GLN:HB2	1:A:136:TYR:HB2	1.98	0.45
1:A:257:ARG:HG2	1:A:289:LEU:HD21	2.00	0.44
2:D:417:ASN:N	5:D:502:HOH:O	2.50	0.44
1:A:249[A]:MET:SD	1:B:329:PHE:HB2	2.58	0.44
3:E:9:G:H1'	3:E:11:G:O4'	2.19	0.43
1:A:301:MET:HE2	1:A:302:ILE:HG13	2.00	0.43
1:B:388:ARG:NH2	3:F:9:G:N7	2.66	0.43
1:A:312:PRO:HG3	1:A:320:LEU:HD22	2.00	0.42
1:A:218:ASN:ND2	3:E:1:M7G:HM73	2.24	0.42
2:C:426:HIS:HB3	2:C:431:ASP:HB2	2.01	0.42
1:B:312:PRO:HG2	1:B:320:LEU:HD22	2.01	0.42
1:B:79:GLU:HG2	2:D:428[B]:GLN:HG2	2.01	0.42
3:E:10:C:H2'	3:E:10:C:O2	2.19	0.42
1:A:37:LEU:O	1:A:41:VAL:HG23	2.20	0.41
1:A:377:GLU:OE1	1:A:416:THR:HG21	2.20	0.41
1:A:25:TRP:O	1:A:26:GLU:C	2.64	0.41
1:A:401:ILE:O	1:A:402:ILE:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:MET:HE3	1:B:34:MET:HB3	1.94	0.41
1:A:437:LEU:HD22	1:A:468:LEU:HD13	2.02	0.41
1:A:445:LEU:HD23	1:A:461:TYR:CE1	2.55	0.41
1:B:153:LYS:NZ	3:F:1:M7G:H5'2	2.35	0.41
1:B:273:LEU:O	1:B:277:LYS:HG2	2.21	0.40
1:B:437:LEU:HD22	1:B:468:LEU:HD13	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLU:OE2	1:B:53:SER:OG[1_455]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	457/465 (98%)	439 (96%)	18 (4%)	0	100	100
1	B	450/465 (97%)	438 (97%)	11 (2%)	1 (0%)	43	56
2	C	42/44 (96%)	42 (100%)	0	0	100	100
2	D	43/44 (98%)	42 (98%)	1 (2%)	0	100	100
All	All	992/1018 (97%)	961 (97%)	30 (3%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	250	SER

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	402/406 (99%)	393 (98%)	9 (2%)	45	64
1	B	398/406 (98%)	389 (98%)	9 (2%)	44	62
2	C	36/36 (100%)	35 (97%)	1 (3%)	38	57
2	D	37/36 (103%)	35 (95%)	2 (5%)	20	30
All	All	873/884 (99%)	852 (98%)	21 (2%)	43	61

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	LEU
1	A	132	ASN
1	A	135	ARG
1	A	171	GLU
1	A	253	THR
1	A	285	THR
1	A	315	GLN
1	A	423	SER
1	A	439	LEU
1	B	85	GLN
1	B	132	ASN
1	B	157	LYS
1	B	252	GLN
1	B	309	LYS
1	B	322	LYS
1	B	354	GLU
1	B	388	ARG
1	B	409	LYS
2	C	441	LYS
2	D	437	LYS
2	D	456	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	125	ASN
1	A	132	ASN
1	A	218	ASN
1	A	300	GLN
1	A	366	GLN
1	A	390	GLN
1	B	215	ASN
1	B	218	ASN
1	B	248	ASN
1	B	300	GLN
1	B	358	HIS
1	B	385	HIS
2	C	428	GLN
2	D	426	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	9/11 (81%)	5 (55%)	1 (11%)
3	F	9/11 (81%)	4 (44%)	0
All	All	18/22 (81%)	9 (50%)	1 (5%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	E	4	A
3	E	8	G
3	E	9	G
3	E	10	C
3	E	11	G
3	F	4	A
3	F	6	G
3	F	8	G
3	F	9	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	E	10	C

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 4 ligands modelled in this entry, 4 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	456/465 (98%)	-0.10	7 (1%) 72 73	14, 36, 76, 127	5 (1%)
1	B	454/465 (97%)	-0.20	5 (1%) 78 79	16, 36, 64, 90	2 (0%)
2	C	44/44 (100%)	-0.02	1 (2%) 61 62	34, 46, 75, 84	0
2	D	44/44 (100%)	0.10	1 (2%) 61 62	20, 45, 65, 81	1 (2%)
3	E	10/11 (90%)	0.43	1 (10%) 12 12	22, 68, 100, 100	0
3	F	10/11 (90%)	0.16	1 (10%) 12 12	23, 69, 95, 99	0
All	All	1018/1040 (97%)	-0.12	16 (1%) 70 71	14, 37, 75, 127	8 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	PHE	5.4
1	A	133	PRO	3.8
1	A	130	LEU	3.2
1	A	92	ALA	3.1
2	D	460	SER	2.9
2	C	460	SER	2.5
1	B	433	ARG	2.5
1	A	472	PHE	2.5
3	E	10	C	2.3
1	B	84	MET	2.2
1	B	203	PHE	2.2
1	B	133	PRO	2.1
3	F	8	G	2.1
1	A	84	MET	2.1
1	A	100	TRP	2.0
1	B	28	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($\text{\AA}^2$)	Q<0.9
4	MG	E	102	1/1	0.91	0.10	53,53,53,53	0
4	MG	E	103	1/1	0.92	0.17	65,65,65,65	0
4	MG	B	501	1/1	0.98	0.20	49,49,49,49	0
4	MG	E	101	1/1	0.98	0.10	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.