W O R L D W I D E
wwPDB
P R O T E I N D A T A B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 11:41 am GMT

PDB ID	:	5M73
Title	:	Structure of the human SRP S domain with SRP72 RNA-binding domain
Authors	:	Becker, M.M.M.; Wild, K.; Sinning, I.
Deposited on	:	2016-10-26
Resolution	:	3.40 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 3.40 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	Percentile Ranks	Value
Rfree		0.280
Clashscore		23
Ramachandran outliers		2.4%
Sidechain outliers		6.3%
RSRZ outliers		4.2%
RNA backbone		0.43

Worse ▪ *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
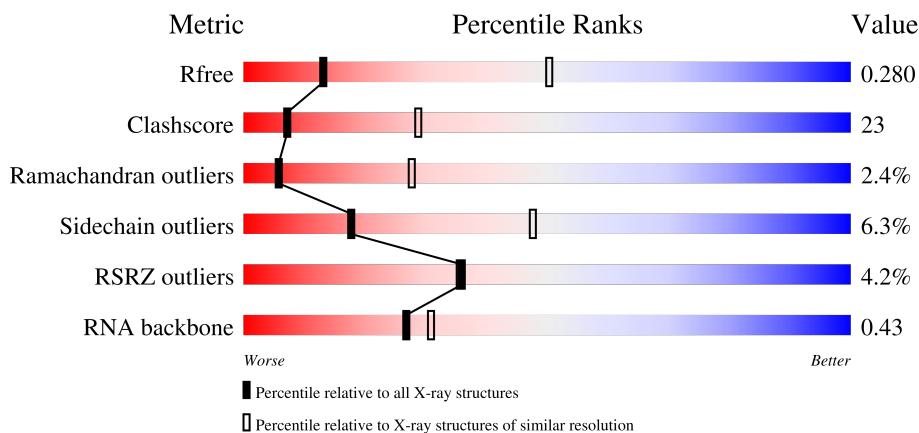
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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 <=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	145	16% 57% 22% 6%
1	E	145	24% 52% 18% 6%
2	B	128	55% 28% • 16%
2	F	128	14% 51% 27% • 19%

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Mol	Chain	Length	Quality of chain
3	C	203	62% · · 32%
3	G	203	63% · · 32%
4	D	158	4% 8% 15% 6% · 70%
4	H	158	8% 8% 13% 5% · 74%
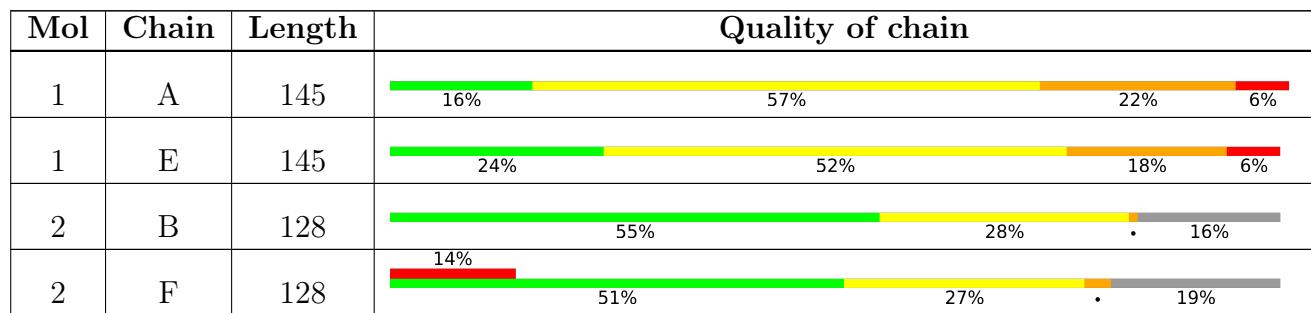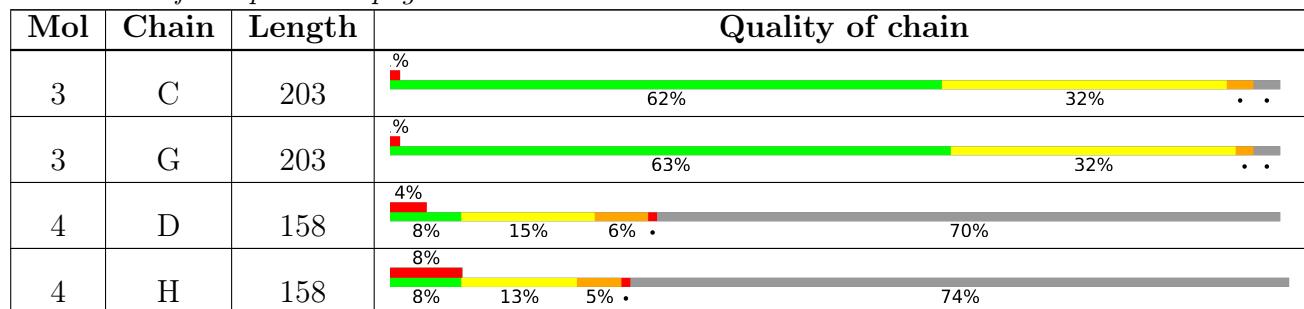
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	A	308	-	-	-	X
5	MG	A	313	-	-	-	X
5	MG	A	320	-	-	-	X
5	MG	A	321	-	-	-	X
5	MG	A	326	-	-	-	X
5	MG	A	327	-	-	-	X
5	MG	E	311	-	-	-	X
6	K	A	330	-	-	-	X
6	K	A	331	-	-	-	X
7	GOL	A	336	-	-	-	X

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 12128 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 Human gene for small cytoplasmic 7SL RNA (7L30.1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	P	0	0	0
			3126	1388	577	1014	147			
1	E	145	Total	C	N	O	P	0	0	0
			3117	1388	577	1007	145			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GTP	-	insertion	GB 23924
A	249	A	-	insertion	GB 23924
E	105	GTP	-	expression tag	GB 23924
E	249	A	-	expression tag	GB 23924

- Molecule 2 is a protein called Signal recognition particle 19 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	108	Total	C	N	O	S	0	0	0
			878	553	160	159	6			
2	F	104	Total	C	N	O	S	0	0	0
			842	534	152	150	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P09132
B	2	ALA	-	expression tag	UNP P09132
B	3	CYS	-	expression tag	UNP P09132
B	4	ALA	-	expression tag	UNP P09132
B	5	ALA	-	expression tag	UNP P09132
B	6	ALA	-	expression tag	UNP P09132
B	7	ARG	-	expression tag	UNP P09132
B	8	SER	-	expression tag	UNP P09132

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	PRO	-	expression tag	UNP P09132
B	10	ALA	-	expression tag	UNP P09132
B	119	THR	-	expression tag	UNP P09132
B	120	GLN	-	expression tag	UNP P09132
B	121	LEU	-	expression tag	UNP P09132
B	122	GLU	-	expression tag	UNP P09132
B	123	HIS	-	expression tag	UNP P09132
B	124	HIS	-	expression tag	UNP P09132
B	125	HIS	-	expression tag	UNP P09132
B	126	HIS	-	expression tag	UNP P09132
B	127	HIS	-	expression tag	UNP P09132
B	128	HIS	-	expression tag	UNP P09132
F	1	MET	-	initiating methionine	UNP P09132
F	2	ALA	-	expression tag	UNP P09132
F	3	CYS	-	expression tag	UNP P09132
F	4	ALA	-	expression tag	UNP P09132
F	5	ALA	-	expression tag	UNP P09132
F	6	ALA	-	expression tag	UNP P09132
F	7	ARG	-	expression tag	UNP P09132
F	8	SER	-	expression tag	UNP P09132
F	9	PRO	-	expression tag	UNP P09132
F	10	ALA	-	expression tag	UNP P09132
F	119	THR	-	expression tag	UNP P09132
F	120	GLN	-	expression tag	UNP P09132
F	121	LEU	-	expression tag	UNP P09132
F	122	GLU	-	expression tag	UNP P09132
F	123	HIS	-	expression tag	UNP P09132
F	124	HIS	-	expression tag	UNP P09132
F	125	HIS	-	expression tag	UNP P09132
F	126	HIS	-	expression tag	UNP P09132
F	127	HIS	-	expression tag	UNP P09132
F	128	HIS	-	expression tag	UNP P09132

- Molecule 3 is a protein called Signal recognition particle subunit SRP68.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	197	Total 1653	C 1036	N 313	O 296	S 8	0	0	0
3	G	197	Total 1656	C 1039	N 316	O 293	S 8	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	MET	-	initiating methionine	UNP Q9UHB9
C	53	GLY	-	expression tag	UNP Q9UHB9
C	54	HIS	-	expression tag	UNP Q9UHB9
C	55	HIS	-	expression tag	UNP Q9UHB9
C	56	HIS	-	expression tag	UNP Q9UHB9
C	57	HIS	-	expression tag	UNP Q9UHB9
C	58	HIS	-	expression tag	UNP Q9UHB9
C	59	HIS	-	expression tag	UNP Q9UHB9
C	116	ASP	GLU	conflict	UNP Q9UHB9
G	52	MET	-	initiating methionine	UNP Q9UHB9
G	53	GLY	-	expression tag	UNP Q9UHB9
G	54	HIS	-	expression tag	UNP Q9UHB9
G	55	HIS	-	expression tag	UNP Q9UHB9
G	56	HIS	-	expression tag	UNP Q9UHB9
G	57	HIS	-	expression tag	UNP Q9UHB9
G	58	HIS	-	expression tag	UNP Q9UHB9
G	59	HIS	-	expression tag	UNP Q9UHB9
G	116	ASP	GLU	conflict	UNP Q9UHB9

- Molecule 4 is a protein called Signal recognition particle subunit SRP72.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	47	Total	C	N	O	S	0	0	0
			395	250	78	66	1			
4	H	41	Total	C	N	O	S	0	0	0
			352	223	71	57	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	511	MET	-	initiating methionine	UNP O76094
D	512	GLY	MET	conflict	UNP O76094
D	663	HIS	LYS	conflict	UNP O76094
D	664	HIS	LYS	conflict	UNP O76094
D	665	HIS	LYS	conflict	UNP O76094
D	666	HIS	GLY	conflict	UNP O76094
D	667	HIS	GLY	conflict	UNP O76094
D	668	HIS	LYS	conflict	UNP O76094
H	511	MET	-	initiating methionine	UNP O76094
H	512	GLY	MET	conflict	UNP O76094
H	663	HIS	LYS	conflict	UNP O76094
H	664	HIS	LYS	conflict	UNP O76094
H	665	HIS	LYS	conflict	UNP O76094

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Chain	Residue	Modelled	Actual	Comment	Reference
H	666	HIS	GLY	conflict	UNP O76094
H	667	HIS	GLY	conflict	UNP O76094
H	668	HIS	LYS	conflict	UNP O76094

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total 27	Mg 27	0	0
5	C	3	Total 3	Mg 3	0	0
5	E	14	Total 14	Mg 14	0	0
5	G	1	Total 1	Mg 1	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total 5	K 5	0	0
6	E	5	Total 5	K 5	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
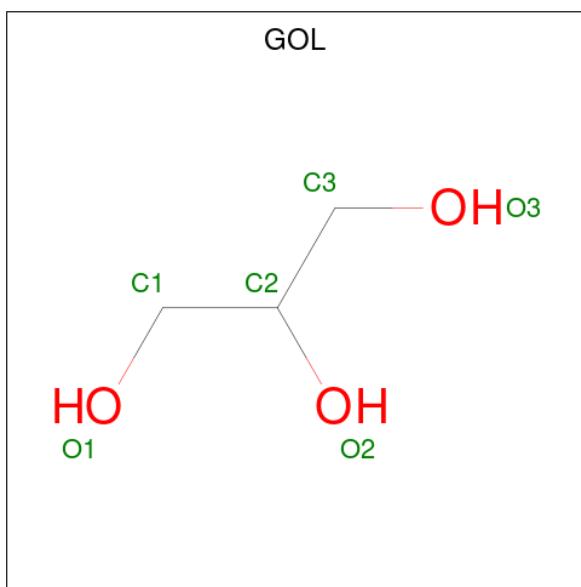
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	E	1	Total 6	C 3	O 3	0	0
7	E	1	Total 6	C 3	O 3	0	0
7	E	1	Total 6	C 3	O 3	0	0

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: Human gene for small cytoplasmic 7SL RNA (7L30.1)
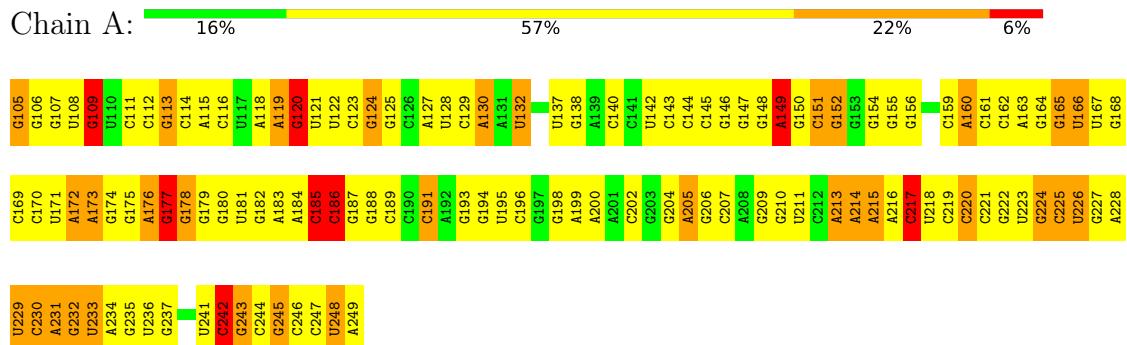
Chain A:

- Molecule 1: Human gene for small cytoplasmic 7SL RNA (7L30.1)

Chain E:

- Molecule 2: Signal recognition particle 19 kDa protein

Chain B:

- Molecule 2: Signal recognition particle 19 kDa protein

Chain F:

• Molecule 3: Signal recognition particle subunit SRP68
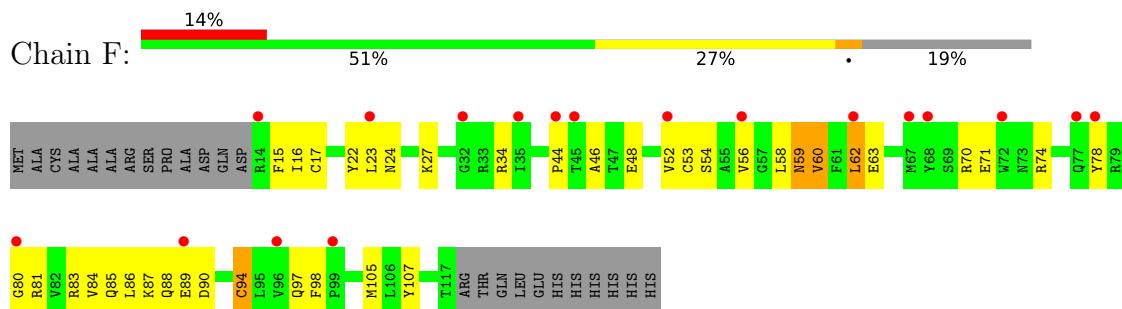
Chain C:
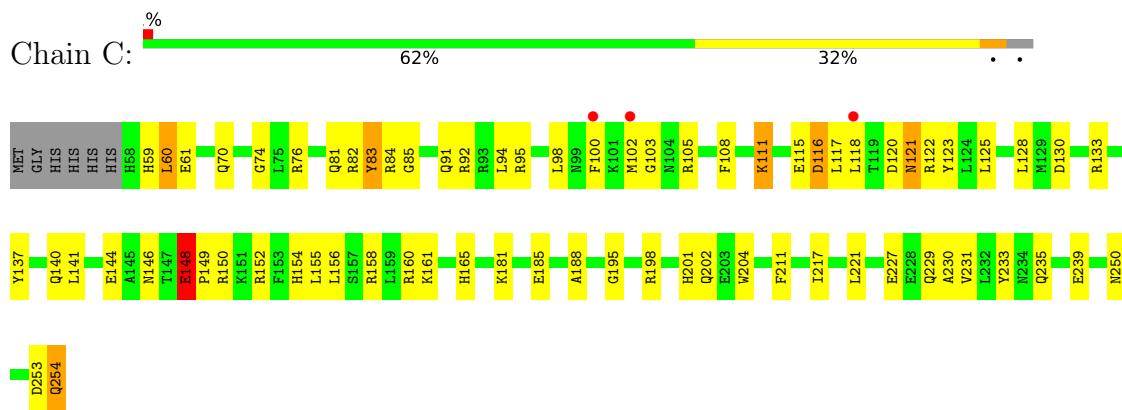
• Molecule 3: Signal recognition particle subunit SRP68
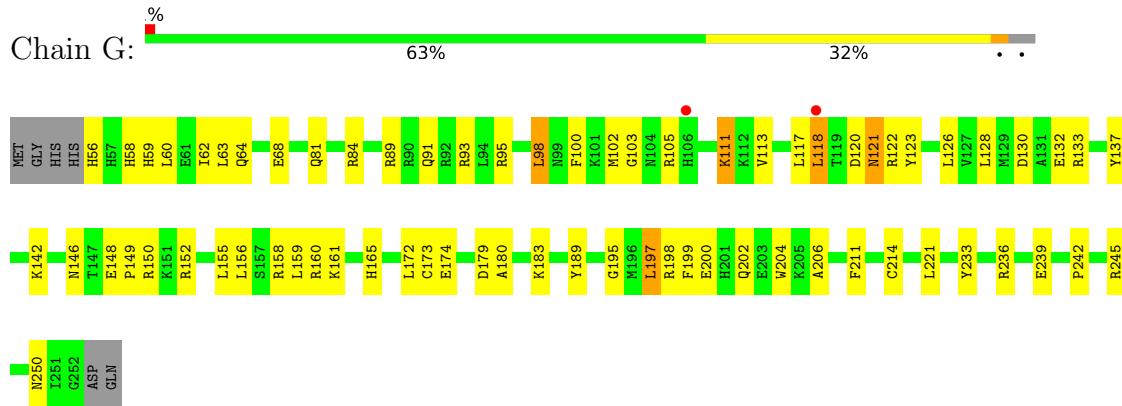
Chain G:

• Molecule 4: Signal recognition particle subunit SRP72
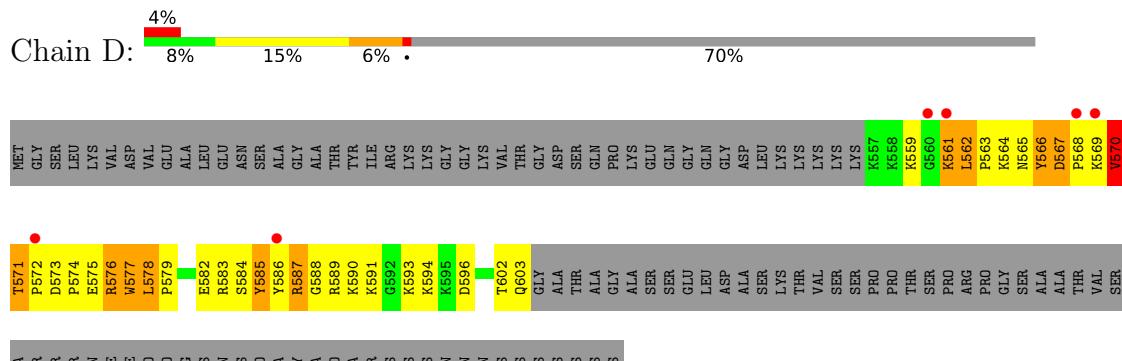
Chain D:

• Molecule 4: Signal recognition particle subunit SRP72

Chain H:
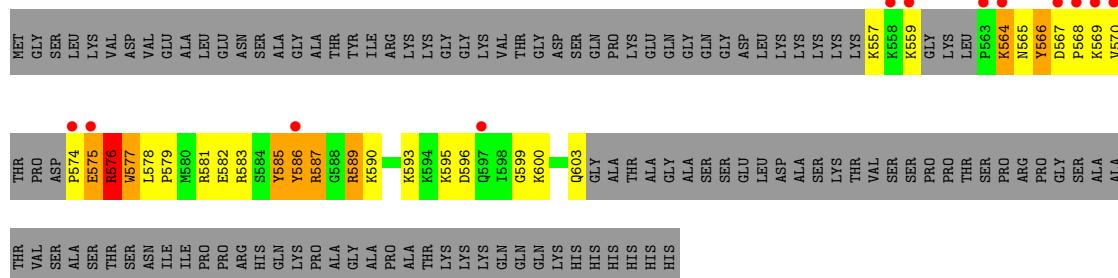
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	134.57Å 139.31Å 152.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 3.40 48.39 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.39-3.40) 82.3 (48.39-3.40)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.91 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.237 , 0.280 0.237 , 0.280	Depositor DCC
R_{free} test set	1921 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	74.2	Xtriage
Anisotropy	0.834	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 7.3	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12128	wwPDB-VP
Average B, all atoms (Å^2)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: K, GTP, GOL, MG

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	0.92	2/3463 (0.1%)	1.56	74/5402 (1.4%)
1	E	0.70	1/3463 (0.0%)	1.35	34/5402 (0.6%)
2	B	0.62	0/892	0.82	0/1200
2	F	0.41	0/856	0.69	1/1152 (0.1%)
3	C	0.55	1/1683 (0.1%)	0.79	1/2254 (0.0%)
3	G	0.64	1/1688 (0.1%)	0.98	5/2261 (0.2%)
4	D	1.26	1/404 (0.2%)	0.78	0/534
4	H	0.83	1/358 (0.3%)	0.63	0/466
All	All	0.75	7/12807 (0.1%)	1.24	115/18671 (0.6%)

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
3	C	0	1
4	D	0	1
4	H	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	567	ASP	C-N	23.47	1.78	1.34
4	H	567	ASP	C-N	13.86	1.60	1.34
1	A	149	A	N9-C4	-9.43	1.32	1.37
1	A	205	A	N9-C4	-6.92	1.33	1.37
1	E	174	G	N9-C4	-6.15	1.33	1.38
3	G	214	CYS	CB-SG	-5.85	1.72	1.81
3	C	83	TYR	CE2-CZ	-5.20	1.31	1.38

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	150	G	OP1-P-O3'	-12.33	78.07	105.20
1	A	185	C	C6-N1-C2	11.19	124.78	120.30
1	A	217	C	C6-N1-C2	-10.14	116.25	120.30
1	A	123	C	C6-N1-C2	9.53	124.11	120.30
1	A	186	C	C6-N1-C2	-9.09	116.66	120.30
1	A	144	C	C2-N1-C1'	8.80	128.48	118.80
3	G	98	LEU	CA-CB-CG	-8.70	95.29	115.30
1	A	185	C	N3-C2-O2	8.57	127.90	121.90
1	A	217	C	C2-N1-C1'	8.38	128.02	118.80
1	A	112	C	C6-N1-C2	8.01	123.50	120.30
1	A	149	A	C8-N9-C4	7.98	108.99	105.80
1	E	217	C	N1-C2-O2	7.98	123.69	118.90
1	E	166	U	C6-N1-C2	7.88	125.73	121.00
1	A	217	C	C5-C6-N1	7.74	124.87	121.00
1	A	186	C	N3-C2-O2	-7.61	116.57	121.90
1	A	186	C	C2-N1-C1'	7.60	127.16	118.80
1	A	217	C	N1-C2-O2	7.51	123.41	118.90
1	E	144	C	C2-N1-C1'	7.48	127.03	118.80
1	A	205	A	C8-N9-C4	7.46	108.78	105.80
1	A	186	C	N1-C2-O2	7.43	123.36	118.90
1	A	217	C	N3-C2-O2	-7.37	116.74	121.90
1	A	140	C	C6-N1-C2	7.34	123.24	120.30
1	E	217	C	C2-N1-C1'	7.31	126.84	118.80
1	A	143	C	C2-N1-C1'	7.12	126.63	118.80
1	E	166	U	C5-C6-N1	-7.07	119.17	122.70
1	E	185	C	C6-N1-C2	-7.04	117.48	120.30
1	A	242	C	C6-N1-C1'	-7.00	112.41	120.80
1	A	124	G	C8-N9-C4	6.81	109.13	106.40
1	E	174	G	N3-C4-C5	6.76	131.98	128.60
1	E	151	C	O5'-P-OP1	6.67	118.70	110.70
1	E	220	C	C6-N1-C2	-6.60	117.66	120.30
1	E	114	C	C2-N1-C1'	6.56	126.02	118.80
1	A	144	C	C6-N1-C1'	-6.55	112.94	120.80
1	E	217	C	C5-C6-N1	6.54	124.27	121.00
1	E	174	G	N3-C4-N9	-6.45	122.13	126.00
1	A	154	G	C4-N9-C1'	-6.43	118.14	126.50
1	A	119	A	N1-C6-N6	6.39	122.43	118.60
1	E	217	C	C6-N1-C1'	-6.31	113.22	120.80
1	E	144	C	C6-N1-C1'	-6.28	113.27	120.80
1	A	220	C	C2-N1-C1'	6.25	125.67	118.80
1	A	154	G	C8-N9-C1'	6.18	135.03	127.00
1	A	152	G	OP1-P-OP2	6.11	128.76	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	G	N1-C6-O6	6.08	123.55	119.90
1	E	150	G	OP2-P-O3'	-6.08	91.82	105.20
1	A	177	G	C6-C5-N7	-6.08	126.75	130.40
1	A	154	G	N3-C4-N9	-6.06	122.36	126.00
1	E	186	C	N3-C2-O2	-6.04	117.67	121.90
1	A	243	G	C4-N9-C1'	5.98	134.27	126.50
1	A	143	C	C6-N1-C1'	-5.95	113.66	120.80
2	F	62	LEU	CA-CB-CG	5.94	128.97	115.30
1	A	143	C	OP2-P-O3'	5.94	118.26	105.20
1	A	242	C	C6-N1-C2	5.93	122.67	120.30
1	E	164	G	C4-N9-C1'	5.91	134.18	126.50
1	A	123	C	N3-C4-C5	5.89	124.25	121.90
1	A	177	G	N3-C4-N9	5.83	129.50	126.00
1	A	185	C	C2-N1-C1'	-5.81	112.41	118.80
1	E	114	C	C6-N1-C1'	-5.76	113.89	120.80
1	A	185	C	N1-C2-N3	-5.73	115.19	119.20
3	G	126	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	124	G	N9-C4-C5	-5.65	103.14	105.40
1	A	114	C	C2-N1-C1'	5.62	124.99	118.80
1	E	186	C	N1-C2-O2	5.61	122.27	118.90
1	A	114	C	C6-N1-C1'	-5.60	114.08	120.80
1	E	194	G	C6-C5-N7	-5.58	127.05	130.40
1	A	152	G	O5'-P-OP1	-5.57	100.68	105.70
1	A	242	C	C2-N1-C1'	5.56	124.92	118.80
1	A	160	A	C8-N9-C4	5.54	108.02	105.80
1	A	177	G	C4-N9-C1'	5.54	133.69	126.50
1	A	114	C	N1-C2-O2	5.53	122.22	118.90
1	A	215	A	N9-C4-C5	-5.49	103.60	105.80
1	A	245	G	C5-C6-O6	5.48	131.89	128.60
1	A	225	C	C6-N1-C2	5.44	122.48	120.30
1	E	234	A	C8-N9-C4	-5.43	103.63	105.80
1	A	144	C	OP2-P-O3'	5.42	117.11	105.20
3	G	197	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	A	111	C	C6-N1-C2	5.40	122.46	120.30
1	E	151	C	OP1-P-OP2	5.39	127.69	119.60
1	A	109	G	C8-N9-C4	-5.39	104.25	106.40
1	A	243	G	C8-N9-C4	-5.38	104.25	106.40
1	A	149	A	C2-N3-C4	-5.38	107.91	110.60
3	C	60	LEU	CA-CB-CG	-5.36	102.97	115.30
1	E	235	G	N9-C4-C5	5.34	107.54	105.40
1	E	185	C	C5'-C4'-O4'	5.33	115.50	109.10
1	A	166	U	C6-N1-C2	5.32	124.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	242	C	C5-C4-N4	-5.29	116.50	120.20
1	A	123	C	C5-C6-N1	-5.27	118.37	121.00
1	A	229	U	OP1-P-OP2	5.26	127.50	119.60
3	G	118	LEU	CA-CB-CG	5.26	127.40	115.30
1	E	233	U	C3'-C2'-C1'	5.26	105.71	101.50
1	E	233	U	O4'-C1'-N1	5.25	112.40	108.20
1	A	124	G	N3-C4-C5	5.24	131.22	128.60
1	A	177	G	C4-C5-N7	5.22	112.89	110.80
1	A	217	C	N3-C4-C5	-5.21	119.81	121.90
1	A	132	U	C2-N1-C1'	5.20	123.94	117.70
1	A	177	G	C8-N9-C1'	-5.19	120.25	127.00
1	A	242	C	C4-C5-C6	-5.19	114.81	117.40
1	E	217	C	C5-C4-N4	-5.18	116.57	120.20
1	E	143	C	C2-N1-C1'	5.17	124.49	118.80
1	A	186	C	C5-C6-N1	5.17	123.58	121.00
1	A	154	G	N3-C4-C5	5.17	131.18	128.60
1	A	220	C	C6-N1-C1'	-5.17	114.60	120.80
1	A	215	A	C8-N9-C4	5.16	107.86	105.80
1	E	164	G	C8-N9-C1'	-5.15	120.31	127.00
1	A	243	G	C6-C5-N7	-5.14	127.31	130.40
1	E	170	C	C2-N1-C1'	-5.14	113.14	118.80
1	E	114	C	N1-C2-O2	5.14	121.98	118.90
1	A	149	A	O4'-C1'-N9	-5.12	104.10	108.20
1	A	146	G	OP2-P-O3'	5.12	116.47	105.20
1	A	224	G	N9-C4-C5	-5.09	103.36	105.40
3	G	152	ARG	CB-CA-C	5.07	120.54	110.40
1	A	242	C	N1-C2-O2	5.07	121.94	118.90
1	E	185	C	N3-C4-C5	-5.06	119.88	121.90
1	A	166	U	C5-C6-N1	-5.05	120.18	122.70
1	E	173	A	C8-N9-C4	-5.05	103.78	105.80
1	A	149	A	N3-C4-C5	5.00	130.30	126.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	148	GLU	Peptide
4	D	569	LYS	Peptide
4	H	575	GLU	Peptide

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	3126	0	1572	139	2
1	E	3117	0	1572	130	1
2	B	878	0	902	38	1
2	F	842	0	873	30	1
3	C	1653	0	1655	77	0
3	G	1656	0	1657	67	0
4	D	395	0	423	41	1
4	H	352	0	378	28	0
5	A	27	0	0	0	0
5	C	3	0	0	0	0
5	E	14	0	0	0	0
5	G	1	0	0	0	0
6	A	5	0	0	0	0
6	E	5	0	0	0	0
7	A	30	0	40	2	0
7	B	6	0	8	1	0
7	E	18	0	20	0	0
All	All	12128	0	9100	474	3

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 23.

All (474) 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)
4:D:567:ASP:C	4:D:568:PRO:N	1.78	1.33
1:A:242:C:OP2	4:D:576:ARG:NH2	1.85	1.09
1:A:242:C:OP2	4:D:559:LYS:NZ	1.89	1.05
1:A:173:A:H5'	3:C:158:ARG:HH12	1.18	1.04
1:E:128:U:H3	1:E:222:G:H1	1.11	0.99
1:E:191:C:N4	1:E:207:C:OP2	2.01	0.94
1:A:226:U:OP2	3:C:95:ARG:NH1	2.04	0.91
1:E:233:U:O2'	1:E:234:A:O5'	1.88	0.89
1:A:242:C:N3	4:D:565:ASN:ND2	2.19	0.89
1:A:227:G:O2'	3:C:105:ARG:NH1	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:C:O2	4:H:557:LYS:NZ	2.07	0.88
3:C:59:HIS:HE1	3:C:181:LYS:HD3	1.38	0.86
1:A:243:G:C6	4:D:577:TRP:HZ2	1.94	0.85
1:A:150:G:OP1	2:B:22:TYR:OH	1.96	0.84
3:C:98:LEU:HG	3:C:123:TYR:HE1	1.44	0.82
1:A:183:A:O4'	1:A:213:A:N6	2.12	0.82
1:A:242:C:P	4:D:576:ARG:HH22	2.03	0.82
3:C:117:LEU:HD23	3:C:123:TYR:HE2	1.46	0.81
2:B:60:VAL:HG12	2:B:84:VAL:HG22	1.62	0.79
1:A:191:C:N4	1:A:207:C:OP2	2.14	0.78
1:A:198:G:OP2	2:B:66:LYS:NZ	2.16	0.78
1:E:120:G:OP2	3:G:89:ARG:NH1	2.15	0.78
3:C:148:GLU:O	3:C:150:ARG:N	2.17	0.78
3:G:195:GLY:HA3	3:G:211:PHE:CE1	2.19	0.77
1:A:242:C:N4	4:D:565:ASN:OD1	2.17	0.77
1:A:108:U:H2'	1:A:109:G:C8	2.19	0.77
1:A:181:U:O4	7:A:335:GOL:O2	2.03	0.75
2:F:54:SER:HA	2:F:58:LEU:HB2	1.69	0.75
1:E:234:A:O2'	1:E:235:G:O5'	2.05	0.74
1:E:231:A:H4'	1:E:232:G:H5''	1.68	0.74
1:E:216:A:HO2'	1:E:217:C:H6	1.36	0.74
1:E:225:C:P	3:G:133:ARG:HH22	2.11	0.73
3:G:81:GLN:HG3	3:G:84:ARG:HH21	1.54	0.73
3:G:198:ARG:HD3	3:G:206:ALA:HB1	1.71	0.73
1:A:108:U:H2'	1:A:109:G:H8	1.53	0.72
4:H:559:LYS:O	4:H:564:LYS:NZ	2.22	0.72
1:A:173:A:H5'	3:C:158:ARG:NH1	2.00	0.71
4:H:574:PRO:HG2	4:H:576:ARG:HB3	1.71	0.71
3:G:117:LEU:HB3	3:G:123:TYR:HE2	1.56	0.70
1:E:226:U:OP2	3:G:95:ARG:NH1	2.24	0.70
1:A:151:C:H41	2:B:34:ARG:HH21	1.40	0.70
1:E:170:C:OP1	3:G:160:ARG:NH2	2.24	0.70
1:E:108:U:H2'	1:E:109:G:C8	2.26	0.69
3:C:81:GLN:HG3	3:C:84:ARG:NH2	2.08	0.69
4:H:579:PRO:HG2	4:H:582:GLU:HG3	1.75	0.67
1:A:171:U:H1'	1:A:174:G:O6	1.94	0.67
1:A:225:C:P	3:C:133:ARG:HH22	2.16	0.67
1:E:233:U:HO2'	1:E:234:A:P	2.18	0.67
1:A:174:G:P	3:C:158:ARG:NH2	2.67	0.67
1:A:180:G:H2'	1:A:181:U:O4'	1.94	0.67
4:D:572:PRO:HG2	4:D:576:ARG:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:59:ASN:ND2	2:F:85:GLN:O	2.27	0.67
3:G:148:GLU:O	3:G:150:ARG:N	2.28	0.67
4:H:575:GLU:HG3	4:H:576:ARG:H	1.60	0.66
2:B:19:TYR:HD1	2:B:22:TYR:CE2	2.14	0.66
3:G:120:ASP:O	3:G:122:ARG:HG3	1.97	0.65
2:B:23:LEU:O	2:B:40:ALA:HB1	1.97	0.65
4:D:575:GLU:OE2	4:D:584:SER:N	2.21	0.65
1:E:115:A:H2'	1:E:116:C:C6	2.32	0.65
3:G:95:ARG:HG2	3:G:100:PHE:HB3	1.78	0.65
4:D:562:LEU:H	4:D:563:PRO:HD2	1.61	0.65
1:E:180:G:H2'	1:E:181:U:O4'	1.97	0.65
2:B:19:TYR:HD1	2:B:22:TYR:HE2	1.44	0.65
1:A:173:A:O5'	3:C:161:LYS:NZ	2.29	0.64
1:E:195:U:H3	1:E:204:G:H1	1.45	0.64
1:A:242:C:O2'	1:A:243:G:H5'	1.98	0.64
1:E:242:C:OP2	4:H:559:LYS:NZ	2.30	0.64
3:G:105:ARG:HA	3:G:105:ARG:NE	2.13	0.64
1:E:241:U:H5''	4:H:559:LYS:HE2	1.81	0.63
1:E:163:A:H3'	1:E:164:G:C8	2.33	0.63
1:A:118:A:H2'	1:A:119:A:C8	2.33	0.63
1:E:225:C:H2'	1:E:226:U:O4'	1.99	0.63
1:A:242:C:P	4:D:559:LYS:HZ1	2.20	0.63
1:E:142:U:H3	1:E:155:G:H1	1.46	0.63
1:E:233:U:C2	1:E:234:A:C8	2.87	0.63
4:D:585:TYR:H	4:D:585:TYR:HD2	1.45	0.62
1:E:172:A:O2'	1:E:224:G:O2'	2.16	0.62
3:C:116:ASP:OD1	3:C:116:ASP:N	2.29	0.62
3:G:98:LEU:HD22	3:G:123:TYR:HE1	1.64	0.62
1:A:185:C:H4'	1:A:186:C:O5'	1.98	0.62
3:C:130:ASP:HB3	3:C:165:HIS:CE1	2.35	0.62
1:A:163:A:H3'	1:A:164:G:C8	2.35	0.61
3:G:102:MET:SD	3:G:111:LYS:HB3	2.40	0.61
1:E:226:U:OP1	3:G:103:GLY:N	2.33	0.61
3:G:98:LEU:HD22	3:G:123:TYR:CE1	2.36	0.61
1:E:233:U:O2'	1:E:234:A:H8	1.84	0.61
4:D:587:ARG:HA	4:D:587:ARG:NE	2.16	0.61
1:A:226:U:OP2	3:C:95:ARG:HD2	2.01	0.61
1:E:185:C:H4'	1:E:186:C:O5'	2.00	0.61
1:A:183:A:O2'	1:A:184:A:OP2	2.16	0.61
1:E:172:A:HO2'	1:E:224:G:HO2'	1.45	0.61
1:E:108:U:H2'	1:E:109:G:H8	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:G:N2	3:G:105:ARG:HH12	1.98	0.60
4:H:589:ARG:O	4:H:593:LYS:N	2.25	0.60
3:G:105:ARG:HA	3:G:105:ARG:HE	1.66	0.60
1:A:170:C:H2'	1:A:171:U:O4'	2.02	0.60
1:E:173:A:OP1	3:G:161:LYS:HD2	2.02	0.60
1:A:221:C:C4	1:A:222:G:N7	2.71	0.59
2:F:23:LEU:HB2	2:F:44:PRO:HG3	1.84	0.59
1:A:216:A:O2'	1:A:217:C:H6	1.86	0.59
1:E:151:C:OP1	1:E:204:G:H4'	2.03	0.59
1:E:183:A:H2'	1:E:184:A:C8	2.37	0.59
1:A:173:A:OP1	3:C:161:LYS:HD2	2.01	0.59
1:A:183:A:H2	1:A:184:A:H62	1.51	0.59
4:H:565:ASN:HB3	4:H:566:TYR:CZ	2.38	0.59
4:D:575:GLU:OE1	4:D:584:SER:OG	2.21	0.58
1:E:235:G:H2'	1:E:236:U:C6	2.38	0.58
1:A:223:U:OP1	3:C:84:ARG:NH1	2.36	0.58
3:G:236:ARG:NH1	3:G:239:GLU:OE1	2.37	0.58
1:A:172:A:H2'	1:A:173:A:C8	2.39	0.58
1:E:183:A:N6	1:E:213:A:C4	2.71	0.58
1:E:150:G:OP1	2:F:22:TYR:OH	2.20	0.57
1:A:151:C:H2'	1:A:152:G:H8	1.69	0.57
1:E:179:G:H2'	1:E:180:G:H8	1.69	0.57
2:F:23:LEU:HD21	2:F:105:MET:HB3	1.86	0.57
1:E:119:A:C6	1:E:120:G:C8	2.93	0.57
4:D:587:ARG:HA	4:D:587:ARG:HE	1.70	0.57
2:F:63:GLU:OE2	2:F:81:ARG:NH2	2.35	0.57
3:C:98:LEU:HG	3:C:123:TYR:CE1	2.32	0.57
1:E:173:A:P	3:G:161:LYS:HZ2	2.28	0.57
1:E:216:A:O2'	1:E:217:C:H6	1.87	0.57
2:F:16:ILE:O	2:F:83:ARG:HA	2.05	0.57
1:A:213:A:O2'	1:A:214:A:H8	1.87	0.56
4:H:583:ARG:HB3	4:H:585:TYR:CD2	2.39	0.56
4:D:593:LYS:O	4:D:596:ASP:N	2.36	0.56
1:E:123:C:H2'	1:E:124:G:H8	1.71	0.56
1:A:194:G:H1	1:A:205:A:H61	1.52	0.56
1:E:173:A:O5'	3:G:161:LYS:NZ	2.37	0.56
1:E:173:A:H5'	3:G:158:ARG:HH12	1.70	0.56
1:E:232:G:HO2'	1:E:233:U:H6	1.52	0.56
3:G:130:ASP:HB3	3:G:165:HIS:ND1	2.20	0.56
4:D:572:PRO:HG2	4:D:576:ARG:CG	2.35	0.56
4:D:571:THR:HG23	4:D:572:PRO:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:577:TRP:O	4:D:577:TRP:HD1	1.89	0.56
1:E:232:G:O2'	1:E:233:U:O5'	2.24	0.56
3:C:185:GLU:OE2	3:C:233:TYR:OH	2.16	0.55
1:A:225:C:OP2	3:C:133:ARG:NH2	2.36	0.55
1:E:234:A:HO2'	1:E:235:G:P	2.29	0.55
1:E:125:G:H21	3:G:105:ARG:HH12	1.55	0.55
1:E:179:G:H2'	1:E:180:G:C8	2.41	0.55
1:A:118:A:H2'	1:A:119:A:H8	1.72	0.55
1:E:173:A:HO2'	1:E:223:U:HO2'	1.31	0.55
1:A:186:C:O2'	1:A:187:G:OP1	2.20	0.55
4:D:564:LYS:O	4:D:568:PRO:HD2	2.06	0.55
1:E:173:A:C5'	3:G:161:LYS:HZ3	2.20	0.55
1:E:185:C:H4'	1:E:186:C:C5'	2.37	0.55
4:H:564:LYS:H	4:H:564:LYS:HD3	1.71	0.55
3:C:195:GLY:HA3	3:C:211:PHE:CE1	2.42	0.54
1:E:148:G:H5"	2:F:16:ILE:HG22	1.89	0.54
2:F:54:SER:HA	2:F:58:LEU:HD13	1.88	0.54
1:A:227:G:H2'	1:A:228:A:O4'	2.08	0.54
1:E:242:C:O2'	1:E:243:G:H5'	2.07	0.54
1:A:125:G:O5'	1:A:125:G:H8	1.89	0.54
4:D:579:PRO:HB2	4:D:582:GLU:HB2	1.89	0.54
2:F:60:VAL:HB	2:F:83:ARG:O	2.07	0.54
1:A:137:U:N3	1:A:138:G:N7	2.56	0.54
3:C:59:HIS:O	3:C:121:ASN:ND2	2.38	0.54
1:E:226:U:P	3:G:102:MET:HB3	2.48	0.54
2:F:53:CYS:O	2:F:56:VAL:HG12	2.07	0.54
1:A:195:U:H2'	1:A:196:C:C6	2.43	0.53
1:A:193:G:H2'	1:A:194:G:O4'	2.08	0.53
4:H:593:LYS:O	4:H:596:ASP:N	2.41	0.53
3:C:221:LEU:HB3	3:C:233:TYR:HE2	1.73	0.53
1:A:163:A:H3'	1:A:164:G:H8	1.74	0.53
1:A:151:C:H2'	1:A:152:G:C8	2.44	0.53
2:B:59:ASN:OD1	7:B:201:GOL:H2	2.09	0.52
4:H:586:TYR:HD1	4:H:586:TYR:O	1.92	0.52
1:A:173:A:C5'	3:C:161:LYS:HZ3	2.22	0.52
1:E:193:G:C8	1:E:194:G:C8	2.97	0.52
3:C:146:ASN:ND2	3:G:146:ASN:HB3	2.25	0.52
1:E:129:C:H5'	1:E:174:G:C2	2.44	0.52
1:E:184:A:O2'	1:E:185:C:H5'	2.09	0.52
1:A:178:G:C2	1:A:179:G:C8	2.97	0.52
1:E:242:C:N4	4:H:570:VAL:HG11	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:24:ASN:HD22	2:F:27:LYS:HE2	1.75	0.52
3:G:221:LEU:HB3	3:G:233:TYR:HE2	1.74	0.52
1:A:198:G:P	2:B:66:LYS:NZ	2.83	0.52
1:A:183:A:C5	1:A:213:A:C5	2.98	0.52
4:D:585:TYR:CD2	4:D:585:TYR:N	2.74	0.52
1:E:173:A:H5'	3:G:158:ARG:NH1	2.24	0.52
3:C:141:LEU:HD13	3:C:154:HIS:HB3	1.92	0.51
3:G:130:ASP:HB3	3:G:165:HIS:CE1	2.46	0.51
1:A:242:C:OP1	4:D:576:ARG:NH1	2.40	0.51
1:E:173:A:P	3:G:161:LYS:NZ	2.83	0.51
3:C:84:ARG:NH2	3:C:140:GLN:OE1	2.42	0.51
2:F:87:LYS:HA	2:F:94:CYS:H	1.76	0.51
3:G:173:CYS:O	3:G:183:LYS:NZ	2.31	0.51
1:A:164:G:N2	1:A:165:G:O6	2.42	0.51
3:C:120:ASP:O	3:C:122:ARG:N	2.44	0.51
1:E:181:U:H2'	1:E:182:G:C8	2.46	0.51
1:A:181:U:H2'	1:A:182:G:C8	2.46	0.51
1:A:221:C:C2	1:A:222:G:C8	2.99	0.51
1:A:243:G:C6	4:D:577:TRP:CZ2	2.86	0.51
4:D:587:ARG:HE	4:D:588:GLY:H	1.59	0.51
3:G:91:GLN:CD	3:G:95:ARG:HH21	2.13	0.50
4:H:587:ARG:HA	4:H:587:ARG:NE	2.26	0.50
1:A:149:A:O2'	2:B:19:TYR:OH	2.25	0.50
1:E:174:G:H3'	1:E:174:G:C8	2.47	0.50
1:E:185:C:N4	1:E:211:U:O4	2.44	0.50
1:A:221:C:OP2	7:A:334:GOL:O2	2.11	0.50
1:A:246:C:H2'	1:A:247:C:H6	1.77	0.50
1:E:195:U:H2'	1:E:196:C:H6	1.75	0.50
2:B:22:TYR:HD1	2:B:34:ARG:CG	2.24	0.50
1:A:147:G:N2	1:A:150:G:OP2	2.42	0.50
3:G:64:GLN:NE2	3:G:68:GLU:OE1	2.31	0.50
1:A:115:A:H2'	1:A:116:C:C6	2.47	0.50
1:A:195:U:H2'	1:A:196:C:H6	1.77	0.50
4:D:562:LEU:O	4:D:565:ASN:HB3	2.12	0.50
3:G:242:PRO:HA	3:G:245:ARG:HG3	1.92	0.50
1:A:173:A:O3'	3:C:158:ARG:NH2	2.45	0.50
3:G:113:VAL:O	3:G:172:LEU:HD21	2.12	0.50
1:A:219:C:C4	1:A:220:C:C5	2.99	0.50
1:E:187:G:N3	1:E:188:G:C8	2.80	0.50
1:E:187:G:H2'	1:E:188:G:H8	1.77	0.50
2:F:87:LYS:HA	2:F:94:CYS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:585:TYR:H	4:H:585:TYR:HD2	1.59	0.49
3:C:95:ARG:HG2	3:C:100:PHE:O	2.12	0.49
1:A:225:C:O3'	3:C:102:MET:HB2	2.13	0.49
1:E:119:A:O5'	3:G:93:ARG:NH1	2.46	0.49
2:F:88:GLN:C	2:F:90:ASP:H	2.15	0.49
1:E:173:A:OP1	3:G:161:LYS:NZ	2.41	0.49
1:E:194:G:H1	1:E:205:A:H61	1.59	0.49
3:C:235:GLN:O	3:C:239:GLU:HB2	2.13	0.49
1:E:225:C:OP2	3:G:133:ARG:NH2	2.45	0.49
3:G:62:ILE:HG23	3:G:128:LEU:CD2	2.42	0.49
2:F:97:GLN:HG2	2:F:98:PHE:CD1	2.47	0.49
3:G:221:LEU:HB3	3:G:233:TYR:CE2	2.47	0.49
1:A:173:A:P	3:C:161:LYS:NZ	2.85	0.48
1:A:219:C:H2'	1:A:220:C:O4'	2.13	0.48
3:C:61:GLU:HG2	3:C:181:LYS:NZ	2.28	0.48
1:A:121:U:H2'	1:A:122:U:C6	2.48	0.48
1:A:151:C:OP1	1:A:204:G:H4'	2.13	0.48
1:E:174:G:O3'	1:E:175:G:H8	1.96	0.48
1:E:124:G:C6	1:E:227:G:C2	3.01	0.48
1:E:182:G:H2'	1:E:213:A:N1	2.28	0.48
1:E:232:G:C5	1:E:233:U:C5	3.01	0.48
1:E:161:C:H2'	1:E:162:C:C6	2.49	0.48
1:E:218:U:H2'	1:E:219:C:C6	2.49	0.48
3:G:204:TRP:CE2	3:G:250:ASN:ND2	2.82	0.48
3:G:81:GLN:HG3	3:G:84:ARG:NH2	2.27	0.48
4:H:583:ARG:HB3	4:H:585:TYR:HD2	1.78	0.48
3:C:117:LEU:HD23	3:C:123:TYR:CE2	2.37	0.48
3:G:58:HIS:HB3	3:G:121:ASN:OD1	2.13	0.48
1:A:198:G:P	2:B:66:LYS:HZ1	2.36	0.48
2:B:24:ASN:OD1	2:B:43:ASN:N	2.46	0.48
3:C:221:LEU:HB3	3:C:233:TYR:CE2	2.49	0.48
3:C:81:GLN:HG3	3:C:84:ARG:HH21	1.79	0.48
1:A:243:G:C6	1:A:244:C:C4	3.02	0.47
4:D:562:LEU:N	4:D:563:PRO:HD2	2.29	0.47
1:E:199:A:H2'	1:E:200:A:O4'	2.14	0.47
1:E:124:G:C4	1:E:227:G:N2	2.81	0.47
3:C:115:GLU:HG2	3:C:118:LEU:HD12	1.95	0.47
3:C:130:ASP:HB3	3:C:165:HIS:ND1	2.29	0.47
1:E:183:A:C5	1:E:213:A:C6	3.01	0.47
3:G:62:ILE:HG23	3:G:128:LEU:HD22	1.96	0.47
4:H:596:ASP:O	4:H:600:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:LEU:O	3:C:144:GLU:N	2.47	0.47
1:E:161:C:H2'	1:E:162:C:H6	1.79	0.47
1:E:183:A:C6	1:E:213:A:C4	3.02	0.47
1:E:232:G:C8	1:E:233:U:C6	3.02	0.47
2:B:32:GLY:HA2	2:B:70:ARG:HH11	1.79	0.47
1:A:199:A:H8	1:A:199:A:OP1	1.97	0.47
2:B:19:TYR:CD1	2:B:22:TYR:HE2	2.30	0.47
2:B:25:ASN:OD1	2:B:26:LYS:HG3	2.15	0.46
1:A:151:C:O2	1:A:152:G:C8	2.67	0.46
1:A:174:G:OP1	3:C:154:HIS:NE2	2.36	0.46
4:D:602:THR:O	4:D:603:GLN:HB3	2.14	0.46
1:E:234:A:O2'	1:E:235:G:H8	1.99	0.46
3:G:132:GLU:OE2	3:G:189:TYR:OH	2.20	0.46
1:A:124:G:H1	1:A:226:U:H3	1.63	0.46
1:A:209:G:H2'	1:A:210:G:O4'	2.15	0.46
4:D:562:LEU:HD12	4:D:565:ASN:CB	2.46	0.46
1:E:125:G:O5'	1:E:125:G:H8	1.98	0.46
2:B:23:LEU:HA	2:B:35:ILE:HD11	1.98	0.46
1:E:226:U:OP1	3:G:102:MET:HB3	2.15	0.46
1:A:174:G:OP1	3:C:158:ARG:NH2	2.49	0.46
1:A:183:A:C5	1:A:213:A:C4	3.04	0.46
4:D:573:ASP:O	4:D:576:ARG:HG3	2.16	0.46
1:E:232:G:O2'	1:E:233:U:H6	1.99	0.46
1:E:133:A:H2'	1:E:134:U:O4'	2.16	0.46
1:E:174:G:H3'	1:E:174:G:H8	1.80	0.46
1:A:129:C:C2	1:A:170:C:O2	2.69	0.46
1:A:194:G:C6	1:A:195:U:C4	3.03	0.46
4:D:562:LEU:H	4:D:563:PRO:CD	2.27	0.46
1:E:223:U:OP1	3:G:84:ARG:NH1	2.37	0.46
3:C:227:GLU:HA	3:C:230:ALA:HB3	1.98	0.45
1:A:179:G:H2'	1:A:180:G:H8	1.81	0.45
2:B:97:GLN:C	2:B:98:PHE:HD1	2.20	0.45
4:D:574:PRO:O	4:D:576:ARG:HB2	2.17	0.45
2:F:71:GLU:HG2	2:F:78:TYR:HB3	1.98	0.45
3:G:63:LEU:HD23	3:G:233:TYR:CD1	2.51	0.45
4:H:577:TRP:HA	4:H:577:TRP:CE3	2.51	0.45
1:A:149:A:H4'	2:B:17:CYS:SG	2.57	0.45
2:B:22:TYR:HD1	2:B:34:ARG:HG3	1.81	0.45
3:C:61:GLU:HG2	3:C:181:LYS:HZ1	1.80	0.45
4:D:591:LYS:O	4:D:591:LYS:HG2	2.16	0.45
1:A:151:C:H41	2:B:34:ARG:NH2	2.10	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:C:H3'	1:A:243:G:H8	1.82	0.45
1:A:248:U:H5"	1:A:248:U:H6	1.82	0.45
3:C:59:HIS:CE1	3:C:181:LYS:HD3	2.31	0.45
3:G:161:LYS:HB3	3:G:161:LYS:HE3	1.71	0.45
1:A:178:G:C2	1:A:179:G:N7	2.84	0.45
1:A:193:G:C8	1:A:194:G:C8	3.05	0.45
2:B:97:GLN:O	2:B:98:PHE:HD1	2.00	0.45
1:E:137:U:C2	1:E:138:G:C8	3.05	0.45
1:E:187:G:C2	1:E:188:G:C8	3.05	0.45
1:E:231:A:N3	1:E:231:A:H2'	2.31	0.45
3:G:156:LEU:HD21	3:G:200:GLU:HB3	1.99	0.45
1:A:221:C:N3	1:A:222:G:C8	2.85	0.45
1:A:234:A:H2'	1:A:235:G:C8	2.52	0.45
1:E:195:U:H2'	1:E:196:C:C6	2.50	0.45
1:A:180:G:N2	1:A:218:U:H1'	2.32	0.45
2:B:22:TYR:CD1	2:B:34:ARG:HG3	2.51	0.45
2:F:88:GLN:O	2:F:90:ASP:N	2.50	0.45
1:A:225:C:H2'	1:A:226:U:O4'	2.17	0.45
2:B:28:THR:N	2:B:31:GLU:OE1	2.30	0.45
1:E:140:C:N3	1:E:141:C:C5	2.85	0.45
1:E:233:U:N3	1:E:234:A:N7	2.64	0.45
3:C:94:LEU:HD11	3:C:125:LEU:HD23	2.00	0.44
3:C:204:TRP:CZ2	3:C:250:ASN:ND2	2.85	0.44
1:E:129:C:H2'	1:E:130:A:O4'	2.17	0.44
1:E:184:A:C5	1:E:187:G:N7	2.85	0.44
1:A:224:G:H5"	3:C:133:ARG:NH2	2.32	0.44
1:A:243:G:C6	1:A:244:C:C5	3.05	0.44
2:B:27:LYS:NZ	2:B:31:GLU:HB3	2.32	0.44
1:E:128:U:O2	1:E:222:G:N2	2.44	0.44
1:E:242:C:OP1	4:H:576:ARG:NH2	2.50	0.44
1:A:113:G:C1'	4:D:589:ARG:HH21	2.30	0.44
3:C:156:LEU:HD22	3:C:201:HIS:CD2	2.52	0.44
1:E:119:A:C2	1:E:120:G:H1'	2.51	0.44
1:A:159:C:N4	1:A:160:A:H62	2.16	0.44
1:A:245:G:C6	1:A:246:C:C4	3.06	0.44
2:B:86:LEU:HA	2:B:86:LEU:HD23	1.62	0.44
2:B:108:ALA:O	2:B:112:ILE:HG13	2.18	0.44
1:E:151:C:P	2:F:70:ARG:HH21	2.40	0.44
1:E:226:U:OP2	3:G:95:ARG:HD2	2.17	0.44
3:C:60:LEU:HD12	3:C:60:LEU:HA	1.65	0.44
3:C:150:ARG:HG3	3:C:150:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:C:C4	1:E:222:G:N7	2.86	0.44
3:C:120:ASP:C	3:C:122:ARG:N	2.71	0.44
2:B:71:GLU:HG2	2:B:78:TYR:HB3	1.99	0.44
1:A:178:G:N3	1:A:179:G:C8	2.85	0.44
1:A:179:G:H2'	1:A:180:G:C8	2.52	0.44
1:A:224:G:H5"	3:C:133:ARG:CZ	2.48	0.44
3:C:74:GLY:O	3:C:76:ARG:N	2.51	0.44
3:C:91:GLN:NE2	3:C:130:ASP:OD1	2.49	0.44
4:H:564:LYS:O	4:H:568:PRO:HD2	2.17	0.44
1:A:172:A:C8	3:C:108:PHE:CZ	3.06	0.43
1:A:183:A:C6	1:A:213:A:C4	3.06	0.43
1:A:235:G:H2'	1:A:236:U:C6	2.53	0.43
3:C:120:ASP:C	3:C:122:ARG:H	2.21	0.43
1:A:188:G:H2'	1:A:189:C:O4'	2.17	0.43
4:D:559:LYS:HB2	4:D:561:LYS:O	2.18	0.43
4:D:571:THR:OG1	4:D:572:PRO:HD2	2.18	0.43
1:E:244:C:H2'	1:E:245:G:H8	1.83	0.43
1:A:119:A:C6	1:A:120:G:C8	3.06	0.43
2:F:46:ALA:HB2	2:F:80:GLY:HA3	2.01	0.43
1:A:176:A:HO2'	1:A:177:G:P	2.40	0.43
2:B:60:VAL:CG1	2:B:84:VAL:HG22	2.42	0.43
1:E:233:U:C2	1:E:234:A:N7	2.86	0.43
1:A:162:C:C2	1:A:163:A:C8	3.07	0.43
1:A:183:A:N7	1:A:213:A:C8	2.87	0.43
1:A:226:U:H4'	3:C:103:GLY:O	2.18	0.43
3:C:70:GLN:HG2	3:C:83:TYR:CZ	2.54	0.43
3:C:254:GLN:N	3:C:254:GLN:OE1	2.52	0.43
1:A:160:A:H2'	1:A:161:C:C6	2.54	0.43
1:A:231:A:H3'	1:A:232:G:H5"	2.00	0.43
3:C:116:ASP:O	3:C:118:LEU:N	2.51	0.43
1:E:148:G:O3'	2:F:16:ILE:HA	2.19	0.43
4:H:583:ARG:HB3	4:H:585:TYR:CE2	2.54	0.43
4:H:596:ASP:O	4:H:600:LYS:HE3	2.18	0.43
1:A:165:G:N1	1:A:166:U:C4	2.86	0.43
3:C:227:GLU:O	3:C:231:VAL:HG23	2.18	0.43
1:E:151:C:H41	2:F:34:ARG:HH21	1.66	0.43
4:H:569:LYS:HD2	4:H:569:LYS:N	2.34	0.43
1:E:243:G:H1'	4:H:576:ARG:HH21	1.83	0.43
1:A:121:U:H2'	1:A:122:U:H6	1.81	0.42
2:B:58:LEU:HD11	2:B:98:PHE:CD2	2.54	0.42
1:E:246:C:O2'	1:E:247:C:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:56:VAL:HG21	2:F:107:TYR:HE1	1.84	0.42
3:C:202:GLN:HB3	3:C:204:TRP:CZ2	2.53	0.42
1:E:124:G:C5	1:E:227:G:N2	2.87	0.42
1:E:159:C:H2'	1:E:160:A:C8	2.54	0.42
3:G:197:LEU:O	3:G:199:PHE:N	2.52	0.42
1:A:105:GTP:H2'	1:A:106:G:C8	2.54	0.42
1:E:107:G:H2'	1:E:108:U:O4'	2.19	0.42
1:E:131:A:C2	1:E:167:U:O2	2.72	0.42
2:F:86:LEU:HD23	2:F:86:LEU:HA	1.76	0.42
1:E:204:G:H2'	1:E:205:A:C8	2.53	0.42
1:A:148:G:O3'	2:B:16:ILE:HA	2.19	0.42
3:C:82:ARG:O	3:C:85:GLY:N	2.52	0.42
2:F:48:GLU:O	2:F:52:VAL:HG22	2.18	0.42
3:G:142:LYS:N	3:G:155:LEU:HD12	2.35	0.42
3:G:180:ALA:HA	3:G:183:LYS:HD2	2.01	0.42
3:C:188:ALA:HB2	3:C:217:ILE:CG2	2.50	0.42
1:E:213:A:O2'	1:E:214:A:O4'	2.38	0.42
1:E:213:A:O2'	1:E:214:A:O5'	2.33	0.42
1:E:221:C:N3	1:E:222:G:C8	2.87	0.42
2:B:97:GLN:C	2:B:98:PHE:CD1	2.93	0.42
3:C:98:LEU:HD13	3:C:98:LEU:HA	1.61	0.42
4:D:562:LEU:HD12	4:D:565:ASN:HB3	2.02	0.42
3:G:58:HIS:HB3	3:G:121:ASN:CG	2.40	0.42
4:H:600:LYS:HG3	4:H:600:LYS:H	1.70	0.42
1:A:232:G:HO2'	1:A:233:U:H6	1.67	0.42
3:C:111:LYS:NZ	3:C:130:ASP:OD2	2.52	0.42
1:A:162:C:H2'	1:A:163:A:O4'	2.20	0.42
4:D:566:TYR:HA	4:D:570:VAL:HA	2.02	0.42
1:A:120:G:C2	1:A:121:U:C6	3.08	0.42
2:B:32:GLY:HA2	2:B:70:ARG:NH1	2.35	0.42
1:A:194:G:C5	1:A:195:U:C5	3.08	0.41
1:A:242:C:H3'	1:A:243:G:C8	2.55	0.41
2:B:67:MET:CE	2:B:79:ARG:HG3	2.50	0.41
1:A:107:G:H2'	1:A:108:U:O4'	2.21	0.41
3:G:98:LEU:HD13	3:G:123:TYR:CD1	2.54	0.41
3:G:98:LEU:HD23	3:G:98:LEU:HA	1.49	0.41
1:A:161:C:C2	1:A:162:C:C5	3.08	0.41
3:G:60:LEU:HD12	3:G:60:LEU:HA	1.84	0.41
1:A:241:U:H5"	4:D:559:LYS:HZ3	1.85	0.41
2:B:115:LEU:HD23	2:B:115:LEU:HA	1.91	0.41
3:C:161:LYS:HB3	3:C:161:LYS:HE3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:C:H2'	1:E:220:C:O4'	2.19	0.41
3:G:159:LEU:HA	3:G:159:LEU:HD23	1.85	0.41
1:A:246:C:H2'	1:A:247:C:C6	2.55	0.41
1:E:149:A:O5'	2:F:17:CYS:HB2	2.21	0.41
2:F:16:ILE:HD11	2:F:84:VAL:HB	2.01	0.41
1:A:183:A:N7	1:A:213:A:N7	2.69	0.41
1:E:213:A:O2'	1:E:214:A:H8	2.04	0.41
3:G:179:ASP:N	3:G:179:ASP:OD1	2.53	0.41
3:G:202:GLN:HB3	3:G:204:TRP:CZ2	2.55	0.41
4:H:578:LEU:HD22	4:H:579:PRO:HD2	2.03	0.41
1:A:130:A:C2	1:A:168:G:C6	3.09	0.41
3:C:98:LEU:N	3:C:98:LEU:HD22	2.35	0.41
1:E:221:C:C2	1:E:222:G:C8	3.09	0.41
2:F:15:PHE:N	2:F:15:PHE:CD1	2.87	0.41
3:G:195:GLY:O	3:G:199:PHE:HB2	2.20	0.41
3:C:152:ARG:O	3:C:155:LEU:HB3	2.21	0.41
3:G:128:LEU:HA	3:G:128:LEU:HD12	1.77	0.41
1:A:161:C:H2'	1:A:162:C:H6	1.86	0.41
1:A:234:A:H2'	1:A:235:G:H8	1.86	0.41
3:C:128:LEU:HD12	3:C:128:LEU:HA	1.68	0.41
1:E:184:A:C5	1:E:187:G:C5	3.09	0.41
1:E:195:U:C2	1:E:196:C:C6	3.08	0.41
1:A:164:G:O2'	1:A:165:G:C8	2.72	0.41
1:A:183:A:C8	1:A:213:A:N7	2.89	0.41
2:B:23:LEU:HD22	2:B:35:ILE:HD13	2.03	0.41
3:C:98:LEU:CG	3:C:123:TYR:HE1	2.22	0.41
1:E:187:G:C2	1:E:188:G:C5	3.09	0.41
2:B:29:ILE:HG13	2:B:33:ARG:NH2	2.36	0.40
3:C:91:GLN:CD	3:C:95:ARG:HH21	2.25	0.40
4:D:577:TRP:O	4:D:577:TRP:CD1	2.71	0.40
4:D:583:ARG:HB3	4:D:585:TYR:CE2	2.56	0.40
1:E:233:U:O2'	1:E:234:A:P	2.75	0.40
4:H:565:ASN:HB3	4:H:566:TYR:CE1	2.55	0.40
1:A:142:U:H3	1:A:155:G:H1	1.68	0.40
1:A:230:C:O2'	1:A:232:G:H5'	2.21	0.40
2:B:19:TYR:H	2:B:22:TYR:HD2	1.69	0.40
3:C:117:LEU:HB3	3:C:123:TYR:CD2	2.57	0.40
1:E:136:G:C6	1:E:137:U:C4	3.09	0.40
1:E:209:G:H2'	1:E:210:G:O4'	2.22	0.40
1:A:165:G:C2	1:A:166:U:C4	3.10	0.40
1:A:227:G:N7	3:C:92:ARG:NH2	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:A:O2'	1:E:223:U:O2'	2.09	0.40
1:E:176:A:HO2'	1:E:177:G:P	2.44	0.40
2:F:60:VAL:HB	2:F:84:VAL:HG22	2.02	0.40
2:F:63:GLU:CD	2:F:81:ARG:HH21	2.22	0.40
1:A:129:C:O2	1:A:170:C:O2	2.40	0.40
3:C:156:LEU:HD23	3:C:156:LEU:HA	1.97	0.40
1:E:242:C:OP1	1:E:243:G:C8	2.74	0.40
3:G:174:GLU:HA	3:G:183:LYS:NZ	2.36	0.40
1:A:127:A:H2	1:A:223:U:H3	1.70	0.40
1:A:210:G:H2'	1:A:211:U:O4'	2.20	0.40
3:C:117:LEU:HB3	3:C:123:TYR:CE2	2.56	0.40
1:E:177:G:N3	1:E:177:G:H2'	2.36	0.40
3:G:195:GLY:CA	3:G:211:PHE:CE1	3.00	0.40

All (3) 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:E:228:A:O2'	2:F:74:ARG:NH1[3_444]	2.13	0.07
1:A:124:G:O5'	2:B:79:ARG:NH2[3_554]	2.14	0.06
1:A:206:G:OP1	4:D:594:LYS:NZ[3_544]	2.15	0.05

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	B	106/128 (83%)	103 (97%)	2 (2%)	1 (1%)	17	49
2	F	102/128 (80%)	99 (97%)	2 (2%)	1 (1%)	15	46
3	C	195/203 (96%)	177 (91%)	14 (7%)	4 (2%)	7	30
3	G	195/203 (96%)	177 (91%)	15 (8%)	3 (2%)	10	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	45/158 (28%)	31 (69%)	10 (22%)	4 (9%)	1	5
4	H	35/158 (22%)	22 (63%)	10 (29%)	3 (9%)	1	5
All	All	678/978 (69%)	609 (90%)	53 (8%)	16 (2%)	6	28

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	121	ASN
3	C	149	PRO
4	D	562	LEU
4	D	570	VAL
4	D	578	LEU
3	G	121	ASN
4	D	590	LYS
2	F	89	GLU
3	G	118	LEU
2	B	115	LEU
4	H	590	LYS
4	H	576	ARG
3	C	198	ARG
3	G	149	PRO
4	H	599	GLY
3	C	148	GLU

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	B	97/112 (87%)	94 (97%)	3 (3%)	40	68
2	F	93/112 (83%)	89 (96%)	4 (4%)	29	59
3	C	173/178 (97%)	166 (96%)	7 (4%)	31	60
3	G	173/178 (97%)	169 (98%)	4 (2%)	50	74
4	D	42/129 (33%)	32 (76%)	10 (24%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	37/129 (29%)	26 (70%)	11 (30%)	0	1
All	All	615/838 (73%)	576 (94%)	39 (6%)	18	47

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	64	LYS
2	B	74	ARG
2	B	118	ARG
3	C	111	LYS
3	C	116	ASP
3	C	137	TYR
3	C	160	ARG
3	C	229	GLN
3	C	253	ASP
3	C	254	GLN
4	D	561	LYS
4	D	566	TYR
4	D	570	VAL
4	D	571	THR
4	D	576	ARG
4	D	577	TRP
4	D	578	LEU
4	D	585	TYR
4	D	586	TYR
4	D	587	ARG
2	F	59	ASN
2	F	60	VAL
2	F	62	LEU
2	F	94	CYS
3	G	56	HIS
3	G	59	HIS
3	G	111	LYS
3	G	137	TYR
4	H	564	LYS
4	H	566	TYR
4	H	576	ARG
4	H	577	TRP
4	H	581	ARG
4	H	585	TYR
4	H	586	TYR
4	H	587	ARG

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Mol	Chain	Res	Type
4	H	589	ARG
4	H	595	LYS
4	H	603	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	59	HIS
4	H	565	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	143/145 (98%)	38 (26%)	4 (2%)
1	E	143/145 (98%)	41 (28%)	6 (4%)
All	All	286/290 (98%)	79 (27%)	10 (3%)

All (79) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	109	G
1	A	113	G
1	A	120	G
1	A	128	U
1	A	130	A
1	A	132	U
1	A	145	C
1	A	149	A
1	A	151	C
1	A	156	G
1	A	165	G
1	A	167	U
1	A	169	C
1	A	172	A
1	A	173	A
1	A	175	G
1	A	176	A
1	A	177	G
1	A	178	G
1	A	185	C

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Mol	Chain	Res	Type
1	A	186	C
1	A	191	C
1	A	200	A
1	A	202	C
1	A	213	A
1	A	214	A
1	A	215	A
1	A	217	C
1	A	226	U
1	A	229	U
1	A	230	C
1	A	231	A
1	A	232	G
1	A	233	U
1	A	237	G
1	A	242	C
1	A	248	U
1	A	249	A
1	E	109	G
1	E	113	G
1	E	114	C
1	E	120	G
1	E	128	U
1	E	130	A
1	E	132	U
1	E	145	C
1	E	149	A
1	E	151	C
1	E	156	G
1	E	165	G
1	E	167	U
1	E	169	C
1	E	172	A
1	E	173	A
1	E	175	G
1	E	176	A
1	E	177	G
1	E	183	A
1	E	185	C
1	E	186	C
1	E	187	G
1	E	191	C

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Mol	Chain	Res	Type
1	E	200	A
1	E	202	C
1	E	213	A
1	E	215	A
1	E	217	C
1	E	226	U
1	E	229	U
1	E	230	C
1	E	231	A
1	E	232	G
1	E	233	U
1	E	234	A
1	E	235	G
1	E	237	G
1	E	242	C
1	E	248	U
1	E	249	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	128	U
1	A	176	A
1	A	185	C
1	A	186	C
1	E	128	U
1	E	176	A
1	E	186	C
1	E	231	A
1	E	233	U
1	E	234	A

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

2 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	A	105	1	26,34,34	1.16	2 (7%)	32,54,54	1.52	6 (18%)
1	GTP	E	105	1	19,25,34	1.03	2 (10%)	18,37,54	0.74	1 (5%)

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	A	105	1	-	9/18/38/38	0/3/3/3
1	GTP	E	105	1	-	1/3/25/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	GTP	C5-C6	-4.02	1.39	1.47
1	E	105	GTP	C5-C6	-2.61	1.42	1.47
1	E	105	GTP	C8-N7	-2.48	1.30	1.35
1	A	105	GTP	C2-N3	2.20	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	GTP	PA-O3A-PB	-3.38	121.23	132.83
1	A	105	GTP	PB-O3B-PG	-3.18	121.93	132.83
1	A	105	GTP	C8-N7-C5	3.10	108.89	102.99
1	A	105	GTP	C5-C6-N1	3.03	119.30	113.95
1	A	105	GTP	C2-N1-C6	-2.59	120.33	125.10
1	A	105	GTP	C3'-C2'-C1'	2.47	104.69	100.98
1	E	105	GTP	O6-C6-C5	2.19	128.64	124.37

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	105	GTP	C5'-O5'-PA-O1A
1	A	105	GTP	C3'-C4'-C5'-O5'
1	A	105	GTP	PA-O3A-PB-O1B
1	A	105	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
1	A	105	GTP	PB-O3A-PA-O5'
1	A	105	GTP	C5'-O5'-PA-O3A
1	A	105	GTP	O4'-C4'-C5'-O5'
1	A	105	GTP	C5'-O5'-PA-O2A
1	E	105	GTP	C3'-C4'-C5'-O5'
1	A	105	GTP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	105	GTP	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 64 ligands modelled in this entry, 55 are monoatomic - leaving 9 for Mogul analysis.

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	$\#|Z| > 2$
7	GOL	A	336	6	5,5,5	0.35	0	5,5,5	0.19	0
7	GOL	A	333	-	5,5,5	0.37	0	5,5,5	0.26	0
7	GOL	A	335	6	5,5,5	0.35	0	5,5,5	0.35	0
7	GOL	E	320	6	5,5,5	0.38	0	5,5,5	0.58	0
7	GOL	A	334	-	5,5,5	0.40	0	5,5,5	0.48	0
7	GOL	A	337	-	5,5,5	0.35	0	5,5,5	0.26	0
7	GOL	E	321	6	5,5,5	0.39	0	5,5,5	0.17	0
7	GOL	E	322	6	5,5,5	0.42	0	5,5,5	0.18	0
7	GOL	B	201	-	5,5,5	0.44	0	5,5,5	0.47	0

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
7	GOL	A	336	6	-	0/4/4/4	-
7	GOL	A	333	-	-	4/4/4/4	-
7	GOL	A	335	6	-	2/4/4/4	-
7	GOL	E	320	6	-	2/4/4/4	-
7	GOL	A	334	-	-	0/4/4/4	-
7	GOL	A	337	-	-	0/4/4/4	-
7	GOL	E	321	6	-	4/4/4/4	-
7	GOL	E	322	6	-	4/4/4/4	-
7	GOL	B	201	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	335	GOL	O1-C1-C2-C3
7	B	201	GOL	O1-C1-C2-C3
7	E	321	GOL	O1-C1-C2-C3
7	E	321	GOL	C1-C2-C3-O3
7	E	322	GOL	O1-C1-C2-C3
7	E	322	GOL	C1-C2-C3-O3
7	E	321	GOL	O2-C2-C3-O3
7	A	333	GOL	C1-C2-C3-O3
7	E	320	GOL	O1-C1-C2-C3
7	E	321	GOL	O1-C1-C2-O2
7	E	322	GOL	O1-C1-C2-O2
7	E	322	GOL	O2-C2-C3-O3
7	A	335	GOL	O1-C1-C2-O2
7	E	320	GOL	O1-C1-C2-O2
7	B	201	GOL	O1-C1-C2-O2
7	A	333	GOL	O1-C1-C2-O2
7	A	333	GOL	O2-C2-C3-O3
7	A	333	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	335	GOL	1	0
7	A	334	GOL	1	0
7	B	201	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	1
4	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	567:ASP	C	568:PRO	N	1.78
1	H	567:ASP	C	568:PRO	N	1.60

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	144/145 (99%)	-0.73	0	100	100	106, 129, 163, 205	0
1	E	144/145 (99%)	-0.79	0	100	100	105, 152, 187, 215	0
2	B	108/128 (84%)	-0.11	0	100	100	72, 108, 134, 181	0
2	F	104/128 (81%)	0.85	18 (17%)	1	1	108, 173, 223, 278	0
3	C	197/203 (97%)	-0.17	3 (1%)	73	72	84, 114, 165, 197	0
3	G	197/203 (97%)	-0.17	2 (1%)	82	81	81, 112, 155, 228	0
4	D	47/158 (29%)	0.81	6 (12%)	3	4	116, 143, 210, 233	0
4	H	41/158 (25%)	1.60	12 (29%)	0	0	131, 149, 209, 246	0
All	All	982/1268 (77%)	-0.11	41 (4%)	36	35	72, 129, 201, 278	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	568	PRO	12.6
4	H	569	LYS	7.2
4	H	567	ASP	7.1
4	D	568	PRO	4.5
4	D	572	PRO	4.5
4	H	558	LYS	4.1
4	H	564	LYS	4.1
3	C	118	LEU	3.8
4	H	559	LYS	3.8
4	H	574	PRO	3.6
4	H	586	TYR	3.5
4	D	569	LYS	3.4
3	G	118	LEU	3.4
2	F	14	ARG	3.2
2	F	89	GLU	3.2
2	F	99	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	35	ILE	3.0
4	D	561	LYS	3.0
4	D	586	TYR	2.9
2	F	56	VAL	2.8
4	D	560	GLY	2.7
4	H	570	VAL	2.7
4	H	563	PRO	2.7
2	F	52	VAL	2.7
2	F	77	GLN	2.7
3	G	106	HIS	2.7
4	H	597	GLN	2.7
3	C	100	PHE	2.6
3	C	102	MET	2.6
2	F	32	GLY	2.5
2	F	23	LEU	2.5
2	F	96	VAL	2.4
2	F	80	GLY	2.4
2	F	68	TYR	2.3
2	F	67	MET	2.2
2	F	72	TRP	2.2
2	F	62	LEU	2.1
2	F	44	PRO	2.1
2	F	78	TYR	2.1
4	H	575	GLU	2.0
2	F	45	THR	2.0

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	GTP	E	105	23/32	0.82	0.12	213,224,235,238	0
1	GTP	A	105	32/32	0.85	0.11	173,207,305,306	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
5	MG	A	308	1/1	0.39	0.41	80,80,80,80	0
5	MG	E	311	1/1	0.42	0.45	101,101,101,101	0
6	K	E	319	1/1	0.48	0.11	175,175,175,175	0
5	MG	A	313	1/1	0.53	0.80	73,73,73,73	0
5	MG	A	303	1/1	0.59	0.14	98,98,98,98	0
5	MG	A	316	1/1	0.60	0.32	90,90,90,90	0
5	MG	E	301	1/1	0.62	0.21	76,76,76,76	0
5	MG	E	302	1/1	0.63	0.18	74,74,74,74	0
5	MG	E	307	1/1	0.66	0.12	88,88,88,88	0
5	MG	A	323	1/1	0.68	0.29	81,81,81,81	0
5	MG	A	304	1/1	0.68	0.21	87,87,87,87	0
6	K	A	331	1/1	0.69	0.82	173,173,173,173	0
5	MG	E	314	1/1	0.69	0.31	75,75,75,75	0
7	GOL	E	321	6/6	0.70	0.33	126,129,138,142	0
6	K	A	332	1/1	0.71	0.11	166,166,166,166	0
7	GOL	E	320	6/6	0.72	0.36	116,124,129,132	0
7	GOL	A	336	6/6	0.72	0.86	138,150,153,156	0
5	MG	A	307	1/1	0.73	0.30	68,68,68,68	0
6	K	A	330	1/1	0.73	0.47	156,156,156,156	0
5	MG	E	313	1/1	0.74	0.25	83,83,83,83	0
5	MG	A	320	1/1	0.74	0.50	69,69,69,69	0
5	MG	A	326	1/1	0.74	0.57	74,74,74,74	0
7	GOL	A	337	6/6	0.76	0.31	101,109,111,111	0
5	MG	A	302	1/1	0.77	0.23	73,73,73,73	0
5	MG	A	321	1/1	0.77	1.42	55,55,55,55	0
5	MG	A	327	1/1	0.79	0.80	78,78,78,78	0
5	MG	A	306	1/1	0.80	0.27	73,73,73,73	0
7	GOL	A	334	6/6	0.80	0.31	117,126,129,135	0
7	GOL	A	333	6/6	0.81	0.24	82,87,92,99	0
5	MG	A	324	1/1	0.81	0.13	81,81,81,81	0
5	MG	E	303	1/1	0.81	0.35	76,76,76,76	0
5	MG	E	310	1/1	0.82	0.11	86,86,86,86	0
5	MG	E	308	1/1	0.82	0.30	87,87,87,87	0
6	K	E	317	1/1	0.83	0.24	144,144,144,144	0
5	MG	E	306	1/1	0.84	0.18	74,74,74,74	0
7	GOL	E	322	6/6	0.84	0.30	102,108,112,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	MG	G	301	1/1	0.85	0.30	73,73,73,73	0
7	GOL	B	201	6/6	0.86	0.22	72,90,91,95	0
5	MG	E	312	1/1	0.86	0.33	97,97,97,97	0
5	MG	A	314	1/1	0.86	0.35	61,61,61,61	0
6	K	A	329	1/1	0.86	0.09	172,172,172,172	0
5	MG	A	312	1/1	0.87	0.43	85,85,85,85	0
5	MG	C	302	1/1	0.87	0.38	60,60,60,60	0
7	GOL	A	335	6/6	0.87	0.25	103,110,115,118	0
5	MG	A	322	1/1	0.88	0.24	78,78,78,78	0
5	MG	E	304	1/1	0.88	0.33	72,72,72,72	0
6	K	E	315	1/1	0.89	0.12	140,140,140,140	0
5	MG	A	309	1/1	0.89	0.19	72,72,72,72	0
6	K	A	328	1/1	0.89	0.10	152,152,152,152	0
5	MG	C	303	1/1	0.89	0.35	60,60,60,60	0
5	MG	A	311	1/1	0.90	0.26	72,72,72,72	0
5	MG	E	309	1/1	0.91	0.08	84,84,84,84	0
5	MG	A	325	1/1	0.91	0.36	74,74,74,74	0
5	MG	E	305	1/1	0.91	0.12	114,114,114,114	0
5	MG	A	318	1/1	0.91	0.10	82,82,82,82	0
5	MG	A	315	1/1	0.91	0.46	88,88,88,88	0
5	MG	A	301	1/1	0.91	0.14	69,69,69,69	0
6	K	E	316	1/1	0.92	0.32	113,113,113,113	0
5	MG	A	319	1/1	0.92	0.20	59,59,59,59	0
5	MG	A	317	1/1	0.92	0.07	80,80,80,80	0
6	K	E	318	1/1	0.94	0.23	129,129,129,129	0
5	MG	C	301	1/1	0.95	0.29	38,38,38,38	0
5	MG	A	310	1/1	0.97	0.27	58,58,58,58	0
5	MG	A	305	1/1	0.98	0.11	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.