



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 01:58 AM UTC

PDB ID : 1QZW / pdb_00001qzw
Title : Crystal structure of the complete core of archaeal SRP and implications for inter-domain communication
Authors : Rosendal, K.R.; Wild, K.; Montoya, G.; Sinning, I.
Deposited on : 2003-09-18
Resolution : 4.10 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
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

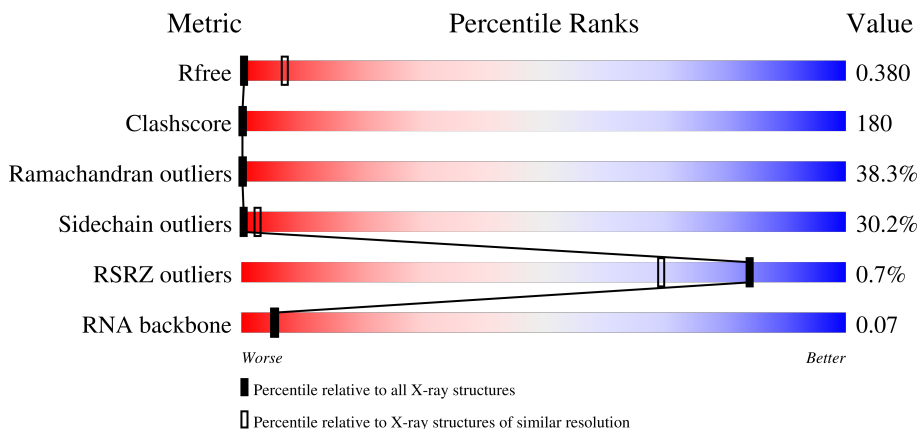
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

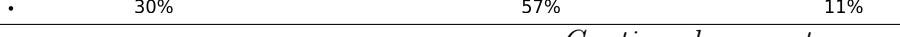
The reported resolution of this entry is 4.10 Å.

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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)
RNA backbone	3983	1026 (5.04-3.10)

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	B	47	
1	D	47	
1	F	47	
1	H	47	

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Mol	Chain	Length	Quality of chain
2	A	440	 37% 46% 13%
2	C	440	 38% 45% 14%
2	E	440	 38% 45% 13%
2	G	440	 38% 45% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	GTP	B	179	X	-	-	-
1	GTP	D	179	X	-	-	-
1	GTP	F	179	X	-	-	-
1	GTP	H	179	X	-	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17720 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 RNA chain called 7S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	47	Total	C	N	O	P	0	0	0
			1031	452	197	332	50			
1	D	47	Total	C	N	O	P	0	0	0
			1031	452	197	332	50			
1	F	47	Total	C	N	O	P	0	0	0
			1031	452	197	332	50			
1	H	47	Total	C	N	O	P	0	0	0
			1031	452	197	332	50			

- Molecule 2 is a protein called Signal recognition 54 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	432	Total	C	N	O	S	0	0	0
			3399	2173	574	637	15			
2	C	432	Total	C	N	O	S	0	0	0
			3399	2173	574	637	15			
2	E	432	Total	C	N	O	S	0	0	0
			3399	2173	574	637	15			
2	G	432	Total	C	N	O	S	0	0	0
			3399	2173	574	637	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q97ZE7
A	-6	GLY	-	expression tag	UNP Q97ZE7
A	-5	HIS	-	expression tag	UNP Q97ZE7
A	-4	HIS	-	expression tag	UNP Q97ZE7
A	-3	HIS	-	expression tag	UNP Q97ZE7
A	-2	HIS	-	expression tag	UNP Q97ZE7
A	-1	HIS	-	expression tag	UNP Q97ZE7
A	0	HIS	-	expression tag	UNP Q97ZE7
C	-7	MET	-	expression tag	UNP Q97ZE7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	expression tag	UNP Q97ZE7
C	-5	HIS	-	expression tag	UNP Q97ZE7
C	-4	HIS	-	expression tag	UNP Q97ZE7
C	-3	HIS	-	expression tag	UNP Q97ZE7
C	-2	HIS	-	expression tag	UNP Q97ZE7
C	-1	HIS	-	expression tag	UNP Q97ZE7
C	0	HIS	-	expression tag	UNP Q97ZE7
E	-7	MET	-	expression tag	UNP Q97ZE7
E	-6	GLY	-	expression tag	UNP Q97ZE7
E	-5	HIS	-	expression tag	UNP Q97ZE7
E	-4	HIS	-	expression tag	UNP Q97ZE7
E	-3	HIS	-	expression tag	UNP Q97ZE7
E	-2	HIS	-	expression tag	UNP Q97ZE7
E	-1	HIS	-	expression tag	UNP Q97ZE7
E	0	HIS	-	expression tag	UNP Q97ZE7
G	-7	MET	-	expression tag	UNP Q97ZE7
G	-6	GLY	-	expression tag	UNP Q97ZE7
G	-5	HIS	-	expression tag	UNP Q97ZE7
G	-4	HIS	-	expression tag	UNP Q97ZE7
G	-3	HIS	-	expression tag	UNP Q97ZE7
G	-2	HIS	-	expression tag	UNP Q97ZE7
G	-1	HIS	-	expression tag	UNP Q97ZE7
G	0	HIS	-	expression tag	UNP Q97ZE7

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: 7S RNA

Chain B: 



• Molecule 1: 7S RNA

Chain D: 



• Molecule 1: 7S RNA

Chain F: 



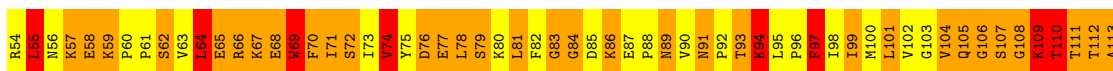
• Molecule 1: 7S RNA

Chain H: 



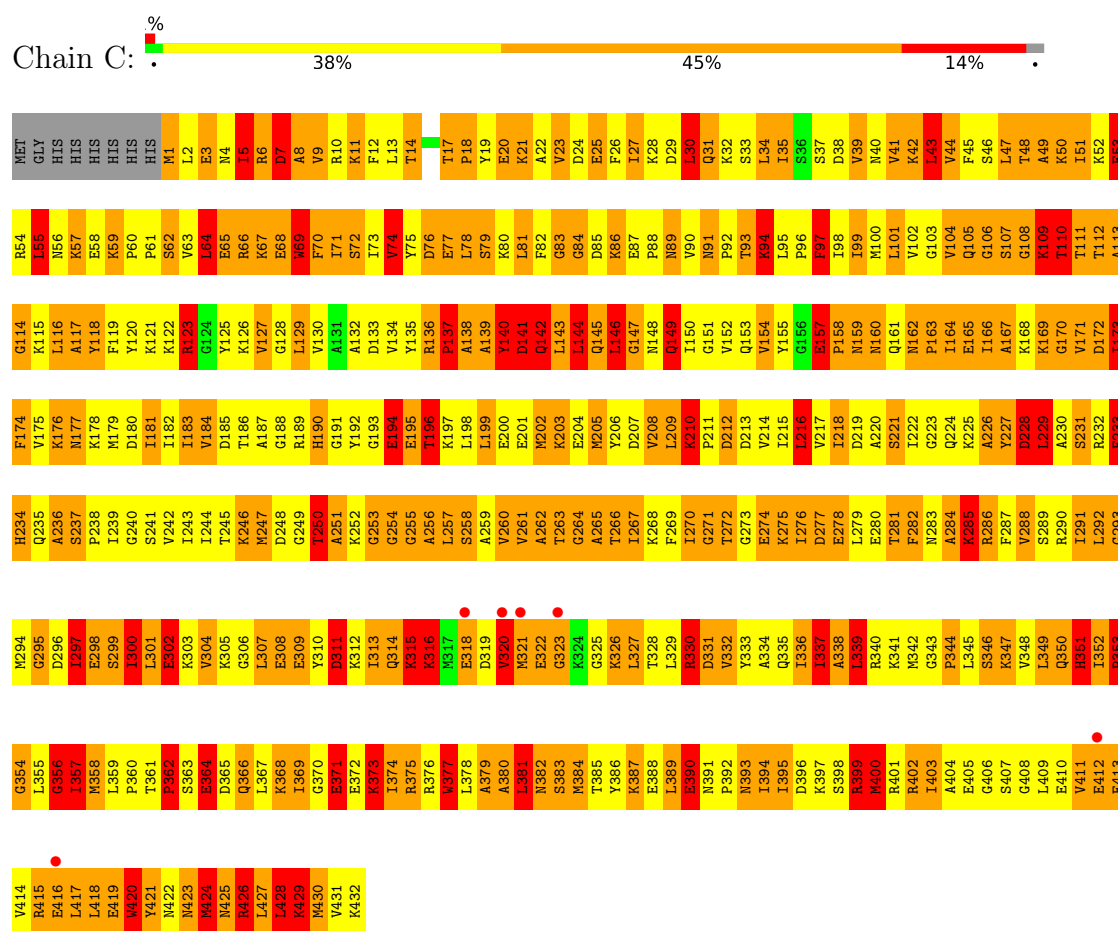
• Molecule 2: Signal recognition 54 kDa protein

Chain A: 

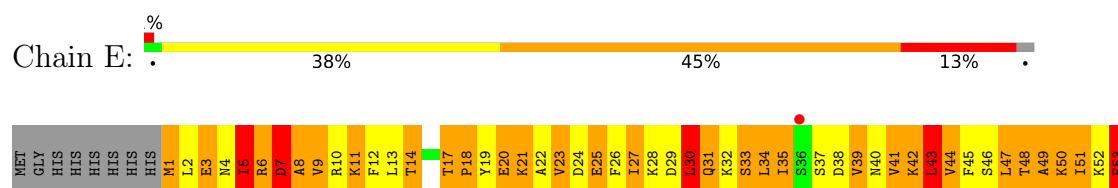


F174	H234	M294	G354	V414
V175	Q235	G295	L355	R415
K176	Q236	D296	G356	E416
N177	S237	I297	I357	L417
K178	P238	E298	M358	L418
M179	T239	S299	L359	E419
D180	G240	I300	P360	R420
I181	S241	L301	T361	Y421
I182	V242	E302	P362	M422
I183	I243	K303	S363	M423
V184	I244	V304	E364	M424
I185	T245	K305	D365	M425
T186	K246	G306	D366	R426
A187	M247	L307	L367	L427
K188	D248	E308	K368	L428
R189	G249	E309	I369	K429
H190	T250	Y310	G370	M430
G191	A251	D311	E371	V431
Y192	K252	K312	E372	K432
G193	G253	I313	K373	
E194	G254	Q314	I374	
E195	G255	K315	R375	
T196	A256	K316	R376	
K197	L257	M317	Y377	
L198	S258	E318	L378	
L199	A259	D319	A379	
E200	V260	R320	A380	
E201	V261	M321	L381	
M202	A262	E322	N382	
K203	T263	G323	S383	
E204	G264	K324	M384	
M205	A265	G325	T385	
Y206	T266	K326	Y386	
D207	I267	L327	K387	
V208	K268	T328	E388	
L209	F269	L329	L389	
K210	I270	R330	E390	
P211	G271	D331	N391	
D212	T272	V332	P392	
D213	G273	Y333	N393	
V214	E274	A334	I394	
I215	K275	Q335	I395	
L216	L276	D336	D396	
V217	D277	K337	K397	
I218	E278	A338	S398	
D219	L279	R399	R399	
A220	E280	R400	R401	
S221	T281	K341	R402	
I222	F282	M342	I403	
G223	N283	G343	A404	
Q224	A284	P344	E405	
K225	R285	L345	G406	
A226	R286	S346	G407	
Y227	F287	K347	S407	
V228	V288	V348	G408	
D229	L229	L349	L409	
A230	R290	Q350	E410	
S231	I291	R351	V411	
R232	L292	I352	E412	
F233	G293	P353	E413	

• Molecule 2: Signal recognition 54 kDa protein



• Molecule 2: Signal recognition 54 kDa protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	137.76Å 137.76Å 307.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.10 30.00 – 4.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-4.10) 98.3 (30.00-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 4.11Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.340 , 0.387 0.348 , 0.380	Depositor DCC
R_{free} test set	4666 reflections (9.26%)	wwPDB-VP
Wilson B-factor (Å ²)	167.7	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 395.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.337 for -h,-k,l 0.339 for h,-h-k,-l 0.377 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17720	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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: GTP, CCC

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	B	0.63	0/1093	1.21	11/1706 (0.6%)
1	D	0.63	0/1093	1.21	11/1706 (0.6%)
1	F	0.63	0/1093	1.21	11/1706 (0.6%)
1	H	0.63	0/1093	1.21	11/1706 (0.6%)
2	A	0.76	0/3450	1.37	63/4636 (1.4%)
2	C	0.76	0/3450	1.37	63/4636 (1.4%)
2	E	0.76	0/3450	1.37	62/4636 (1.3%)
2	G	0.76	0/3450	1.37	62/4636 (1.3%)
All	All	0.73	0/18172	1.33	294/25368 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	D	1	0
1	F	1	0
1	H	1	0
All	All	4	0

There are no bond length outliers.

The worst 5 of 294 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	217	U	C5'-C4'-C3'	-15.93	92.11	116.00
1	F	217	U	C5'-C4'-C3'	-15.90	92.15	116.00
1	B	217	U	C5'-C4'-C3'	-15.89	92.16	116.00
1	D	217	U	C5'-C4'-C3'	-15.88	92.18	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	U	O3'-P-O5'	15.72	127.58	104.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	179	GTP	C3'
1	D	179	GTP	C3'
1	F	179	GTP	C3'
1	H	179	GTP	C3'

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	B	1031	0	514	95	1
1	D	1031	0	514	94	0
1	F	1031	0	514	92	1
1	H	1031	0	514	92	1
2	A	3399	0	3543	1448	5
2	C	3399	0	3543	1483	15
2	E	3399	0	3543	1492	17
2	G	3399	0	3543	1438	4
All	All	17720	0	16228	6119	22

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 180.

The worst 5 of 6119 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)
2:A:59:LYS:O	2:A:59:LYS:HD3	1.18	1.34
2:A:151:GLY:HA2	2:G:151:GLY:CA	1.68	1.23
2:A:151:GLY:CA	2:G:151:GLY:HA2	1.73	1.18
2:C:177:ASN:CG	2:E:144:LEU:CD1	2.18	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:48:THR:HA	2:E:51:ILE:HD12	1.29	1.15

The worst 5 of 22 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)
2:C:59:LYS:O	2:E:361:THR:O[2_655]	1.08	1.12
2:C:315:LYS:CG	2:E:312:LYS:NZ[2_655]	1.56	0.64
2:C:61:PRO:CB	2:E:359:LEU:O[2_655]	1.59	0.61
2:C:361:THR:O	2:E:59:LYS:O[2_655]	1.59	0.61
2:A:59:LYS:CD	2:G:361:THR:O[2_665]	1.73	0.47

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	
2	A	430/440 (98%)	142 (33%)	123 (29%)	165 (38%)	0	0
2	C	430/440 (98%)	143 (33%)	123 (29%)	164 (38%)	0	0
2	E	430/440 (98%)	143 (33%)	122 (28%)	165 (38%)	0	0
2	G	430/440 (98%)	142 (33%)	123 (29%)	165 (38%)	0	0
All	All	1720/1760 (98%)	570 (33%)	491 (28%)	659 (38%)	0	0

5 of 659 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	18	PRO
2	A	20	GLU
2	A	23	VAL
2	A	33	SER
2	A	39	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	
2	A	370/377 (98%)	258 (70%)	112 (30%)	0	2
2	C	370/377 (98%)	257 (70%)	113 (30%)	0	2
2	E	370/377 (98%)	259 (70%)	111 (30%)	0	3
2	G	370/377 (98%)	259 (70%)	111 (30%)	0	3
All	All	1480/1508 (98%)	1033 (70%)	447 (30%)	0	3

5 of 447 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	31	GLN
2	G	427	LEU
2	E	266	THR
2	G	420	TRP
2	G	277	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	31	GLN
2	G	425	ASN
2	E	177	ASN
2	G	351	HIS
2	G	177	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	46/47 (97%)	31 (67%)	3 (6%)
1	D	46/47 (97%)	31 (67%)	3 (6%)
1	F	46/47 (97%)	31 (67%)	3 (6%)
1	H	46/47 (97%)	31 (67%)	3 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	184/188 (97%)	124 (67%)	12 (6%)

5 of 124 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	181	C
1	B	182	C
1	B	184	G
1	B	185	G
1	B	186	G

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	F	210	G
1	F	217	U
1	H	217	U
1	H	179	GTP
1	D	179	GTP

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are 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
1	GTP	D	179	1	33,34,34	4.55	4 (12%)	50,54,54	1.87	11 (22%)
1	GTP	H	179	1	33,34,34	4.53	4 (12%)	50,54,54	1.87	10 (20%)
1	CCC	D	225	1	20,25,26	0.61	0	27,38,41	1.19	3 (11%)
1	GTP	F	179	1	33,34,34	4.54	4 (12%)	50,54,54	1.87	11 (22%)
1	CCC	H	225	1	20,25,26	0.62	0	27,38,41	1.19	3 (11%)
1	CCC	F	225	1	20,25,26	0.62	0	27,38,41	1.19	3 (11%)
1	GTP	B	179	1	33,34,34	4.53	4 (12%)	50,54,54	1.87	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CCC	B	225	1	20,25,26	0.62	0	27,38,41	1.19	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GTP	D	179	1	1/1/7/7	4/22/38/38	0/3/3/3
1	GTP	H	179	1	1/1/7/7	4/22/38/38	0/3/3/3
1	CCC	D	225	1	-	7/7/35/36	0/3/3/3
1	GTP	F	179	1	1/1/7/7	4/22/38/38	0/3/3/3
1	CCC	H	225	1	-	7/7/35/36	0/3/3/3
1	CCC	F	225	1	-	7/7/35/36	0/3/3/3
1	GTP	B	179	1	1/1/7/7	4/22/38/38	0/3/3/3
1	CCC	B	225	1	-	7/7/35/36	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	179	GTP	PB-O3A	-24.88	1.32	1.59
1	F	179	GTP	PB-O3A	-24.85	1.32	1.59
1	B	179	GTP	PB-O3A	-24.81	1.32	1.59
1	H	179	GTP	PB-O3A	-24.81	1.32	1.59
1	F	179	GTP	PB-O3B	-5.73	1.53	1.59

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	GTP	O3G-PG-O2G	6.51	132.21	107.80
1	D	179	GTP	O3G-PG-O2G	6.51	132.20	107.80
1	F	179	GTP	O3G-PG-O2G	6.51	132.20	107.80
1	H	179	GTP	O3G-PG-O2G	6.50	132.19	107.80
1	F	179	GTP	O3A-PB-O1B	-5.32	94.71	110.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	179	GTP	C3'
1	D	179	GTP	C3'

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Mol	Chain	Res	Type	Atom
1	F	179	GTP	C3'
1	H	179	GTP	C3'

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	179	GTP	C5'-O5'-PA-O3A
1	B	179	GTP	C5'-O5'-PA-O1A
1	B	225	CCC	O4'-C1'-N1-C2
1	B	225	CCC	O4'-C1'-N1-C6
1	B	225	CCC	C2'-C1'-N1-C2

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	179	GTP	2	0
1	H	179	GTP	2	0
1	D	225	CCC	1	0
1	F	179	GTP	2	0
1	H	225	CCC	1	0
1	F	225	CCC	1	0
1	B	179	GTP	2	0
1	B	225	CCC	1	0

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 ⓘ

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	B	45/47 (95%)	-0.54	0 100 100	71, 71, 71, 71	0
1	D	45/47 (95%)	-0.53	0 100 100	71, 71, 71, 71	0
1	F	45/47 (95%)	-0.58	0 100 100	71, 71, 71, 71	0
1	H	45/47 (95%)	-0.61	0 100 100	71, 71, 71, 71	0
2	A	432/440 (98%)	-0.61	0 100 100	71, 71, 71, 71	0
2	C	432/440 (98%)	-0.55	6 (1%) 73 56	71, 71, 71, 71	0
2	E	432/440 (98%)	-0.52	6 (1%) 73 56	71, 71, 71, 71	0
2	G	432/440 (98%)	-0.58	1 (0%) 91 82	71, 71, 71, 71	0
All	All	1908/1948 (97%)	-0.56	13 (0%) 84 69	71, 71, 71, 71	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	321	MET	4.3
2	E	320	VAL	4.2
2	C	323	GLY	3.9
2	C	320	VAL	3.5
2	E	319	ASP	3.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	CCC	D	225	23/24	0.93	0.09	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CCC	F	225	23/24	0.95	0.07	70,70,70,70	0
1	GTP	F	179	32/32	0.96	0.06	70,70,70,70	0
1	GTP	D	179	32/32	0.96	0.09	70,70,70,70	0
1	GTP	B	179	32/32	0.97	0.08	70,70,70,70	0
1	CCC	B	225	23/24	0.97	0.05	70,70,70,70	0
1	GTP	H	179	32/32	0.97	0.09	70,70,70,70	0
1	CCC	H	225	23/24	0.97	0.06	70,70,70,70	0

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.