



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:43 PM GMT

PDB ID : 1UVK
Title : The structural basis for RNA specificity and Ca²⁺ inhibition of an RNA-dependent RNA polymerase phi6p2 dead-end complex
Authors : Salgado, P.S.; Makeyev, E.V.; Butcher, S.; Bamford, D.; Stuart, D.I.; Grimes, J.M.
Deposited on : 2004-01-21
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

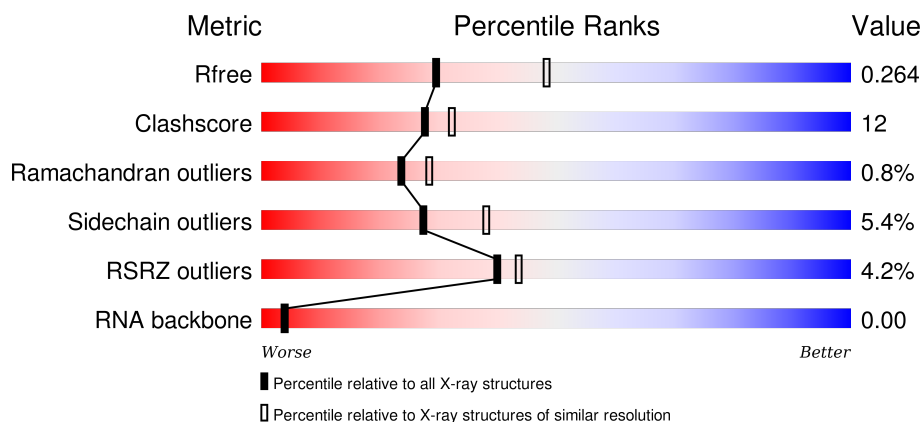
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)
RNA backbone	2183	1004 (2.92-2.00)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	664	<div> <div>3%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
1	C	664	<div> <div>2%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
1	E	664	<div> <div>7%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
2	B	2	<div> <div>50%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	2	<div><div></div><div>50%</div><div></div><div>100%</div></div>
2	F	2	<div><div></div><div>100%</div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16257 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called P2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	C	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	E	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	CONFLICT	UNP P11124
C	456	MET	ILE	CONFLICT	UNP P11124
E	456	MET	ILE	CONFLICT	UNP P11124

- Molecule 2 is a RNA chain called 5'-D(*GP*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	P	0	0	0
			55	20	10	21	4			
2	D	2	Total	C	N	O	P	0	0	0
			55	20	10	21	4			
2	F	2	Total	C	N	O	P	0	0	0
			55	20	10	21	4			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

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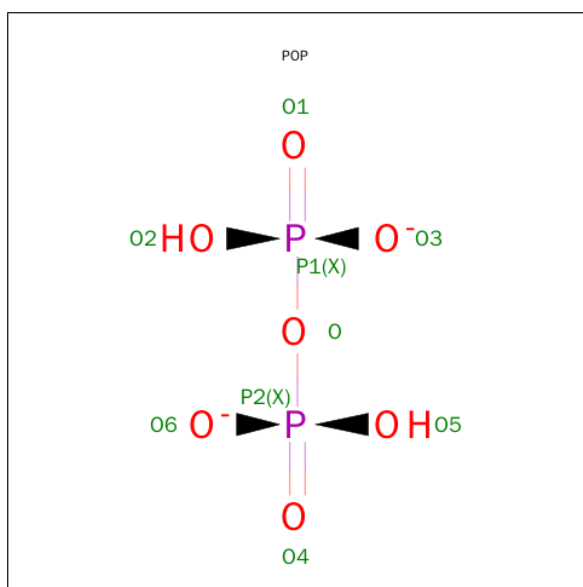
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Mn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	E	2	Total	Mg	0	0
			2	2		

- Molecule 5 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			9	7	2		
5	C	1	Total	O	P	0	0
			9	7	2		
5	E	1	Total	O	P	0	0
			9	7	2		

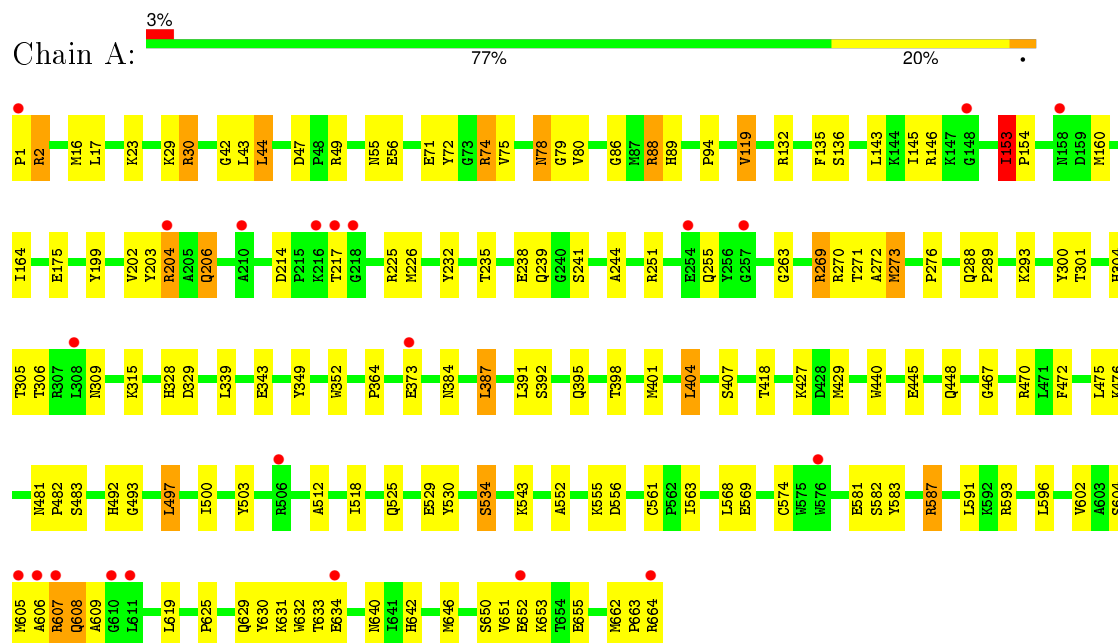
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	83	Total 83	O 83	0	0
6	B	1	Total 1	O 1	0	0
6	C	86	Total 86	O 86	0	0
6	D	1	Total 1	O 1	0	0
6	E	89	Total 89	O 89	0	0
6	F	1	Total 1	O 1	0	0

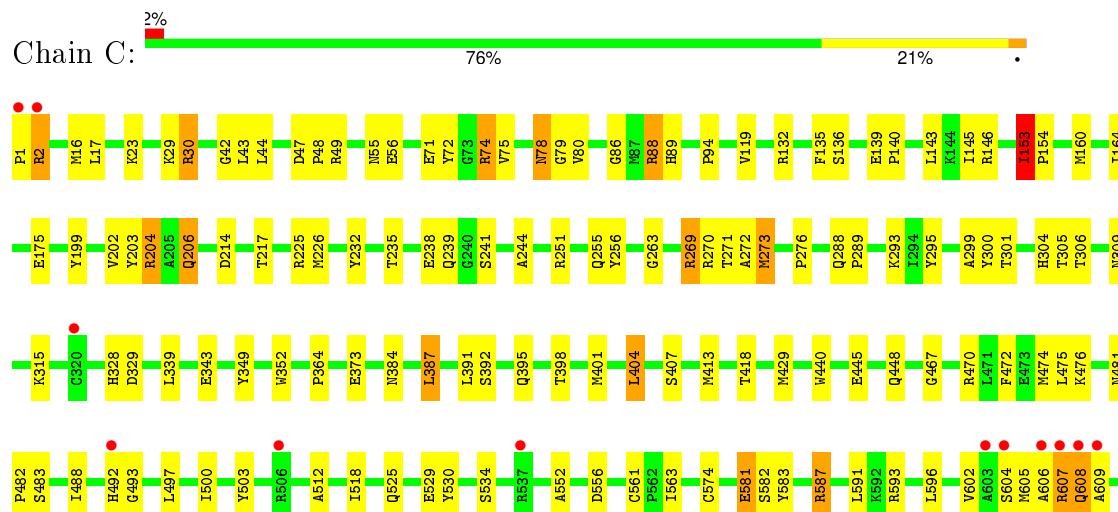
3 Residue-property plots [i](#)

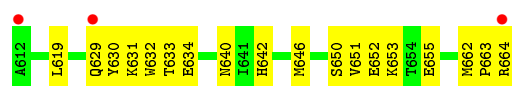
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: P2 PROTEIN

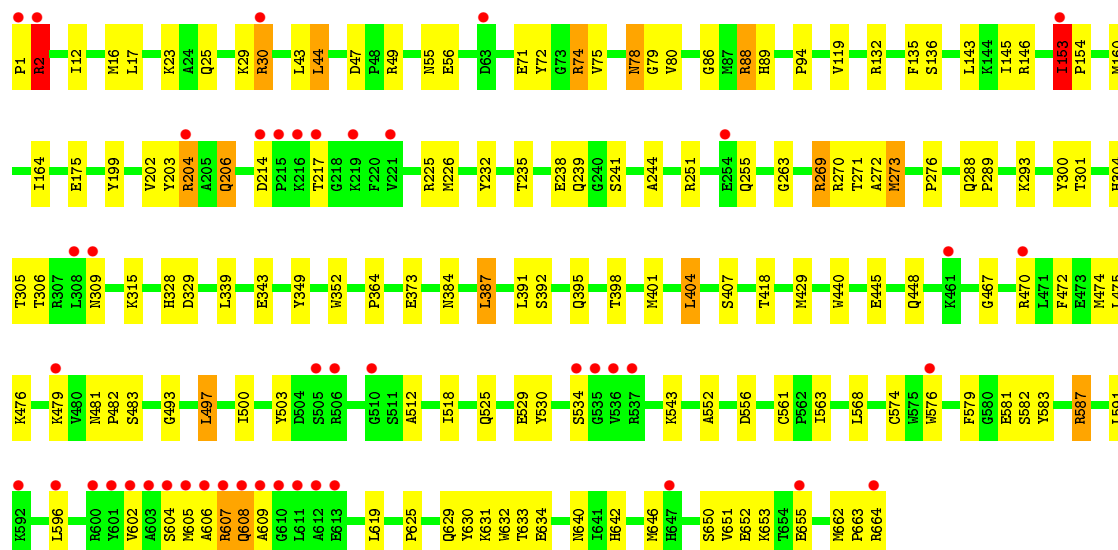
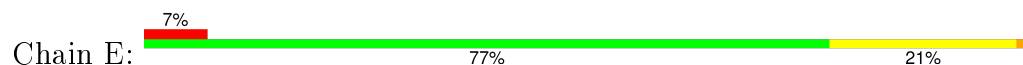


• Molecule 1: P2 PROTEIN





• Molecule 1: P2 PROTEIN



• Molecule 2: 5'-D(*GP*GP)-3'



• Molecule 2: 5'-D(*GP*GP)-3'



• Molecule 2: 5'-D(*GP*GP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.29Å 93.80Å 140.77Å 90.00° 101.35° 90.00°	Depositor
Resolution (Å)	19.98 – 2.45 20.02 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.98-2.45) 97.5 (20.02-2.45)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.68 (at 2.47Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.265 0.240 , 0.264	Depositor DCC
R_{free} test set	4874 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 97100 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16257	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, MN, POP

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	0.77	1/5396 (0.0%)	0.90	9/7297 (0.1%)
1	C	0.77	1/5396 (0.0%)	0.90	9/7297 (0.1%)
1	E	0.77	1/5396 (0.0%)	0.90	9/7297 (0.1%)
2	B	0.87	0/25	0.94	0/37
2	D	0.87	0/25	0.93	0/37
2	F	0.87	0/25	0.94	0/37
All	All	0.77	3/16263 (0.0%)	0.90	27/22002 (0.1%)

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	A	0	1
1	C	0	1
1	E	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	153	ILE	CA-CB	-9.66	1.32	1.54
1	C	153	ILE	CA-CB	-9.65	1.32	1.54
1	A	153	ILE	CA-CB	-9.64	1.32	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	153	ILE	C-N-CD	11.76	153.09	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ILE	C-N-CD	11.75	153.08	128.40
1	C	153	ILE	C-N-CD	11.75	153.07	128.40
1	E	153	ILE	CG1-CB-CG2	9.46	132.22	111.40
1	A	153	ILE	CG1-CB-CG2	9.46	132.21	111.40
1	C	153	ILE	CG1-CB-CG2	9.46	132.21	111.40
1	A	153	ILE	C-N-CA	-8.51	86.24	122.00
1	E	153	ILE	C-N-CA	-8.51	86.24	122.00
1	C	153	ILE	C-N-CA	-8.50	86.29	122.00
1	A	153	ILE	N-CA-C	8.45	133.80	111.00
1	C	153	ILE	N-CA-C	8.44	133.79	111.00
1	E	153	ILE	N-CA-C	8.44	133.78	111.00
1	A	153	ILE	CB-CA-C	-6.86	97.89	111.60
1	E	153	ILE	CB-CA-C	-6.86	97.89	111.60
1	C	153	ILE	CB-CA-C	-6.84	97.91	111.60
1	C	88	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	206	GLN	N-CA-C	-6.72	92.84	111.00
1	E	88	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	C	206	GLN	N-CA-C	-6.72	92.86	111.00
1	A	88	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	E	206	GLN	N-CA-C	-6.71	92.87	111.00
1	C	153	ILE	CA-CB-CG1	-5.94	99.71	111.00
1	A	153	ILE	CA-CB-CG1	-5.94	99.72	111.00
1	E	153	ILE	CA-CB-CG1	-5.94	99.72	111.00
1	A	404	LEU	CA-CB-CG	5.43	127.79	115.30
1	C	404	LEU	CA-CB-CG	5.43	127.78	115.30
1	E	404	LEU	CA-CB-CG	5.42	127.77	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	TYR	Sidechain
1	C	199	TYR	Sidechain
1	E	199	TYR	Sidechain

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	A	5265	0	5165	124	2
1	C	5265	0	5165	128	1
1	E	5265	0	5165	124	7
2	B	55	0	23	5	0
2	D	55	0	23	5	0
2	F	55	0	23	5	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
5	A	9	0	0	0	0
5	C	9	0	0	0	0
5	E	9	0	0	0	0
6	A	83	0	0	4	1
6	B	1	0	0	0	0
6	C	86	0	0	6	2
6	D	1	0	0	0	0
6	E	89	0	0	11	1
6	F	1	0	0	0	0
All	All	16257	0	15564	373	9

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 12.

All (373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ILE:HG23	1:C:154:PRO:CD	1.50	1.41
1:A:153:ILE:HG23	1:A:154:PRO:CD	1.50	1.39
1:E:153:ILE:HG23	1:E:154:PRO:CD	1.50	1.38
1:A:153:ILE:HG23	1:A:154:PRO:N	1.61	1.14
1:A:608:GLN:HE22	1:C:593:ARG:CZ	1.58	1.14
1:A:206:GLN:NE2	1:A:270:ARG:HE	1.51	1.09
1:C:206:GLN:NE2	1:C:270:ARG:HE	1.51	1.09
1:A:153:ILE:HG23	1:A:154:PRO:HD2	1.35	1.08
1:E:576:TRP:CE3	6:E:2075:HOH:O	2.03	1.08
1:E:206:GLN:NE2	1:E:270:ARG:HE	1.51	1.07
1:E:153:ILE:HG23	1:E:154:PRO:N	1.61	1.06
1:C:153:ILE:HG23	1:C:154:PRO:HD2	1.34	1.05
1:E:153:ILE:HG23	1:E:154:PRO:HD2	1.34	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ILE:HG23	1:C:154:PRO:N	1.61	1.03
1:E:153:ILE:CG2	1:E:154:PRO:CD	2.37	1.03
1:C:153:ILE:CG2	1:C:154:PRO:CD	2.37	1.03
1:A:153:ILE:CG2	1:A:154:PRO:CD	2.37	1.02
1:C:251:ARG:HH11	1:C:255:GLN:HE22	1.12	0.95
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.12	0.95
1:C:581:GLU:OE1	6:C:2073:HOH:O	1.89	0.90
1:E:576:TRP:HB3	6:E:2075:HOH:O	1.71	0.90
1:A:561:CYS:HB3	6:A:2068:HOH:O	1.73	0.89
1:C:561:CYS:HB3	6:C:2070:HOH:O	1.73	0.89
1:E:251:ARG:HH11	1:E:255:GLN:HE22	1.12	0.89
1:E:561:CYS:HB3	6:E:2072:HOH:O	1.73	0.89
1:C:153:ILE:CG2	1:C:154:PRO:N	2.37	0.88
1:A:153:ILE:CG2	1:A:154:PRO:N	2.37	0.87
1:E:576:TRP:HE3	6:E:2075:HOH:O	1.45	0.86
1:E:206:GLN:HE21	1:E:270:ARG:HE	1.23	0.85
1:E:364:PRO:HA	1:E:387:LEU:HD22	1.59	0.84
1:C:206:GLN:HE21	1:C:270:ARG:HE	1.23	0.84
1:A:206:GLN:HE21	1:A:270:ARG:HE	1.23	0.84
1:C:364:PRO:HA	1:C:387:LEU:HD22	1.59	0.83
1:A:608:GLN:NE2	1:C:593:ARG:CZ	2.40	0.83
1:A:364:PRO:HA	1:A:387:LEU:HD22	1.59	0.83
2:F:1:GTP:N7	2:F:1:GTP:O1G	2.12	0.82
2:B:1:GTP:N7	2:B:1:GTP:O1G	2.12	0.82
2:D:1:GTP:N7	2:D:1:GTP:O1G	2.12	0.82
1:A:555:LYS:NZ	6:A:2066:HOH:O	2.01	0.81
1:E:49:ARG:NH1	6:E:2012:HOH:O	2.14	0.79
1:E:153:ILE:CG2	1:E:154:PRO:N	2.37	0.79
1:A:74:ARG:HB3	1:A:503:TYR:CD2	2.19	0.77
1:E:74:ARG:HB3	1:E:503:TYR:CD2	2.19	0.77
1:C:74:ARG:HB3	1:C:503:TYR:CD2	2.19	0.77
1:C:301:THR:HG23	1:C:440:TRP:O	1.85	0.76
1:C:226:MET:HE1	1:C:244:ALA:HB2	1.66	0.76
1:A:301:THR:HG23	1:A:440:TRP:O	1.85	0.76
1:E:301:THR:HG23	1:E:440:TRP:O	1.85	0.75
1:C:55:ASN:OD1	1:C:88:ARG:NH2	2.19	0.75
1:A:55:ASN:OD1	1:A:88:ARG:NH2	2.19	0.75
1:E:55:ASN:OD1	1:E:88:ARG:NH2	2.19	0.75
1:C:629:GLN:HG2	1:C:629:GLN:O	1.87	0.74
1:A:629:GLN:O	1:A:629:GLN:HG2	1.87	0.74
1:E:629:GLN:O	1:E:629:GLN:HG2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:GLU:OE2	2:D:1:GTP:O2G	2.08	0.71
1:A:529:GLU:OE2	2:B:1:GTP:O2G	2.08	0.71
1:E:529:GLU:OE2	2:F:1:GTP:O2G	2.08	0.70
1:A:206:GLN:NE2	1:A:270:ARG:NE	2.35	0.69
1:E:153:ILE:CG2	1:E:154:PRO:HD2	2.17	0.69
1:A:226:MET:HE1	1:A:244:ALA:HB2	1.74	0.68
1:C:153:ILE:CG2	1:C:154:PRO:HD2	2.17	0.68
1:C:206:GLN:NE2	1:C:270:ARG:NE	2.35	0.68
1:A:206:GLN:HE21	1:A:270:ARG:NE	1.92	0.68
1:C:206:GLN:HE21	1:C:270:ARG:NE	1.92	0.68
1:E:226:MET:HE1	1:E:244:ALA:HB2	1.74	0.67
2:F:1:GTP:O2G	2:F:2:G:O6	2.14	0.66
2:D:1:GTP:O2G	2:D:2:G:O6	2.14	0.66
2:B:1:GTP:O2G	2:B:2:G:O6	2.14	0.65
1:E:206:GLN:HE21	1:E:270:ARG:NE	1.92	0.65
1:E:206:GLN:HE22	1:E:270:ARG:HE	1.41	0.65
1:E:78:ASN:ND2	1:E:80:VAL:H	1.94	0.65
1:C:206:GLN:HE22	1:C:270:ARG:HE	1.41	0.64
1:E:206:GLN:NE2	1:E:270:ARG:NE	2.35	0.64
1:C:78:ASN:ND2	1:C:80:VAL:H	1.94	0.64
1:C:288:GLN:HB3	1:C:289:PRO:HD3	1.80	0.64
1:A:78:ASN:ND2	1:A:80:VAL:H	1.94	0.64
1:A:206:GLN:HE22	1:A:270:ARG:HE	1.41	0.63
1:A:153:ILE:CG2	1:A:154:PRO:HD2	2.17	0.62
1:A:288:GLN:HB3	1:A:289:PRO:HD3	1.80	0.62
1:E:288:GLN:HB3	1:E:289:PRO:HD3	1.80	0.62
1:C:581:GLU:CG	6:C:2073:HOH:O	2.47	0.62
1:E:78:ASN:HD22	1:E:79:GLY:N	1.98	0.61
1:A:203:TYR:CE1	1:A:271:THR:HG22	2.36	0.61
1:C:78:ASN:HD22	1:C:79:GLY:N	1.98	0.60
1:E:203:TYR:CE1	1:E:271:THR:HG22	2.36	0.60
1:A:78:ASN:HD22	1:A:79:GLY:N	1.98	0.60
1:A:153:ILE:CG2	1:A:154:PRO:HD3	2.32	0.60
1:C:203:TYR:CE1	1:C:271:THR:HG22	2.36	0.60
1:C:75:VAL:HG12	1:C:493:GLY:HA2	1.84	0.60
1:A:427:LYS:HE3	1:E:12:ILE:HG21	1.84	0.59
1:A:608:GLN:HE22	1:C:593:ARG:NE	1.98	0.59
1:C:642:HIS:CE1	1:C:646:MET:HG3	2.38	0.59
1:A:75:VAL:HG12	1:A:493:GLY:HA2	1.84	0.59
1:E:75:VAL:HG12	1:E:493:GLY:HA2	1.84	0.59
1:A:642:HIS:CE1	1:A:646:MET:HG3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:CD	1:A:71:GLU:H	2.06	0.59
1:A:226:MET:HE2	1:A:244:ALA:HA	1.83	0.59
1:E:642:HIS:CE1	1:E:646:MET:HG3	2.38	0.59
1:C:71:GLU:H	1:C:71:GLU:CD	2.06	0.59
1:A:608:GLN:HE22	1:C:593:ARG:NH1	1.99	0.58
1:E:579:PHE:HE2	6:E:2012:HOH:O	1.86	0.58
1:A:608:GLN:NE2	1:C:593:ARG:NH1	2.50	0.58
1:E:226:MET:HE2	1:E:244:ALA:HA	1.84	0.58
1:E:71:GLU:H	1:E:71:GLU:CD	2.06	0.58
1:C:203:TYR:HE1	1:C:271:THR:HG22	1.69	0.58
1:A:119:VAL:O	1:E:25:GLN:HG3	2.04	0.57
1:E:576:TRP:CD2	6:E:2075:HOH:O	2.43	0.57
1:E:203:TYR:HE1	1:E:271:THR:HG22	1.69	0.57
1:A:301:THR:HB	1:A:448:GLN:O	2.06	0.56
1:E:304:HIS:HA	1:E:309:ASN:HD21	1.71	0.56
1:A:304:HIS:HA	1:A:309:ASN:HD21	1.71	0.56
1:A:418:THR:HG22	1:A:467:GLY:C	2.26	0.56
1:A:203:TYR:HE1	1:A:271:THR:HG22	1.69	0.56
1:C:304:HIS:HA	1:C:309:ASN:HD21	1.70	0.56
1:E:418:THR:HG22	1:E:467:GLY:C	2.26	0.56
1:A:606:ALA:C	1:A:608:GLN:H	2.09	0.56
1:C:301:THR:HB	1:C:448:GLN:O	2.06	0.56
1:C:418:THR:HG22	1:C:467:GLY:C	2.26	0.56
1:C:606:ALA:HB3	1:C:609:ALA:HB2	1.88	0.55
1:C:606:ALA:C	1:C:608:GLN:H	2.09	0.55
1:E:153:ILE:CG2	1:E:154:PRO:HD3	2.32	0.55
1:E:606:ALA:C	1:E:608:GLN:H	2.09	0.55
1:A:606:ALA:HB3	1:A:609:ALA:HB2	1.88	0.55
1:C:153:ILE:CG2	1:C:154:PRO:HD3	2.32	0.55
1:E:301:THR:HB	1:E:448:GLN:O	2.06	0.55
1:C:300:TYR:HD1	1:C:301:THR:HG22	1.71	0.54
1:E:606:ALA:HB3	1:E:609:ALA:HB2	1.88	0.54
1:E:300:TYR:HD1	1:E:301:THR:HG22	1.71	0.54
1:A:300:TYR:HD1	1:A:301:THR:HG22	1.71	0.54
1:A:17:LEU:O	1:A:153:ILE:O	2.26	0.54
1:E:576:TRP:CG	6:E:2075:HOH:O	2.61	0.53
1:C:17:LEU:O	1:C:153:ILE:O	2.26	0.53
1:A:407:SER:HA	1:A:448:GLN:HE22	1.74	0.53
1:E:132:ARG:HH11	1:E:429:MET:HE2	1.74	0.53
1:C:475:LEU:HD21	1:C:482:PRO:HG3	1.91	0.53
1:C:251:ARG:NH1	1:C:255:GLN:HE22	1.95	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:LEU:O	1:E:153:ILE:O	2.26	0.52
1:A:175:GLU:HA	1:A:352:TRP:CE3	2.45	0.52
1:E:587:ARG:NH1	6:E:2076:HOH:O	2.43	0.52
1:A:136:SER:OG	1:A:293:LYS:NZ	2.43	0.52
1:C:136:SER:OG	1:C:293:LYS:NZ	2.43	0.52
1:A:475:LEU:HD21	1:A:482:PRO:HG3	1.91	0.52
1:E:136:SER:OG	1:E:293:LYS:NZ	2.43	0.52
1:C:175:GLU:HA	1:C:352:TRP:CE3	2.45	0.52
1:E:175:GLU:HA	1:E:352:TRP:CE3	2.45	0.52
1:A:88:ARG:HD3	1:A:263:GLY:O	2.10	0.52
1:E:364:PRO:HA	1:E:387:LEU:CD2	2.37	0.52
1:C:88:ARG:HD3	1:C:263:GLY:O	2.10	0.52
1:E:475:LEU:HD21	1:E:482:PRO:HG3	1.91	0.52
1:E:407:SER:HA	1:E:448:GLN:HE22	1.74	0.52
1:E:88:ARG:HD3	1:E:263:GLY:O	2.10	0.51
1:C:407:SER:HA	1:C:448:GLN:HE22	1.74	0.51
1:A:2:ARG:HD2	1:A:2:ARG:O	2.11	0.51
1:A:587:ARG:NH1	6:A:2070:HOH:O	2.43	0.51
1:C:481:ASN:ND2	1:C:483:SER:O	2.44	0.51
1:C:587:ARG:NH1	6:C:2074:HOH:O	2.43	0.51
1:C:175:GLU:HA	1:C:352:TRP:CD2	2.46	0.51
1:E:481:ASN:ND2	1:E:483:SER:O	2.44	0.51
1:E:576:TRP:CB	6:E:2075:HOH:O	2.41	0.51
1:A:481:ASN:ND2	1:A:483:SER:O	2.44	0.51
1:C:2:ARG:O	1:C:2:ARG:HD2	2.11	0.51
1:C:602:VAL:HG11	1:C:605:MET:HG3	1.93	0.50
1:A:175:GLU:HA	1:A:352:TRP:CD2	2.46	0.50
1:E:2:ARG:HD2	1:E:2:ARG:O	2.11	0.50
1:C:581:GLU:HG3	6:C:2073:HOH:O	2.11	0.50
1:C:78:ASN:HD22	1:C:78:ASN:C	2.14	0.50
1:A:401:MET:HA	1:A:401:MET:HE2	1.94	0.50
1:E:78:ASN:C	1:E:78:ASN:HD22	2.14	0.50
1:E:175:GLU:HA	1:E:352:TRP:CD2	2.46	0.49
1:C:72:TYR:CZ	1:C:476:LYS:HD3	2.47	0.49
1:A:47:ASP:OD1	1:A:49:ARG:HD3	2.12	0.49
1:E:72:TYR:CZ	1:E:476:LYS:HD3	2.47	0.49
1:A:593:ARG:CG	1:C:42:GLY:HA2	2.43	0.49
1:C:1:PRO:HD2	1:C:238:GLU:OE2	2.13	0.49
1:A:534:SER:O	1:C:48:PRO:HG2	2.13	0.49
2:D:1:GTP:N7	2:D:1:GTP:PG	2.85	0.49
1:E:47:ASP:OD1	1:E:49:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:ARG:NH1	1:E:255:GLN:HE22	1.95	0.49
1:A:78:ASN:C	1:A:78:ASN:HD22	2.14	0.49
1:E:602:VAL:HG11	1:E:605:MET:HG3	1.93	0.49
1:C:339:LEU:HD23	1:C:339:LEU:C	2.33	0.49
1:A:72:TYR:CZ	1:A:476:LYS:HD3	2.47	0.49
1:A:339:LEU:C	1:A:339:LEU:HD23	2.33	0.49
1:A:1:PRO:HD2	1:A:238:GLU:OE2	2.13	0.49
1:E:1:PRO:HD2	1:E:238:GLU:OE2	2.13	0.49
2:B:1:GTP:N7	2:B:1:GTP:PG	2.85	0.48
2:F:1:GTP:N7	2:F:1:GTP:PG	2.85	0.48
1:E:339:LEU:C	1:E:339:LEU:HD23	2.33	0.48
1:A:602:VAL:HG11	1:A:605:MET:HG3	1.94	0.48
1:E:401:MET:CE	1:E:401:MET:HA	2.43	0.48
1:E:72:TYR:CE1	1:E:476:LYS:HD3	2.48	0.48
1:A:72:TYR:CE1	1:A:476:LYS:HD3	2.48	0.48
1:C:401:MET:CE	1:C:401:MET:HA	2.43	0.48
1:C:47:ASP:OD1	1:C:49:ARG:HD3	2.12	0.48
1:E:56:GLU:HG2	1:E:574:CYS:SG	2.54	0.48
1:C:56:GLU:HG2	1:C:574:CYS:SG	2.54	0.48
1:A:401:MET:HA	1:A:401:MET:CE	2.43	0.48
1:A:56:GLU:HG2	1:A:574:CYS:SG	2.54	0.48
1:A:364:PRO:HA	1:A:387:LEU:CD2	2.37	0.47
1:C:72:TYR:CE1	1:C:476:LYS:HD3	2.48	0.47
1:A:305:THR:OG1	1:A:306:THR:N	2.47	0.47
1:E:602:VAL:CG1	1:E:605:MET:HG3	2.45	0.47
1:C:602:VAL:CG1	1:C:605:MET:HG3	2.45	0.47
1:A:602:VAL:CG1	1:A:605:MET:HG3	2.45	0.47
1:A:153:ILE:HD12	1:A:153:ILE:HA	1.41	0.47
1:C:86:GLY:O	1:C:89:HIS:HD2	1.98	0.47
1:A:427:LYS:HE3	1:E:12:ILE:CG2	2.45	0.47
1:C:235:THR:O	1:C:238:GLU:HG3	2.15	0.47
1:E:305:THR:OG1	1:E:306:THR:N	2.47	0.47
1:C:132:ARG:HH11	1:C:429:MET:HE2	1.80	0.47
1:C:606:ALA:O	1:C:608:GLN:N	2.45	0.47
1:A:235:THR:O	1:A:238:GLU:HG3	2.15	0.46
1:E:235:THR:O	1:E:238:GLU:HG3	2.14	0.46
1:E:606:ALA:O	1:E:608:GLN:N	2.45	0.46
1:E:145:ILE:HD12	1:E:164:ILE:HD13	1.98	0.46
1:A:145:ILE:HD12	1:A:164:ILE:HD13	1.98	0.46
1:E:204:ARG:HD2	1:E:530:TYR:OH	2.15	0.46
1:C:304:HIS:HA	1:C:309:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:GLY:O	1:E:89:HIS:HD2	1.98	0.46
1:E:304:HIS:HA	1:E:309:ASN:ND2	2.30	0.46
1:C:401:MET:HE2	1:C:401:MET:HA	1.97	0.46
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.77	0.46
1:E:232:TYR:HA	1:E:239:GLN:O	2.15	0.46
1:A:86:GLY:O	1:A:89:HIS:HD2	1.98	0.46
1:C:145:ILE:HD12	1:C:164:ILE:HD13	1.98	0.46
1:A:304:HIS:HA	1:A:309:ASN:ND2	2.30	0.45
1:A:232:TYR:HA	1:A:239:GLN:O	2.15	0.45
1:C:226:MET:HE2	1:C:244:ALA:HA	1.97	0.45
1:C:305:THR:OG1	1:C:306:THR:N	2.47	0.45
1:C:2:ARG:O	1:C:2:ARG:CD	2.65	0.45
1:A:132:ARG:HH12	1:A:429:MET:HG3	1.82	0.45
1:C:395:GLN:HB3	1:C:398:THR:HG22	1.98	0.45
1:C:204:ARG:HD2	1:C:530:TYR:OH	2.15	0.45
1:E:640:ASN:N	1:E:640:ASN:OD1	2.48	0.45
1:C:662:MET:HB3	1:C:663:PRO:CD	2.47	0.45
1:E:395:GLN:HB3	1:E:398:THR:HG22	1.98	0.45
1:C:232:TYR:HA	1:C:239:GLN:O	2.15	0.45
1:A:395:GLN:HB3	1:A:398:THR:HG22	1.98	0.45
1:A:204:ARG:HD2	1:A:530:TYR:OH	2.15	0.45
1:A:315:LYS:HE3	1:A:512:ALA:O	2.17	0.45
1:A:607:ARG:O	1:A:608:GLN:HG3	2.16	0.45
1:E:607:ARG:O	1:E:608:GLN:HG3	2.16	0.45
1:E:132:ARG:HH12	1:E:429:MET:HG3	1.82	0.45
1:C:132:ARG:HH12	1:C:429:MET:HG3	1.82	0.45
1:E:315:LYS:HE3	1:E:512:ALA:O	2.17	0.45
1:C:226:MET:HE1	1:C:244:ALA:CB	2.44	0.44
1:C:135:PHE:HB3	1:C:349:TYR:OH	2.16	0.44
1:E:135:PHE:HB3	1:E:349:TYR:OH	2.16	0.44
1:C:587:ARG:HA	1:C:587:ARG:HD2	1.77	0.44
1:E:2:ARG:CD	1:E:2:ARG:O	2.64	0.44
1:A:662:MET:HB3	1:A:663:PRO:CD	2.47	0.44
1:A:135:PHE:HB3	1:A:349:TYR:OH	2.16	0.44
1:E:662:MET:HB3	1:E:663:PRO:CD	2.47	0.44
1:A:270:ARG:NH2	2:B:2:G:O2'	2.50	0.44
1:E:270:ARG:NH2	2:F:2:G:O2'	2.50	0.44
1:C:607:ARG:O	1:C:608:GLN:HG3	2.16	0.44
1:C:474:MET:HB2	1:C:474:MET:HE2	1.83	0.44
1:A:2:ARG:CD	1:A:2:ARG:O	2.65	0.44
1:A:160:MET:O	1:A:164:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:650:SER:OG	1:E:653:LYS:CG	2.66	0.44
1:C:270:ARG:NH2	2:D:2:G:O2'	2.50	0.44
1:C:364:PRO:HA	1:C:387:LEU:CD2	2.37	0.44
1:E:328:HIS:HD2	1:E:329:ASP:OD1	2.01	0.44
1:A:525:GLN:NE2	1:A:583:TYR:OH	2.51	0.44
1:C:640:ASN:N	1:C:640:ASN:OD1	2.48	0.44
1:C:315:LYS:HE3	1:C:512:ALA:O	2.17	0.44
1:E:652:GLU:H	1:E:652:GLU:CD	2.21	0.44
1:A:407:SER:OG	1:A:448:GLN:NE2	2.51	0.43
1:E:160:MET:O	1:E:164:ILE:HG12	2.18	0.43
1:C:204:ARG:HE	1:C:204:ARG:HB3	1.56	0.43
1:C:650:SER:OG	1:C:653:LYS:CG	2.66	0.43
1:A:328:HIS:HD2	1:A:329:ASP:OD1	2.01	0.43
1:C:407:SER:OG	1:C:448:GLN:NE2	2.51	0.43
1:A:273:MET:HE2	1:A:392:SER:HA	2.00	0.43
1:C:652:GLU:CD	1:C:652:GLU:H	2.21	0.43
1:E:202:VAL:CG2	1:E:272:ALA:HB3	2.48	0.43
1:A:29:LYS:O	1:A:30:ARG:C	2.57	0.43
1:A:640:ASN:N	1:A:640:ASN:OD1	2.48	0.43
1:C:413:MET:HE1	1:C:488:ILE:HG13	2.01	0.43
1:C:328:HIS:HD2	1:C:329:ASP:OD1	2.01	0.43
1:C:251:ARG:HB2	1:C:255:GLN:NE2	2.33	0.43
1:A:251:ARG:NH1	1:A:255:GLN:HE22	1.95	0.43
1:E:387:LEU:HA	1:E:387:LEU:HD12	1.75	0.43
1:A:75:VAL:HG21	1:A:500:ILE:HG21	2.01	0.43
1:C:525:GLN:NE2	1:C:583:TYR:OH	2.51	0.43
1:E:587:ARG:HD2	1:E:587:ARG:HA	1.77	0.43
1:E:525:GLN:NE2	1:E:583:TYR:OH	2.51	0.43
1:A:214:ASP:HB3	1:A:217:THR:OG1	2.18	0.43
1:C:251:ARG:HB2	1:C:255:GLN:HE21	1.84	0.43
1:E:407:SER:OG	1:E:448:GLN:NE2	2.51	0.43
1:E:75:VAL:HG21	1:E:500:ILE:HG21	2.01	0.43
1:C:160:MET:O	1:C:164:ILE:HG12	2.18	0.43
1:E:650:SER:OG	1:E:653:LYS:HG3	2.19	0.43
1:E:214:ASP:HB3	1:E:217:THR:OG1	2.18	0.43
1:A:650:SER:OG	1:A:653:LYS:HG3	2.18	0.43
1:E:251:ARG:HB2	1:E:255:GLN:NE2	2.34	0.43
1:E:497:LEU:HD12	1:E:497:LEU:HA	1.77	0.43
1:A:251:ARG:HB2	1:A:255:GLN:NE2	2.34	0.43
1:E:78:ASN:HD22	1:E:80:VAL:H	1.64	0.43
1:A:305:THR:H	1:A:309:ASN:ND2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ASP:HB3	1:C:217:THR:OG1	2.18	0.43
1:C:663:PRO:HD2	1:C:664:ARG:H	1.83	0.43
1:E:663:PRO:HD2	1:E:664:ARG:H	1.83	0.43
1:A:651:VAL:O	1:A:655:GLU:HB2	2.19	0.43
1:C:202:VAL:CG2	1:C:272:ALA:HB3	2.48	0.43
1:A:251:ARG:HB2	1:A:255:GLN:HE21	1.84	0.43
1:E:305:THR:H	1:E:309:ASN:ND2	2.17	0.43
1:A:650:SER:OG	1:A:653:LYS:CG	2.66	0.43
1:E:251:ARG:HB2	1:E:255:GLN:HE21	1.84	0.42
1:A:78:ASN:HD22	1:A:80:VAL:H	1.64	0.42
1:E:132:ARG:CZ	1:E:343:GLU:OE2	2.67	0.42
1:A:663:PRO:HD2	1:A:664:ARG:H	1.83	0.42
1:A:132:ARG:CZ	1:A:343:GLU:OE2	2.68	0.42
1:C:29:LYS:O	1:C:30:ARG:C	2.57	0.42
1:C:633:THR:O	1:C:634:GLU:C	2.58	0.42
1:A:652:GLU:CD	1:A:652:GLU:H	2.21	0.42
1:E:273:MET:HE2	1:E:392:SER:HA	2.00	0.42
1:A:42:GLY:O	1:C:256:TYR:HB3	2.20	0.42
1:E:568:LEU:HA	1:E:568:LEU:HD23	1.82	0.42
1:E:518:ILE:HG21	1:E:563:ILE:HD11	2.01	0.42
1:A:202:VAL:CG2	1:A:272:ALA:HB3	2.48	0.42
1:C:651:VAL:O	1:C:655:GLU:HB2	2.19	0.42
1:E:633:THR:O	1:E:634:GLU:C	2.58	0.42
1:A:86:GLY:O	1:A:89:HIS:CD2	2.73	0.42
1:E:474:MET:HE2	1:E:474:MET:HB2	1.84	0.42
1:E:651:VAL:O	1:E:655:GLU:HB2	2.19	0.42
1:A:631:LYS:HE3	1:A:632:TRP:CZ2	2.55	0.42
1:A:633:THR:O	1:A:634:GLU:C	2.58	0.42
1:C:153:ILE:HB	1:C:276:PRO:HB3	2.02	0.42
1:A:606:ALA:O	1:A:608:GLN:N	2.45	0.42
1:A:593:ARG:HG2	1:C:42:GLY:HA2	2.02	0.42
1:E:153:ILE:HA	1:E:153:ILE:HD12	1.41	0.42
1:C:305:THR:H	1:C:309:ASN:ND2	2.17	0.42
1:C:273:MET:HE2	1:C:392:SER:HA	2.00	0.42
1:A:153:ILE:HB	1:A:276:PRO:HB3	2.02	0.42
1:C:132:ARG:CZ	1:C:343:GLU:OE2	2.67	0.42
1:C:650:SER:OG	1:C:653:LYS:HG3	2.19	0.42
1:E:225:ARG:HA	1:E:225:ARG:HD3	1.87	0.42
1:E:29:LYS:O	1:E:30:ARG:C	2.57	0.42
1:E:401:MET:HA	1:E:401:MET:HE2	2.02	0.41
1:C:86:GLY:O	1:C:89:HIS:CD2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:ARG:HD3	1:C:225:ARG:HA	1.87	0.41
1:E:631:LYS:HE3	1:E:632:TRP:CZ2	2.55	0.41
1:C:631:LYS:HE3	1:C:632:TRP:CZ2	2.55	0.41
1:C:518:ILE:HG21	1:C:563:ILE:HD11	2.01	0.41
1:C:75:VAL:HG21	1:C:500:ILE:HG21	2.01	0.41
1:E:94:PRO:CB	1:E:269:ARG:HG3	2.51	0.41
1:E:49:ARG:CZ	6:E:2012:HOH:O	2.59	0.41
1:A:225:ARG:HD3	1:A:225:ARG:HA	1.87	0.41
1:A:552:ALA:HB3	1:A:619:LEU:HD13	2.03	0.41
1:E:153:ILE:HB	1:E:276:PRO:HB3	2.02	0.41
1:C:596:LEU:CD2	1:C:608:GLN:HG2	2.51	0.41
1:C:552:ALA:HB3	1:C:619:LEU:HD13	2.03	0.41
1:A:492:HIS:HB2	6:A:2056:HOH:O	2.21	0.41
1:C:202:VAL:O	1:C:202:VAL:HG23	2.21	0.41
1:C:295:TYR:O	1:C:299:ALA:HB2	2.21	0.41
1:A:518:ILE:HG21	1:A:563:ILE:HD11	2.01	0.41
1:A:94:PRO:CB	1:A:269:ARG:HG3	2.51	0.41
1:A:596:LEU:CD2	1:A:608:GLN:HG2	2.51	0.41
1:C:392:SER:O	1:C:398:THR:HG21	2.21	0.41
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.92	0.41
1:C:492:HIS:HB2	6:C:2059:HOH:O	2.21	0.41
1:A:392:SER:O	1:A:398:THR:HG21	2.21	0.40
1:E:202:VAL:HG23	1:E:202:VAL:O	2.21	0.40
1:A:543:LYS:O	1:A:625:PRO:HD2	2.21	0.40
1:C:153:ILE:HA	1:C:153:ILE:HD12	1.41	0.40
1:C:78:ASN:HD22	1:C:80:VAL:H	1.64	0.40
1:E:596:LEU:CD2	1:E:608:GLN:HG2	2.51	0.40
1:A:568:LEU:HD23	1:A:568:LEU:HA	1.81	0.40
1:E:552:ALA:HB3	1:E:619:LEU:HD13	2.03	0.40
1:C:94:PRO:CB	1:C:269:ARG:HG3	2.51	0.40
1:C:139:GLU:HA	1:C:140:PRO:HD3	1.96	0.40
1:E:543:LYS:O	1:E:625:PRO:HD2	2.21	0.40

All (9) 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)
6:A:2008:HOH:O	6:C:2019:HOH:O[2_646]	0.65	1.55
6:C:2008:HOH:O	6:E:2020:HOH:O[2_555]	1.48	0.72
1:E:479:LYS:NZ	1:E:607:ARG:C[2_445]	1.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:LYS:NZ	1:E:608:GLN:N[2_445]	1.93	0.27
1:A:569:GLU:OE2	1:E:1:PRO:CB[2_555]	2.08	0.12
1:E:479:LYS:CD	1:E:608:GLN:CB[2_445]	2.12	0.08
1:C:607:ARG:CD	1:E:44:LEU:CD1[1_655]	2.12	0.08
1:A:652:GLU:OE2	1:E:664:ARG:NH2[2_545]	2.15	0.05
1:E:479:LYS:NZ	1:E:607:ARG:O[2_445]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	662/664 (100%)	629 (95%)	28 (4%)	5 (1%)	24	28
1	C	662/664 (100%)	630 (95%)	27 (4%)	5 (1%)	24	28
1	E	662/664 (100%)	629 (95%)	27 (4%)	6 (1%)	21	25
All	All	1986/1992 (100%)	1888 (95%)	82 (4%)	16 (1%)	24	28

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ILE
1	A	608	GLN
1	C	153	ILE
1	C	608	GLN
1	E	153	ILE
1	E	608	GLN
1	A	607	ARG
1	A	630	TYR
1	C	607	ARG
1	C	630	TYR
1	E	607	ARG
1	E	630	TYR
1	A	604	SER

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Mol	Chain	Res	Type
1	C	604	SER
1	E	604	SER
1	E	2	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	557/557 (100%)	527 (95%)	30 (5%)	27	38
1	C	557/557 (100%)	527 (95%)	30 (5%)	27	38
1	E	557/557 (100%)	527 (95%)	30 (5%)	27	38
All	All	1671/1671 (100%)	1581 (95%)	90 (5%)	27	38

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	16	MET
1	A	23	LYS
1	A	30	ARG
1	A	43	LEU
1	A	44	LEU
1	A	74	ARG
1	A	78	ASN
1	A	119	VAL
1	A	143	LEU
1	A	146	ARG
1	A	204	ARG
1	A	241	SER
1	A	269	ARG
1	A	273	MET
1	A	373	GLU
1	A	384	ASN
1	A	387	LEU
1	A	391	LEU

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Mol	Chain	Res	Type
1	A	404	LEU
1	A	445	GLU
1	A	470	ARG
1	A	472	PHE
1	A	497	LEU
1	A	534	SER
1	A	556	ASP
1	A	581	GLU
1	A	582	SER
1	A	587	ARG
1	A	591	LEU
1	C	2	ARG
1	C	16	MET
1	C	23	LYS
1	C	30	ARG
1	C	43	LEU
1	C	44	LEU
1	C	74	ARG
1	C	78	ASN
1	C	119	VAL
1	C	143	LEU
1	C	146	ARG
1	C	204	ARG
1	C	241	SER
1	C	269	ARG
1	C	273	MET
1	C	373	GLU
1	C	384	ASN
1	C	387	LEU
1	C	391	LEU
1	C	404	LEU
1	C	445	GLU
1	C	470	ARG
1	C	472	PHE
1	C	497	LEU
1	C	534	SER
1	C	556	ASP
1	C	581	GLU
1	C	582	SER
1	C	587	ARG
1	C	591	LEU
1	E	2	ARG

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Mol	Chain	Res	Type
1	E	16	MET
1	E	23	LYS
1	E	30	ARG
1	E	43	LEU
1	E	44	LEU
1	E	74	ARG
1	E	78	ASN
1	E	119	VAL
1	E	143	LEU
1	E	146	ARG
1	E	204	ARG
1	E	241	SER
1	E	269	ARG
1	E	273	MET
1	E	373	GLU
1	E	384	ASN
1	E	387	LEU
1	E	391	LEU
1	E	404	LEU
1	E	445	GLU
1	E	470	ARG
1	E	472	PHE
1	E	497	LEU
1	E	534	SER
1	E	556	ASP
1	E	581	GLU
1	E	582	SER
1	E	587	ARG
1	E	591	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	26	GLN
1	A	78	ASN
1	A	89	HIS
1	A	91	ASN
1	A	191	GLN
1	A	206	GLN
1	A	255	GLN
1	A	309	ASN

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Mol	Chain	Res	Type
1	A	328	HIS
1	A	448	GLN
1	A	525	GLN
1	A	608	GLN
1	C	15	GLN
1	C	26	GLN
1	C	78	ASN
1	C	89	HIS
1	C	91	ASN
1	C	191	GLN
1	C	206	GLN
1	C	255	GLN
1	C	309	ASN
1	C	328	HIS
1	C	448	GLN
1	C	525	GLN
1	E	26	GLN
1	E	78	ASN
1	E	89	HIS
1	E	91	ASN
1	E	191	GLN
1	E	206	GLN
1	E	255	GLN
1	E	309	ASN
1	E	328	HIS
1	E	448	GLN
1	E	525	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	0/2	-	-
2	D	0/2	-	-
2	F	0/2	-	-
All	All	0/6	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

3 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
2	GTP	B	1	2,4	25,34,34	1.10	2 (8%)	34,54,54	2.09	3 (8%)
2	GTP	D	1	2,4	25,34,34	1.10	2 (8%)	34,54,54	2.09	3 (8%)
2	GTP	F	1	2,4	25,34,34	1.10	2 (8%)	34,54,54	2.09	3 (8%)

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
2	GTP	B	1	2,4	-	0/18/38/38	0/3/3/3
2	GTP	D	1	2,4	-	0/18/38/38	0/3/3/3
2	GTP	F	1	2,4	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	GTP	C8-N7	-2.21	1.30	1.34
2	B	1	GTP	C8-N7	-2.19	1.30	1.34
2	F	1	GTP	C8-N7	-2.16	1.30	1.34
2	D	1	GTP	C6-N1	3.59	1.39	1.33
2	F	1	GTP	C6-N1	3.60	1.39	1.33
2	B	1	GTP	C6-N1	3.60	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GTP	C5-C6-N1	-9.03	111.24	123.59
2	F	1	GTP	C5-C6-N1	-9.03	111.25	123.59
2	B	1	GTP	C5-C6-N1	-9.02	111.25	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GTP	N3-C2-N1	-2.15	124.17	127.44
2	D	1	GTP	N3-C2-N1	-2.13	124.21	127.44
2	F	1	GTP	N3-C2-N1	-2.12	124.21	127.44
2	F	1	GTP	C6-N1-C2	6.52	124.99	115.94
2	B	1	GTP	C6-N1-C2	6.54	125.02	115.94
2	D	1	GTP	C6-N1-C2	6.54	125.02	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	GTP	4	0
2	D	1	GTP	4	0
2	F	1	GTP	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\# Z > 2$
5	POP	A	1670	4	8,8,8	1.33	0	13,13,13	0.71	0
5	POP	C	1667	4	8,8,8	1.34	0	13,13,13	0.71	0
5	POP	E	1667	4	8,8,8	1.34	0	13,13,13	0.71	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
5	POP	A	1670	4	-	0/6/6/6	0/0/0/0
5	POP	C	1667	4	-	0/6/6/6	0/0/0/0
5	POP	E	1667	4	-	0/6/6/6	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	664/664 (100%)	0.05	22 (3%) 50 53	22, 38, 66, 119	0
1	C	664/664 (100%)	0.13	15 (2%) 64 66	22, 38, 66, 119	0
1	E	664/664 (100%)	0.29	45 (6%) 20 22	22, 38, 66, 119	0
2	B	1/2 (50%)	2.78	1 (100%) 0 0	74, 74, 74, 74	0
2	D	1/2 (50%)	2.48	1 (100%) 0 0	74, 74, 74, 74	0
2	F	1/2 (50%)	1.57	0 100 100	74, 74, 74, 74	0
All	All	1995/1998 (99%)	0.16	84 (4%) 40 43	22, 38, 66, 119	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	607	ARG	12.0
1	E	608	GLN	11.3
1	C	608	GLN	9.7
1	C	607	ARG	9.0
1	E	1	PRO	7.9
1	E	609	ALA	7.9
1	E	664	ARG	7.8
1	C	664	ARG	7.0
1	E	604	SER	6.8
1	E	603	ALA	6.7
1	A	664	ARG	6.7
1	E	610	GLY	6.6
1	A	1	PRO	6.5
1	E	606	ALA	6.3
1	C	603	ALA	5.8
1	E	537	ARG	5.6
1	C	609	ALA	5.2
1	A	606	ALA	4.8
1	A	257	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	604	SER	4.4
1	E	215	PRO	4.3
1	A	607	ARG	4.2
1	C	606	ALA	4.2
1	E	535	GLY	4.1
1	E	536	VAL	4.1
1	E	612	ALA	4.0
1	C	537	ARG	3.9
1	E	506	ARG	3.7
1	C	1	PRO	3.6
1	A	216	LYS	3.6
1	E	510	GLY	3.6
1	E	308	LEU	3.5
1	E	576	TRP	3.5
1	E	596	LEU	3.4
1	E	605	MET	3.4
1	E	505	SER	3.3
1	A	610	GLY	3.3
1	C	2	ARG	3.2
1	E	611	LEU	3.2
1	E	254	GLU	3.1
1	A	506	ARG	3.1
1	A	576	TRP	3.1
1	E	600	ARG	3.1
1	E	602	VAL	3.0
1	E	216	LYS	3.0
1	C	629	GLN	3.0
1	E	613	GLU	2.9
1	C	612	ALA	2.9
1	A	217	THR	2.9
1	E	214	ASP	2.9
1	E	2	ARG	2.9
1	E	219	LYS	2.9
1	E	204	ARG	2.9
1	C	506	ARG	2.8
1	E	461	LYS	2.8
2	B	2	G	2.8
1	A	254	GLU	2.7
1	A	652	GLU	2.6
1	A	611	LEU	2.6
1	E	479	LYS	2.5
1	C	320	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	2	G	2.5
1	E	470	ARG	2.5
1	E	217	THR	2.4
1	A	204	ARG	2.4
1	A	218	GLY	2.4
1	E	30	ARG	2.4
1	E	63	ASP	2.4
1	E	221	VAL	2.4
1	E	534	SER	2.3
1	A	605	MET	2.3
1	E	592	LYS	2.3
1	E	309	ASN	2.2
1	E	153	ILE	2.2
1	E	601	TYR	2.1
1	A	373	GLU	2.1
1	E	647	HIS	2.1
1	E	655	GLU	2.1
1	A	158	ASN	2.1
1	A	634	GLU	2.1
1	A	210	ALA	2.1
1	A	148	GLY	2.1
1	C	492	HIS	2.1
1	A	308	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	GTP	B	1	32/32	0.88	0.20	0.45	53,63,70,74	0
2	GTP	D	1	32/32	0.91	0.18	0.19	53,63,70,74	0
2	GTP	F	1	32/32	0.91	0.17	0.17	53,63,70,74	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	POP	A	1670	9/9	0.77	0.31	1.67	108,111,113,113	0
5	POP	E	1667	9/9	0.86	0.22	0.95	108,111,113,113	0
5	POP	C	1667	9/9	0.90	0.19	0.04	108,111,113,113	0
4	MG	A	1669	1/1	0.82	0.10	-1.83	35,35,35,35	0
4	MG	C	1669	1/1	0.80	0.12	-2.04	35,35,35,35	0
4	MG	E	1669	1/1	0.85	0.10	-2.12	35,35,35,35	0
3	MN	C	1670	1/1	0.97	0.10	-2.46	50,50,50,50	0
3	MN	A	1667	1/1	0.97	0.06	-3.07	50,50,50,50	0
3	MN	E	1670	1/1	0.93	0.05	-4.70	50,50,50,50	0
4	MG	E	1668	1/1	0.75	0.14	-	58,58,58,58	0
4	MG	C	1668	1/1	0.78	0.17	-	58,58,58,58	0
4	MG	A	1668	1/1	0.83	0.11	-	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.