Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:01 PM GMT

PDB ID	:	1N3S
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	:	2.55 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 (i) symbol.

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

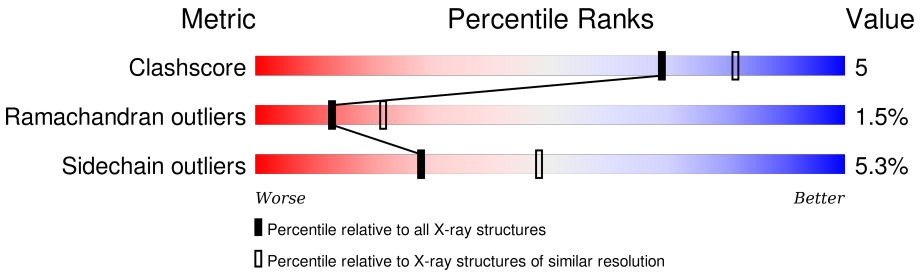
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)

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 <=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	83% 15% •
1	B	221	86% 14% •
1	C	221	84% 14% •
1	D	221	83% 16% •
1	E	221	85% 15%
1	F	221	78% 19% •
1	G	221	85% 13% •

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Mol	Chain	Length	Quality of chain
1	H	221	87% 12%
1	I	221	88% 11%
1	J	221	82% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17795 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
			1729	1085	307	328	9			
1	B	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	C	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	D	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	E	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	F	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	G	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	H	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	I	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	J	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	SER	HIS	ENGINEERED	UNP P0A6T5
B	113	SER	HIS	ENGINEERED	UNP P0A6T5
C	113	SER	HIS	ENGINEERED	UNP P0A6T5
D	113	SER	HIS	ENGINEERED	UNP P0A6T5
E	113	SER	HIS	ENGINEERED	UNP P0A6T5
F	113	SER	HIS	ENGINEERED	UNP P0A6T5
G	113	SER	HIS	ENGINEERED	UNP P0A6T5
H	113	SER	HIS	ENGINEERED	UNP P0A6T5
I	113	SER	HIS	ENGINEERED	UNP P0A6T5

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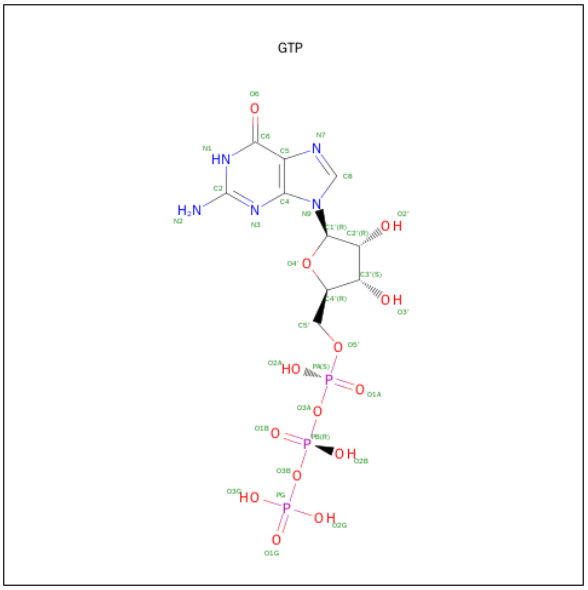
Chain	Residue	Modelled	Actual	Comment	Reference
J	113	SER	HIS	ENGINEERED	UNP P0A6T5

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 23 23	0	0
3	B	34	Total O 34 34	0	0
3	C	16	Total O 16 16	0	0
3	D	24	Total O 24 24	0	0
3	E	9	Total O 9 9	0	0
3	F	18	Total O 18 18	0	0
3	G	13	Total O 13 13	0	0
3	H	9	Total O 9 9	0	0
3	I	18	Total O 18 18	0	0
3	J	21	Total O 21 21	0	0

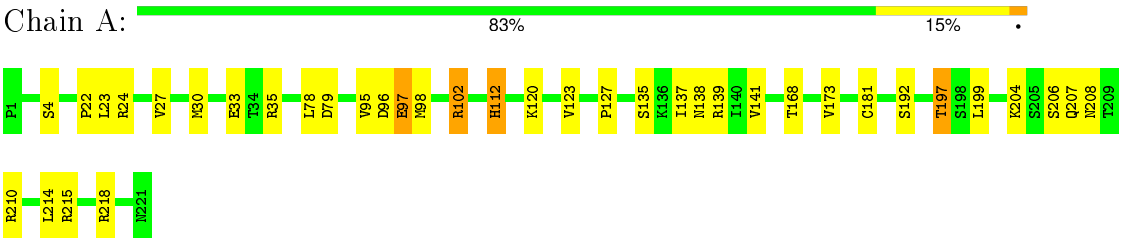
3 Residue-property plots (i)

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.

Note EDS was not executed.

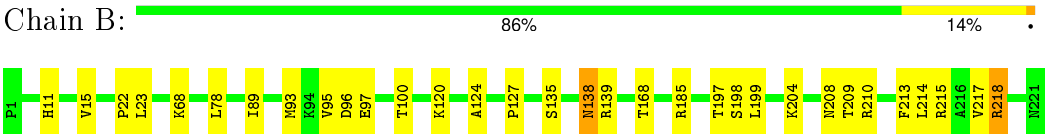
• Molecule 1: GTP cyclohydrolase I

Chain A:



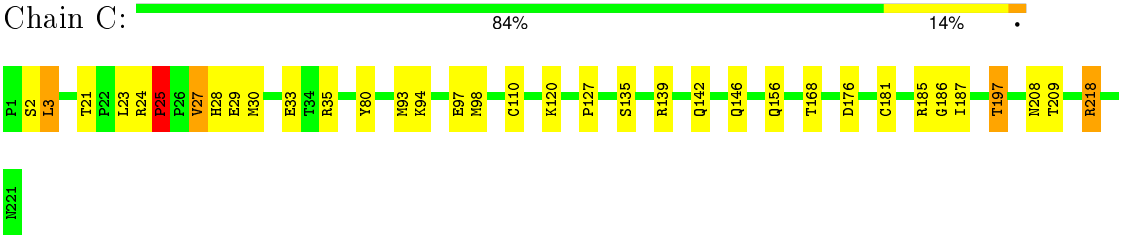
• Molecule 1: GTP cyclohydrolase I

Chain B:



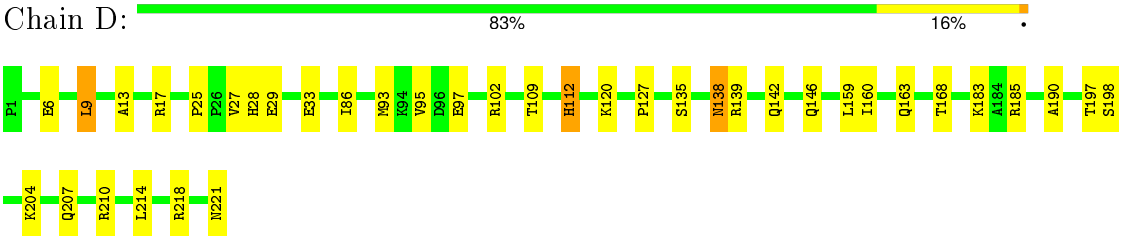
• Molecule 1: GTP cyclohydrolase I

Chain C:



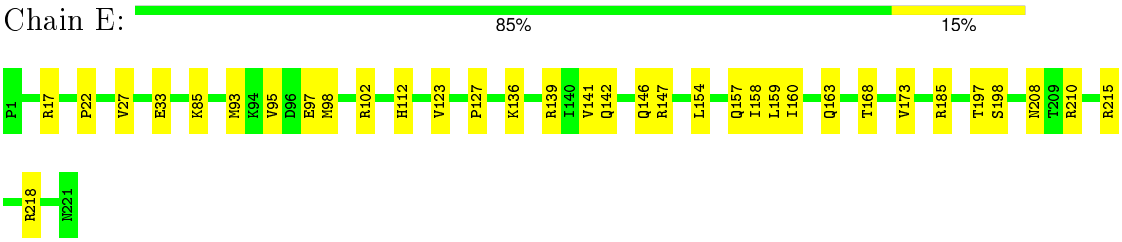
• Molecule 1: GTP cyclohydrolase I

Chain D:



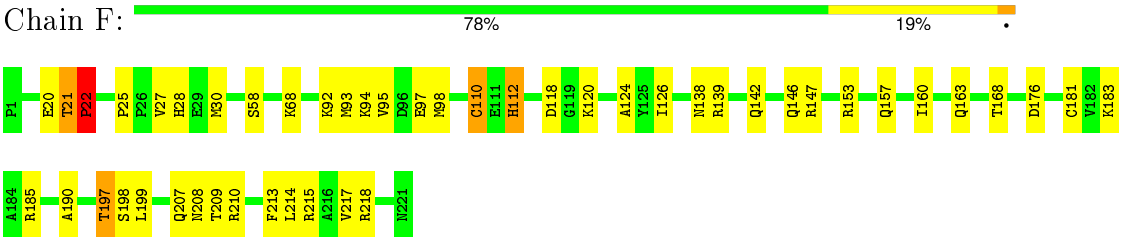
• Molecule 1: GTP cyclohydrolase I

Chain E:



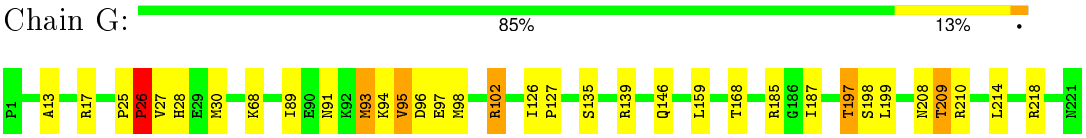
• Molecule 1: GTP cyclohydrolase I

Chain F:



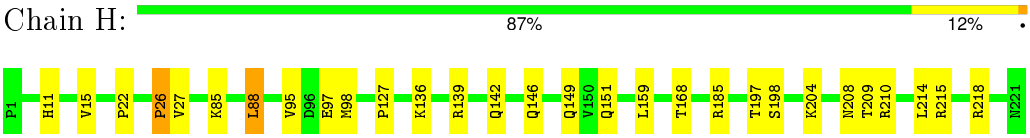
• Molecule 1: GTP cyclohydrolase I

Chain G:



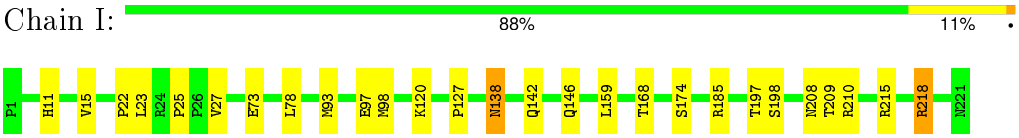
• Molecule 1: GTP cyclohydrolase I

Chain H:



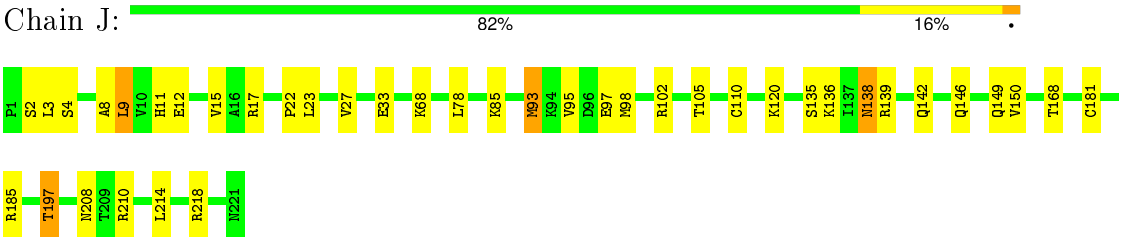
• Molecule 1: GTP cyclohydrolase I

Chain I:



• Molecule 1: GTP cyclohydrolase I

Chain J:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	124.30Å 124.30Å 389.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.55)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.262 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17795	wwPDB-VP
Average B, all atoms (Å^2)	64.0	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	0.61	0/1756	0.84	0/2377
1	B	0.59	0/1756	0.83	0/2377
1	C	0.67	0/1756	1.00	8/2377 (0.3%)
1	D	0.59	0/1756	0.86	1/2377 (0.0%)
1	E	0.60	0/1756	0.83	1/2377 (0.0%)
1	F	0.62	0/1756	1.01	5/2377 (0.2%)
1	G	0.61	0/1756	0.86	2/2377 (0.1%)
1	H	0.60	0/1756	0.83	3/2377 (0.1%)
1	I	0.57	0/1756	0.81	2/2377 (0.1%)
1	J	0.62	0/1756	0.88	6/2377 (0.3%)
All	All	0.61	0/17560	0.88	28/23770 (0.1%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	21	THR	C-N-CD	-19.65	77.36	120.60
1	C	24	ARG	C-N-CD	-18.21	80.55	120.60
1	F	21	THR	C-N-CA	12.01	172.42	122.00
1	C	24	ARG	C-N-CA	10.42	165.77	122.00
1	F	22	PRO	CA-N-CD	-8.33	99.84	111.50
1	C	25	PRO	CA-N-CD	-8.02	100.28	111.50
1	J	110	CYS	CA-CB-SG	7.92	128.26	114.00
1	C	110	CYS	CA-CB-SG	7.59	127.66	114.00
1	J	9	LEU	CA-CB-CG	7.04	131.50	115.30
1	D	9	LEU	CA-CB-CG	6.95	131.28	115.30
1	F	110	CYS	CA-CB-SG	6.85	126.33	114.00
1	J	98	MET	N-CA-C	6.48	128.50	111.00
1	G	98	MET	N-CA-C	6.34	128.12	111.00
1	G	26	PRO	N-CA-C	6.20	128.21	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	181	CYS	CA-CB-SG	6.19	125.15	114.00
1	E	98	MET	N-CA-C	6.09	127.45	111.00
1	H	98	MET	N-CA-C	5.97	127.11	111.00
1	J	181	CYS	CA-CB-SG	5.89	124.60	114.00
1	F	181	CYS	CA-CB-SG	5.88	124.58	114.00
1	C	98	MET	N-CA-C	5.77	126.57	111.00
1	C	25	PRO	C-N-CD	-5.65	108.17	120.60
1	H	149	GLN	N-CA-C	5.42	125.63	111.00
1	I	98	MET	N-CA-C	5.35	125.46	111.00
1	C	25	PRO	C-N-CA	5.30	144.26	122.00
1	H	88	LEU	CA-CB-CG	5.30	127.48	115.30
1	J	149	GLN	N-CA-C	5.21	125.07	111.00
1	I	73	GLU	N-CA-C	5.09	124.74	111.00
1	J	150	VAL	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1729	0	1766	16	0
1	B	1729	0	1766	22	0
1	C	1729	0	1764	22	0
1	D	1729	0	1766	24	0
1	E	1729	0	1766	20	0
1	F	1729	0	1764	25	0
1	G	1729	0	1766	21	0
1	H	1729	0	1766	17	0
1	I	1729	0	1766	16	0
1	J	1729	0	1764	22	0
2	A	32	0	11	1	0
2	B	32	0	11	0	0
2	C	32	0	11	2	0
2	D	32	0	11	2	0
2	E	32	0	11	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	32	0	11	3	0
2	G	32	0	11	1	0
2	H	32	0	11	3	0
2	I	32	0	11	1	0
2	J	32	0	11	2	0
3	A	23	0	0	0	0
3	B	34	0	0	1	0
3	C	16	0	0	0	1
3	D	24	0	0	1	1
3	E	9	0	0	0	0
3	F	18	0	0	1	0
3	G	13	0	0	0	0
3	H	9	0	0	1	0
3	I	18	0	0	0	1
3	J	21	0	0	1	1
All	All	17795	0	17764	164	2

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 5.

All (164) 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:D:210:ARG:HE	1:E:208:ASN:HD21	1.07	1.02
1:B:210:ARG:HE	1:C:208:ASN:HD21	1.02	0.92
1:F:93:MET:HG2	1:J:17:ARG:O	1.72	0.89
1:D:210:ARG:NE	1:E:208:ASN:HD21	1.71	0.87
1:B:210:ARG:NE	1:C:208:ASN:HD21	1.75	0.83
1:H:139:ARG:HH12	2:H:6411:GTP:PG	2.06	0.79
1:I:218:ARG:HH21	1:J:102:ARG:HH22	1.36	0.73
1:C:156:GLN:HG3	1:D:95:VAL:HG21	1.69	0.73
1:J:138:ASN:H	1:J:138:ASN:HD22	1.38	0.72
1:I:138:ASN:HD22	1:I:138:ASN:H	1.39	0.71
1:A:208:ASN:HD21	1:E:210:ARG:NE	1.90	0.69
2:F:9411:GTP:PG	1:J:185:ARG:HH22	2.16	0.68
1:F:110:CYS:SG	1:F:112:HIS:ND1	2.61	0.68
1:C:27:VAL:HG12	1:C:28:HIS:H	1.60	0.66
1:I:185:ARG:HH22	2:J:8411:GTP:PG	2.19	0.66
1:D:210:ARG:HE	1:E:208:ASN:ND2	1.87	0.64
1:G:210:ARG:NE	1:H:208:ASN:HD21	1.97	0.63
1:B:204:LYS:HA	1:B:210:ARG:HH11	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:GLU:O	1:B:127:PRO:HD2	1.99	0.62
1:H:139:ARG:NH1	2:H:6411:GTP:O2G	2.33	0.61
1:J:8:ALA:O	1:J:12:GLU:HG3	1.99	0.61
1:F:197:THR:O	1:G:97:GLU:HB3	2.01	0.61
2:A:4411:GTP:PG	1:E:185:ARG:HH22	2.23	0.60
1:E:160:ILE:HD13	1:E:163:GLN:NE2	2.15	0.60
1:J:85:LYS:O	1:J:136:LYS:HE2	2.01	0.60
1:I:23:LEU:HD11	1:I:78:LEU:HD22	1.84	0.60
1:B:23:LEU:HD11	1:B:78:LEU:HD22	1.83	0.60
1:D:93:MET:HB3	1:D:95:VAL:HG23	1.84	0.60
1:G:93:MET:HB2	1:G:95:VAL:HG23	1.82	0.60
1:H:210:ARG:NE	1:I:208:ASN:HD21	2.01	0.59
1:A:204:LYS:HA	1:A:210:ARG:HH11	1.67	0.59
1:B:185:ARG:HH22	2:C:1411:GTP:PG	2.26	0.58
1:H:159:LEU:HD22	1:H:198:SER:HB3	1.85	0.58
1:C:185:ARG:HH22	2:D:2411:GTP:PG	2.26	0.57
1:D:135:SER:O	1:D:139:ARG:HG3	2.04	0.57
1:J:23:LEU:HD11	1:J:78:LEU:HD22	1.86	0.57
1:G:199:LEU:H	1:H:97:GLU:HG3	1.68	0.57
1:E:85:LYS:O	1:E:136:LYS:HE2	2.05	0.57
1:I:159:LEU:HD22	1:I:198:SER:HB3	1.86	0.57
1:A:102:ARG:HG3	1:A:102:ARG:HH11	1.70	0.57
1:H:85:LYS:O	1:H:136:LYS:HE2	2.05	0.57
1:F:142:GLN:O	1:F:146:GLN:HG2	2.04	0.57
1:B:138:ASN:H	1:B:138:ASN:HD22	1.52	0.57
1:B:197:THR:O	1:C:97:GLU:HB3	2.05	0.56
1:D:204:LYS:HA	1:D:210:ARG:HH11	1.70	0.56
1:D:138:ASN:HD22	1:D:138:ASN:H	1.51	0.56
1:H:185:ARG:HH22	2:I:7411:GTP:PG	2.29	0.55
1:E:154:LEU:O	1:E:158:ILE:HG12	2.05	0.55
1:G:185:ARG:HH22	2:H:6411:GTP:PG	2.30	0.55
1:I:138:ASN:HD22	1:I:138:ASN:N	2.05	0.54
1:D:159:LEU:HD22	1:D:198:SER:HB3	1.89	0.54
1:A:30:MET:HB2	1:A:35:ARG:HE	1.72	0.54
1:F:207:GLN:HE22	1:G:208:ASN:HB2	1.72	0.54
1:F:210:ARG:HD3	1:G:208:ASN:OD1	2.07	0.54
1:F:138:ASN:HD22	1:F:138:ASN:H	1.56	0.54
1:G:214:LEU:HB3	1:H:215:ARG:NH2	2.24	0.53
1:C:135:SER:O	1:C:139:ARG:HG3	2.09	0.53
1:D:197:THR:O	1:E:97:GLU:HB3	2.09	0.53
1:H:204:LYS:HA	1:H:210:ARG:HH11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:LEU:HD22	1:E:198:SER:HB3	1.91	0.53
1:D:142:GLN:O	1:D:146:GLN:HG2	2.09	0.52
1:I:97:GLU:O	1:I:127:PRO:HD2	2.09	0.52
1:G:197:THR:O	1:H:97:GLU:HB3	2.09	0.52
1:H:214:LEU:HB3	1:I:215:ARG:NH2	2.25	0.52
1:I:197:THR:O	1:J:97:GLU:HB3	2.09	0.52
1:A:135:SER:O	1:A:139:ARG:HG3	2.10	0.51
1:F:118:ASP:HB3	3:F:9412:HOH:O	2.08	0.51
1:F:199:LEU:HD11	1:F:214:LEU:HD11	1.92	0.51
1:D:160:ILE:HD13	1:D:163:GLN:NE2	2.26	0.51
1:B:185:ARG:NH2	2:C:1411:GTP:O3G	2.44	0.51
1:F:139:ARG:NH1	2:F:9411:GTP:PG	2.84	0.51
1:F:160:ILE:HD13	1:F:163:GLN:NE2	2.26	0.51
1:F:28:HIS:C	1:F:30:MET:H	2.13	0.50
1:G:102:ARG:HG3	1:G:102:ARG:HH11	1.76	0.50
1:D:214:LEU:HB3	1:E:215:ARG:NH2	2.26	0.50
1:G:210:ARG:CZ	1:H:208:ASN:HD21	2.24	0.50
1:A:197:THR:O	1:B:97:GLU:HB3	2.11	0.50
1:C:218:ARG:HH21	1:D:102:ARG:HH22	1.57	0.50
1:J:142:GLN:O	1:J:146:GLN:HG2	2.12	0.49
1:D:97:GLU:O	1:D:127:PRO:HD2	2.12	0.49
1:F:208:ASN:HD21	1:J:210:ARG:NE	2.10	0.49
1:D:185:ARG:HH22	2:E:3411:GTP:PG	2.36	0.49
1:A:214:LEU:HB3	1:B:215:ARG:NH2	2.28	0.49
1:A:97:GLU:O	1:A:127:PRO:HD2	2.13	0.49
1:B:23:LEU:HD22	3:B:417:HOH:O	2.12	0.48
1:I:11:HIS:O	1:I:15:VAL:HG23	2.12	0.48
1:E:160:ILE:HD13	1:E:163:GLN:HE22	1.77	0.48
1:E:141:VAL:HA	1:E:158:ILE:HD12	1.93	0.48
1:B:11:HIS:O	1:B:15:VAL:HG23	2.14	0.48
1:J:11:HIS:O	1:J:15:VAL:HG23	2.13	0.48
1:E:139:ARG:NH1	2:E:3411:GTP:PG	2.87	0.47
1:A:123:VAL:HG22	1:A:173:VAL:HG22	1.96	0.47
1:J:138:ASN:N	1:J:138:ASN:HD22	2.11	0.47
1:H:11:HIS:O	1:H:15:VAL:HG23	2.14	0.47
1:G:135:SER:O	1:G:139:ARG:HG3	2.15	0.47
1:J:105:THR:HG21	3:J:8425:HOH:O	2.13	0.47
1:F:20:GLU:CD	1:F:147:ARG:HH12	2.17	0.47
1:J:135:SER:O	1:J:139:ARG:HG3	2.15	0.47
1:F:92:LYS:O	1:F:93:MET:SD	2.73	0.47
1:E:142:GLN:O	1:E:146:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ARG:NE	1:C:208:ASN:ND2	2.55	0.47
1:F:198:SER:HA	1:G:97:GLU:HG3	1.97	0.47
1:A:204:LYS:HA	1:A:210:ARG:NH1	2.29	0.47
1:D:183:LYS:HG3	1:D:190:ALA:HA	1.97	0.46
1:G:13:ALA:O	1:G:17:ARG:HD2	2.16	0.46
1:C:187:ILE:HG22	3:D:2432:HOH:O	2.14	0.46
1:H:97:GLU:O	1:H:127:PRO:HD2	2.15	0.46
1:F:153:ARG:O	1:F:157:GLN:HG3	2.15	0.46
1:H:197:THR:O	1:I:97:GLU:HB3	2.16	0.46
1:C:185:ARG:NH2	2:D:2411:GTP:O3G	2.47	0.46
1:J:93:MET:HB2	1:J:95:VAL:HG23	1.97	0.45
1:G:91:ASN:HD21	1:G:94:LYS:HA	1.81	0.45
1:D:210:ARG:NE	1:E:208:ASN:ND2	2.54	0.45
1:H:142:GLN:O	1:H:146:GLN:HG2	2.17	0.45
1:F:185:ARG:NH2	2:G:5411:GTP:O3G	2.45	0.45
1:C:142:GLN:O	1:C:146:GLN:HG2	2.17	0.45
1:G:159:LEU:HD22	1:G:198:SER:HB3	1.99	0.45
1:A:137:ILE:O	1:A:141:VAL:HG23	2.18	0.44
1:I:142:GLN:O	1:I:146:GLN:HG2	2.17	0.44
1:G:187:ILE:HG22	3:H:6416:HOH:O	2.17	0.44
1:F:213:PHE:O	1:F:217:VAL:HG23	2.17	0.44
1:J:138:ASN:ND2	1:J:138:ASN:H	2.10	0.44
1:F:98:MET:HE1	1:F:124:ALA:HB1	1.98	0.44
1:E:147:ARG:NH1	1:E:157:GLN:HE22	2.15	0.44
1:B:199:LEU:H	1:C:97:GLU:HG3	1.82	0.44
1:B:210:ARG:O	1:B:214:LEU:HD12	2.18	0.44
1:E:97:GLU:O	1:E:127:PRO:HD2	2.18	0.44
1:J:3:LEU:HB3	1:J:4:SER:H	1.57	0.44
2:J:8411:GTP:H5'	2:J:8411:GTP:O2B	2.17	0.43
1:A:23:LEU:HD21	1:A:78:LEU:HD22	2.01	0.43
1:C:30:MET:SD	1:C:35:ARG:HG2	2.57	0.43
1:C:185:ARG:HG2	1:C:186:GLY:N	2.33	0.43
1:C:197:THR:O	1:D:97:GLU:HB2	2.19	0.43
1:G:96:ASP:N	1:G:96:ASP:OD1	2.45	0.43
1:F:97:GLU:HB2	1:J:197:THR:O	2.18	0.43
1:A:112:HIS:HE1	1:A:181:CYS:SG	2.42	0.43
1:F:215:ARG:NH2	1:J:214:LEU:HB3	2.34	0.43
1:D:112:HIS:ND1	2:E:3411:GTP:H8	2.17	0.43
1:D:6:GLU:HG2	1:D:86:ILE:HB	2.01	0.43
1:I:138:ASN:N	1:I:138:ASN:ND2	2.66	0.42
1:C:97:GLU:O	1:C:127:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:NE	1:B:208:ASN:HD21	2.16	0.42
1:B:198:SER:HA	1:C:97:GLU:HG3	2.01	0.42
1:A:138:ASN:HD22	1:A:138:ASN:H	1.66	0.42
1:I:210:ARG:NE	1:J:208:ASN:HD21	2.17	0.42
1:F:183:LYS:HG3	1:F:190:ALA:HA	2.01	0.42
1:F:126:ILE:HD11	1:F:209:THR:HG21	2.02	0.42
1:I:174:SER:OG	1:I:197:THR:HG22	2.20	0.42
1:C:218:ARG:NH2	1:D:221:ASN:O	2.53	0.42
1:G:126:ILE:HD11	1:G:209:THR:HG21	2.02	0.42
1:D:13:ALA:O	1:D:17:ARG:HD2	2.20	0.41
2:F:9411:GTP:O3G	1:J:185:ARG:NH2	2.51	0.41
1:B:213:PHE:O	1:B:217:VAL:HG23	2.20	0.41
1:C:185:ARG:HG2	1:C:186:GLY:H	1.85	0.41
1:C:28:HIS:O	1:C:28:HIS:ND1	2.54	0.41
1:G:97:GLU:O	1:G:127:PRO:HD2	2.21	0.41
1:D:198:SER:HA	1:E:97:GLU:HG3	2.02	0.41
1:E:123:VAL:HG22	1:E:173:VAL:HG22	2.03	0.41
1:J:138:ASN:ND2	1:J:138:ASN:N	2.68	0.40
1:F:176:ASP:OD2	1:G:102:ARG:NH2	2.55	0.40
1:A:214:LEU:HB3	1:B:215:ARG:HH22	1.85	0.40
1:B:100:THR:HG23	1:B:124:ALA:HB2	2.02	0.40
1:B:135:SER:O	1:B:139:ARG:HG3	2.21	0.40
1:C:3:LEU:HD21	1:C:80:TYR:HB3	2.03	0.40

All (2) 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)
3:C:1423:HOH:O	3:J:8425:HOH:O[8_655]	2.04	0.16
3:D:2421:HOH:O	3:I:7429:HOH:O[8_655]	2.15	0.05

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	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	14	23
1	B	219/221 (99%)	203 (93%)	13 (6%)	3 (1%)	14	23
1	C	219/221 (99%)	199 (91%)	16 (7%)	4 (2%)	11	17
1	D	219/221 (99%)	199 (91%)	17 (8%)	3 (1%)	14	23
1	E	219/221 (99%)	201 (92%)	15 (7%)	3 (1%)	14	23
1	F	219/221 (99%)	194 (89%)	21 (10%)	4 (2%)	11	17
1	G	219/221 (99%)	203 (93%)	12 (6%)	4 (2%)	11	17
1	H	219/221 (99%)	201 (92%)	14 (6%)	4 (2%)	11	17
1	I	219/221 (99%)	203 (93%)	14 (6%)	2 (1%)	21	36
1	J	219/221 (99%)	201 (92%)	15 (7%)	3 (1%)	14	23
All	All	2190/2210 (99%)	2008 (92%)	149 (7%)	33 (2%)	13	22

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	C	23	LEU
1	C	25	PRO
1	C	27	VAL
1	C	29	GLU
1	D	27	VAL
1	D	28	HIS
1	F	22	PRO
1	F	25	PRO
1	F	27	VAL
1	F	94	LYS
1	G	26	PRO
1	D	29	GLU
1	G	27	VAL
1	H	27	VAL
1	I	22	PRO
1	I	27	VAL
1	A	22	PRO
1	A	218	ARG
1	B	22	PRO
1	E	22	PRO
1	E	27	VAL
1	J	22	PRO

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Mol	Chain	Res	Type
1	J	27	VAL
1	G	28	HIS
1	H	22	PRO
1	H	26	PRO
1	B	218	ARG
1	E	95	VAL
1	J	2	SER
1	H	95	VAL
1	B	95	VAL
1	G	95	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/194 (100%)	176 (91%)	18 (9%)	11	19
1	B	194/194 (100%)	185 (95%)	9 (5%)	33	55
1	C	194/194 (100%)	181 (93%)	13 (7%)	20	35
1	D	194/194 (100%)	184 (95%)	10 (5%)	29	49
1	E	194/194 (100%)	186 (96%)	8 (4%)	37	61
1	F	194/194 (100%)	184 (95%)	10 (5%)	29	49
1	G	194/194 (100%)	182 (94%)	12 (6%)	23	39
1	H	194/194 (100%)	188 (97%)	6 (3%)	47	73
1	I	194/194 (100%)	187 (96%)	7 (4%)	42	67
1	J	194/194 (100%)	185 (95%)	9 (5%)	33	55
All	All	1940/1940 (100%)	1838 (95%)	102 (5%)	28	48

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	24	ARG
1	A	33	GLU

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Mol	Chain	Res	Type
1	A	79	ASP
1	A	95	VAL
1	A	96	ASP
1	A	97	GLU
1	A	98	MET
1	A	102	ARG
1	A	112	HIS
1	A	120	LYS
1	A	168	THR
1	A	192	SER
1	A	197	THR
1	A	199	LEU
1	A	206	SER
1	A	207	GLN
1	A	215	ARG
1	B	68	LYS
1	B	89	ILE
1	B	93	MET
1	B	96	ASP
1	B	120	LYS
1	B	138	ASN
1	B	168	THR
1	B	209	THR
1	B	218	ARG
1	C	2	SER
1	C	3	LEU
1	C	21	THR
1	C	25	PRO
1	C	33	GLU
1	C	93	MET
1	C	94	LYS
1	C	120	LYS
1	C	168	THR
1	C	176	ASP
1	C	197	THR
1	C	209	THR
1	C	218	ARG
1	D	9	LEU
1	D	25	PRO
1	D	33	GLU
1	D	109	THR
1	D	112	HIS

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Mol	Chain	Res	Type
1	D	120	LYS
1	D	138	ASN
1	D	168	THR
1	D	207	GLN
1	D	218	ARG
1	E	17	ARG
1	E	33	GLU
1	E	93	MET
1	E	102	ARG
1	E	112	HIS
1	E	168	THR
1	E	197	THR
1	E	218	ARG
1	F	21	THR
1	F	22	PRO
1	F	58	SER
1	F	68	LYS
1	F	95	VAL
1	F	112	HIS
1	F	120	LYS
1	F	168	THR
1	F	197	THR
1	F	218	ARG
1	G	25	PRO
1	G	26	PRO
1	G	30	MET
1	G	68	LYS
1	G	89	ILE
1	G	93	MET
1	G	102	ARG
1	G	146	GLN
1	G	168	THR
1	G	197	THR
1	G	209	THR
1	G	218	ARG
1	H	26	PRO
1	H	88	LEU
1	H	151	GLN
1	H	168	THR
1	H	209	THR
1	H	218	ARG
1	I	25	PRO

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Mol	Chain	Res	Type
1	I	93	MET
1	I	120	LYS
1	I	138	ASN
1	I	168	THR
1	I	209	THR
1	I	218	ARG
1	J	9	LEU
1	J	33	GLU
1	J	68	LYS
1	J	93	MET
1	J	120	LYS
1	J	138	ASN
1	J	168	THR
1	J	197	THR
1	J	218	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	138	ASN
1	A	163	GLN
1	B	163	GLN
1	C	138	ASN
1	C	163	GLN
1	C	208	ASN
1	D	138	ASN
1	D	146	GLN
1	D	163	GLN
1	E	163	GLN
1	E	208	ASN
1	F	138	ASN
1	F	163	GLN
1	F	207	GLN
1	F	208	ASN
1	G	163	GLN
1	H	138	ASN
1	H	163	GLN
1	H	207	GLN
1	I	82	ASN
1	I	138	ASN
1	I	146	GLN

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Mol	Chain	Res	Type
1	I	163	GLN
1	I	208	ASN
1	J	138	ASN
1	J	163	GLN
1	J	208	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 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	4411	-	25,34,34	3.61	10 (40%)	34,54,54	2.57	11 (32%)
2	GTP	B	411	-	25,34,34	3.66	10 (40%)	34,54,54	2.65	11 (32%)
2	GTP	C	1411	-	25,34,34	3.54	8 (32%)	34,54,54	2.75	11 (32%)
2	GTP	D	2411	-	25,34,34	3.61	10 (40%)	34,54,54	2.75	9 (26%)
2	GTP	E	3411	-	25,34,34	3.57	10 (40%)	34,54,54	2.52	11 (32%)
2	GTP	F	9411	-	25,34,34	3.72	10 (40%)	34,54,54	2.67	11 (32%)
2	GTP	G	5411	-	25,34,34	3.51	9 (36%)	34,54,54	2.69	11 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GTP	H	6411	-	25,34,34	3.67	9 (36%)	34,54,54	2.63	11 (32%)
2	GTP	I	7411	-	25,34,34	3.65	9 (36%)	34,54,54	2.62	10 (29%)
2	GTP	J	8411	-	25,34,34	3.52	10 (40%)	34,54,54	2.70	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	4411	-	-	0/18/38/38	0/3/3/3
2	GTP	B	411	-	-	0/18/38/38	0/3/3/3
2	GTP	C	1411	-	-	0/18/38/38	0/3/3/3
2	GTP	D	2411	-	-	0/18/38/38	0/3/3/3
2	GTP	E	3411	-	-	0/18/38/38	0/3/3/3
2	GTP	F	9411	-	-	0/18/38/38	0/3/3/3
2	GTP	G	5411	-	-	0/18/38/38	0/3/3/3
2	GTP	H	6411	-	-	0/18/38/38	0/3/3/3
2	GTP	I	7411	-	-	0/18/38/38	0/3/3/3
2	GTP	J	8411	-	-	0/18/38/38	0/3/3/3

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	9411	GTP	C6-C5	-7.78	1.25	1.41
2	J	8411	GTP	C6-C5	-7.38	1.26	1.41
2	I	7411	GTP	C6-C5	-7.27	1.26	1.41
2	D	2411	GTP	C6-C5	-7.25	1.26	1.41
2	H	6411	GTP	C6-C5	-7.20	1.26	1.41
2	E	3411	GTP	C6-C5	-7.03	1.27	1.41
2	B	411	GTP	C6-C5	-6.60	1.28	1.41
2	A	4411	GTP	C6-C5	-6.57	1.28	1.41
2	C	1411	GTP	C6-C5	-6.56	1.28	1.41
2	G	5411	GTP	C6-C5	-6.35	1.28	1.41
2	B	411	GTP	O2'-C2'	-4.66	1.31	1.43
2	H	6411	GTP	O2'-C2'	-4.56	1.32	1.43
2	I	7411	GTP	O2'-C2'	-4.50	1.32	1.43
2	A	4411	GTP	O2'-C2'	-4.48	1.32	1.43
2	G	5411	GTP	O2'-C2'	-4.44	1.32	1.43
2	E	3411	GTP	O2'-C2'	-4.42	1.32	1.43
2	C	1411	GTP	O2'-C2'	-4.40	1.32	1.43
2	J	8411	GTP	O2'-C2'	-4.40	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2411	GTP	O2'-C2'	-4.32	1.32	1.43
2	F	9411	GTP	O2'-C2'	-4.16	1.33	1.43
2	D	2411	GTP	C5-C4	-3.97	1.31	1.40
2	F	9411	GTP	C5-C4	-3.92	1.31	1.40
2	E	3411	GTP	C5-C4	-3.72	1.32	1.40
2	A	4411	GTP	C5-C4	-3.65	1.32	1.40
2	I	7411	GTP	C5-C4	-3.62	1.32	1.40
2	J	8411	GTP	C5-C4	-3.56	1.32	1.40
2	C	1411	GTP	C5-C4	-3.53	1.32	1.40
2	G	5411	GTP	C5-C4	-3.50	1.32	1.40
2	H	6411	GTP	C5-C4	-3.45	1.32	1.40
2	B	411	GTP	C5-C4	-3.37	1.32	1.40
2	B	411	GTP	C2-N1	-3.23	1.29	1.35
2	J	8411	GTP	C2-N1	-3.11	1.29	1.35
2	E	3411	GTP	C2-N1	-3.02	1.30	1.35
2	G	5411	GTP	PG-O3G	-2.99	1.44	1.54
2	A	4411	GTP	C2-N1	-2.92	1.30	1.35
2	C	1411	GTP	PG-O3G	-2.91	1.44	1.54
2	F	9411	GTP	PG-O3G	-2.90	1.44	1.54
2	H	6411	GTP	PG-O3G	-2.82	1.44	1.54
2	J	8411	GTP	PG-O3G	-2.77	1.44	1.54
2	B	411	GTP	PG-O3G	-2.77	1.44	1.54
2	D	2411	GTP	PG-O3G	-2.74	1.44	1.54
2	F	9411	GTP	C2-N1	-2.74	1.30	1.35
2	E	3411	GTP	PG-O3G	-2.66	1.45	1.54
2	A	4411	GTP	C3'-C4'	-2.65	1.45	1.53
2	D	2411	GTP	C2-N1	-2.62	1.30	1.35
2	A	4411	GTP	PG-O3G	-2.54	1.45	1.54
2	I	7411	GTP	PG-O3G	-2.52	1.45	1.54
2	B	411	GTP	C3'-C4'	-2.51	1.46	1.53
2	C	1411	GTP	C2-N1	-2.48	1.31	1.35
2	H	6411	GTP	C3'-C4'	-2.47	1.46	1.53
2	I	7411	GTP	C3'-C4'	-2.43	1.46	1.53
2	J	8411	GTP	C3'-C4'	-2.43	1.46	1.53
2	G	5411	GTP	C2-N1	-2.38	1.31	1.35
2	I	7411	GTP	C2-N1	-2.36	1.31	1.35
2	F	9411	GTP	C3'-C4'	-2.31	1.46	1.53
2	B	411	GTP	PB-O2B	-2.29	1.45	1.54
2	H	6411	GTP	C2-N1	-2.28	1.31	1.35
2	E	3411	GTP	C3'-C4'	-2.27	1.46	1.53
2	D	2411	GTP	PB-O2B	-2.26	1.45	1.54
2	E	3411	GTP	PB-O2B	-2.25	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	9411	GTP	PB-O2B	-2.12	1.45	1.54
2	D	2411	GTP	C3'-C4'	-2.07	1.47	1.53
2	A	4411	GTP	PB-O2B	-2.06	1.46	1.54
2	J	8411	GTP	PB-O2B	-2.04	1.46	1.54
2	G	5411	GTP	C3'-C4'	-2.04	1.47	1.53
2	J	8411	GTP	C5'-C4'	2.07	1.58	1.51
2	C	1411	GTP	C5'-C4'	2.34	1.59	1.51
2	D	2411	GTP	C5'-C4'	2.37	1.59	1.51
2	B	411	GTP	C5'-C4'	2.40	1.59	1.51
2	G	5411	GTP	C5'-C4'	2.43	1.59	1.51
2	E	3411	GTP	C5'-C4'	2.46	1.59	1.51
2	H	6411	GTP	C5'-C4'	2.62	1.60	1.51
2	I	7411	GTP	C5'-C4'	2.66	1.60	1.51
2	A	4411	GTP	C5'-C4'	2.72	1.60	1.51
2	F	9411	GTP	C5'-C4'	3.04	1.61	1.51
2	J	8411	GTP	C2-N2	7.21	1.48	1.34
2	E	3411	GTP	C2-N2	7.36	1.49	1.34
2	G	5411	GTP	C2-N2	7.49	1.49	1.34
2	B	411	GTP	C2-N2	7.53	1.49	1.34
2	C	1411	GTP	C2-N2	7.78	1.50	1.34
2	F	9411	GTP	C2-N2	7.79	1.50	1.34
2	D	2411	GTP	C2-N2	7.80	1.50	1.34
2	A	4411	GTP	C2-N2	7.87	1.50	1.34
2	I	7411	GTP	C2-N2	8.01	1.50	1.34
2	H	6411	GTP	C2-N2	8.09	1.50	1.34
2	J	8411	GTP	C6-N1	11.28	1.54	1.33
2	D	2411	GTP	C6-N1	11.60	1.54	1.33
2	G	5411	GTP	C6-N1	11.61	1.54	1.33
2	C	1411	GTP	C6-N1	11.62	1.54	1.33
2	E	3411	GTP	C6-N1	11.75	1.54	1.33
2	I	7411	GTP	C6-N1	11.76	1.55	1.33
2	A	4411	GTP	C6-N1	11.77	1.55	1.33
2	H	6411	GTP	C6-N1	11.88	1.55	1.33
2	F	9411	GTP	C6-N1	11.98	1.55	1.33
2	B	411	GTP	C6-N1	12.26	1.55	1.33

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1411	GTP	C5-C6-N1	-9.11	111.13	123.59
2	B	411	GTP	C5-C6-N1	-8.98	111.31	123.59
2	G	5411	GTP	C5-C6-N1	-8.95	111.35	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2411	GTP	C5-C6-N1	-8.92	111.40	123.59
2	J	8411	GTP	C5-C6-N1	-8.87	111.47	123.59
2	H	6411	GTP	C5-C6-N1	-8.82	111.53	123.59
2	F	9411	GTP	C5-C6-N1	-8.79	111.57	123.59
2	I	7411	GTP	C5-C6-N1	-8.74	111.64	123.59
2	A	4411	GTP	C5-C6-N1	-8.61	111.81	123.59
2	E	3411	GTP	C5-C6-N1	-8.55	111.89	123.59
2	G	5411	GTP	C4-C5-N7	-5.87	104.08	109.48
2	A	4411	GTP	C4-C5-N7	-5.79	104.16	109.48
2	J	8411	GTP	C4-C5-N7	-5.72	104.21	109.48
2	B	411	GTP	C4-C5-N7	-5.69	104.25	109.48
2	I	7411	GTP	C4-C5-N7	-5.57	104.35	109.48
2	C	1411	GTP	C4-C5-N7	-5.57	104.36	109.48
2	H	6411	GTP	C4-C5-N7	-5.55	104.37	109.48
2	D	2411	GTP	C4-C5-N7	-5.49	104.43	109.48
2	E	3411	GTP	C4-C5-N7	-5.32	104.58	109.48
2	I	7411	GTP	C1'-N9-C4	-5.25	119.03	126.94
2	F	9411	GTP	C4-C5-N7	-5.15	104.74	109.48
2	G	5411	GTP	C1'-N9-C4	-4.98	119.43	126.94
2	D	2411	GTP	C2'-C1'-N9	-4.71	107.09	114.29
2	J	8411	GTP	O5'-C5'-C4'	-4.65	91.98	109.12
2	A	4411	GTP	C1'-N9-C4	-4.63	119.95	126.94
2	F	9411	GTP	C1'-N9-C4	-4.58	120.03	126.94
2	C	1411	GTP	C1'-N9-C4	-4.50	120.15	126.94
2	J	8411	GTP	C1'-N9-C4	-4.44	120.25	126.94
2	D	2411	GTP	O5'-C5'-C4'	-4.40	92.91	109.12
2	I	7411	GTP	O5'-C5'-C4'	-4.39	92.94	109.12
2	H	6411	GTP	C1'-N9-C4	-4.36	120.36	126.94
2	B	411	GTP	C1'-N9-C4	-4.36	120.37	126.94
2	H	6411	GTP	O5'-C5'-C4'	-4.34	93.11	109.12
2	E	3411	GTP	C1'-N9-C4	-4.32	120.43	126.94
2	F	9411	GTP	O5'-C5'-C4'	-4.13	93.89	109.12
2	C	1411	GTP	O5'-C5'-C4'	-4.10	94.00	109.12
2	D	2411	GTP	C1'-N9-C4	-3.93	121.00	126.94
2	E	3411	GTP	O5'-C5'-C4'	-3.82	95.04	109.12
2	F	9411	GTP	C2'-C1'-N9	-3.77	108.53	114.29
2	G	5411	GTP	O5'-C5'-C4'	-3.54	96.08	109.12
2	B	411	GTP	O5'-C5'-C4'	-3.52	96.13	109.12
2	H	6411	GTP	C2'-C1'-N9	-3.39	109.11	114.29
2	F	9411	GTP	N2-C2-N3	-3.39	111.30	117.80
2	J	8411	GTP	N2-C2-N3	-3.38	111.31	117.80
2	I	7411	GTP	N2-C2-N3	-3.26	111.55	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	5411	GTP	N2-C2-N3	-3.21	111.64	117.80
2	B	411	GTP	N2-C2-N3	-3.20	111.66	117.80
2	A	4411	GTP	O5'-C5'-C4'	-3.18	97.39	109.12
2	A	4411	GTP	N2-C2-N3	-3.15	111.76	117.80
2	C	1411	GTP	C2'-C1'-N9	-3.12	109.52	114.29
2	E	3411	GTP	N2-C2-N3	-3.10	111.84	117.80
2	H	6411	GTP	N2-C2-N3	-3.08	111.90	117.80
2	C	1411	GTP	N2-C2-N3	-3.06	111.93	117.80
2	D	2411	GTP	N2-C2-N3	-3.04	111.96	117.80
2	J	8411	GTP	C2'-C1'-N9	-3.02	109.68	114.29
2	A	4411	GTP	C2'-C1'-N9	-2.93	109.82	114.29
2	B	411	GTP	C2'-C1'-N9	-2.90	109.86	114.29
2	G	5411	GTP	C2'-C1'-N9	-2.89	109.88	114.29
2	I	7411	GTP	C2'-C1'-N9	-2.64	110.25	114.29
2	E	3411	GTP	C2'-C1'-N9	-2.34	110.72	114.29
2	F	9411	GTP	O3A-PA-O5'	2.00	108.25	102.94
2	B	411	GTP	C2'-C3'-C4'	2.07	106.86	102.61
2	A	4411	GTP	C2'-C3'-C4'	2.08	106.89	102.61
2	E	3411	GTP	O4'-C4'-C5'	2.10	116.82	109.32
2	F	9411	GTP	O4'-C4'-C5'	2.13	116.94	109.32
2	C	1411	GTP	O4'-C4'-C5'	2.16	117.04	109.32
2	E	3411	GTP	C2'-C3'-C4'	2.18	107.09	102.61
2	A	4411	GTP	O4'-C4'-C5'	2.21	117.24	109.32
2	H	6411	GTP	O4'-C4'-C5'	2.22	117.25	109.32
2	G	5411	GTP	O4'-C4'-C5'	2.26	117.39	109.32
2	G	5411	GTP	C2'-C3'-C4'	2.26	107.26	102.61
2	I	7411	GTP	O4'-C4'-C5'	2.39	117.87	109.32
2	B	411	GTP	O4'-C4'-C5'	2.40	117.91	109.32
2	H	6411	GTP	C2'-C3'-C4'	2.45	107.64	102.61
2	H	6411	GTP	O4'-C1'-N9	2.45	113.22	108.10
2	E	3411	GTP	O4'-C1'-N9	2.66	113.66	108.10
2	J	8411	GTP	O4'-C4'-C5'	2.69	118.93	109.32
2	J	8411	GTP	O4'-C1'-N9	2.72	113.80	108.10
2	C	1411	GTP	O3A-PA-O5'	2.83	110.44	102.94
2	I	7411	GTP	O4'-C1'-N9	2.84	114.05	108.10
2	F	9411	GTP	O4'-C1'-N9	2.86	114.09	108.10
2	A	4411	GTP	O4'-C1'-N9	3.09	114.56	108.10
2	I	7411	GTP	N3-C2-N1	3.22	132.35	127.44
2	H	6411	GTP	N3-C2-N1	3.30	132.47	127.44
2	D	2411	GTP	N3-C2-N1	3.36	132.56	127.44
2	F	9411	GTP	N3-C2-N1	3.42	132.66	127.44
2	A	4411	GTP	N3-C2-N1	3.45	132.69	127.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	3411	GTP	N3-C2-N1	3.47	132.73	127.44
2	G	5411	GTP	N3-C2-N1	3.58	132.90	127.44
2	B	411	GTP	N3-C2-N1	3.63	132.97	127.44
2	J	8411	GTP	N3-C2-N1	3.69	133.06	127.44
2	C	1411	GTP	N3-C2-N1	3.72	133.12	127.44
2	B	411	GTP	O4'-C1'-N9	3.74	115.92	108.10
2	D	2411	GTP	O4'-C1'-N9	3.75	115.95	108.10
2	C	1411	GTP	O4'-C1'-N9	3.82	116.09	108.10
2	G	5411	GTP	O4'-C1'-N9	3.89	116.23	108.10
2	A	4411	GTP	C6-C5-C4	4.29	126.02	120.90
2	I	7411	GTP	C6-C5-C4	4.30	126.03	120.90
2	E	3411	GTP	C6-C5-C4	4.36	126.11	120.90
2	B	411	GTP	C6-C5-C4	4.46	126.23	120.90
2	G	5411	GTP	C6-C5-C4	4.47	126.25	120.90
2	F	9411	GTP	C6-C5-C4	4.66	126.47	120.90
2	J	8411	GTP	C6-C5-C4	4.71	126.53	120.90
2	C	1411	GTP	C6-C5-C4	4.78	126.61	120.90
2	H	6411	GTP	C6-C5-C4	4.81	126.64	120.90
2	D	2411	GTP	C6-C5-C4	4.94	126.81	120.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4411	GTP	1	0
2	C	1411	GTP	2	0
2	D	2411	GTP	2	0
2	E	3411	GTP	3	0
2	F	9411	GTP	3	0
2	G	5411	GTP	1	0
2	H	6411	GTP	3	0
2	I	7411	GTP	1	0
2	J	8411	GTP	2	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

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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