



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:04 PM GMT

PDB ID : 1N3R
Title : Biosynthesis of pteridins. Reaction mechanism of GTP cyclohydrolase I
Authors : Rebelo, J.; Auerbach, G.; Bader, G.; Bracher, A.; Nar, H.; Hoesl, C.; Schramek, N.; Kaiser, J.; Bacher, A.; Huber, R.; Fischer, M.
Deposited on : 2002-10-29
Resolution : 2.80 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

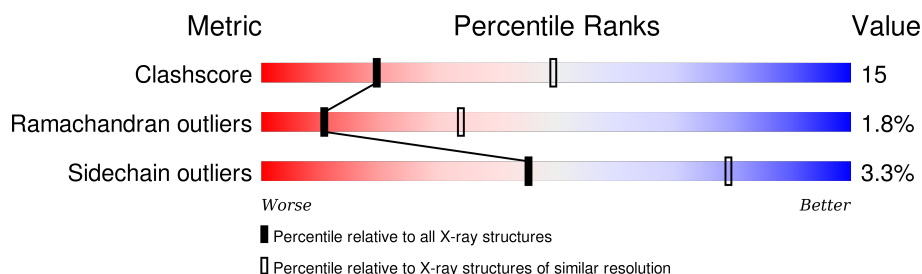
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	
1	B	221	
1	C	221	
1	D	221	
1	E	221	
1	F	221	
1	G	221	

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Mol	Chain	Length	Quality of chain
1	H	221	 61% 38% .
1	I	221	 65% 33% .
1	J	221	 68% 30% .
1	K	221	 65% 33% .
1	L	221	 71% 29% .
1	M	221	 71% 25% .
1	N	221	 69% 28% .
1	O	221	 66% 32% .

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
2	GTP	I	1418	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26471 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.

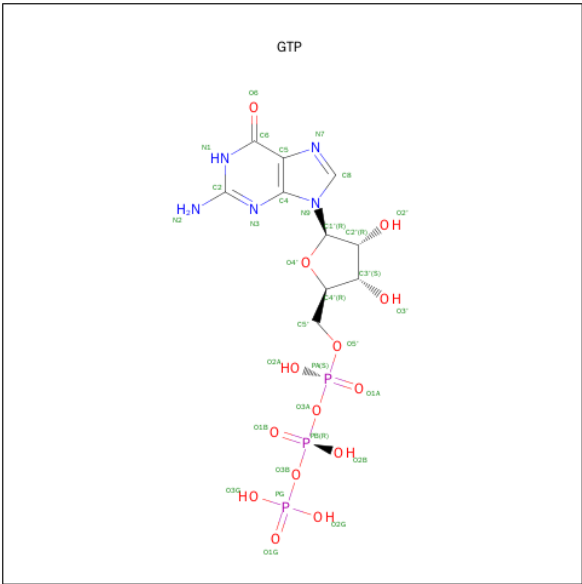
- Molecule 1 is a protein called GTP cyclohydrolase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1728	1085	307	327	9			
1	B	221	Total	C	N	O	S	0	0	0
			1728	1085	307	327	9			
1	C	221	Total	C	N	O	S	0	0	0
			1728	1085	307	327	9			
1	D	221	Total	C	N	O	S	0	0	0
			1728	1085	307	327	9			
1	E	220	Total	C	N	O	S	0	0	0
			1720	1081	305	325	9			
1	F	221	Total	C	N	O	S	0	0	0
			1728	1085	307	327	9			
1	G	221	Total	C	N	O	S	0	0	0
			1728	1085	307	327	9			
1	H	221	Total	C	N	O	S	0	0	0
			1728	1085	307	327	9			
1	I	221	Total	C	N	O	S	0	0	0
			1728	1085	307	327	9			
1	J	221	Total	C	N	O	S	0	0	0
			1728	1085	307	327	9			
1	K	221	Total	C	N	O	S	0	0	0
			1728	1085	307	327	9			
1	L	221	Total	C	N	O	S	21	0	0
			1728	1085	307	327	9			
1	M	221	Total	C	N	O	S	21	0	0
			1728	1085	307	327	9			
1	N	221	Total	C	N	O	S	0	0	0
			1728	1085	307	327	9			
1	O	221	Total	C	N	O	S	0	0	0
			1728	1085	307	327	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	SER	HIS	ENGINEERED	UNP P0A6T5
B	112	SER	HIS	ENGINEERED	UNP P0A6T5
C	112	SER	HIS	ENGINEERED	UNP P0A6T5
D	112	SER	HIS	ENGINEERED	UNP P0A6T5
E	112	SER	HIS	ENGINEERED	UNP P0A6T5
F	112	SER	HIS	ENGINEERED	UNP P0A6T5
G	112	SER	HIS	ENGINEERED	UNP P0A6T5
H	112	SER	HIS	ENGINEERED	UNP P0A6T5
I	112	SER	HIS	ENGINEERED	UNP P0A6T5
J	112	SER	HIS	ENGINEERED	UNP P0A6T5
K	112	SER	HIS	ENGINEERED	UNP P0A6T5
L	112	SER	HIS	ENGINEERED	UNP P0A6T5
M	112	SER	HIS	ENGINEERED	UNP P0A6T5
N	112	SER	HIS	ENGINEERED	UNP P0A6T5
O	112	SER	HIS	ENGINEERED	UNP P0A6T5

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	I	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	J	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	L	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	M	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	N	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	O	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	K	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	4	Total	O	0	0
			4	4		
3	C	4	Total	O	0	0
			4	4		
3	D	7	Total	O	0	0
			7	7		
3	E	2	Total	O	0	0
			2	2		
3	F	6	Total	O	0	0
			6	6		
3	G	5	Total	O	0	0
			5	5		
3	H	6	Total	O	0	0
			6	6		

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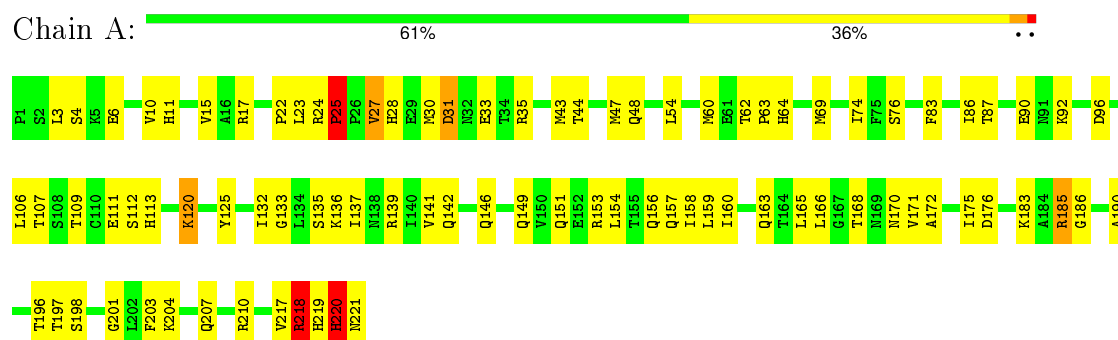
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	4	Total 4	O 4	0	0
3	J	2	Total 2	O 2	0	0
3	K	7	Total 7	O 7	0	0
3	L	5	Total 5	O 5	0	0
3	M	13	Total 13	O 13	0	0
3	N	9	Total 9	O 9	0	0
3	O	3	Total 3	O 3	0	0

3 Residue-property plots

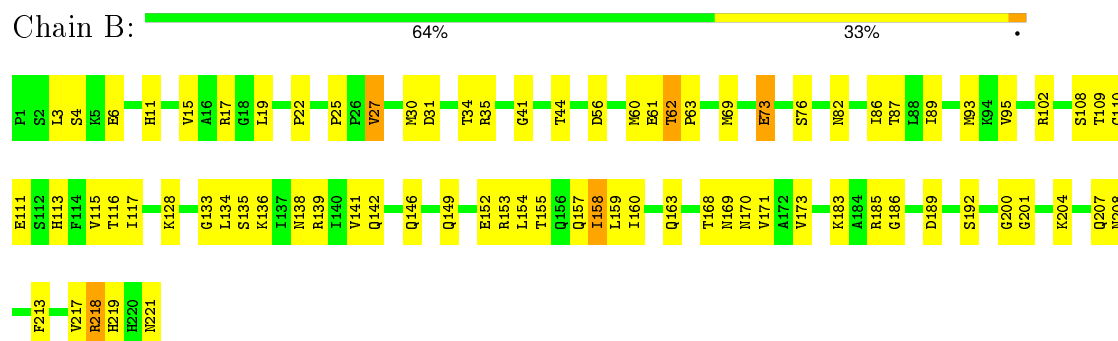
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

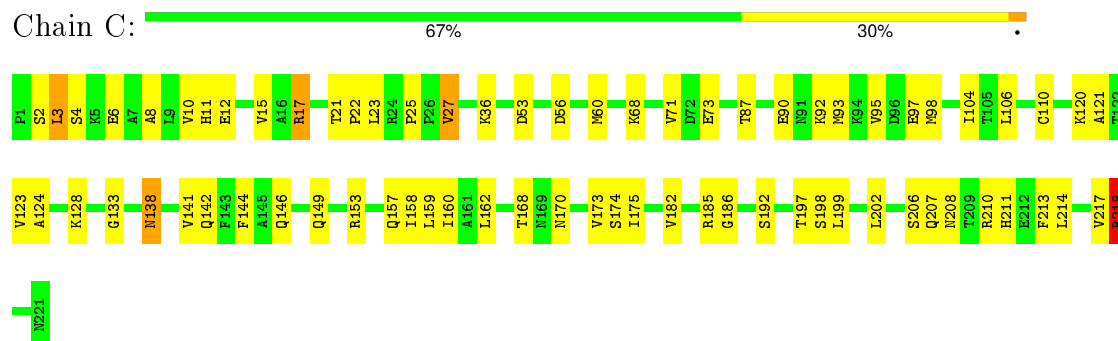
• Molecule 1: GTP cyclohydrolase I



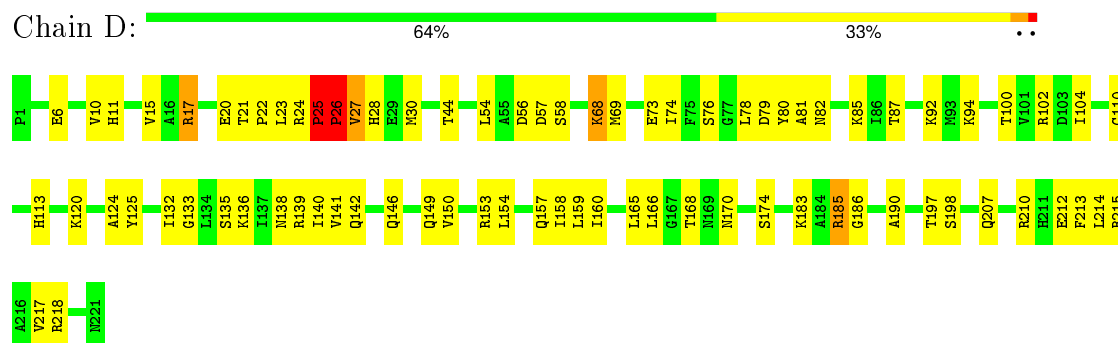
• Molecule 1: GTP cyclohydrolase I



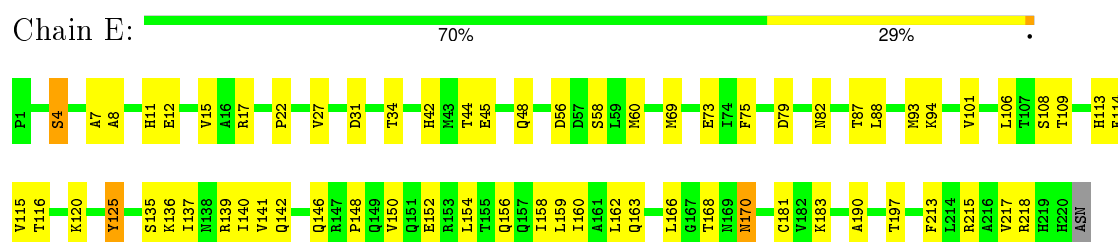
• Molecule 1: GTP cyclohydrolase I



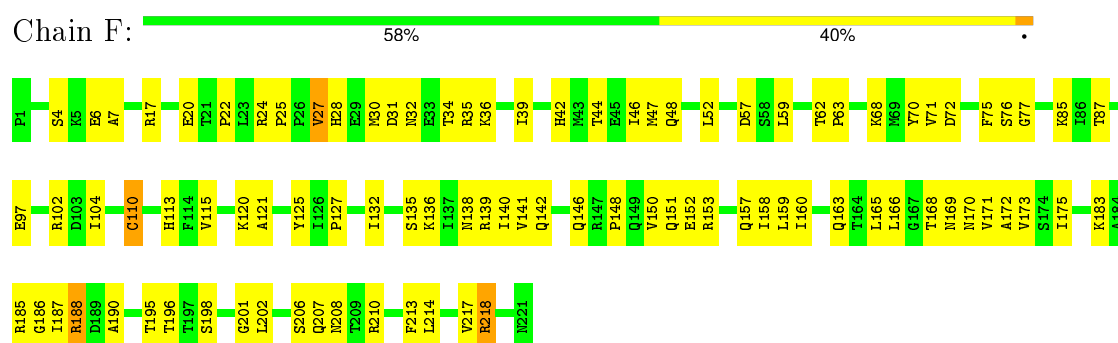
- Molecule 1: GTP cyclohydrolase I



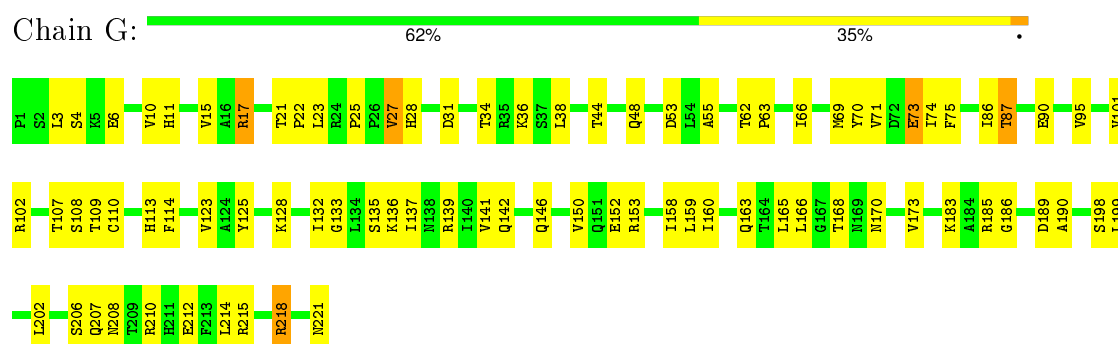
- Molecule 1: GTP cyclohydrolase I



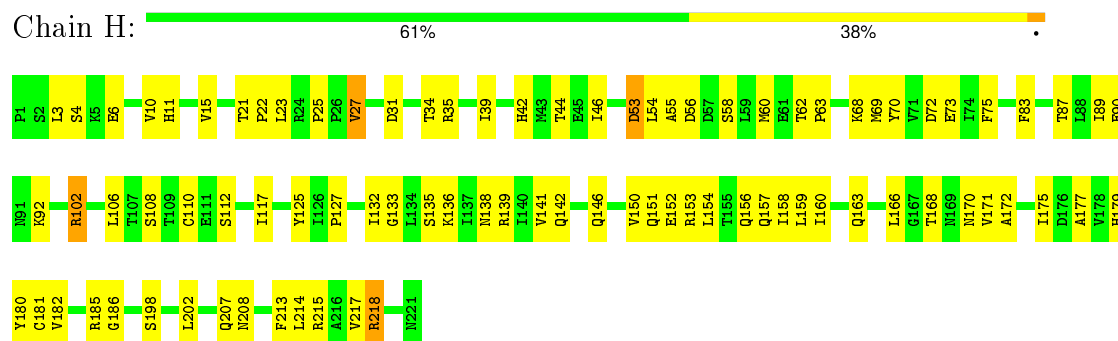
- Molecule 1: GTP cyclohydrolase I



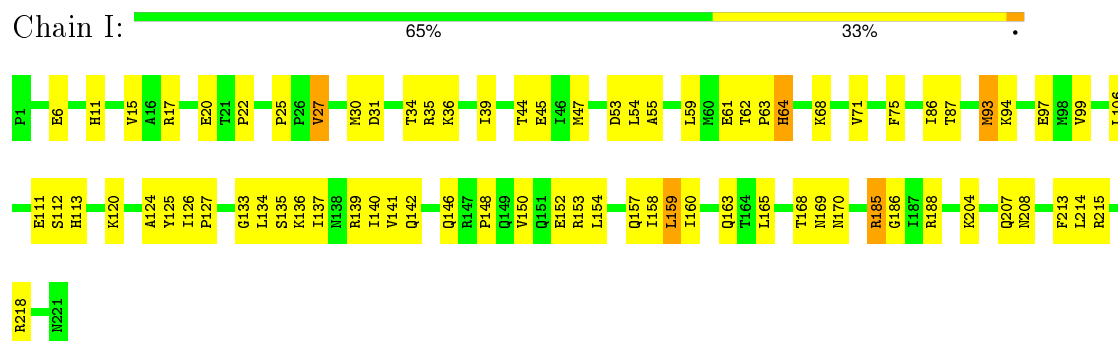
- Molecule 1: GTP cyclohydrolase I



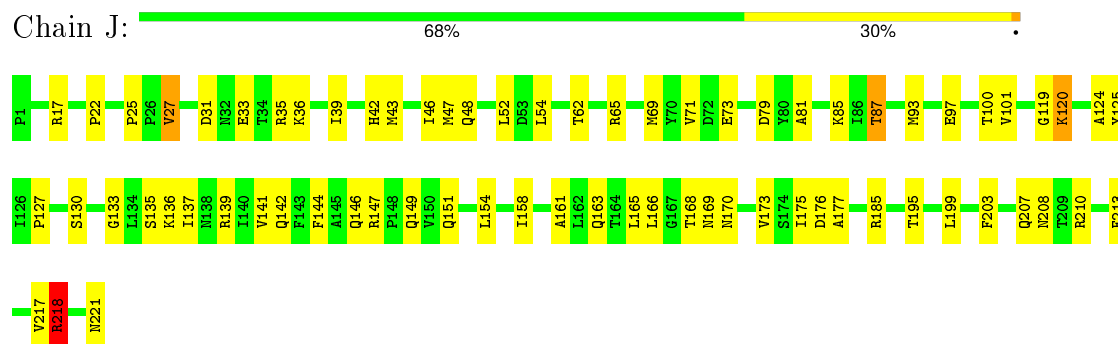
- Molecule 1: GTP cyclohydrolase I



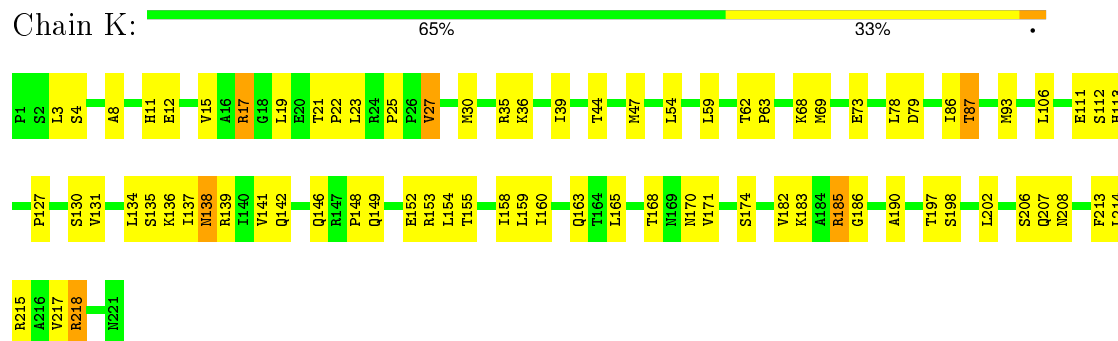
- Molecule 1: GTP cyclohydrolase I



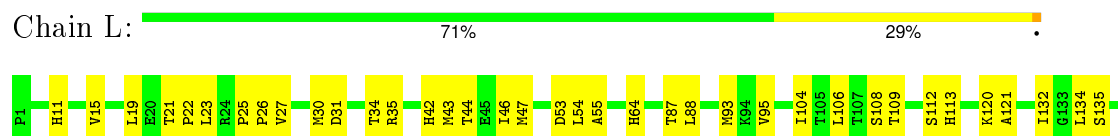
- Molecule 1: GTP cyclohydrolase I



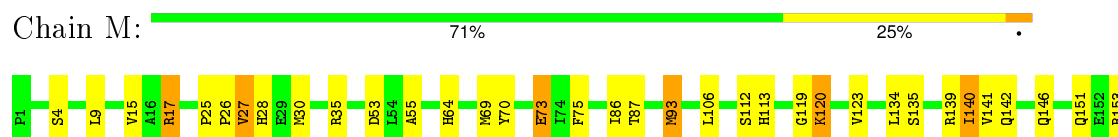
- Molecule 1: GTP cyclohydrolase I



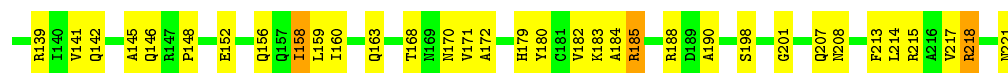
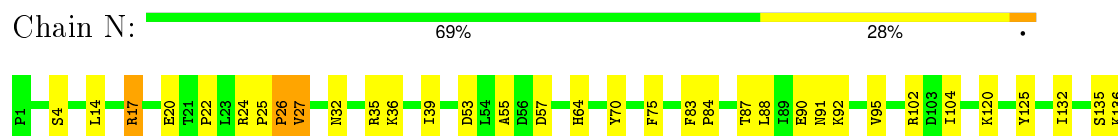
- Molecule 1: GTP cyclohydrolase I



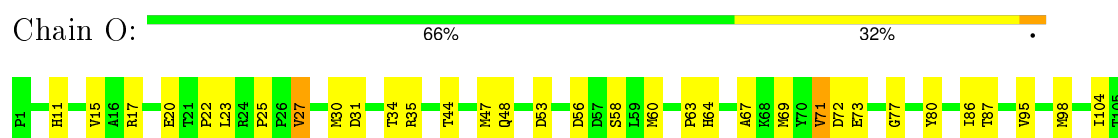
- Molecule 1: GTP cyclohydrolase I



- Molecule 1: GTP cyclohydrolase I



- Molecule 1: GTP cyclohydrolase I



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	224.47Å 313.26Å 130.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26471	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.40	0/1755	0.70	0/2377
1	B	0.38	0/1755	0.66	0/2377
1	C	0.38	0/1755	0.68	0/2377
1	D	0.40	0/1755	0.71	3/2377 (0.1%)
1	E	0.35	0/1747	0.63	0/2366
1	F	0.39	0/1755	0.67	0/2377
1	G	0.36	0/1755	0.66	0/2377
1	H	0.35	0/1755	0.65	0/2377
1	I	0.39	0/1755	0.67	1/2377 (0.0%)
1	J	0.36	0/1755	0.64	0/2377
1	K	0.39	0/1755	0.67	1/2377 (0.0%)
1	L	0.45	0/1755	0.70	1/2377 (0.0%)
1	M	0.48	0/1755	0.75	0/2377
1	N	0.42	0/1755	0.70	1/2377 (0.0%)
1	O	0.37	0/1755	0.67	1/2377 (0.0%)
All	All	0.39	0/26317	0.68	8/35644 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	150	VAL	N-CA-C	-6.08	94.58	111.00
1	D	26	PRO	N-CA-C	5.65	126.80	112.10
1	D	25	PRO	C-N-CD	-5.54	108.42	120.60
1	D	150	VAL	N-CA-C	-5.54	96.05	111.00
1	K	148	PRO	N-CA-C	-5.46	97.89	112.10
1	N	148	PRO	N-CA-C	-5.36	98.17	112.10
1	L	150	VAL	N-CA-C	-5.29	96.72	111.00
1	O	148	PRO	N-CA-C	-5.28	98.37	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1728	0	1766	71	0
1	B	1728	0	1766	64	0
1	C	1728	0	1766	53	0
1	D	1728	0	1766	58	0
1	E	1720	0	1760	39	0
1	F	1728	0	1766	71	0
1	G	1728	0	1766	68	0
1	H	1728	0	1766	60	0
1	I	1728	0	1766	61	0
1	J	1728	0	1766	57	0
1	K	1728	0	1766	56	0
1	L	1728	0	1766	47	0
1	M	1728	0	1766	51	0
1	N	1728	0	1766	53	0
1	O	1728	0	1766	53	0
2	A	32	0	11	5	0
2	B	32	0	11	5	0
2	C	32	0	11	4	0
2	D	32	0	11	5	0
2	E	32	0	11	2	0
2	F	32	0	11	3	0
2	G	32	0	11	5	0
2	H	32	0	11	3	0
2	I	32	0	11	9	0
2	J	32	0	11	3	0
2	K	32	0	11	3	0
2	L	32	0	11	3	0
2	M	32	0	11	2	0
2	N	32	0	11	2	0
2	O	32	0	11	3	0
3	A	2	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	7	0	0	3	0
3	E	2	0	0	0	0
3	F	6	0	0	1	0
3	G	5	0	0	1	0
3	H	6	0	0	0	0
3	I	4	0	0	1	0
3	J	2	0	0	0	0
3	K	7	0	0	0	0
3	L	5	0	0	0	0
3	M	13	0	0	3	0
3	N	9	0	0	2	0
3	O	3	0	0	0	0
All	All	26471	0	26649	796	0

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 15.

All (796) 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:O:185:ARG:HG2	1:O:185:ARG:HH11	0.97	1.12
1:M:207:GLN:HE22	1:N:208:ASN:HB2	1.17	1.09
1:N:168:THR:HG22	1:N:170:ASN:H	1.27	0.95
1:C:168:THR:HG22	1:C:170:ASN:H	1.31	0.95
1:A:24:ARG:HG2	1:A:25:PRO:HD2	1.47	0.94
1:F:168:THR:HG22	1:F:170:ASN:H	1.30	0.94
1:G:207:GLN:HE22	1:H:208:ASN:HB2	1.33	0.93
1:N:87:THR:HG21	2:N:1423:GTP:O1A	1.67	0.92
1:O:185:ARG:HH11	1:O:185:ARG:CG	1.82	0.92
1:I:168:THR:HG22	1:I:170:ASN:H	1.35	0.91
1:F:208:ASN:HB2	1:J:207:GLN:HE22	1.37	0.90
1:G:69:MET:HA	1:G:73:GLU:HG3	1.50	0.90
1:O:185:ARG:HG2	1:O:185:ARG:NH1	1.76	0.89
1:B:207:GLN:HE22	1:C:208:ASN:HB2	1.38	0.88
1:I:207:GLN:HE22	1:J:208:ASN:HB2	1.36	0.88
1:K:208:ASN:HB2	1:O:207:GLN:HE22	1.37	0.87
1:G:168:THR:HG22	1:G:170:ASN:H	1.41	0.86
1:L:168:THR:HG22	1:L:170:ASN:H	1.37	0.85
1:A:207:GLN:HE22	1:B:208:ASN:HB2	1.41	0.85
1:D:168:THR:HG22	1:D:170:ASN:H	1.40	0.84
1:D:87:THR:HG21	2:D:1413:GTP:O1A	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ASN:HD22	1:C:138:ASN:H	1.26	0.83
1:K:87:THR:HG21	2:K:1425:GTP:O1A	1.78	0.83
1:G:87:THR:HG21	2:G:1416:GTP:O1A	1.79	0.82
1:C:87:THR:HG21	2:C:1412:GTP:O1A	1.80	0.82
1:D:85:LYS:O	1:D:136:LYS:HE3	1.80	0.81
1:I:87:THR:HG21	2:I:1418:GTP:O1A	1.81	0.81
1:N:207:GLN:HE22	1:O:208:ASN:HB2	1.46	0.81
1:O:142:GLN:O	1:O:146:GLN:HG2	1.82	0.80
1:M:168:THR:HG22	1:M:170:ASN:H	1.47	0.79
1:A:120:LYS:HD3	1:A:220:HIS:HB2	1.64	0.79
1:H:168:THR:HG22	1:H:170:ASN:H	1.47	0.79
1:G:17:ARG:NH2	1:G:160:ILE:HD12	1.98	0.79
1:M:159:LEU:HG	1:M:163:GLN:NE2	1.98	0.79
1:G:137:ILE:O	1:G:141:VAL:HG23	1.83	0.78
1:O:199:LEU:HD12	1:O:210:ARG:NH1	1.99	0.78
1:A:132:ILE:HB	1:A:166:LEU:HD21	1.66	0.78
1:O:87:THR:HG21	2:O:1424:GTP:O1A	1.83	0.78
1:O:168:THR:HG22	1:O:170:ASN:H	1.49	0.77
1:J:87:THR:HG21	2:J:1419:GTP:O1A	1.84	0.77
1:M:207:GLN:NE2	1:N:208:ASN:HB2	1.99	0.76
1:B:142:GLN:O	1:B:146:GLN:HG2	1.86	0.76
1:F:159:LEU:HD22	1:F:198:SER:HB3	1.68	0.75
1:F:207:GLN:HE22	1:G:208:ASN:HB2	1.50	0.75
1:M:207:GLN:HE22	1:N:208:ASN:CB	1.98	0.74
1:H:87:THR:HG21	2:H:1417:GTP:O1A	1.87	0.74
1:N:135:SER:O	1:N:139:ARG:HG3	1.87	0.74
1:B:168:THR:HG22	1:B:170:ASN:H	1.50	0.73
1:J:100:THR:HG23	1:J:124:ALA:HB2	1.69	0.73
1:H:207:GLN:HE22	1:I:208:ASN:HB2	1.52	0.73
1:M:141:VAL:HA	1:M:158:ILE:HD12	1.70	0.73
1:K:185:ARG:HG2	1:K:186:GLY:N	2.04	0.73
1:L:87:THR:HG21	2:L:1421:GTP:O1A	1.88	0.73
1:L:207:GLN:HE22	1:M:208:ASN:HB2	1.52	0.72
1:A:220:HIS:ND1	1:A:221:ASN:N	2.38	0.72
1:K:86:ILE:HG13	1:K:165:LEU:HD13	1.71	0.72
1:O:47:MET:SD	1:O:63:PRO:HG3	2.30	0.71
1:F:87:THR:HG21	2:F:1420:GTP:O1A	1.89	0.71
1:E:79:ASP:HB3	1:E:82:ASN:ND2	2.05	0.71
1:J:142:GLN:O	1:J:146:GLN:HG2	1.90	0.71
1:B:87:THR:HG21	2:B:1411:GTP:O1A	1.89	0.70
1:A:159:LEU:O	1:A:163:GLN:HG3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:HIS:O	1:H:15:VAL:HG23	1.90	0.70
1:J:168:THR:HG22	1:J:170:ASN:H	1.55	0.70
1:E:135:SER:O	1:E:139:ARG:HG3	1.92	0.70
1:B:69:MET:HA	1:B:73:GLU:HG3	1.74	0.69
1:K:214:LEU:HB3	1:L:215:ARG:HH22	1.56	0.69
1:K:214:LEU:HB3	1:L:215:ARG:NH2	2.06	0.69
1:C:218:ARG:HH21	1:D:102:ARG:HH22	1.40	0.69
1:D:69:MET:HA	1:D:73:GLU:HG3	1.73	0.69
1:I:61:GLU:OE1	1:I:64:HIS:HD2	1.75	0.69
1:M:112:SER:OG	1:M:113:HIS:HD2	1.76	0.69
1:H:213:PHE:O	1:H:217:VAL:HG23	1.93	0.69
1:G:11:HIS:O	1:G:15:VAL:HG23	1.92	0.69
1:M:142:GLN:O	1:M:146:GLN:HG2	1.92	0.69
1:I:135:SER:O	1:I:139:ARG:HG3	1.94	0.69
1:L:138:ASN:H	1:L:138:ASN:HD22	1.41	0.69
1:A:219:HIS:O	1:A:220:HIS:HB3	1.93	0.68
1:E:154:LEU:O	1:E:158:ILE:HG12	1.94	0.68
1:K:168:THR:HG22	1:K:170:ASN:H	1.57	0.68
1:A:24:ARG:HG2	1:A:25:PRO:CD	2.23	0.68
1:D:141:VAL:HA	1:D:158:ILE:HD12	1.76	0.68
1:E:87:THR:HG21	2:E:1414:GTP:O1A	1.95	0.68
1:B:135:SER:O	1:B:139:ARG:HG3	1.95	0.67
1:K:213:PHE:O	1:K:217:VAL:HG23	1.93	0.67
1:F:141:VAL:HA	1:F:158:ILE:HD12	1.77	0.67
1:L:112:SER:OG	1:L:113:HIS:HD2	1.78	0.66
1:L:11:HIS:O	1:L:15:VAL:HG23	1.95	0.66
1:I:142:GLN:O	1:I:146:GLN:HG2	1.95	0.66
1:N:142:GLN:O	1:N:146:GLN:HG2	1.95	0.66
1:G:90:GLU:HG3	3:G:1418:HOH:O	1.95	0.66
1:B:207:GLN:HE22	1:C:208:ASN:CB	2.09	0.66
1:E:213:PHE:O	1:E:217:VAL:HG23	1.96	0.65
1:J:141:VAL:HA	1:J:158:ILE:HD12	1.78	0.65
1:G:69:MET:HA	1:G:73:GLU:CG	2.27	0.65
1:A:160:ILE:HD13	1:A:163:GLN:NE2	2.12	0.65
1:J:149:GLN:HE21	1:J:154:LEU:HD13	1.59	0.65
1:H:102:ARG:HH11	1:H:102:ARG:HG3	1.60	0.65
1:F:208:ASN:CB	1:J:207:GLN:HE22	2.09	0.64
1:E:159:LEU:O	1:E:163:GLN:HG3	1.97	0.64
1:A:185:ARG:HG2	1:A:186:GLY:N	2.11	0.64
1:M:217:VAL:HG12	1:M:218:ARG:N	2.13	0.64
1:C:141:VAL:HA	1:C:158:ILE:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:GLN:HE22	1:H:208:ASN:CB	2.10	0.64
1:C:8:ALA:O	1:C:12:GLU:HG3	1.97	0.64
1:A:220:HIS:CG	1:A:221:ASN:N	2.66	0.64
1:E:141:VAL:HA	1:E:158:ILE:HD12	1.80	0.64
1:M:213:PHE:O	1:M:217:VAL:HG23	1.98	0.63
1:F:142:GLN:O	1:F:146:GLN:HG2	1.98	0.63
1:G:141:VAL:HA	1:G:158:ILE:HD12	1.80	0.63
1:A:86:ILE:HG13	1:A:165:LEU:HD13	1.80	0.63
1:I:134:LEU:HG	2:I:1418:GTP:C2	2.34	0.63
1:H:159:LEU:HD22	1:H:198:SER:HB3	1.81	0.63
1:C:138:ASN:ND2	1:C:138:ASN:H	1.97	0.63
1:M:87:THR:HG21	2:M:1422:GTP:O1A	1.98	0.63
1:J:149:GLN:NE2	1:J:154:LEU:HD13	2.14	0.63
1:F:6:GLU:HB3	1:F:165:LEU:HD21	1.80	0.63
1:K:142:GLN:O	1:K:146:GLN:HG2	1.98	0.63
1:K:185:ARG:HH22	2:L:1421:GTP:PG	2.21	0.62
1:A:141:VAL:HA	1:A:158:ILE:HD12	1.80	0.62
1:I:134:LEU:HG	2:I:1418:GTP:N2	2.15	0.62
1:A:160:ILE:HA	1:A:163:GLN:HE21	1.65	0.62
1:C:6:GLU:O	1:C:10:VAL:HG23	2.00	0.62
1:K:87:THR:HG23	1:K:136:LYS:HE2	1.80	0.62
1:O:11:HIS:O	1:O:15:VAL:HG23	1.99	0.62
1:D:139:ARG:NH1	2:D:1413:GTP:O2G	2.32	0.62
1:H:142:GLN:O	1:H:146:GLN:HG2	1.99	0.62
1:K:155:THR:HG22	1:K:198:SER:OG	2.00	0.62
1:H:25:PRO:O	1:H:27:VAL:HG23	2.00	0.61
1:J:217:VAL:HG12	1:J:218:ARG:N	2.15	0.61
1:C:11:HIS:O	1:C:15:VAL:HG23	1.99	0.61
2:G:1416:GTP:O2B	2:G:1416:GTP:H5'	1.99	0.61
1:M:70:TYR:O	1:M:75:PHE:HB2	2.01	0.61
1:K:138:ASN:N	1:K:138:ASN:HD22	1.98	0.61
1:D:213:PHE:O	1:D:217:VAL:HG23	2.00	0.61
1:D:153:ARG:O	1:D:157:GLN:HG3	2.00	0.61
1:I:137:ILE:O	1:I:141:VAL:HG23	2.00	0.61
1:K:154:LEU:O	1:K:158:ILE:HG12	2.01	0.61
1:O:159:LEU:O	1:O:163:GLN:HG3	2.01	0.61
1:A:87:THR:HG21	2:A:1415:GTP:O1A	2.00	0.61
1:K:141:VAL:HA	1:K:158:ILE:HD12	1.82	0.61
1:D:76:SER:O	1:D:82:ASN:ND2	2.33	0.61
1:L:213:PHE:O	1:L:217:VAL:HG23	2.01	0.61
1:A:220:HIS:CG	1:A:221:ASN:H	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:VAL:HA	1:I:158:ILE:HD12	1.81	0.61
1:O:159:LEU:HD22	1:O:198:SER:HB3	1.81	0.61
1:K:202:LEU:O	1:K:206:SER:HB3	2.00	0.61
1:D:17:ARG:NH2	1:D:160:ILE:HD12	2.16	0.61
1:D:159:LEU:HD22	1:D:198:SER:HB3	1.82	0.60
1:F:185:ARG:HG2	1:F:186:GLY:N	2.16	0.60
1:A:218:ARG:NH2	1:B:102:ARG:HH22	1.99	0.60
1:J:136:LYS:HA	1:J:139:ARG:HG3	1.83	0.60
1:F:141:VAL:HA	1:F:158:ILE:CD1	2.30	0.60
1:F:70:TYR:O	1:F:75:PHE:HB2	2.02	0.60
1:A:137:ILE:O	1:A:141:VAL:HG23	2.02	0.60
1:J:119:GLY:O	1:J:120:LYS:HD2	2.02	0.60
1:O:183:LYS:HG3	1:O:190:ALA:HA	1.83	0.60
1:E:4:SER:HB3	1:E:7:ALA:HB3	1.82	0.60
1:F:36:LYS:HG2	1:F:71:VAL:HG21	1.83	0.60
1:H:135:SER:O	1:H:139:ARG:HG3	2.02	0.59
1:A:44:THR:HG23	1:A:54:LEU:CD1	2.32	0.59
1:I:207:GLN:HE22	1:J:208:ASN:CB	2.11	0.59
1:N:213:PHE:O	1:N:217:VAL:HG23	2.03	0.59
1:A:218:ARG:NH2	1:B:102:ARG:NH2	2.51	0.59
1:C:123:VAL:HG11	1:C:162:LEU:CD1	2.31	0.59
1:F:44:THR:O	1:F:48:GLN:HG3	2.02	0.59
1:D:185:ARG:HH11	1:D:185:ARG:CG	2.15	0.59
1:F:208:ASN:HB2	1:J:207:GLN:NE2	2.14	0.59
1:B:213:PHE:O	1:B:217:VAL:HG23	2.03	0.59
1:H:53:ASP:OD1	1:H:55:ALA:HB3	2.03	0.59
1:E:142:GLN:O	1:E:146:GLN:HG2	2.03	0.59
1:A:6:GLU:HB3	1:A:165:LEU:HD21	1.85	0.59
1:F:213:PHE:O	1:F:217:VAL:HG23	2.03	0.58
1:H:170:ASN:OD1	1:H:202:LEU:HG	2.02	0.58
1:C:214:LEU:HB3	1:D:215:ARG:NH2	2.18	0.58
1:L:185:ARG:HG2	1:L:186:GLY:N	2.18	0.58
1:E:69:MET:HA	1:E:73:GLU:HG3	1.85	0.58
1:O:156:GLN:O	1:O:160:ILE:HG12	2.03	0.58
1:A:159:LEU:HD22	1:A:198:SER:HB3	1.86	0.58
1:F:153:ARG:O	1:F:157:GLN:HG3	2.04	0.58
1:K:134:LEU:HG	2:K:1425:GTP:C2	2.39	0.58
1:F:185:ARG:HG2	1:F:186:GLY:H	1.69	0.58
1:K:208:ASN:CB	1:O:207:GLN:HE22	2.13	0.57
1:I:185:ARG:HG2	1:I:186:GLY:N	2.17	0.57
1:N:17:ARG:NH2	1:N:160:ILE:HD12	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:THR:HG23	1:G:136:LYS:HE2	1.86	0.57
1:L:31:ASP:HB3	1:L:34:THR:OG1	2.04	0.57
1:F:31:ASP:HB3	1:F:34:THR:OG1	2.04	0.57
1:M:30:MET:SD	1:M:35:ARG:HG2	2.44	0.57
1:M:186:GLY:HA3	3:M:1428:HOH:O	2.04	0.57
1:I:133:GLY:HA2	2:I:1418:GTP:H1'	1.86	0.57
1:L:141:VAL:HA	1:L:158:ILE:CD1	2.34	0.57
1:N:159:LEU:O	1:N:163:GLN:HG3	2.04	0.57
1:C:56:ASP:O	1:C:60:MET:HB2	2.04	0.57
1:A:90:GLU:HB3	1:A:92:LYS:HE3	1.86	0.57
1:J:199:LEU:HD13	1:J:203:PHE:O	2.05	0.57
1:I:133:GLY:CA	2:I:1418:GTP:H1'	2.34	0.57
1:M:168:THR:HG21	3:M:1433:HOH:O	2.03	0.57
1:N:185:ARG:HA	1:N:188:ARG:NH1	2.20	0.57
1:L:141:VAL:HA	1:L:158:ILE:HD13	1.87	0.57
1:B:108:SER:HB3	1:B:117:ILE:HB	1.87	0.57
1:N:25:PRO:O	1:N:27:VAL:HG23	2.05	0.57
1:D:212:GLU:HA	1:D:215:ARG:HH12	1.68	0.57
1:N:159:LEU:HD22	1:N:198:SER:HB3	1.86	0.57
1:K:8:ALA:O	1:K:12:GLU:HG3	2.05	0.57
1:J:135:SER:O	1:J:139:ARG:HG3	2.04	0.56
1:F:24:ARG:HD3	1:N:24:ARG:HD3	1.86	0.56
1:O:56:ASP:O	1:O:60:MET:HB2	2.05	0.56
1:K:159:LEU:HD22	1:K:198:SER:HB3	1.86	0.56
1:H:112:SER:HB3	2:I:1418:GTP:H8	1.69	0.56
1:F:158:ILE:HG22	1:F:173:VAL:HG21	1.86	0.56
1:A:44:THR:O	1:A:48:GLN:HG3	2.06	0.56
1:F:35:ARG:O	1:F:39:ILE:HG13	2.05	0.56
1:H:102:ARG:NH1	1:H:102:ARG:HG3	2.21	0.56
1:A:142:GLN:O	1:A:146:GLN:HG2	2.05	0.56
1:N:152:GLU:HB3	1:O:95:VAL:HG21	1.87	0.56
1:I:218:ARG:NH2	1:J:221:ASN:O	2.39	0.56
1:M:151:GLN:NE2	1:M:196:THR:HG23	2.20	0.56
1:I:207:GLN:NE2	1:J:208:ASN:HB2	2.15	0.56
1:F:185:ARG:HA	1:F:188:ARG:NH1	2.20	0.56
1:D:44:THR:HG23	1:D:54:LEU:CD1	2.35	0.56
1:K:159:LEU:O	1:K:163:GLN:HG3	2.06	0.56
1:B:93:MET:HB2	1:B:95:VAL:HG23	1.88	0.56
1:L:142:GLN:O	1:L:146:GLN:HG2	2.06	0.56
1:C:159:LEU:HD22	1:C:198:SER:HB3	1.88	0.55
1:M:86:ILE:HD11	1:M:140:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:THR:O	1:C:23:LEU:HD13	2.06	0.55
1:I:153:ARG:O	1:I:157:GLN:HG3	2.06	0.55
1:O:69:MET:HA	1:O:73:GLU:HG2	1.87	0.55
1:D:21:THR:O	1:D:23:LEU:HD13	2.07	0.55
1:H:154:LEU:O	1:H:158:ILE:HG12	2.07	0.55
1:B:185:ARG:NH2	2:C:1412:GTP:O3G	2.40	0.55
1:D:185:ARG:HG2	1:D:186:GLY:N	2.21	0.55
1:A:183:LYS:HG3	1:A:190:ALA:HA	1.89	0.55
1:I:30:MET:SD	1:I:35:ARG:HG2	2.47	0.55
1:N:156:GLN:O	1:N:160:ILE:HG12	2.07	0.55
1:G:123:VAL:HG22	1:G:173:VAL:HG22	1.89	0.55
1:E:160:ILE:HA	1:E:163:GLN:HE21	1.71	0.55
1:H:150:VAL:HA	2:I:1418:GTP:O6	2.06	0.55
1:B:110:CYS:SG	1:B:113:HIS:HB2	2.47	0.55
1:E:168:THR:HG22	1:E:170:ASN:H	1.71	0.55
1:F:207:GLN:HE22	1:G:208:ASN:CB	2.19	0.55
1:H:69:MET:HA	1:H:73:GLU:HG3	1.89	0.55
1:F:159:LEU:O	1:F:163:GLN:HG3	2.07	0.54
1:D:24:ARG:O	1:D:26:PRO:HD3	2.08	0.54
1:G:139:ARG:NH1	2:G:1416:GTP:O2G	2.32	0.54
1:A:132:ILE:HB	1:A:166:LEU:CD2	2.37	0.54
1:J:47:MET:O	1:J:52:LEU:HB2	2.07	0.54
1:F:27:VAL:HG12	1:F:28:HIS:N	2.22	0.54
1:A:43:MET:O	1:A:47:MET:HG3	2.07	0.54
1:K:182:VAL:HG22	1:L:135:SER:HB3	1.89	0.54
1:A:135:SER:O	1:A:139:ARG:HG3	2.08	0.54
1:E:79:ASP:HB3	1:E:82:ASN:HD21	1.70	0.54
1:L:53:ASP:OD1	1:L:55:ALA:HB3	2.07	0.54
1:M:64:HIS:HB2	3:M:1423:HOH:O	2.06	0.54
1:K:138:ASN:H	1:K:138:ASN:HD22	1.54	0.54
1:F:125:TYR:CD2	1:F:166:LEU:HD13	2.43	0.54
1:H:160:ILE:HA	1:H:163:GLN:HE21	1.72	0.53
1:H:151:GLN:OE1	1:H:177:ALA:HB3	2.08	0.53
1:I:159:LEU:O	1:I:163:GLN:HG3	2.07	0.53
1:C:185:ARG:HG2	1:C:186:GLY:N	2.23	0.53
1:H:185:ARG:HH22	2:I:1418:GTP:PG	2.30	0.53
1:L:185:ARG:CG	1:L:185:ARG:HH11	2.22	0.53
1:H:133:GLY:O	1:H:136:LYS:HB2	2.07	0.53
1:A:27:VAL:HG12	1:A:28:HIS:N	2.23	0.53
1:B:30:MET:SD	1:B:35:ARG:HG2	2.47	0.53
1:H:125:TYR:CE2	1:H:127:PRO:HG3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:VAL:HA	1:C:158:ILE:CD1	2.38	0.53
1:A:217:VAL:O	1:A:218:ARG:HB2	2.08	0.53
1:C:144:PHE:O	1:C:149:GLN:NE2	2.34	0.53
1:M:159:LEU:HG	1:M:163:GLN:HE21	1.69	0.53
1:I:185:ARG:CG	1:I:185:ARG:HH11	2.20	0.53
1:A:153:ARG:O	1:A:157:GLN:HG3	2.07	0.53
1:F:47:MET:SD	1:F:63:PRO:HG3	2.48	0.53
1:J:213:PHE:O	1:J:217:VAL:HG23	2.09	0.53
1:N:70:TYR:O	1:N:75:PHE:HB2	2.08	0.53
1:A:207:GLN:HE22	1:B:208:ASN:CB	2.18	0.53
1:H:207:GLN:HE22	1:I:208:ASN:CB	2.21	0.53
1:O:25:PRO:O	1:O:27:VAL:HG23	2.08	0.53
1:K:11:HIS:O	1:K:15:VAL:HG23	2.08	0.53
1:K:17:ARG:HB2	1:K:17:ARG:HH11	1.74	0.53
1:O:135:SER:O	1:O:139:ARG:HG3	2.09	0.53
1:D:154:LEU:O	1:D:158:ILE:HG12	2.09	0.53
1:B:159:LEU:HD11	1:B:171:VAL:O	2.08	0.53
1:I:61:GLU:OE1	1:I:64:HIS:CD2	2.60	0.53
1:B:155:THR:HG23	1:B:173:VAL:HG12	1.91	0.53
1:I:31:ASP:HB3	1:I:34:THR:OG1	2.08	0.53
1:B:134:LEU:HG	2:B:1411:GTP:C2	2.44	0.53
1:J:119:GLY:C	1:J:120:LYS:HD2	2.29	0.53
1:G:31:ASP:HB3	1:G:34:THR:OG1	2.09	0.53
1:J:163:GLN:HG2	1:J:169:ASN:HA	1.91	0.52
1:F:214:LEU:HB3	1:G:215:ARG:NH2	2.23	0.52
1:D:100:THR:HG23	1:D:124:ALA:HB2	1.92	0.52
1:J:133:GLY:O	1:J:136:LYS:HB2	2.09	0.52
1:L:187:ILE:HD13	1:M:139:ARG:HG2	1.92	0.52
1:A:218:ARG:NH2	1:B:221:ASN:O	2.42	0.52
1:L:30:MET:SD	1:L:35:ARG:HG2	2.49	0.52
1:G:132:ILE:HB	1:G:166:LEU:HD21	1.91	0.52
1:D:214:LEU:HB3	1:E:215:ARG:NH2	2.24	0.52
1:E:150:VAL:HG12	1:E:152:GLU:OE1	2.10	0.52
1:E:109:THR:CG2	1:E:114:PHE:HA	2.40	0.52
1:G:66:ILE:O	1:G:69:MET:HB3	2.10	0.52
1:J:79:ASP:OD2	1:J:81:ALA:HB3	2.10	0.52
1:D:125:TYR:CD2	1:D:166:LEU:HD13	2.45	0.52
1:M:69:MET:HA	1:M:73:GLU:CG	2.40	0.52
1:I:44:THR:HG23	1:I:54:LEU:HD13	1.92	0.52
1:A:133:GLY:HA2	2:A:1415:GTP:N3	2.25	0.52
1:B:141:VAL:HA	1:B:158:ILE:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:THR:O	1:G:48:GLN:HG3	2.09	0.52
1:A:218:ARG:HG3	1:B:219:HIS:CE1	2.45	0.52
1:H:108:SER:HB3	1:H:117:ILE:HB	1.92	0.52
1:K:47:MET:CE	1:K:59:LEU:HD22	2.40	0.52
1:I:160:ILE:HD13	1:I:163:GLN:HE21	1.75	0.51
1:F:42:HIS:O	1:F:46:ILE:HG13	2.10	0.51
1:N:35:ARG:O	1:N:39:ILE:HG13	2.11	0.51
1:B:128:LYS:HB2	1:B:168:THR:OG1	2.10	0.51
1:E:58:SER:C	1:E:60:MET:H	2.14	0.51
1:H:152:GLU:O	1:H:156:GLN:HG2	2.10	0.51
1:O:141:VAL:HA	1:O:158:ILE:HD12	1.92	0.51
1:M:185:ARG:HH22	2:N:1423:GTP:PG	2.34	0.51
1:K:69:MET:HA	1:K:73:GLU:HG3	1.93	0.51
1:M:154:LEU:O	1:M:158:ILE:HG12	2.11	0.51
1:C:142:GLN:O	1:C:146:GLN:HG2	2.11	0.51
1:A:62:THR:HB	1:A:63:PRO:HD3	1.92	0.51
1:L:138:ASN:H	1:L:138:ASN:ND2	2.08	0.51
1:C:36:LYS:HG2	1:C:71:VAL:HG21	1.92	0.51
1:L:156:GLN:O	1:L:160:ILE:HG12	2.10	0.51
1:D:212:GLU:HA	1:D:215:ARG:NH1	2.25	0.51
1:L:44:THR:HG23	1:L:54:LEU:HD13	1.91	0.51
1:K:127:PRO:HB3	1:K:131:VAL:HG22	1.92	0.51
1:B:31:ASP:HB3	1:B:34:THR:OG1	2.11	0.51
1:F:135:SER:O	1:F:139:ARG:HG3	2.11	0.51
1:G:70:TYR:O	1:G:75:PHE:HB2	2.09	0.51
1:F:187:ILE:HG22	3:F:1426:HOH:O	2.11	0.51
1:G:135:SER:O	1:G:139:ARG:HG3	2.11	0.51
1:M:153:ARG:O	1:M:157:GLN:HG3	2.11	0.51
1:F:132:ILE:HB	1:F:166:LEU:HD21	1.93	0.51
1:O:44:THR:O	1:O:48:GLN:HG3	2.10	0.51
1:C:106:LEU:C	1:C:106:LEU:HD23	2.32	0.51
1:C:133:GLY:HA2	2:C:1412:GTP:N3	2.26	0.50
1:H:141:VAL:HA	1:H:158:ILE:HD12	1.93	0.50
1:J:217:VAL:CG1	1:J:218:ARG:N	2.74	0.50
1:E:44:THR:O	1:E:48:GLN:HG3	2.11	0.50
1:H:138:ASN:HD22	1:H:138:ASN:H	1.60	0.50
1:K:25:PRO:O	1:K:27:VAL:HG23	2.10	0.50
1:F:152:GLU:HB3	1:G:95:VAL:HG21	1.94	0.50
1:G:185:ARG:HG2	1:G:186:GLY:N	2.27	0.50
1:B:141:VAL:HA	1:B:158:ILE:HD13	1.94	0.50
1:O:213:PHE:O	1:O:217:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:LYS:O	1:D:94:LYS:HD2	2.11	0.50
1:A:125:TYR:CD2	1:A:166:LEU:HD13	2.46	0.50
1:J:199:LEU:HB3	1:J:203:PHE:O	2.11	0.50
1:H:153:ARG:O	1:H:157:GLN:HG3	2.12	0.50
1:A:11:HIS:O	1:A:15:VAL:HG23	2.12	0.50
1:F:218:ARG:NH2	1:G:221:ASN:O	2.45	0.50
1:K:112:SER:OG	1:K:113:HIS:HD2	1.93	0.50
1:K:135:SER:O	1:K:139:ARG:HG3	2.11	0.50
1:L:93:MET:HB2	1:L:95:VAL:HG23	1.93	0.50
1:G:152:GLU:OE1	1:G:152:GLU:N	2.44	0.50
1:K:174:SER:CB	1:K:197:THR:HG22	2.42	0.49
1:N:64:HIS:HB2	3:N:1428:HOH:O	2.12	0.49
1:K:137:ILE:O	1:K:141:VAL:HG23	2.12	0.49
1:H:31:ASP:HB3	1:H:34:THR:OG1	2.12	0.49
1:G:53:ASP:OD2	1:G:55:ALA:HB3	2.12	0.49
1:M:214:LEU:HD13	1:N:215:ARG:HH22	1.77	0.49
2:H:1417:GTP:O2B	2:H:1417:GTP:H5'	2.12	0.49
1:F:25:PRO:O	1:F:27:VAL:HG23	2.12	0.49
1:B:160:ILE:HA	1:B:163:GLN:HE21	1.78	0.49
1:J:85:LYS:O	1:J:136:LYS:HE2	2.11	0.49
1:G:142:GLN:O	1:G:146:GLN:HG2	2.12	0.49
1:H:6:GLU:O	1:H:10:VAL:HG23	2.12	0.49
1:F:207:GLN:NE2	1:G:208:ASN:HB2	2.23	0.49
1:B:25:PRO:O	1:B:27:VAL:HG23	2.12	0.49
1:H:56:ASP:O	1:H:60:MET:HB2	2.11	0.49
1:D:102:ARG:HD3	3:D:1419:HOH:O	2.11	0.49
1:J:36:LYS:HG2	1:J:71:VAL:HG21	1.93	0.49
1:J:125:TYR:CE2	1:J:127:PRO:HG3	2.47	0.49
1:N:87:THR:HG23	1:N:136:LYS:HE3	1.94	0.49
1:A:160:ILE:HD13	1:A:163:GLN:HE21	1.75	0.49
1:O:202:LEU:O	1:O:206:SER:HB3	2.12	0.49
1:H:214:LEU:HB3	1:I:215:ARG:NH2	2.26	0.49
1:B:11:HIS:O	1:B:15:VAL:HG23	2.12	0.49
1:F:75:PHE:CE1	1:F:148:PRO:HG3	2.48	0.49
1:I:126:ILE:HD12	1:I:170:ASN:HB3	1.95	0.49
1:K:86:ILE:HG13	1:K:165:LEU:CD1	2.41	0.49
1:L:19:LEU:CD1	1:L:160:ILE:HG13	2.43	0.49
1:F:102:ARG:NH2	1:J:176:ASP:OD2	2.46	0.49
1:C:199:LEU:HD12	1:C:210:ARG:NH1	2.27	0.49
1:G:108:SER:OG	1:G:109:THR:N	2.45	0.49
1:B:56:ASP:O	1:B:60:MET:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:88:LEU:HD23	1:N:132:ILE:HA	1.94	0.48
1:O:22:PRO:O	1:O:23:LEU:HD12	2.12	0.48
1:K:207:GLN:HE22	1:L:208:ASN:HB2	1.78	0.48
1:N:207:GLN:NE2	1:O:208:ASN:HB2	2.21	0.48
1:G:36:LYS:HG2	1:G:71:VAL:HG21	1.95	0.48
1:D:135:SER:O	1:D:138:ASN:HB2	2.13	0.48
1:A:133:GLY:CA	2:A:1415:GTP:H1'	2.44	0.48
1:A:28:HIS:ND1	1:A:28:HIS:O	2.44	0.48
1:N:168:THR:HG22	1:N:170:ASN:N	2.10	0.48
2:F:1420:GTP:O3G	1:J:185:ARG:NH2	2.44	0.48
1:B:76:SER:O	1:B:82:ASN:ND2	2.44	0.48
1:F:150:VAL:HA	2:G:1416:GTP:O6	2.13	0.48
1:B:217:VAL:HG12	1:B:218:ARG:N	2.28	0.48
1:G:86:ILE:HG13	1:G:165:LEU:HD13	1.96	0.48
1:B:139:ARG:NH1	2:B:1411:GTP:PG	2.87	0.48
1:K:159:LEU:HD11	1:K:171:VAL:O	2.14	0.48
1:F:169:ASN:O	1:F:201:GLY:N	2.46	0.48
1:G:87:THR:CG2	1:G:136:LYS:HE2	2.44	0.48
1:E:217:VAL:HG12	1:E:218:ARG:N	2.29	0.48
1:A:217:VAL:HG12	1:A:218:ARG:N	2.29	0.48
1:A:30:MET:SD	1:A:35:ARG:HG2	2.53	0.48
1:O:139:ARG:NH1	2:O:1424:GTP:PG	2.87	0.48
1:C:106:LEU:HD11	1:C:175:ILE:HD13	1.95	0.48
1:J:31:ASP:OD2	1:J:33:GLU:HB2	2.14	0.48
1:O:64:HIS:O	1:O:67:ALA:HB3	2.14	0.48
1:N:185:ARG:CG	1:N:185:ARG:HH11	2.27	0.48
1:I:185:ARG:HA	1:I:188:ARG:NH1	2.29	0.48
1:G:199:LEU:HD13	1:G:210:ARG:HG3	1.95	0.48
1:I:106:LEU:HD23	1:I:106:LEU:C	2.33	0.48
1:C:185:ARG:HG2	1:C:186:GLY:H	1.79	0.47
1:K:142:GLN:HA	1:K:142:GLN:OE1	2.13	0.47
1:I:141:VAL:HA	1:I:158:ILE:CD1	2.44	0.47
1:H:138:ASN:ND2	1:H:138:ASN:H	2.12	0.47
1:C:213:PHE:O	1:C:217:VAL:HG23	2.14	0.47
1:O:155:THR:HG23	1:O:173:VAL:HG12	1.96	0.47
1:J:125:TYR:CD2	1:J:166:LEU:HD13	2.49	0.47
1:M:159:LEU:HD22	1:M:198:SER:HB3	1.96	0.47
1:B:139:ARG:HH11	2:B:1411:GTP:PG	2.37	0.47
1:I:125:TYR:CE2	1:I:127:PRO:HG3	2.48	0.47
1:B:153:ARG:O	1:B:157:GLN:HG3	2.14	0.47
1:L:42:HIS:O	1:L:46:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:VAL:CG1	1:B:116:THR:N	2.77	0.47
1:D:174:SER:OG	1:D:197:THR:HG22	2.14	0.47
1:O:135:SER:O	1:O:138:ASN:HB2	2.15	0.47
1:G:34:THR:O	1:G:38:LEU:HG	2.14	0.47
1:J:69:MET:HA	1:J:73:GLU:HG3	1.95	0.47
1:F:110:CYS:SG	1:F:113:HIS:HB2	2.55	0.47
1:H:89:ILE:HG13	1:H:89:ILE:O	2.14	0.47
1:B:185:ARG:HG2	1:B:186:GLY:H	1.79	0.47
2:F:1420:GTP:PG	1:J:185:ARG:HH22	2.38	0.47
1:D:27:VAL:HG12	1:D:28:HIS:N	2.29	0.47
1:O:30:MET:SD	1:O:35:ARG:HG2	2.54	0.47
1:G:101:VAL:HG21	1:G:137:ILE:HD12	1.95	0.47
1:A:87:THR:HG23	1:A:136:LYS:HE3	1.95	0.47
1:L:135:SER:O	1:L:139:ARG:HG3	2.14	0.47
1:B:138:ASN:HD22	1:B:138:ASN:H	1.63	0.47
1:H:68:LYS:HG2	1:H:72:ASP:OD2	2.15	0.47
1:A:111:GLU:HG2	1:A:149:GLN:O	2.14	0.47
1:F:104:ILE:HG23	1:F:138:ASN:OD1	2.14	0.47
1:E:56:ASP:O	1:E:60:MET:HB2	2.15	0.47
1:C:185:ARG:NH2	2:D:1413:GTP:O3G	2.48	0.47
1:A:44:THR:HG23	1:A:54:LEU:HD11	1.95	0.47
1:A:170:ASN:OD1	1:A:201:GLY:HA3	2.15	0.47
1:E:125:TYR:CD2	1:E:166:LEU:HD13	2.50	0.47
1:M:217:VAL:HG12	1:M:218:ARG:H	1.78	0.47
1:O:106:LEU:O	1:O:106:LEU:HD23	2.15	0.47
1:M:217:VAL:CG1	1:M:218:ARG:N	2.77	0.46
1:M:69:MET:HA	1:M:73:GLU:HG3	1.97	0.46
1:C:90:GLU:HB3	1:C:92:LYS:HG3	1.97	0.46
1:D:142:GLN:O	1:D:146:GLN:HG2	2.15	0.46
1:L:185:ARG:NH1	1:L:185:ARG:HG2	2.29	0.46
1:E:113:HIS:O	1:E:114:PHE:HB2	2.15	0.46
1:O:111:GLU:HB3	1:O:148:PRO:C	2.36	0.46
1:C:68:LYS:HD2	1:C:73:GLU:OE1	2.16	0.46
1:J:101:VAL:HG21	1:J:137:ILE:HD12	1.97	0.46
1:H:110:CYS:SG	1:H:181:CYS:SG	3.13	0.46
1:H:179:HIS:HB3	1:H:181:CYS:SG	2.55	0.46
1:D:79:ASP:OD2	1:D:81:ALA:HB3	2.14	0.46
1:N:179:HIS:HB2	1:N:182:VAL:HG23	1.97	0.46
1:K:106:LEU:C	1:K:106:LEU:HD23	2.36	0.46
1:L:185:ARG:NH1	1:L:185:ARG:CG	2.78	0.46
1:G:21:THR:O	1:G:23:LEU:HD13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:ARG:O	1:H:39:ILE:HG13	2.15	0.46
1:D:135:SER:O	1:D:139:ARG:HG3	2.16	0.46
1:C:22:PRO:O	1:C:23:LEU:HD12	2.15	0.46
1:G:159:LEU:HD22	1:G:198:SER:HB3	1.98	0.46
1:C:17:ARG:NH2	1:C:160:ILE:HD12	2.30	0.46
1:E:11:HIS:O	1:E:15:VAL:HG23	2.15	0.46
1:B:185:ARG:HH22	2:C:1412:GTP:PG	2.39	0.46
1:L:155:THR:HG22	1:L:198:SER:OG	2.15	0.46
1:K:62:THR:HB	1:K:63:PRO:HD3	1.96	0.46
1:C:173:VAL:HG12	1:C:174:SER:N	2.31	0.46
1:N:207:GLN:HE22	1:O:208:ASN:CB	2.23	0.46
1:E:108:SER:OG	1:E:109:THR:N	2.49	0.46
1:M:180:TYR:CE2	1:M:183:LYS:HD3	2.51	0.46
1:G:62:THR:HB	1:G:63:PRO:HD3	1.98	0.46
1:B:62:THR:O	1:B:63:PRO:C	2.54	0.46
1:N:104:ILE:O	1:N:120:LYS:HA	2.15	0.46
1:G:125:TYR:CD2	1:G:166:LEU:HD13	2.50	0.46
1:E:140:ILE:HD13	1:E:162:LEU:HD23	1.98	0.46
1:A:185:ARG:HH22	2:B:1411:GTP:PG	2.38	0.46
1:I:111:GLU:HB3	1:I:148:PRO:C	2.36	0.46
1:A:203:PHE:O	1:A:210:ARG:HG3	2.16	0.46
1:I:53:ASP:OD1	1:I:55:ALA:HB3	2.16	0.46
1:O:107:THR:O	1:O:146:GLN:NE2	2.49	0.46
1:A:218:ARG:HD3	1:A:218:ARG:C	2.35	0.46
1:B:19:LEU:HD12	1:B:160:ILE:HG13	1.98	0.46
1:J:62:THR:OG1	1:J:65:ARG:NH2	2.48	0.46
1:D:140:ILE:HD13	1:D:165:LEU:HD12	1.98	0.46
1:C:168:THR:HG22	1:C:170:ASN:N	2.14	0.45
1:J:87:THR:HG23	1:J:136:LYS:HE2	1.97	0.45
1:F:32:ASN:O	1:F:36:LYS:HG3	2.16	0.45
1:I:75:PHE:CE1	1:I:148:PRO:HG3	2.51	0.45
1:M:15:VAL:C	1:M:17:ARG:H	2.20	0.45
1:F:183:LYS:HG3	1:F:190:ALA:HA	1.98	0.45
1:G:168:THR:HG22	1:G:170:ASN:N	2.22	0.45
1:M:160:ILE:HD13	1:M:163:GLN:NE2	2.31	0.45
1:O:69:MET:HA	1:O:73:GLU:CG	2.45	0.45
1:F:171:VAL:HG12	1:F:172:ALA:N	2.31	0.45
1:I:204:LYS:NZ	1:J:97:GLU:OE2	2.49	0.45
1:H:70:TYR:O	1:H:75:PHE:HB2	2.16	0.45
1:J:175:ILE:O	1:J:195:THR:HA	2.17	0.45
1:N:17:ARG:HH21	1:N:160:ILE:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LEU:HD13	1:C:175:ILE:HG23	1.97	0.45
1:F:102:ARG:HH21	1:J:176:ASP:CG	2.20	0.45
1:L:159:LEU:HD22	1:L:198:SER:HB3	1.98	0.45
1:O:185:ARG:NH1	1:O:185:ARG:CG	2.53	0.45
1:J:139:ARG:HD2	2:J:1419:GTP:O2G	2.16	0.45
1:I:112:SER:OG	1:I:113:HIS:HD2	2.00	0.45
1:L:21:THR:O	1:L:23:LEU:HD13	2.16	0.45
1:N:141:VAL:HA	1:N:158:ILE:HD13	1.99	0.45
1:O:86:ILE:HG13	1:O:165:LEU:HD13	1.96	0.45
1:I:136:LYS:O	1:I:140:ILE:HG13	2.16	0.45
1:N:125:TYR:HB2	1:N:171:VAL:HG22	1.99	0.45
1:A:112:SER:OG	1:A:113:HIS:HD2	1.99	0.45
1:I:47:MET:HE1	1:I:59:LEU:HD22	1.99	0.45
1:G:70:TYR:HD1	1:G:74:ILE:HD11	1.81	0.45
2:K:1425:GTP:H5'	2:K:1425:GTP:O2B	2.17	0.45
1:I:185:ARG:NH2	2:J:1419:GTP:O3G	2.49	0.45
1:B:19:LEU:CD1	1:B:160:ILE:HG13	2.46	0.45
1:J:161:ALA:O	1:J:165:LEU:HG	2.16	0.45
1:G:158:ILE:HG22	1:G:173:VAL:HG21	1.97	0.45
1:F:30:MET:HG2	1:F:35:ARG:HG2	1.99	0.45
1:D:92:LYS:HB2	3:D:1416:HOH:O	2.16	0.45
1:O:151:GLN:OE1	1:O:194:THR:HB	2.17	0.45
1:E:8:ALA:O	1:E:12:GLU:HG3	2.16	0.45
1:D:23:LEU:HD11	1:D:78:LEU:HD22	1.99	0.45
1:H:69:MET:HG2	1:H:69:MET:O	2.17	0.45
1:K:44:THR:HG23	1:K:54:LEU:HD13	1.98	0.45
1:D:110:CYS:SG	1:D:113:HIS:HB2	2.57	0.45
1:N:183:LYS:HG3	1:N:190:ALA:HA	1.99	0.45
1:A:106:LEU:HD11	1:A:175:ILE:HD13	1.99	0.45
1:I:35:ARG:O	1:I:39:ILE:HG13	2.16	0.45
1:K:215:ARG:NH2	1:O:214:LEU:HB3	2.31	0.45
1:N:180:TYR:HD2	1:N:184:ALA:HB2	1.81	0.45
1:H:42:HIS:O	1:H:46:ILE:HG13	2.17	0.45
1:J:35:ARG:O	1:J:39:ILE:HG13	2.16	0.45
1:E:136:LYS:NZ	2:E:1414:GTP:O2G	2.49	0.45
1:I:97:GLU:HG2	3:I:1419:HOH:O	2.15	0.45
1:I:6:GLU:HB3	1:I:165:LEU:HD21	1.99	0.45
1:O:31:ASP:HB3	1:O:34:THR:OG1	2.17	0.45
1:N:185:ARG:NH1	1:N:185:ARG:CG	2.80	0.45
1:M:112:SER:OG	1:M:113:HIS:CD2	2.63	0.45
1:K:138:ASN:N	1:K:138:ASN:ND2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:44:THR:HG23	1:L:54:LEU:CD1	2.47	0.45
1:B:152:GLU:HB3	1:C:95:VAL:HG21	1.99	0.45
1:M:53:ASP:OD1	1:M:55:ALA:HB3	2.17	0.45
1:G:135:SER:HB3	2:G:1416:GTP:O2'	2.17	0.44
1:A:220:HIS:C	1:A:220:HIS:ND1	2.70	0.44
1:K:160:ILE:HA	1:K:163:GLN:HE21	1.82	0.44
1:D:185:ARG:HG2	1:D:185:ARG:NH1	2.31	0.44
1:L:88:LEU:HD23	1:L:132:ILE:HA	1.99	0.44
1:E:113:HIS:CD2	1:E:181:CYS:HB2	2.52	0.44
1:E:183:LYS:HG3	1:E:190:ALA:HA	1.99	0.44
1:B:133:GLY:O	1:B:136:LYS:HB2	2.17	0.44
1:B:41:GLY:O	1:B:44:THR:HB	2.17	0.44
1:C:2:SER:O	1:C:3:LEU:O	2.35	0.44
1:L:43:MET:O	1:L:47:MET:HG3	2.17	0.44
1:H:180:TYR:C	1:H:182:VAL:N	2.71	0.44
1:M:176:ASP:CG	1:N:102:ARG:HH21	2.20	0.44
1:D:133:GLY:CA	2:D:1413:GTP:H1'	2.48	0.44
1:F:158:ILE:CG2	1:F:173:VAL:HG21	2.48	0.44
1:B:154:LEU:HD12	1:B:154:LEU:O	2.17	0.44
1:F:151:GLN:HE21	1:F:196:THR:HG23	1.83	0.44
1:L:134:LEU:HG	2:L:1421:GTP:C2	2.52	0.44
1:O:58:SER:C	1:O:60:MET:N	2.71	0.44
1:B:153:ARG:HB2	1:C:93:MET:HG2	1.99	0.44
1:H:21:THR:O	1:H:23:LEU:HD13	2.17	0.44
1:J:42:HIS:O	1:J:46:ILE:HG13	2.18	0.44
1:B:111:GLU:HG2	1:B:149:GLN:O	2.18	0.44
1:A:207:GLN:NE2	1:B:208:ASN:HB2	2.21	0.44
1:H:112:SER:CB	2:I:1418:GTP:H8	2.30	0.44
1:B:62:THR:HB	1:B:63:PRO:HD3	1.99	0.44
1:F:4:SER:HB2	1:F:7:ALA:H	1.83	0.44
1:L:106:LEU:C	1:L:106:LEU:HD23	2.38	0.44
1:G:160:ILE:HA	1:G:163:GLN:NE2	2.33	0.44
1:E:156:GLN:O	1:E:160:ILE:HG12	2.18	0.44
1:M:86:ILE:CD1	1:M:140:ILE:HD11	2.47	0.44
1:C:218:ARG:HE	1:D:102:ARG:NH2	2.16	0.44
1:J:154:LEU:O	1:J:158:ILE:HG12	2.17	0.44
1:D:22:PRO:O	1:D:23:LEU:HD12	2.18	0.44
1:D:210:ARG:O	1:D:214:LEU:HG	2.17	0.44
1:K:153:ARG:HB2	1:L:93:MET:HG2	2.00	0.44
1:J:48:GLN:HG3	1:J:54:LEU:HD11	2.00	0.44
1:M:106:LEU:C	1:M:106:LEU:HD23	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LYS:HB2	1:C:168:THR:OG1	2.18	0.43
1:L:171:VAL:HG12	1:L:172:ALA:N	2.33	0.43
1:N:32:ASN:O	1:N:36:LYS:HG3	2.17	0.43
1:H:44:THR:HG23	1:H:54:LEU:HD13	1.99	0.43
1:E:106:LEU:HD23	1:E:106:LEU:C	2.38	0.43
1:D:139:ARG:NH1	2:D:1413:GTP:PG	2.91	0.43
1:I:185:ARG:CG	1:I:185:ARG:NH1	2.78	0.43
1:D:92:LYS:HE3	3:D:1416:HOH:O	2.17	0.43
1:K:111:GLU:HG2	1:K:149:GLN:O	2.18	0.43
1:E:75:PHE:CE1	1:E:148:PRO:HG3	2.53	0.43
1:M:28:HIS:O	1:M:28:HIS:ND1	2.50	0.43
1:B:69:MET:HA	1:B:73:GLU:CG	2.45	0.43
1:N:213:PHE:CD2	1:N:214:LEU:HD23	2.53	0.43
1:D:185:ARG:CG	1:D:185:ARG:NH1	2.74	0.43
1:N:185:ARG:HH21	2:O:1424:GTP:PG	2.42	0.43
1:H:217:VAL:CG1	1:H:218:ARG:N	2.81	0.43
1:F:140:ILE:HD11	1:F:165:LEU:CD1	2.48	0.43
1:B:159:LEU:HD12	1:B:171:VAL:HG12	2.01	0.43
1:B:61:GLU:O	1:B:62:THR:C	2.57	0.43
1:L:108:SER:OG	1:L:109:THR:N	2.52	0.43
1:H:207:GLN:NE2	1:I:208:ASN:HB2	2.28	0.43
1:A:27:VAL:HG12	1:A:28:HIS:CG	2.53	0.43
1:N:83:PHE:CD1	1:N:84:PRO:HD2	2.54	0.43
1:C:153:ARG:O	1:C:157:GLN:HG3	2.18	0.43
1:B:169:ASN:O	1:B:200:GLY:HA3	2.19	0.43
1:G:70:TYR:CD1	1:G:74:ILE:HD11	2.54	0.43
1:C:182:VAL:HG22	1:D:135:SER:HB3	2.00	0.43
1:G:208:ASN:O	1:G:212:GLU:HG3	2.19	0.43
1:F:97:GLU:OE1	1:J:210:ARG:NH2	2.47	0.43
1:N:14:LEU:CB	1:N:20:GLU:HG2	2.49	0.43
1:E:115:VAL:HG12	1:E:116:THR:N	2.33	0.43
1:I:11:HIS:O	1:I:15:VAL:HG23	2.19	0.43
1:I:25:PRO:O	1:I:27:VAL:HG23	2.18	0.43
1:J:163:GLN:HG2	1:J:168:THR:O	2.18	0.43
1:I:163:GLN:OE1	1:I:169:ASN:HA	2.18	0.43
1:B:61:GLU:O	1:B:63:PRO:N	2.52	0.43
1:O:71:VAL:HG12	1:O:72:ASP:N	2.34	0.43
1:A:151:GLN:NE2	1:A:196:THR:HG23	2.34	0.43
1:E:217:VAL:CG1	1:E:218:ARG:N	2.82	0.43
1:J:158:ILE:HB	1:J:173:VAL:HG11	2.00	0.43
1:A:133:GLY:HA2	2:A:1415:GTP:HI'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:86:ILE:HG13	1:I:165:LEU:HD13	2.01	0.43
1:K:35:ARG:O	1:K:39:ILE:HG13	2.18	0.43
1:H:217:VAL:HG12	1:H:218:ARG:N	2.34	0.43
1:K:3:LEU:HB3	1:K:4:SER:H	1.45	0.43
1:O:98:MET:HE3	1:O:124:ALA:HB1	2.01	0.43
1:A:171:VAL:HG12	1:A:172:ALA:N	2.32	0.43
1:A:31:ASP:OD2	1:A:33:GLU:HB2	2.18	0.43
1:A:3:LEU:HB3	1:A:4:SER:H	1.62	0.43
1:M:119:GLY:O	1:M:120:LYS:HD2	2.19	0.43
1:M:123:VAL:HG11	1:M:162:LEU:CD1	2.49	0.43
1:G:69:MET:HG2	1:G:74:ILE:HG12	2.00	0.42
1:A:156:GLN:O	1:A:160:ILE:HG12	2.19	0.42
1:F:30:MET:HG2	1:F:35:ARG:CG	2.48	0.42
1:I:213:PHE:O	1:I:215:ARG:N	2.52	0.42
1:N:141:VAL:HA	1:N:158:ILE:CD1	2.49	0.42
1:M:25:PRO:O	1:M:27:VAL:HG23	2.19	0.42
1:G:183:LYS:HA	1:G:189:ASP:O	2.19	0.42
1:H:106:LEU:HD11	1:H:175:ILE:HD13	1.99	0.42
1:F:85:LYS:O	1:F:136:LYS:HE3	2.19	0.42
1:O:104:ILE:HB	1:O:121:ALA:HB3	2.01	0.42
1:K:152:GLU:HB3	1:L:95:VAL:HG21	2.00	0.42
1:M:175:ILE:O	1:M:195:THR:HA	2.19	0.42
1:H:3:LEU:HB3	1:H:4:SER:H	1.61	0.42
1:M:139:ARG:NH1	2:M:1422:GTP:PG	2.92	0.42
1:A:133:GLY:O	1:A:136:LYS:HB2	2.19	0.42
1:F:218:ARG:HH21	1:G:102:ARG:NH2	2.17	0.42
1:D:25:PRO:HA	1:D:26:PRO:HD2	1.66	0.42
1:B:109:THR:HA	1:B:115:VAL:O	2.19	0.42
1:N:102:ARG:HH11	1:N:102:ARG:HG3	1.85	0.42
1:F:68:LYS:HG2	1:F:72:ASP:OD2	2.19	0.42
1:G:202:LEU:O	1:G:206:SER:HB3	2.19	0.42
1:D:6:GLU:O	1:D:10:VAL:HG23	2.19	0.42
1:I:99:VAL:O	1:I:124:ALA:HA	2.20	0.42
1:F:160:ILE:HD13	1:F:163:GLN:NE2	2.35	0.42
1:I:44:THR:HG23	1:I:54:LEU:CD1	2.49	0.42
1:I:106:LEU:HD23	1:I:106:LEU:O	2.18	0.42
1:L:104:ILE:HB	1:L:121:ALA:HB3	2.02	0.42
1:I:62:THR:HB	1:I:63:PRO:HD3	2.01	0.42
1:I:31:ASP:O	1:I:34:THR:HB	2.20	0.42
1:H:62:THR:N	1:H:63:PRO:CD	2.83	0.42
1:K:93:MET:N	1:K:93:MET:SD	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:GLN:NE2	1:D:154:LEU:HD13	2.35	0.42
1:A:141:VAL:HA	1:A:158:ILE:CD1	2.49	0.42
1:C:123:VAL:HG11	1:C:162:LEU:HD13	2.00	0.42
1:N:24:ARG:HG2	1:N:25:PRO:HD2	2.02	0.42
1:D:132:ILE:HB	1:D:166:LEU:CD2	2.50	0.42
1:H:90:GLU:HB3	1:H:92:LYS:HE3	2.01	0.42
1:C:25:PRO:O	1:C:27:VAL:HG23	2.19	0.42
1:M:202:LEU:O	1:M:206:SER:HB3	2.20	0.42
1:B:192:SER:HB3	1:C:104:ILE:HA	2.02	0.42
1:G:185:ARG:HG2	1:G:186:GLY:H	1.84	0.42
1:F:202:LEU:O	1:F:206:SER:HB3	2.19	0.42
1:O:126:ILE:HD12	1:O:170:ASN:HB3	2.01	0.42
1:F:210:ARG:HE	1:G:212:GLU:CD	2.22	0.42
1:A:10:VAL:HG21	1:A:83:PHE:CZ	2.55	0.42
1:G:102:ARG:HG3	1:G:102:ARG:HH11	1.84	0.42
1:N:171:VAL:HG12	1:N:172:ALA:N	2.34	0.42
1:D:56:ASP:OD2	1:D:58:SER:HB3	2.20	0.42
1:F:168:THR:HG22	1:F:170:ASN:N	2.14	0.42
1:G:128:LYS:HB2	1:G:168:THR:OG1	2.20	0.42
1:G:133:GLY:O	1:G:136:LYS:HB2	2.19	0.42
1:G:136:LYS:HA	1:G:136:LYS:HD3	1.87	0.42
1:J:43:MET:O	1:J:47:MET:HG3	2.19	0.42
1:G:183:LYS:HG3	1:G:190:ALA:HA	2.01	0.42
1:F:72:ASP:O	1:F:76:SER:HB3	2.20	0.42
1:B:183:LYS:HA	1:B:189:ASP:O	2.19	0.42
1:M:218:ARG:NH2	1:N:221:ASN:O	2.53	0.41
1:H:132:ILE:HB	1:H:166:LEU:HD21	2.02	0.41
1:B:154:LEU:HD11	1:B:158:ILE:HD11	2.02	0.41
1:K:183:LYS:HG3	1:K:190:ALA:HA	2.01	0.41
1:H:185:ARG:HG2	1:H:186:GLY:N	2.35	0.41
1:F:175:ILE:O	1:F:195:THR:HA	2.21	0.41
1:K:23:LEU:HD11	1:K:78:LEU:HD22	2.02	0.41
1:O:20:GLU:OE2	1:O:80:TYR:OH	2.31	0.41
1:G:113:HIS:O	1:G:114:PHE:HB2	2.20	0.41
1:A:6:GLU:O	1:A:10:VAL:HG23	2.21	0.41
1:D:217:VAL:HG12	1:D:218:ARG:N	2.35	0.41
1:N:26:PRO:O	1:N:27:VAL:HB	2.21	0.41
1:D:132:ILE:HB	1:D:166:LEU:HD21	2.02	0.41
1:E:58:SER:C	1:E:60:MET:N	2.73	0.41
1:O:141:VAL:HA	1:O:158:ILE:CD1	2.50	0.41
1:H:10:VAL:HG21	1:H:83:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:GLU:OE2	1:D:80:TYR:OH	2.33	0.41
1:E:42:HIS:O	1:E:45:GLU:HB2	2.21	0.41
1:B:204:LYS:NZ	1:C:97:GLU:OE2	2.50	0.41
1:C:110:CYS:O	1:C:110:CYS:SG	2.78	0.41
1:J:135:SER:O	1:J:139:ARG:CG	2.68	0.41
1:M:217:VAL:CG1	1:M:218:ARG:H	2.33	0.41
1:J:144:PHE:HE2	1:J:161:ALA:CB	2.34	0.41
1:L:25:PRO:HA	1:L:26:PRO:HD3	1.96	0.41
1:H:171:VAL:HG12	1:H:172:ALA:N	2.35	0.41
1:N:142:GLN:HA	1:N:145:ALA:HB3	2.02	0.41
1:F:125:TYR:CE2	1:F:127:PRO:HG3	2.55	0.41
1:H:125:TYR:CD2	1:H:166:LEU:HD13	2.55	0.41
1:D:140:ILE:CD1	1:D:165:LEU:HD12	2.50	0.41
1:I:47:MET:CE	1:I:59:LEU:HD22	2.50	0.41
1:G:150:VAL:HB	1:G:153:ARG:HB3	2.03	0.41
1:O:125:TYR:CE2	1:O:127:PRO:HG3	2.56	0.41
1:M:141:VAL:HA	1:M:158:ILE:CD1	2.47	0.41
1:I:154:LEU:O	1:I:158:ILE:HG12	2.21	0.41
1:C:192:SER:HB3	1:D:104:ILE:HA	2.03	0.41
1:G:28:HIS:O	1:G:28:HIS:ND1	2.53	0.41
1:A:136:LYS:HG2	2:A:1415:GTP:O3'	2.21	0.41
1:L:31:ASP:O	1:L:34:THR:HB	2.21	0.41
1:E:101:VAL:HG21	1:E:137:ILE:HD12	2.03	0.41
1:B:6:GLU:HG2	1:B:86:ILE:HB	2.01	0.41
1:L:153:ARG:HB2	1:M:93:MET:HG2	2.03	0.41
1:G:3:LEU:HB3	1:G:4:SER:H	1.63	0.41
1:D:11:HIS:O	1:D:15:VAL:HG23	2.20	0.41
1:O:113:HIS:CE1	1:O:185:ARG:NH2	2.89	0.41
1:L:168:THR:HG22	1:L:170:ASN:N	2.20	0.41
1:K:19:LEU:HD12	1:K:160:ILE:HG13	2.03	0.41
1:F:62:THR:HB	1:F:63:PRO:HD3	2.02	0.41
1:O:217:VAL:HG12	1:O:218:ARG:N	2.35	0.41
1:C:174:SER:OG	1:C:197:THR:HG22	2.20	0.41
1:M:180:TYR:HA	1:M:183:LYS:HB3	2.03	0.41
1:F:68:LYS:HE2	1:F:68:LYS:HB3	1.96	0.41
1:K:21:THR:O	1:K:23:LEU:HD13	2.20	0.41
1:L:140:ILE:CD1	1:L:165:LEU:HD12	2.51	0.41
1:C:202:LEU:HD22	1:C:206:SER:HB2	2.03	0.41
1:K:36:LYS:HD2	1:K:68:LYS:HA	2.02	0.41
1:B:89:ILE:O	1:B:89:ILE:HG13	2.21	0.41
1:F:75:PHE:C	1:F:77:GLY:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:91:ASN:OD1	1:N:95:VAL:HG23	2.21	0.41
1:C:207:GLN:NE2	1:C:211:HIS:CE1	2.89	0.41
1:F:52:LEU:HB3	1:F:59:LEU:HD13	2.03	0.41
1:D:183:LYS:HG3	1:D:190:ALA:HA	2.02	0.41
1:F:160:ILE:HD13	1:F:163:GLN:HE21	1.86	0.40
1:F:217:VAL:HG12	1:F:218:ARG:N	2.35	0.40
1:G:107:THR:O	1:G:146:GLN:NE2	2.54	0.40
1:K:78:LEU:HD23	1:K:78:LEU:HA	1.85	0.40
1:J:25:PRO:O	1:J:27:VAL:HG23	2.21	0.40
1:O:77:GLY:HA3	1:O:143:PHE:O	2.21	0.40
1:I:36:LYS:HG2	1:I:71:VAL:HG21	2.02	0.40
1:C:98:MET:HE3	1:C:124:ALA:HB1	2.03	0.40
1:I:93:MET:O	1:I:94:LYS:C	2.59	0.40
1:M:134:LEU:O	1:M:135:SER:C	2.57	0.40
1:E:152:GLU:O	1:E:156:GLN:HG2	2.22	0.40
1:A:176:ASP:CG	1:B:102:ARG:HH21	2.24	0.40
1:N:17:ARG:HG2	3:N:1427:HOH:O	2.21	0.40
1:C:106:LEU:HD12	1:C:121:ALA:HB2	2.02	0.40
1:N:90:GLU:OE2	1:N:92:LYS:HE2	2.20	0.40
1:A:69:MET:HG2	1:A:74:ILE:HG23	2.03	0.40
1:N:53:ASP:OD1	1:N:55:ALA:HB3	2.22	0.40
1:K:218:ARG:C	1:K:218:ARG:HD3	2.42	0.40
1:G:214:LEU:HB3	1:H:215:ARG:NH2	2.36	0.40
1:G:152:GLU:OE2	2:H:1417:GTP:N2	2.52	0.40
1:J:218:ARG:C	1:J:218:ARG:HD3	2.42	0.40
1:A:204:LYS:HA	1:A:210:ARG:NH1	2.37	0.40
1:G:25:PRO:O	1:G:27:VAL:HG23	2.21	0.40
1:B:3:LEU:HB3	1:B:4:SER:H	1.56	0.40
1:D:68:LYS:HE2	1:D:68:LYS:HB3	1.81	0.40
1:J:151:GLN:OE1	1:J:177:ALA:HB3	2.22	0.40
1:N:159:LEU:CD2	1:N:198:SER:HB3	2.50	0.40
1:A:149:GLN:NE2	1:A:154:LEU:HD13	2.36	0.40
1:I:15:VAL:HG22	1:I:20:GLU:HG3	2.04	0.40
1:G:6:GLU:O	1:G:10:VAL:HG23	2.21	0.40
1:I:152:GLU:N	1:I:152:GLU:OE1	2.44	0.40
1:F:104:ILE:HB	1:F:121:ALA:HB3	2.03	0.40
1:E:31:ASP:HB3	1:E:34:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/221 (99%)	196 (90%)	16 (7%)	7 (3%)	5	17
1	B	219/221 (99%)	196 (90%)	19 (9%)	4 (2%)	11	34
1	C	219/221 (99%)	197 (90%)	18 (8%)	4 (2%)	11	34
1	D	219/221 (99%)	197 (90%)	17 (8%)	5 (2%)	8	26
1	E	218/221 (99%)	189 (87%)	24 (11%)	5 (2%)	8	26
1	F	219/221 (99%)	191 (87%)	25 (11%)	3 (1%)	14	42
1	G	219/221 (99%)	199 (91%)	17 (8%)	3 (1%)	14	42
1	H	219/221 (99%)	196 (90%)	19 (9%)	4 (2%)	11	34
1	I	219/221 (99%)	193 (88%)	22 (10%)	4 (2%)	11	34
1	J	219/221 (99%)	195 (89%)	21 (10%)	3 (1%)	14	42
1	K	219/221 (99%)	200 (91%)	17 (8%)	2 (1%)	21	55
1	L	219/221 (99%)	199 (91%)	18 (8%)	2 (1%)	21	55
1	M	219/221 (99%)	197 (90%)	19 (9%)	3 (1%)	14	42
1	N	219/221 (99%)	197 (90%)	16 (7%)	6 (3%)	6	21
1	O	219/221 (99%)	200 (91%)	16 (7%)	3 (1%)	14	42
All	All	3284/3315 (99%)	2942 (90%)	284 (9%)	58 (2%)	11	34

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ARG
1	A	220	HIS
1	C	3	LEU
1	D	26	PRO
1	B	27	VAL
1	B	62	THR
1	C	27	VAL
1	D	27	VAL

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Mol	Chain	Res	Type
1	E	27	VAL
1	E	170	ASN
1	G	27	VAL
1	I	27	VAL
1	I	214	LEU
1	L	27	VAL
1	M	26	PRO
1	M	27	VAL
1	N	201	GLY
1	O	53	ASP
1	O	71	VAL
1	A	76	SER
1	B	22	PRO
1	C	53	ASP
1	D	74	ILE
1	E	4	SER
1	F	27	VAL
1	F	57	ASP
1	K	22	PRO
1	K	27	VAL
1	N	27	VAL
1	O	27	VAL
1	C	218	ARG
1	G	22	PRO
1	H	53	ASP
1	H	58	SER
1	J	218	ARG
1	N	57	ASP
1	A	22	PRO
1	A	60	MET
1	D	57	ASP
1	E	22	PRO
1	E	94	LYS
1	G	218	ARG
1	I	159	LEU
1	J	22	PRO
1	N	218	ARG
1	F	22	PRO
1	H	22	PRO
1	A	27	VAL
1	H	27	VAL
1	I	22	PRO

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Mol	Chain	Res	Type
1	A	25	PRO
1	B	201	GLY
1	D	25	PRO
1	M	201	GLY
1	N	22	PRO
1	J	27	VAL
1	L	22	PRO
1	N	26	PRO

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	194/194 (100%)	180 (93%)	14 (7%)	18	45
1	B	194/194 (100%)	190 (98%)	4 (2%)	61	90
1	C	194/194 (100%)	189 (97%)	5 (3%)	54	86
1	D	194/194 (100%)	187 (96%)	7 (4%)	42	76
1	E	193/194 (100%)	187 (97%)	6 (3%)	47	81
1	F	194/194 (100%)	187 (96%)	7 (4%)	42	76
1	G	194/194 (100%)	189 (97%)	5 (3%)	54	86
1	H	194/194 (100%)	192 (99%)	2 (1%)	82	96
1	I	194/194 (100%)	187 (96%)	7 (4%)	42	76
1	J	194/194 (100%)	187 (96%)	7 (4%)	42	76
1	K	194/194 (100%)	186 (96%)	8 (4%)	37	72
1	L	194/194 (100%)	189 (97%)	5 (3%)	54	86
1	M	194/194 (100%)	185 (95%)	9 (5%)	33	67
1	N	194/194 (100%)	189 (97%)	5 (3%)	54	86
1	O	194/194 (100%)	190 (98%)	4 (2%)	61	90
All	All	2909/2910 (100%)	2814 (97%)	95 (3%)	45	79

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	23	LEU
1	A	25	PRO
1	A	31	ASP
1	A	64	HIS
1	A	96	ASP
1	A	107	THR
1	A	109	THR
1	A	120	LYS
1	A	168	THR
1	A	185	ARG
1	A	197	THR
1	A	218	ARG
1	A	220	HIS
1	B	17	ARG
1	B	73	GLU
1	B	158	ILE
1	B	218	ARG
1	C	4	SER
1	C	17	ARG
1	C	120	LYS
1	C	138	ASN
1	C	218	ARG
1	D	17	ARG
1	D	26	PRO
1	D	30	MET
1	D	68	LYS
1	D	120	LYS
1	D	185	ARG
1	D	207	GLN
1	E	17	ARG
1	E	88	LEU
1	E	93	MET
1	E	120	LYS
1	E	125	TYR
1	E	197	THR
1	F	17	ARG
1	F	20	GLU
1	F	110	CYS
1	F	115	VAL
1	F	120	LYS
1	F	188	ARG
1	F	218	ARG

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Mol	Chain	Res	Type
1	G	17	ARG
1	G	73	GLU
1	G	87	THR
1	G	110	CYS
1	G	218	ARG
1	H	102	ARG
1	H	218	ARG
1	I	17	ARG
1	I	45	GLU
1	I	64	HIS
1	I	68	LYS
1	I	93	MET
1	I	120	LYS
1	I	185	ARG
1	J	17	ARG
1	J	87	THR
1	J	93	MET
1	J	120	LYS
1	J	130	SER
1	J	147	ARG
1	J	218	ARG
1	K	17	ARG
1	K	30	MET
1	K	79	ASP
1	K	87	THR
1	K	130	SER
1	K	138	ASN
1	K	185	ARG
1	K	218	ARG
1	L	64	HIS
1	L	120	LYS
1	L	139	ARG
1	L	185	ARG
1	L	218	ARG
1	M	4	SER
1	M	9	LEU
1	M	17	ARG
1	M	73	GLU
1	M	93	MET
1	M	120	LYS
1	M	140	ILE
1	M	199	LEU

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Mol	Chain	Res	Type
1	M	218	ARG
1	N	4	SER
1	N	17	ARG
1	N	158	ILE
1	N	185	ARG
1	N	218	ARG
1	O	17	ARG
1	O	185	ARG
1	O	194	THR
1	O	218	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	163	GLN
1	A	207	GLN
1	B	113	HIS
1	B	138	ASN
1	B	163	GLN
1	C	113	HIS
1	C	138	ASN
1	C	163	GLN
1	C	211	HIS
1	D	64	HIS
1	D	113	HIS
1	D	163	GLN
1	E	82	ASN
1	E	113	HIS
1	E	146	GLN
1	E	163	GLN
1	F	163	GLN
1	G	113	HIS
1	G	146	GLN
1	G	163	GLN
1	H	113	HIS
1	H	138	ASN
1	H	146	GLN
1	H	163	GLN
1	I	64	HIS
1	I	113	HIS
1	I	207	GLN

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Mol	Chain	Res	Type
1	J	113	HIS
1	J	163	GLN
1	J	207	GLN
1	K	113	HIS
1	K	138	ASN
1	K	146	GLN
1	K	163	GLN
1	L	113	HIS
1	L	138	ASN
1	M	113	HIS
1	M	163	GLN
1	N	113	HIS
1	N	207	GLN
1	O	146	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 ligands 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	A	1415	-	25,34,34	3.63	11 (44%)	34,54,54	2.70	12 (35%)
2	GTP	B	1411	-	25,34,34	3.49	11 (44%)	34,54,54	2.65	11 (32%)
2	GTP	C	1412	-	25,34,34	3.71	11 (44%)	34,54,54	2.72	9 (26%)
2	GTP	D	1413	-	25,34,34	3.63	11 (44%)	34,54,54	2.57	10 (29%)
2	GTP	E	1414	-	25,34,34	3.55	9 (36%)	34,54,54	2.64	10 (29%)
2	GTP	F	1420	-	25,34,34	3.63	9 (36%)	34,54,54	2.62	10 (29%)
2	GTP	G	1416	-	25,34,34	3.60	12 (48%)	34,54,54	2.62	10 (29%)
2	GTP	H	1417	-	25,34,34	3.61	11 (44%)	34,54,54	2.75	11 (32%)
2	GTP	I	1418	-	25,34,34	3.49	10 (40%)	34,54,54	2.58	10 (29%)
2	GTP	J	1419	-	25,34,34	3.59	11 (44%)	34,54,54	2.70	10 (29%)
2	GTP	K	1425	-	25,34,34	3.52	9 (36%)	34,54,54	2.74	11 (32%)
2	GTP	L	1421	-	25,34,34	3.58	9 (36%)	34,54,54	2.68	9 (26%)
2	GTP	M	1422	-	25,34,34	3.71	11 (44%)	34,54,54	2.72	9 (26%)
2	GTP	N	1423	-	25,34,34	3.69	12 (48%)	34,54,54	2.56	10 (29%)
2	GTP	O	1424	-	25,34,34	3.62	11 (44%)	34,54,54	2.61	10 (29%)

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	A	1415	-	-	0/18/38/38	0/3/3/3
2	GTP	B	1411	-	-	0/18/38/38	0/3/3/3
2	GTP	C	1412	-	-	0/18/38/38	0/3/3/3
2	GTP	D	1413	-	-	0/18/38/38	0/3/3/3
2	GTP	E	1414	-	-	0/18/38/38	0/3/3/3
2	GTP	F	1420	-	-	0/18/38/38	0/3/3/3
2	GTP	G	1416	-	-	0/18/38/38	0/3/3/3
2	GTP	H	1417	-	-	0/18/38/38	0/3/3/3
2	GTP	I	1418	-	-	0/18/38/38	0/3/3/3
2	GTP	J	1419	-	-	0/18/38/38	0/3/3/3
2	GTP	K	1425	-	-	0/18/38/38	0/3/3/3
2	GTP	L	1421	-	-	0/18/38/38	0/3/3/3
2	GTP	M	1422	-	-	0/18/38/38	0/3/3/3
2	GTP	N	1423	-	-	0/18/38/38	0/3/3/3
2	GTP	O	1424	-	-	0/18/38/38	0/3/3/3

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1422	GTP	C6-C5	-7.06	1.27	1.41
2	F	1420	GTP	C6-C5	-6.49	1.28	1.41
2	J	1419	GTP	C6-C5	-6.43	1.28	1.41
2	A	1415	GTP	C6-C5	-6.39	1.28	1.41
2	G	1416	GTP	C6-C5	-6.35	1.28	1.41
2	D	1413	GTP	C6-C5	-6.28	1.28	1.41
2	I	1418	GTP	C6-C5	-6.23	1.28	1.41
2	O	1424	GTP	C6-C5	-6.13	1.29	1.41
2	N	1423	GTP	C6-C5	-6.12	1.29	1.41
2	C	1412	GTP	C6-C5	-6.12	1.29	1.41
2	B	1411	GTP	C6-C5	-6.05	1.29	1.41
2	H	1417	GTP	C6-C5	-5.96	1.29	1.41
2	E	1414	GTP	C6-C5	-5.78	1.29	1.41
2	K	1425	GTP	C6-C5	-5.73	1.29	1.41
2	L	1421	GTP	C6-C5	-5.49	1.30	1.41
2	N	1423	GTP	O2'-C2'	-4.85	1.31	1.43
2	J	1419	GTP	O2'-C2'	-4.56	1.32	1.43
2	I	1418	GTP	O2'-C2'	-4.56	1.32	1.43
2	H	1417	GTP	O2'-C2'	-4.48	1.32	1.43
2	K	1425	GTP	O2'-C2'	-4.46	1.32	1.43
2	F	1420	GTP	O2'-C2'	-4.42	1.32	1.43
2	B	1411	GTP	O2'-C2'	-4.39	1.32	1.43
2	O	1424	GTP	O2'-C2'	-4.34	1.32	1.43
2	A	1415	GTP	O2'-C2'	-4.32	1.32	1.43
2	D	1413	GTP	O2'-C2'	-4.31	1.32	1.43
2	E	1414	GTP	O2'-C2'	-4.26	1.32	1.43
2	G	1416	GTP	O2'-C2'	-4.26	1.32	1.43
2	C	1412	GTP	O2'-C2'	-4.26	1.32	1.43
2	L	1421	GTP	O2'-C2'	-4.07	1.33	1.43
2	M	1422	GTP	O2'-C2'	-3.95	1.33	1.43
2	C	1412	GTP	C5-C4	-3.47	1.32	1.40
2	G	1416	GTP	C5-C4	-3.40	1.32	1.40
2	M	1422	GTP	C5-C4	-3.39	1.32	1.40
2	A	1415	GTP	C5-C4	-3.37	1.32	1.40
2	J	1419	GTP	C5-C4	-3.35	1.32	1.40
2	K	1425	GTP	C5-C4	-3.27	1.33	1.40
2	O	1424	GTP	C5-C4	-3.24	1.33	1.40
2	B	1411	GTP	C5-C4	-3.19	1.33	1.40
2	H	1417	GTP	C5-C4	-3.18	1.33	1.40
2	E	1414	GTP	C5-C4	-3.16	1.33	1.40
2	D	1413	GTP	C5-C4	-3.13	1.33	1.40
2	I	1418	GTP	C5-C4	-3.10	1.33	1.40
2	B	1411	GTP	PG-O3G	-3.08	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1423	GTP	PG-O3G	-3.01	1.43	1.54
2	I	1418	GTP	C2-N1	-3.00	1.30	1.35
2	J	1419	GTP	C2-N1	-2.95	1.30	1.35
2	F	1420	GTP	C5-C4	-2.95	1.33	1.40
2	D	1413	GTP	PG-O3G	-2.88	1.44	1.54
2	B	1411	GTP	C2-N1	-2.85	1.30	1.35
2	I	1418	GTP	C3'-C4'	-2.82	1.45	1.53
2	A	1415	GTP	C2-N1	-2.82	1.30	1.35
2	H	1417	GTP	PG-O3G	-2.81	1.44	1.54
2	A	1415	GTP	PG-O3G	-2.80	1.44	1.54
2	L	1421	GTP	C5-C4	-2.75	1.34	1.40
2	K	1425	GTP	C3'-C4'	-2.74	1.45	1.53
2	O	1424	GTP	PG-O3G	-2.72	1.44	1.54
2	K	1425	GTP	PG-O3G	-2.71	1.45	1.54
2	G	1416	GTP	C2-N1	-2.67	1.30	1.35
2	D	1413	GTP	C2-N1	-2.67	1.30	1.35
2	N	1423	GTP	C5-C4	-2.66	1.34	1.40
2	J	1419	GTP	C3'-C4'	-2.63	1.45	1.53
2	M	1422	GTP	PG-O3G	-2.62	1.45	1.54
2	I	1418	GTP	PG-O3G	-2.61	1.45	1.54
2	C	1412	GTP	PG-O3G	-2.61	1.45	1.54
2	F	1420	GTP	PG-O3G	-2.58	1.45	1.54
2	E	1414	GTP	C2-N1	-2.54	1.30	1.35
2	L	1421	GTP	PG-O3G	-2.53	1.45	1.54
2	E	1414	GTP	PG-O3G	-2.50	1.45	1.54
2	G	1416	GTP	PG-O3G	-2.49	1.45	1.54
2	O	1424	GTP	C2-N1	-2.49	1.31	1.35
2	F	1420	GTP	C2-N1	-2.41	1.31	1.35
2	M	1422	GTP	C3'-C4'	-2.34	1.46	1.53
2	K	1425	GTP	C2-N1	-2.34	1.31	1.35
2	C	1412	GTP	C2-N1	-2.31	1.31	1.35
2	N	1423	GTP	PA-O1A	-2.31	1.42	1.51
2	J	1419	GTP	PG-O3G	-2.29	1.46	1.54
2	H	1417	GTP	C2-N1	-2.27	1.31	1.35
2	G	1416	GTP	C3'-C4'	-2.25	1.46	1.53
2	N	1423	GTP	C2-N1	-2.24	1.31	1.35
2	O	1424	GTP	C3'-C4'	-2.21	1.47	1.53
2	B	1411	GTP	C3'-C4'	-2.18	1.47	1.53
2	H	1417	GTP	C3'-C4'	-2.12	1.47	1.53
2	A	1415	GTP	C3'-C4'	-2.10	1.47	1.53
2	N	1423	GTP	C3'-C4'	-2.06	1.47	1.53
2	D	1413	GTP	C3'-C4'	-2.04	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1422	GTP	C2-N1	-2.01	1.31	1.35
2	L	1421	GTP	C2-N1	-2.01	1.31	1.35
2	G	1416	GTP	PB-O2B	-2.00	1.46	1.54
2	M	1422	GTP	C2'-C3'	2.03	1.58	1.53
2	D	1413	GTP	PA-O5'	2.05	1.68	1.59
2	A	1415	GTP	PA-O5'	2.08	1.68	1.59
2	B	1411	GTP	PA-O5'	2.09	1.68	1.59
2	B	1411	GTP	O4'-C1'	2.10	1.43	1.41
2	E	1414	GTP	O4'-C1'	2.13	1.43	1.41
2	O	1424	GTP	PA-O5'	2.13	1.68	1.59
2	C	1412	GTP	PA-O5'	2.23	1.69	1.59
2	H	1417	GTP	PA-O5'	2.23	1.69	1.59
2	O	1424	GTP	O4'-C1'	2.24	1.44	1.41
2	M	1422	GTP	C5'-C4'	2.26	1.59	1.51
2	J	1419	GTP	O4'-C4'	2.26	1.50	1.45
2	A	1415	GTP	O4'-C1'	2.32	1.44	1.41
2	G	1416	GTP	PA-O5'	2.32	1.69	1.59
2	N	1423	GTP	PA-O5'	2.32	1.69	1.59
2	J	1419	GTP	PA-O5'	2.32	1.69	1.59
2	C	1412	GTP	O4'-C4'	2.39	1.50	1.45
2	L	1421	GTP	O4'-C1'	2.47	1.44	1.41
2	G	1416	GTP	O4'-C1'	2.52	1.44	1.41
2	M	1422	GTP	C4-N3	2.54	1.39	1.35
2	K	1425	GTP	C5'-C4'	2.62	1.60	1.51
2	F	1420	GTP	O4'-C1'	2.67	1.44	1.41
2	L	1421	GTP	C5'-C4'	2.70	1.60	1.51
2	D	1413	GTP	O4'-C1'	2.78	1.44	1.41
2	G	1416	GTP	C5'-C4'	2.81	1.60	1.51
2	I	1418	GTP	C5'-C4'	2.86	1.60	1.51
2	D	1413	GTP	C5'-C4'	2.88	1.61	1.51
2	E	1414	GTP	C5'-C4'	2.90	1.61	1.51
2	H	1417	GTP	O4'-C1'	2.92	1.44	1.41
2	A	1415	GTP	C5'-C4'	2.96	1.61	1.51
2	O	1424	GTP	C5'-C4'	2.96	1.61	1.51
2	F	1420	GTP	C5'-C4'	3.05	1.61	1.51
2	C	1412	GTP	C5'-C4'	3.09	1.61	1.51
2	H	1417	GTP	C5'-C4'	3.13	1.61	1.51
2	J	1419	GTP	C5'-C4'	3.16	1.61	1.51
2	N	1423	GTP	O4'-C1'	3.17	1.45	1.41
2	N	1423	GTP	C5'-C4'	3.20	1.62	1.51
2	B	1411	GTP	C5'-C4'	3.22	1.62	1.51
2	C	1412	GTP	O4'-C1'	3.30	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1418	GTP	O4'-C1'	3.34	1.45	1.41
2	I	1418	GTP	C2-N2	7.29	1.49	1.34
2	B	1411	GTP	C2-N2	7.62	1.49	1.34
2	H	1417	GTP	C2-N2	7.63	1.49	1.34
2	A	1415	GTP	C2-N2	7.90	1.50	1.34
2	K	1425	GTP	C2-N2	7.93	1.50	1.34
2	L	1421	GTP	C2-N2	8.00	1.50	1.34
2	O	1424	GTP	C2-N2	8.13	1.50	1.34
2	N	1423	GTP	C2-N2	8.20	1.50	1.34
2	G	1416	GTP	C2-N2	8.21	1.50	1.34
2	J	1419	GTP	C2-N2	8.27	1.51	1.34
2	D	1413	GTP	C2-N2	8.30	1.51	1.34
2	F	1420	GTP	C2-N2	8.32	1.51	1.34
2	E	1414	GTP	C2-N2	8.52	1.51	1.34
2	C	1412	GTP	C2-N2	9.23	1.53	1.34
2	M	1422	GTP	C2-N2	9.35	1.53	1.34
2	I	1418	GTP	C6-N1	10.96	1.53	1.33
2	J	1419	GTP	C6-N1	11.04	1.53	1.33
2	M	1422	GTP	C6-N1	11.14	1.53	1.33
2	B	1411	GTP	C6-N1	11.22	1.54	1.33
2	C	1412	GTP	C6-N1	11.24	1.54	1.33
2	E	1414	GTP	C6-N1	11.36	1.54	1.33
2	G	1416	GTP	C6-N1	11.48	1.54	1.33
2	F	1420	GTP	C6-N1	11.62	1.54	1.33
2	D	1413	GTP	C6-N1	11.66	1.54	1.33
2	K	1425	GTP	C6-N1	11.71	1.54	1.33
2	N	1423	GTP	C6-N1	11.80	1.55	1.33
2	A	1415	GTP	C6-N1	11.82	1.55	1.33
2	O	1424	GTP	C6-N1	11.91	1.55	1.33
2	H	1417	GTP	C6-N1	11.98	1.55	1.33
2	L	1421	GTP	C6-N1	12.22	1.55	1.33

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1417	GTP	C5-C6-N1	-9.31	110.86	123.59
2	K	1425	GTP	C5-C6-N1	-9.29	110.88	123.59
2	F	1420	GTP	C5-C6-N1	-9.29	110.89	123.59
2	C	1412	GTP	C5-C6-N1	-9.23	110.97	123.59
2	L	1421	GTP	C5-C6-N1	-9.11	111.14	123.59
2	G	1416	GTP	C5-C6-N1	-9.05	111.22	123.59
2	M	1422	GTP	C5-C6-N1	-9.05	111.22	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1419	GTP	C5-C6-N1	-9.04	111.23	123.59
2	E	1414	GTP	C5-C6-N1	-9.04	111.23	123.59
2	A	1415	GTP	C5-C6-N1	-8.98	111.32	123.59
2	O	1424	GTP	C5-C6-N1	-8.95	111.35	123.59
2	B	1411	GTP	C5-C6-N1	-8.94	111.36	123.59
2	D	1413	GTP	C5-C6-N1	-8.88	111.45	123.59
2	N	1423	GTP	C5-C6-N1	-8.88	111.45	123.59
2	I	1418	GTP	C5-C6-N1	-8.77	111.61	123.59
2	M	1422	GTP	C4-C5-N7	-7.37	102.70	109.48
2	C	1412	GTP	C4-C5-N7	-6.86	103.17	109.48
2	J	1419	GTP	C4-C5-N7	-6.46	103.54	109.48
2	K	1425	GTP	C4-C5-N7	-6.35	103.63	109.48
2	E	1414	GTP	C4-C5-N7	-6.28	103.70	109.48
2	I	1418	GTP	C4-C5-N7	-6.23	103.75	109.48
2	H	1417	GTP	C4-C5-N7	-6.19	103.78	109.48
2	F	1420	GTP	C4-C5-N7	-6.13	103.84	109.48
2	B	1411	GTP	C4-C5-N7	-6.09	103.88	109.48
2	L	1421	GTP	C4-C5-N7	-6.05	103.91	109.48
2	A	1415	GTP	C4-C5-N7	-5.95	104.00	109.48
2	O	1424	GTP	C4-C5-N7	-5.94	104.02	109.48
2	G	1416	GTP	C4-C5-N7	-5.89	104.06	109.48
2	D	1413	GTP	C4-C5-N7	-5.59	104.33	109.48
2	N	1423	GTP	C4-C5-N7	-5.50	104.42	109.48
2	E	1414	GTP	C1'-N9-C4	-4.68	119.89	126.94
2	L	1421	GTP	C1'-N9-C4	-4.61	119.98	126.94
2	K	1425	GTP	O5'-C5'-C4'	-4.60	92.17	109.12
2	M	1422	GTP	C1'-N9-C4	-4.55	120.07	126.94
2	K	1425	GTP	C1'-N9-C4	-4.48	120.18	126.94
2	H	1417	GTP	C1'-N9-C4	-4.37	120.34	126.94
2	A	1415	GTP	C1'-N9-C4	-4.27	120.50	126.94
2	L	1421	GTP	O5'-C5'-C4'	-4.25	93.46	109.12
2	O	1424	GTP	O5'-C5'-C4'	-4.22	93.56	109.12
2	M	1422	GTP	O5'-C5'-C4'	-4.22	93.57	109.12
2	B	1411	GTP	O5'-C5'-C4'	-4.20	93.65	109.12
2	C	1412	GTP	C1'-N9-C4	-4.13	120.72	126.94
2	O	1424	GTP	C1'-N9-C4	-4.05	120.84	126.94
2	D	1413	GTP	O5'-C5'-C4'	-4.03	94.27	109.12
2	J	1419	GTP	O5'-C5'-C4'	-4.01	94.35	109.12
2	G	1416	GTP	C1'-N9-C4	-4.01	120.90	126.94
2	E	1414	GTP	O5'-C5'-C4'	-3.96	94.52	109.12
2	I	1418	GTP	O5'-C5'-C4'	-3.95	94.54	109.12
2	D	1413	GTP	C1'-N9-C4	-3.94	120.99	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1417	GTP	O5'-C5'-C4'	-3.84	94.97	109.12
2	G	1416	GTP	O5'-C5'-C4'	-3.83	95.00	109.12
2	F	1420	GTP	C1'-N9-C4	-3.81	121.19	126.94
2	A	1415	GTP	O5'-C5'-C4'	-3.76	95.27	109.12
2	C	1412	GTP	O5'-C5'-C4'	-3.73	95.37	109.12
2	B	1411	GTP	C1'-N9-C4	-3.72	121.33	126.94
2	F	1420	GTP	O5'-C5'-C4'	-3.72	95.40	109.12
2	N	1423	GTP	C1'-N9-C4	-3.66	121.42	126.94
2	J	1419	GTP	C1'-N9-C4	-3.64	121.44	126.94
2	N	1423	GTP	O5'-C5'-C4'	-3.62	95.76	109.12
2	H	1417	GTP	N2-C2-N3	-3.56	110.97	117.80
2	K	1425	GTP	N2-C2-N3	-3.48	111.12	117.80
2	L	1421	GTP	N2-C2-N3	-3.33	111.42	117.80
2	I	1418	GTP	C1'-N9-C4	-3.31	121.95	126.94
2	I	1418	GTP	N2-C2-N3	-3.18	111.71	117.80
2	O	1424	GTP	N2-C2-N3	-3.12	111.81	117.80
2	G	1416	GTP	N2-C2-N3	-3.08	111.90	117.80
2	B	1411	GTP	N2-C2-N3	-3.07	111.92	117.80
2	M	1422	GTP	N2-C2-N3	-3.06	111.94	117.80
2	F	1420	GTP	N2-C2-N3	-3.00	112.04	117.80
2	D	1413	GTP	N2-C2-N3	-3.00	112.05	117.80
2	C	1412	GTP	N2-C2-N3	-2.98	112.08	117.80
2	E	1414	GTP	N2-C2-N3	-2.97	112.10	117.80
2	J	1419	GTP	N2-C2-N3	-2.96	112.12	117.80
2	A	1415	GTP	N2-C2-N3	-2.94	112.16	117.80
2	N	1423	GTP	N2-C2-N3	-2.87	112.30	117.80
2	A	1415	GTP	C2'-C1'-N9	-2.81	110.00	114.29
2	H	1417	GTP	C2'-C1'-N9	-2.73	110.12	114.29
2	J	1419	GTP	C2'-C1'-N9	-2.28	110.80	114.29
2	K	1425	GTP	C2'-C1'-N9	-2.23	110.89	114.29
2	B	1411	GTP	C2'-C1'-N9	-2.07	111.14	114.29
2	N	1423	GTP	C2'-C1'-N9	-2.03	111.18	114.29
2	O	1424	GTP	C2'-C3'-C4'	2.03	106.78	102.61
2	A	1415	GTP	C2'-C3'-C4'	2.07	106.87	102.61
2	A	1415	GTP	O3A-PA-O5'	2.09	108.47	102.94
2	O	1424	GTP	O4'-C1'-N9	2.11	112.51	108.10
2	F	1420	GTP	C2'-C3'-C4'	2.12	106.97	102.61
2	B	1411	GTP	C2'-C3'-C4'	2.13	107.00	102.61
2	I	1418	GTP	O4'-C1'-N9	2.14	112.59	108.10
2	G	1416	GTP	C2'-C3'-C4'	2.15	107.02	102.61
2	K	1425	GTP	O4'-C1'-N9	2.23	112.78	108.10
2	G	1416	GTP	O4'-C1'-N9	2.24	112.79	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1414	GTP	C2'-C3'-C4'	2.29	107.33	102.61
2	I	1418	GTP	C2'-C3'-C4'	2.31	107.36	102.61
2	K	1425	GTP	C2'-C3'-C4'	2.31	107.37	102.61
2	M	1422	GTP	O4'-C4'-C5'	2.34	117.68	109.32
2	H	1417	GTP	C2'-C3'-C4'	2.36	107.46	102.61
2	D	1413	GTP	C2'-C3'-C4'	2.36	107.47	102.61
2	F	1420	GTP	O4'-C4'-C5'	2.43	118.01	109.32
2	D	1413	GTP	O4'-C4'-C5'	2.53	118.36	109.32
2	D	1413	GTP	O4'-C1'-N9	2.54	113.42	108.10
2	B	1411	GTP	O4'-C1'-N9	2.58	113.50	108.10
2	L	1421	GTP	O4'-C4'-C5'	2.61	118.65	109.32
2	G	1416	GTP	O4'-C4'-C5'	2.61	118.65	109.32
2	I	1418	GTP	O4'-C4'-C5'	2.62	118.71	109.32
2	O	1424	GTP	O4'-C4'-C5'	2.63	118.72	109.32
2	K	1425	GTP	O4'-C4'-C5'	2.63	118.73	109.32
2	F	1420	GTP	O4'-C1'-N9	2.67	113.69	108.10
2	H	1417	GTP	O4'-C1'-N9	2.69	113.73	108.10
2	H	1417	GTP	O4'-C4'-C5'	2.69	118.95	109.32
2	B	1411	GTP	O4'-C4'-C5'	2.69	118.96	109.32
2	A	1415	GTP	O4'-C4'-C5'	2.72	119.07	109.32
2	N	1423	GTP	O4'-C4'-C5'	2.73	119.08	109.32
2	E	1414	GTP	O4'-C4'-C5'	2.87	119.58	109.32
2	M	1422	GTP	O4'-C1'-N9	2.91	114.18	108.10
2	C	1412	GTP	O4'-C4'-C5'	3.01	120.09	109.32
2	E	1414	GTP	O4'-C1'-N9	3.05	114.48	108.10
2	M	1422	GTP	N3-C2-N1	3.12	132.19	127.44
2	J	1419	GTP	O4'-C4'-C5'	3.17	120.66	109.32
2	N	1423	GTP	O4'-C1'-N9	3.18	114.75	108.10
2	L	1421	GTP	O4'-C1'-N9	3.20	114.80	108.10
2	J	1419	GTP	O4'-C1'-N9	3.34	115.08	108.10
2	C	1412	GTP	N3-C2-N1	3.42	132.65	127.44
2	D	1413	GTP	N3-C2-N1	3.47	132.73	127.44
2	E	1414	GTP	N3-C2-N1	3.47	132.73	127.44
2	A	1415	GTP	O4'-C1'-N9	3.54	115.50	108.10
2	C	1412	GTP	O4'-C1'-N9	3.54	115.51	108.10
2	F	1420	GTP	N3-C2-N1	3.59	132.91	127.44
2	N	1423	GTP	N3-C2-N1	3.61	132.95	127.44
2	L	1421	GTP	N3-C2-N1	3.63	132.97	127.44
2	G	1416	GTP	N3-C2-N1	3.63	132.97	127.44
2	A	1415	GTP	N3-C2-N1	3.64	133.00	127.44
2	K	1425	GTP	N3-C2-N1	3.69	133.06	127.44
2	J	1419	GTP	N3-C2-N1	3.71	133.10	127.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1424	GTP	N3-C2-N1	3.74	133.15	127.44
2	I	1418	GTP	N3-C2-N1	3.80	133.24	127.44
2	H	1417	GTP	N3-C2-N1	3.91	133.40	127.44
2	B	1411	GTP	N3-C2-N1	4.03	133.58	127.44
2	E	1414	GTP	C6-C5-C4	4.18	125.89	120.90
2	L	1421	GTP	C6-C5-C4	4.20	125.92	120.90
2	K	1425	GTP	C6-C5-C4	4.38	126.13	120.90
2	D	1413	GTP	C6-C5-C4	4.42	126.18	120.90
2	H	1417	GTP	C6-C5-C4	4.55	126.34	120.90
2	M	1422	GTP	C6-C5-C4	4.56	126.35	120.90
2	I	1418	GTP	C6-C5-C4	4.58	126.37	120.90
2	G	1416	GTP	C6-C5-C4	4.63	126.43	120.90
2	N	1423	GTP	C6-C5-C4	4.64	126.44	120.90
2	A	1415	GTP	C6-C5-C4	4.66	126.47	120.90
2	O	1424	GTP	C6-C5-C4	4.68	126.50	120.90
2	F	1420	GTP	C6-C5-C4	4.71	126.53	120.90
2	J	1419	GTP	C6-C5-C4	4.72	126.54	120.90
2	B	1411	GTP	C6-C5-C4	4.75	126.58	120.90
2	C	1412	GTP	C6-C5-C4	4.77	126.61	120.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1415	GTP	5	0
2	B	1411	GTP	5	0
2	C	1412	GTP	4	0
2	D	1413	GTP	5	0
2	E	1414	GTP	2	0
2	F	1420	GTP	3	0
2	G	1416	GTP	5	0
2	H	1417	GTP	3	0
2	I	1418	GTP	9	0
2	J	1419	GTP	3	0
2	K	1425	GTP	3	0
2	L	1421	GTP	3	0
2	M	1422	GTP	2	0
2	N	1423	GTP	2	0
2	O	1424	GTP	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.