



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 06:04 am BST

PDB ID : 1QZW
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

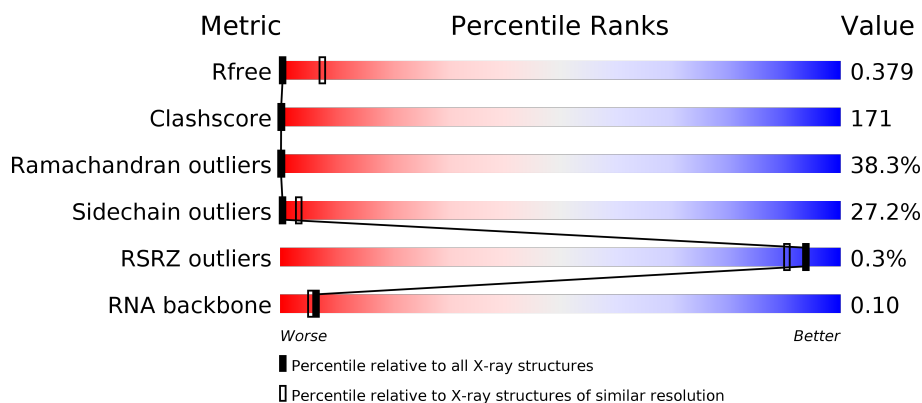
1 Overall quality at a glance ⓘ

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}	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)
RNA backbone	3102	1049 (5.04-3.00)

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 on 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	<div> <div></div> <div> <div></div> <div>32%</div> <div>60%</div> <div>6%</div> </div> </div>
1	D	47	<div> <div></div> <div> <div></div> <div>32%</div> <div>57%</div> <div>6%</div> </div> </div>
1	F	47	<div> <div></div> <div> <div></div> <div>32%</div> <div>60%</div> <div>6%</div> </div> </div>
1	H	47	<div> <div></div> <div> <div></div> <div>32%</div> <div>57%</div> <div>6%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	A	440	45% 41% 9%
2	C	440	45% 41% 9%
2	E	440	45% 41% 9%
2	G	440	45% 40% 9%

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

Continued on next page...

Continued from previous page...

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 and DNA 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: 



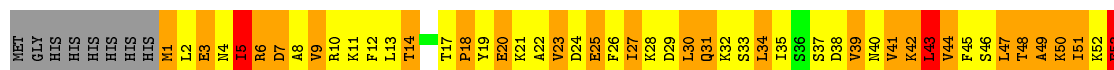
• Molecule 1: 7S RNA

Chain H: 



• Molecule 2: Signal recognition 54 kDa protein

Chain A: 



V175	Q235	G295	G356	E416
K176	A236	D296	I357	L417
M177	S237	I297	R358	L418
K178	P238	E298	H15	E419
M179	I239	L359	H15	E420
D180	G240	S299	H15	E421
I181	S241	I300	T361	E422
I182	I242	L301	P362	E423
I183	I243	S302	S363	E424
D184	I244	K303	E364	E425
D185	T245	V304	G365	E426
L186	T246	K305	Q366	E427
A187	K247	G306	L367	E428
A188	K248	L307	K368	E429
G188	I249	E308	I369	E430
R189	G249	E309	G370	E431
H190	T250	Y310	E371	E432
G191	A251	D311	K372	K432
Y192	K252	K312	E373	
G193	G253	I313	I374	
E194	G254	Q314	R375	
E195	G255	K315	R376	
T196	A256	R316	W377	
K197	L257	M317	L378	
L198	S258	E318	A379	
L199	A259	D319	A380	
E200	V260	V320	L381	
E201	V261	M321	N382	
M202	A262	E322	S383	
K203	T263	G323	N384	
E204	G264	T385	T386	
M205	A265	G386	D24	
D206	T266	K387	E25	
D207	I267	E388	F26	
V208	K268	L389	E37	
L209	F269	R390	K28	
K210	I270	D391	N391	
P211	G271	V392	P392	
D212	T272	X393	N393	
D213	G273	A394	I394	
V214	E274	Q395	I395	
I215	K275	D396	D396	
L216	I276	K397	K397	
V217	D277	A398	S398	
L218	E278	L399	R399	
D219	L279	R340	M400	
A220	E280	R341	R401	
S221	T281	M342	R402	
I222	F282	G343	I403	
G223	N283	A404	A404	
Q224	A284	E405	E405	
K225	R285	S346	G406	
A226	R286	R347	S407	
Y227	F287	V348	G408	
D228	V288	L349	L409	
L229	S289	Q350	E410	
A230	R290	H351	V411	
S231	I291	I352	E412	
R232	L292	P353	E413	
F233	G293	V414	V414	
H234	M294	L355	R415	

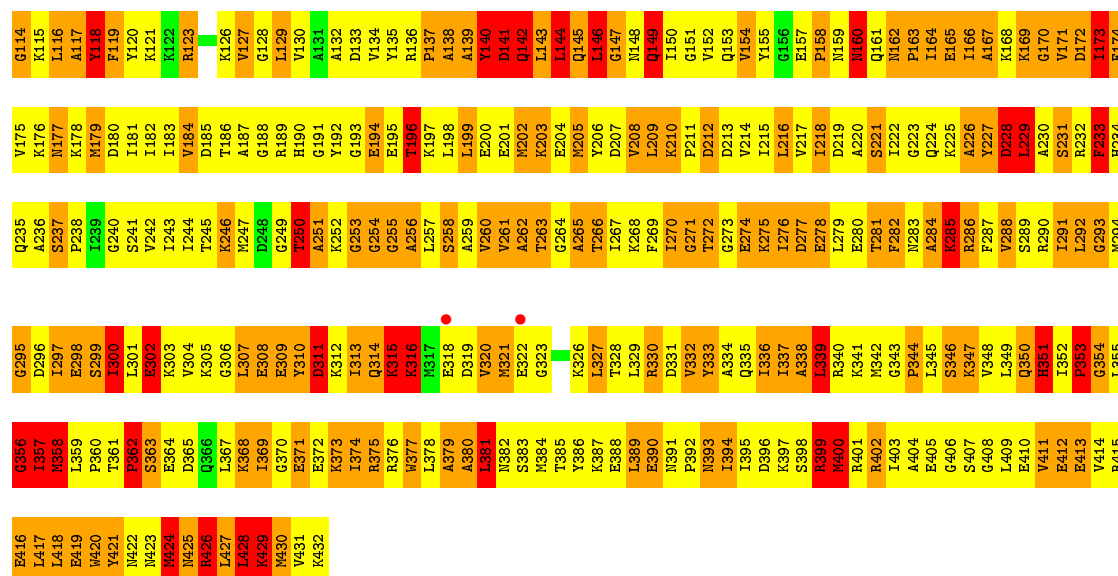
• Molecule 2: Signal recognition 54 kDa protein



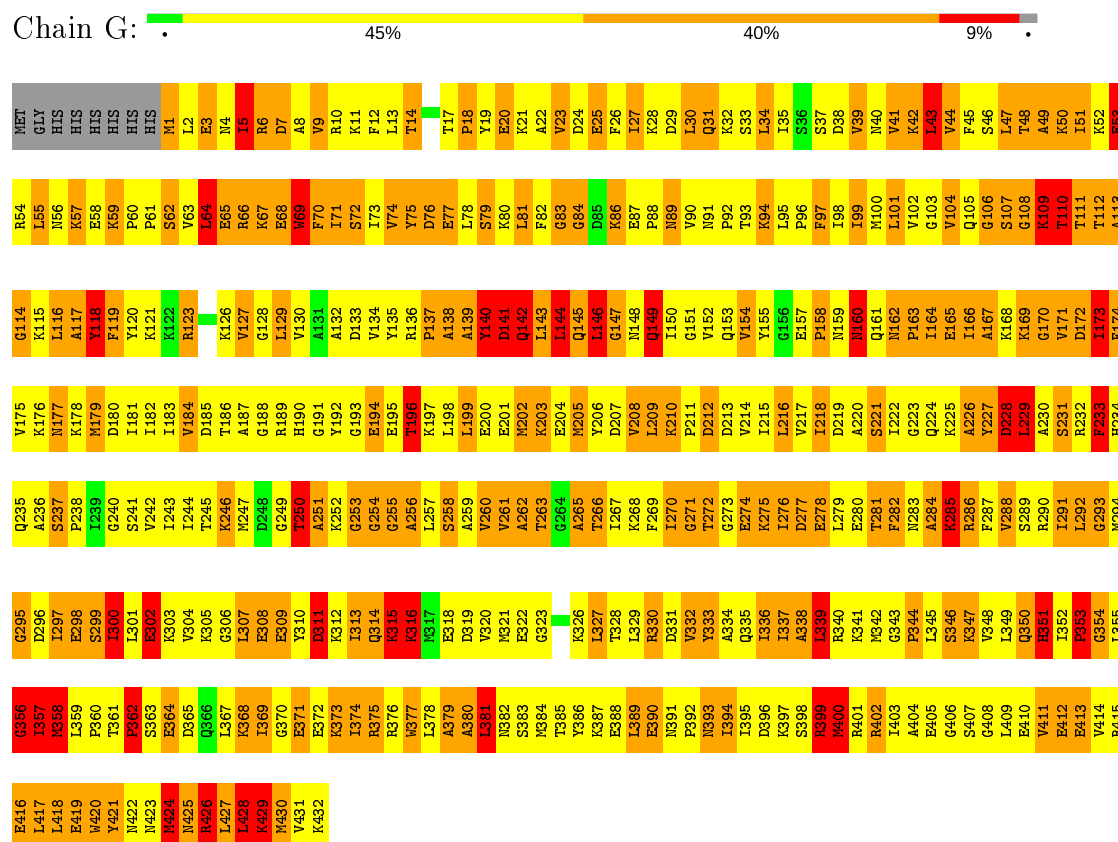
WET	GLY	GLY	G114	B54	V175	Q235	G295	G356	E416
HIS	HIS	HIS	K115	L55	K176	A236	D296	I357	L417
HIS	HIS	HIS	A117	L56	M177	S237	I297	R358	L418
HIS	HIS	HIS	E57	L57	D178	P238	E298	H15	E419
HIS	HIS	HIS	F118	E58	M179	I239	S299	P360	E420
HIS	HIS	HIS	F119	E59	D180	G240	I300	T361	E421
HIS	HIS	HIS	F120	P60	I181	S241	L301	P362	E422
HIS	HIS	HIS	K122	P61	I182	I242	S302	S363	E423
M1	L2	L2	K123	S62	I183	I243	K303	E364	E424
E3	E3	E3	L64	L64	D184	I244	V304	G365	E425
N4	N4	N4	B65	B65	L186	T245	K305	Q366	E426
I5	I5	I5	V127	B66	A187	K246	G306	L367	E427
R6	R6	R6	G128	K67	G188	K247	L307	K368	E428
D7	D7	D7	G129	E68	R189	I248	E308	I369	E429
A8	A8	A8	V130	E69	H190	G249	Y310	G370	E430
V9	V9	V9	A131	F70	H191	T250	D311	E371	E431
R10	R10	R10	A132	I71	Y192	K251	K312	E372	E432
K11	K11	K11	D133	S72	G193	K252	I313	E373	
F12	F12	F12	V134	I73	E194	G253	Q314	I374	
L13	L13	L13	Y135	V74	E195	G254	R315	R375	
T14	T14	T14	R136	Y75	T196	A256	K316	W377	
T17	T17	T17	P137	D76	K197	L257	M317	L378	
P18	P18	P18	A138	E77	L198	S258	E318	A379	
Y19	Y19	Y19	A139	L78	L199	A259	D319	A380	
E20	E20	E20	Y140	S79	E200	V260	V320	L381	
K21	K21	K21	D141	R80	E201	V261	M321	N382	
A22	A22	A22	E142	L81	M202	A262	E322	S383	
G23	G23	G23	L143	F82	K203	T263	G323	N384	
D24	D24	D24	L144	G83	E204	G264	T385	T386	
E25	E25	E25	Q145	G84	M205	A265	G386	D24	
F26	F26	F26	L146	R85	Y206	T266	K387	E25	
I27	I27	I27	G147	R86	D207	I267	E388	F26	
K28	K28	K28	N148	E37	V208	K268	L389	E37	
D29	D29	D29	Q149	P88	L209	F269	R390	K28	
L30	L30	L30	I150	N89	K210	I270	D391	N391	
Q31	Q31	Q31	G151	V90	P211	G271	V392	P392	
K32	K32	K32	V152	N91	D212	T272	X393	N393	
S33	S33	S33	Q153	P92	D213	G273	A394	I394	
L34	L34	L34	V154	T93	V214	E274	Q395	I395	
I35	I35	I35	Y155	R94	L215	K275	D396	D396	
P96	P96	P96	G156	L95	L216	I276	K397	K397	
S37	S37	S37	E157	P96	V217	D277	A398	S398	
D38	D38	D38	P158	P97	L218	E278	L399	R399	
V39	V39	V39	N159	I98	D219	L279	R340	M400	
M100	M100	M100	N160	I99	A220	E280	R341	R401	
L101	L101	L101	Q161	N100	S221	T281	M342	R402	
V102	V102	V102	N162	L101	I222	F282	G343	I403	
G103	G103	G103	P163	K42	G223	N283	A404	A404	
V104	V104	V104	L164	G103	Q224	A284	E405	E405	
Q105	Q105	Q105	E165	V104	K225	R285	S346	G406	
S46	S46	S46	I166	F45	A226	R286	R347	S407	
L47	L47	L47	A167	S46	Y227	F287	V348	G408	
T48	T48	T48	K168	S107	D228	V288	L349	L409	
K109	K109	K109	K169	G108	S289	R290	Q350	E410	
T110	T110	T110	G170	E109	L229	R290	H351	V411	
T111	T111	T111	V171	K50	S231	I291	I352	E412	
K52	K52	K52	I172	L51	R232	L292	P353	E413	
E53	E53	E53	I173	T112	F233	G293	V414	V414	
			F174	A113	H234	M294	R415	R415	

• 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	137.76 Å 137.76 Å 307.89 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.10 29.81 – 4.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-4.10) 98.3 (29.81-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 4.11 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.340 , 0.387 0.348 , 0.379	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)	0.21 , 98.9	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	0.89	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.88	0/1093	1.14	7/1706 (0.4%)
1	D	0.88	0/1093	1.14	7/1706 (0.4%)
1	F	0.88	0/1093	1.14	7/1706 (0.4%)
1	H	0.88	0/1093	1.14	7/1706 (0.4%)
2	A	0.63	0/3450	0.95	7/4636 (0.2%)
2	C	0.62	0/3450	0.96	7/4636 (0.2%)
2	E	0.62	0/3450	0.95	7/4636 (0.2%)
2	G	0.63	0/3450	0.95	7/4636 (0.2%)
All	All	0.69	0/18172	1.01	56/25368 (0.2%)

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 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	217	U	C5'-C4'-C3'	-14.93	92.11	116.00
1	F	217	U	C5'-C4'-C3'	-14.90	92.15	116.00
1	B	217	U	C5'-C4'-C3'	-14.90	92.16	116.00
1	D	217	U	C5'-C4'-C3'	-14.89	92.18	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	U	N1-C1'-C2'	13.30	131.29	114.00

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	96	1
1	D	1031	0	514	94	0
1	F	1031	0	514	93	1
1	H	1031	0	514	92	1
2	A	3399	0	3543	1366	5
2	C	3399	0	3543	1401	15
2	E	3399	0	3543	1413	17
2	G	3399	0	3543	1356	4
All	All	17720	0	16228	5797	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 171.

The worst 5 of 5797 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:HD3	2:A:59:LYS:O	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:E:48:THR:HA	2:E:51:ILE:HD12	1.29	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:153:GLN:HG3	2:E:153:GLN:CG	1.76	1.14

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 [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	
2	A	370/377 (98%)	270 (73%)	100 (27%)	0	3
2	C	370/377 (98%)	269 (73%)	101 (27%)	0	3
2	E	370/377 (98%)	269 (73%)	101 (27%)	0	3
2	G	370/377 (98%)	270 (73%)	100 (27%)	0	3
All	All	1480/1508 (98%)	1078 (73%)	402 (27%)	0	3

5 of 402 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	362	PRO
2	E	101	LEU
2	G	319	ASP
2	C	393	ASN
2	E	7	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	350	GLN
2	E	153	GLN
2	G	283	ASN
2	C	351	HIS
2	E	31	GLN

5.3.3 RNA [i](#)

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%)

Continued on next page...

Continued from previous page...

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	D	217	U
1	F	179	GTP
1	H	179	GTP
1	D	210	G
1	F	217	U

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	CCC	H	225	1	16,25,26	0.94	0	18,38,41	1.80	5 (27%)
1	CCC	F	225	1	16,25,26	0.95	0	18,38,41	1.81	5 (27%)
1	CCC	D	225	1	16,25,26	0.94	0	18,38,41	1.81	5 (27%)
1	CCC	B	225	1	16,25,26	0.94	0	18,38,41	1.81	5 (27%)
1	GTP	H	179	1	26,34,34	1.44	3 (11%)	33,54,54	2.85	12 (36%)
1	GTP	D	179	1	26,34,34	1.44	3 (11%)	33,54,54	2.84	12 (36%)
1	GTP	F	179	1	26,34,34	1.44	3 (11%)	33,54,54	2.85	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GTP	B	179	1	26,34,34	1.44	3 (11%)	33,54,54	2.84	12 (36%)

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	CCC	H	225	1	-	3/5/35/36	0/3/3/3
1	CCC	F	225	1	-	3/5/35/36	0/3/3/3
1	CCC	D	225	1	-	3/5/35/36	0/3/3/3
1	CCC	B	225	1	-	3/5/35/36	0/3/3/3
1	GTP	H	179	1	1/1/7/7	4/18/38/38	0/3/3/3
1	GTP	D	179	1	1/1/7/7	4/18/38/38	0/3/3/3
1	GTP	F	179	1	1/1/7/7	4/18/38/38	0/3/3/3
1	GTP	B	179	1	1/1/7/7	4/18/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	179	GTP	C6-N1	4.20	1.40	1.33
1	B	179	GTP	C6-N1	4.20	1.40	1.33
1	F	179	GTP	C6-N1	4.18	1.40	1.33
1	H	179	GTP	C6-N1	4.17	1.40	1.33
1	H	179	GTP	PG-O1G	3.02	1.60	1.50

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	179	GTP	C5-C6-N1	-8.81	111.38	123.43
1	B	179	GTP	C5-C6-N1	-8.81	111.38	123.43
1	H	179	GTP	C5-C6-N1	-8.80	111.39	123.43
1	F	179	GTP	C5-C6-N1	-8.80	111.39	123.43
1	F	179	GTP	PA-O3A-PB	-6.49	110.54	132.83

All (4) chirality outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	225	CCC	O4'-C4'-C5'-O5'
1	F	225	CCC	O4'-C4'-C5'-O5'
1	D	225	CCC	O4'-C4'-C5'-O5'
1	B	225	CCC	O4'-C4'-C5'-O5'
1	H	179	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

8 monomers are involved in 12 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	B	45/47 (95%)	-0.26	0 100 100	71, 71, 71, 71	0
1	D	45/47 (95%)	-0.22	0 100 100	71, 71, 71, 71	0
1	F	45/47 (95%)	-0.27	0 100 100	71, 71, 71, 71	0
1	H	45/47 (95%)	-0.31	0 100 100	71, 71, 71, 71	0
2	A	432/440 (98%)	-0.66	0 100 100	71, 71, 71, 71	0
2	C	432/440 (98%)	-0.66	3 (0%) 87 82	71, 71, 71, 71	0
2	E	432/440 (98%)	-0.66	2 (0%) 91 85	71, 71, 71, 71	0
2	G	432/440 (98%)	-0.65	0 100 100	71, 71, 71, 71	0
All	All	1908/1948 (97%)	-0.62	5 (0%) 94 90	71, 71, 71, 71	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	323	GLY	3.1
2	E	318	GLU	2.7
2	C	318	GLU	2.3
2	C	322	GLU	2.1
2	E	322	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CCC	B	225	23/24	0.84	0.23	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CCC	H	225	23/24	0.88	0.27	70,70,70,70	0
1	CCC	D	225	23/24	0.89	0.23	70,70,70,70	0
1	GTP	D	179	32/32	0.89	0.14	70,70,70,70	0
1	CCC	F	225	23/24	0.91	0.25	70,70,70,70	0
1	GTP	F	179	32/32	0.92	0.12	70,70,70,70	0
1	GTP	H	179	32/32	0.93	0.12	70,70,70,70	0
1	GTP	B	179	32/32	0.93	0.11	70,70,70,70	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.