Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 08:25 AM GMT

PDB ID	:	3EK5
Title	:	Unique GTP-binding Pocket and Allostery of UMP Kinase from a Gram-Negative Phytopathogen Bacterium
Authors	:	Tu, J.-L.; Chin, K.-H.; Wang, A.H.-J.; Chou, S.-H.
Deposited on	:	2008-09-18
Resolution	:	2.56 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 (1)) were used in the production of this report:

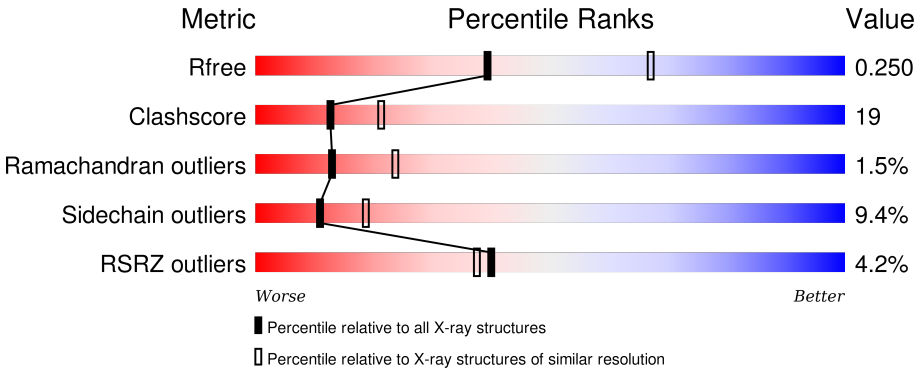
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

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.

Mol	Chain	Length	Quality of chain
1	A	243	2% 75% 22% •
1	B	243	3% 67% 27% 5% •
1	C	243	3% 73% 21% • •
1	D	243	2% 62% 30% 6% •
1	E	243	7% 56% 36% 6% • •

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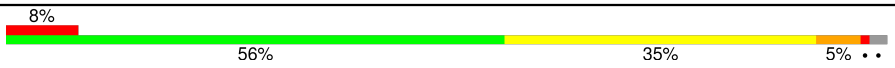
Mol	Chain	Length	Quality of chain
1	F	243	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11484 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 Uridylate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	1
			1811	1135	327	338	11			
1	B	239	Total	C	N	O	S	0	0	0
			1796	1126	323	337	10			
1	C	239	Total	C	N	O	S	0	0	0
			1796	1126	323	337	10			
1	D	239	Total	C	N	O	S	0	0	0
			1796	1126	323	337	10			
1	E	239	Total	C	N	O	S	0	0	0
			1796	1126	323	337	10			
1	F	239	Total	C	N	O	S	0	0	1
			1790	1123	323	334	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP P59009
A	-1	ASN	-	EXPRESSION TAG	UNP P59009
A	0	ALA	-	EXPRESSION TAG	UNP P59009
B	-2	SER	-	EXPRESSION TAG	UNP P59009
B	-1	ASN	-	EXPRESSION TAG	UNP P59009
B	0	ALA	-	EXPRESSION TAG	UNP P59009
C	-2	SER	-	EXPRESSION TAG	UNP P59009
C	-1	ASN	-	EXPRESSION TAG	UNP P59009
C	0	ALA	-	EXPRESSION TAG	UNP P59009
D	-2	SER	-	EXPRESSION TAG	UNP P59009
D	-1	ASN	-	EXPRESSION TAG	UNP P59009
D	0	ALA	-	EXPRESSION TAG	UNP P59009
E	-2	SER	-	EXPRESSION TAG	UNP P59009
E	-1	ASN	-	EXPRESSION TAG	UNP P59009
E	0	ALA	-	EXPRESSION TAG	UNP P59009
F	-2	SER	-	EXPRESSION TAG	UNP P59009
F	-1	ASN	-	EXPRESSION TAG	UNP P59009

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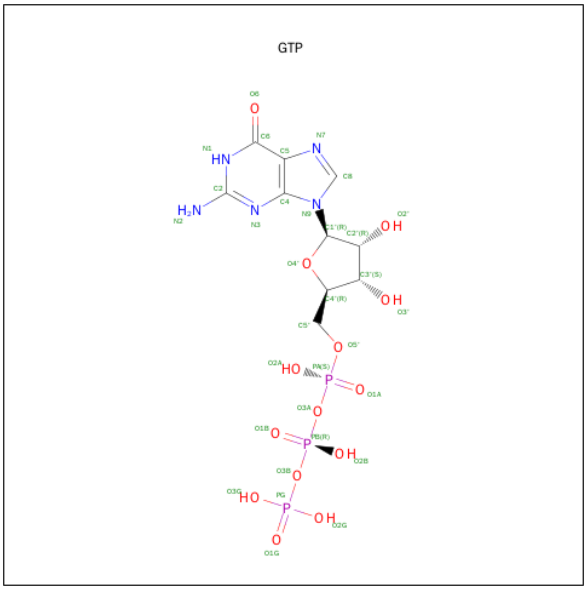
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	EXPRESSION TAG	UNP P59009

- 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	E	6	Total	C	N	O	P	0	0
			192	60	30	84	18		

- Molecule 3 is water.

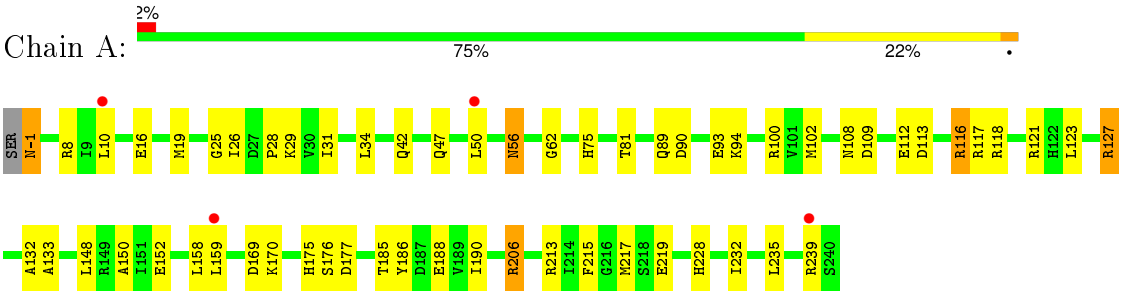
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total	O	0	0
			101	101		
3	B	82	Total	O	0	0
			82	82		
3	C	91	Total	O	0	0
			91	91		
3	D	75	Total	O	0	0
			75	75		
3	E	79	Total	O	0	0
			79	79		
3	F	79	Total	O	0	0
			79	79		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

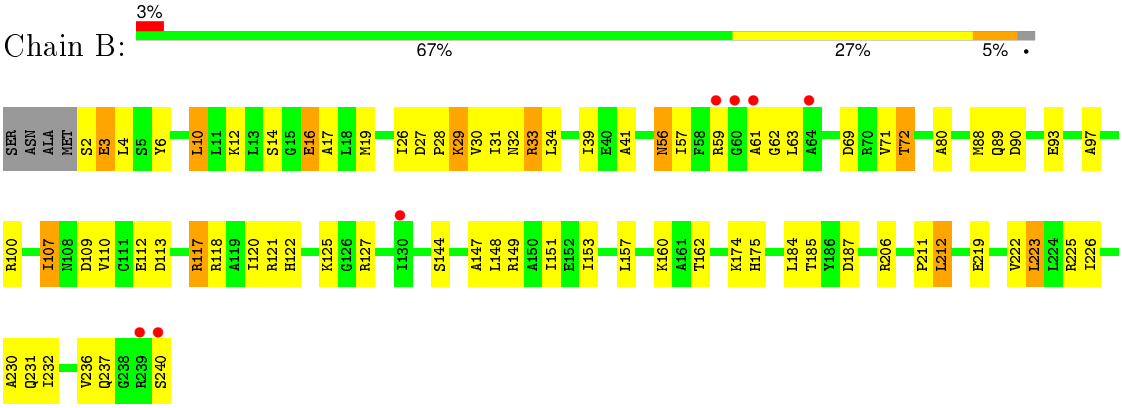
- Molecule 1: Uridylate kinase

Chain A:



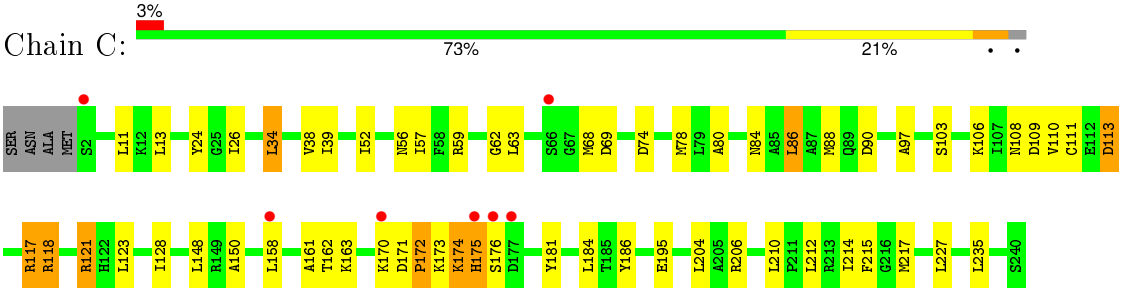
- Molecule 1: Uridylate kinase

Chain B:



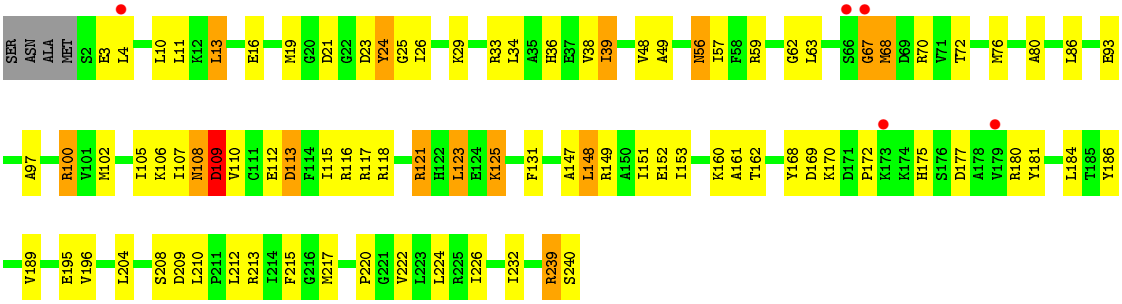
- Molecule 1: Uridylate kinase

Chain C:



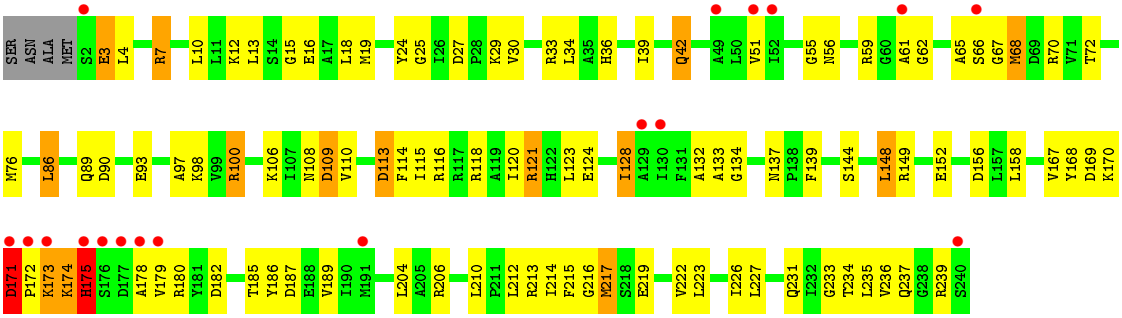
- Molecule 1: Uridylate kinase

Chain D:



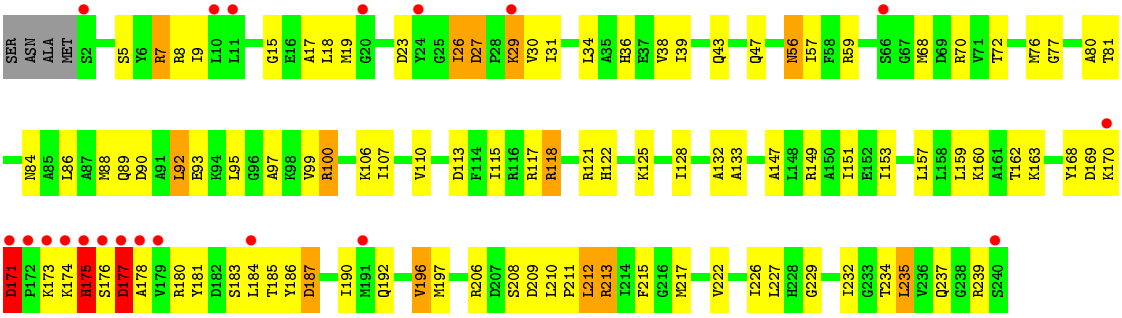
- Molecule 1: Uridylate kinase

Chain E:



- Molecule 1: Uridylate kinase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.63Å 119.64Å 125.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.30 – 2.56 27.30 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.0 (27.30-2.56) 98.8 (27.30-2.54)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.252 0.205 , 0.250	Depositor DCC
R_{free} test set	2764 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	53.5	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.5	EDS
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 55327 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11484	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.63	0/1832	0.77	3/2466 (0.1%)
1	B	0.55	0/1817	0.74	3/2444 (0.1%)
1	C	0.60	0/1817	0.81	5/2444 (0.2%)
1	D	0.60	0/1817	0.81	5/2444 (0.2%)
1	E	0.51	0/1817	0.74	6/2444 (0.2%)
1	F	0.53	0/1811	0.66	0/2438
All	All	0.57	0/10911	0.76	22/14680 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	109	ASP	CB-CA-C	10.24	130.88	110.40
1	C	108	ASN	CA-CB-CG	8.31	131.69	113.40
1	E	121	ARG	CG-CD-NE	8.14	128.88	111.80
1	C	118	ARG	CG-CD-NE	8.05	128.71	111.80
1	A	109	ASP	CB-CA-C	7.60	125.60	110.40
1	B	117	ARG	CG-CD-NE	7.46	127.48	111.80
1	C	117	ARG	CA-CB-CG	6.97	128.74	113.40
1	D	125	LYS	CA-CB-CG	6.97	128.74	113.40
1	C	121	ARG	CD-NE-CZ	6.72	133.01	123.60
1	E	100	ARG	CD-NE-CZ	6.68	132.96	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ASN	CA-CB-CG	6.24	127.12	113.40
1	B	109	ASP	CB-CA-C	6.23	122.87	110.40
1	D	121	ARG	CG-CD-NE	6.00	124.40	111.80
1	D	108	ASN	CA-CB-CG	5.88	126.33	113.40
1	A	127	ARG	CG-CD-NE	-5.86	99.49	111.80
1	E	100	ARG	CB-CG-CD	5.62	126.20	111.60
1	C	108	ASN	CB-CA-C	5.54	121.49	110.40
1	E	100	ARG	CA-CB-CG	5.39	125.27	113.40
1	D	109	ASP	CA-C-O	5.25	131.12	120.10
1	E	118	ARG	CD-NE-CZ	-5.21	116.31	123.60
1	B	127	ARG	CD-NE-CZ	5.05	130.67	123.60
1	E	109	ASP	CB-CA-C	5.03	120.46	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	109	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1811	0	1858	54	0
1	B	1796	0	1840	69	0
1	C	1796	0	1840	56	0
1	D	1796	0	1840	70	0
1	E	1796	0	1840	96	0
1	F	1790	0	1835	106	0
2	E	192	0	72	16	0
3	A	101	0	0	10	0
3	B	82	0	0	2	0
3	C	91	0	0	8	0
3	D	75	0	0	6	0
3	E	79	0	0	8	0
3	F	79	0	0	12	0
All	All	11484	0	11125	427	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 19.

All (427) 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:A:10:LEU:HB3	3:A:2668:HOH:O	1.34	1.26
1:D:29:LYS:HB2	3:D:2628:HOH:O	1.46	1.14
1:B:117:ARG:NH2	1:F:89:GLN:CD	2.01	1.14
1:F:174:LYS:O	1:F:175:HIS:HB2	1.63	0.98
1:A:81:THR:HG21	1:A:133:ALA:H	1.31	0.95
1:C:63:LEU:HD12	3:C:2464:HOH:O	1.67	0.93
1:F:97:ALA:HA	3:F:2516:HOH:O	1.67	0.92
1:F:234:THR:HG22	1:F:235:LEU:H	1.33	0.91
1:F:56:ASN:ND2	1:F:84:ASN:HD21	1.68	0.91
1:E:7:ARG:HB3	1:E:7:ARG:HH11	1.35	0.90
1:D:10:LEU:HD12	1:D:49:ALA:HB3	1.52	0.90
1:F:56:ASN:HD21	1:F:84:ASN:HD21	0.94	0.90
1:D:39:ILE:HD11	1:D:97:ALA:HB2	1.55	0.88
1:C:56:ASN:HD21	1:C:84:ASN:HD21	1.19	0.86
1:F:39:ILE:O	1:F:43:GLN:HG2	1.74	0.86
1:F:213:ARG:NH2	3:F:2702:HOH:O	2.07	0.86
1:D:56:ASN:H	1:D:56:ASN:HD22	1.24	0.86
1:B:39:ILE:HD11	1:B:97:ALA:HB2	1.58	0.85
1:A:28:PRO:HA	1:A:31:ILE:HG22	1.57	0.85
1:F:168:TYR:HA	3:F:2123:HOH:O	1.76	0.85
1:F:185:THR:HA	1:F:237:GLN:O	1.78	0.83
1:F:56:ASN:HD21	1:F:84:ASN:ND2	1.75	0.82
1:D:184:LEU:HD23	1:D:189:VAL:HG22	1.61	0.82
3:C:2694:HOH:O	1:D:68:MET:HE3	1.78	0.82
1:C:106:LYS:H	1:C:106:LYS:HD2	1.44	0.82
1:E:100:ARG:CZ	2:E:2006:GTP:H3'	2.10	0.82
1:F:170:LYS:O	1:F:171:ASP:HB3	1.77	0.82
1:A:206:ARG:NH2	3:A:2308:HOH:O	2.13	0.81
1:E:219:GLU:O	1:E:222:VAL:HG23	1.81	0.81
1:B:93:GLU:OE2	1:C:117:ARG:NH2	2.14	0.80
1:C:24:TYR:HB3	3:C:2040:HOH:O	1.80	0.79
1:F:234:THR:HG22	1:F:235:LEU:N	1.97	0.79
1:B:56:ASN:HD22	1:B:56:ASN:H	1.30	0.79
1:A:56:ASN:HD22	1:A:56:ASN:H	1.30	0.79
1:B:117:ARG:HH22	1:F:89:GLN:CD	1.85	0.79
1:B:117:ARG:NH2	1:F:89:GLN:NE2	2.30	0.78
1:D:10:LEU:HD12	1:D:49:ALA:CB	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:LYS:HE3	1:E:174:LYS:HA	1.65	0.77
1:A:81:THR:HG22	1:A:132:ALA:HB1	1.66	0.77
1:C:162:THR:HG22	1:C:163:LYS:H	1.49	0.76
1:B:121:ARG:HG3	1:B:125:LYS:HE3	1.65	0.76
1:D:175:HIS:HB3	1:D:177:ASP:OD1	1.86	0.75
1:B:31:ILE:HG13	1:B:88:MET:CE	2.17	0.74
1:F:159:LEU:CD2	1:F:213:ARG:HG2	2.17	0.73
1:F:147:ALA:O	1:F:151:ILE:HG12	1.87	0.73
1:E:7:ARG:NH1	1:E:7:ARG:HB3	2.03	0.73
1:F:159:LEU:HD23	1:F:213:ARG:HG2	1.69	0.73
1:B:117:ARG:HH22	1:F:89:GLN:NE2	1.85	0.73
1:C:121:ARG:HG2	2:E:2001:GTP:O2G	1.88	0.73
1:F:169:ASP:HB3	1:F:181:TYR:OH	1.89	0.73
1:F:56:ASN:HD22	1:F:56:ASN:H	1.36	0.72
1:C:39:ILE:CD1	1:C:97:ALA:HB2	2.20	0.72
1:B:93:GLU:CD	1:C:117:ARG:HH22	1.92	0.72
1:B:39:ILE:CD1	1:B:97:ALA:HB2	2.20	0.72
1:B:93:GLU:CD	1:C:117:ARG:NH2	2.43	0.72
1:A:239:ARG:HD3	3:A:2308:HOH:O	1.90	0.71
1:A:89:GLN:O	1:A:93:GLU:HG3	1.90	0.71
1:E:171:ASP:OD1	1:E:174:LYS:HB3	1.89	0.71
1:E:216:GLY:O	1:E:217:MET:HB3	1.90	0.71
1:D:13:LEU:N	1:D:13:LEU:HD22	2.05	0.71
1:D:70:ARG:HH11	1:D:70:ARG:HG3	1.53	0.71
1:A:239:ARG:O	3:A:2565:HOH:O	2.08	0.71
1:F:117:ARG:HG3	3:F:2023:HOH:O	1.89	0.71
1:B:117:ARG:NH2	1:F:89:GLN:OE1	2.22	0.71
1:A:28:PRO:HA	1:A:31:ILE:CG2	2.21	0.70
1:E:171:ASP:OD2	1:E:171:ASP:N	2.25	0.70
1:B:147:ALA:O	1:B:151:ILE:HG13	1.92	0.70
1:A:26:ILE:O	1:B:62:GLY:HA3	1.93	0.69
1:E:3:GLU:HA	1:E:3:GLU:OE1	1.90	0.69
1:B:31:ILE:CG1	1:B:88:MET:HE2	2.22	0.69
1:A:56:ASN:HD22	1:A:56:ASN:N	1.89	0.68
1:B:149:ARG:O	1:B:153:ILE:HG12	1.94	0.68
1:B:31:ILE:HG13	1:B:88:MET:HE2	1.75	0.68
1:E:86:LEU:HD21	1:E:110:VAL:CG1	2.23	0.68
1:F:100:ARG:HG3	1:F:122:HIS:ND1	2.09	0.68
1:B:19:MET:O	1:B:27:ASP:HB2	1.94	0.67
1:B:93:GLU:OE1	1:C:117:ARG:NH2	2.26	0.67
1:B:219:GLU:O	1:B:222:VAL:HG23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:LEU:HB2	1:E:236:VAL:HB	1.77	0.66
1:E:128:ILE:HD12	1:E:128:ILE:N	2.09	0.66
1:B:56:ASN:HD22	1:B:56:ASN:N	1.92	0.66
1:E:216:GLY:O	1:E:217:MET:CB	2.44	0.66
1:E:106:LYS:HG2	1:E:113:ASP:OD1	1.96	0.66
1:C:106:LYS:N	1:C:106:LYS:HD2	2.10	0.65
1:A:8:ARG:HE	1:A:47:GLN:NE2	1.95	0.65
1:B:211:PRO:HG3	1:B:237:GLN:NE2	2.11	0.65
1:F:234:THR:CG2	1:F:235:LEU:H	2.07	0.65
1:A:62:GLY:HA3	1:B:26:ILE:O	1.95	0.65
1:E:19:MET:CE	1:E:24:TYR:HA	2.27	0.65
1:D:72:THR:HG22	3:F:2632:HOH:O	1.97	0.65
1:B:59:ARG:O	1:B:63:LEU:HD13	1.96	0.64
1:D:147:ALA:O	1:D:151:ILE:HG13	1.96	0.64
1:E:100:ARG:NH1	2:E:2006:GTP:H3'	2.11	0.64
1:D:169:ASP:HB3	1:D:181:TYR:OH	1.97	0.64
1:D:36:HIS:HB3	3:D:2323:HOH:O	1.96	0.64
1:E:213:ARG:HH21	1:E:226:ILE:HG23	1.62	0.64
1:C:26:ILE:O	1:D:62:GLY:HA3	1.97	0.64
1:D:215:PHE:CE1	1:D:217:MET:HG3	2.33	0.63
1:C:162:THR:HG22	1:C:163:LYS:N	2.12	0.63
1:D:63:LEU:HD22	1:D:76:MET:HE2	1.81	0.63
1:A:-1:ASN:N	3:A:2635:HOH:O	2.31	0.63
1:F:56:ASN:HD22	1:F:56:ASN:N	1.97	0.63
1:C:109:ASP:OD1	3:C:2296:HOH:O	2.15	0.63
1:F:157:LEU:HD12	1:F:159:LEU:HG	1.79	0.63
1:A:121:ARG:HG2	2:E:2005:GTP:O2G	1.99	0.62
1:F:26:ILE:HG13	1:F:31:ILE:HD11	1.81	0.62
1:F:27:ASP:OD1	1:F:30:VAL:HG22	1.99	0.62
1:A:8:ARG:HH21	1:A:47:GLN:HE22	1.47	0.62
1:C:39:ILE:HD11	1:C:97:ALA:HB2	1.80	0.61
1:B:117:ARG:HH21	1:F:89:GLN:CD	1.98	0.61
1:F:27:ASP:OD2	1:F:29:LYS:HB3	2.00	0.61
1:B:29:LYS:HA	1:B:29:LYS:HE3	1.81	0.61
1:E:100:ARG:NH1	2:E:2006:GTP:O2A	2.34	0.61
1:C:170:LYS:HB2	1:C:175:HIS:CD2	2.35	0.61
1:E:171:ASP:HB3	3:E:2686:HOH:O	2.01	0.60
1:F:192:GLN:HB2	3:F:2177:HOH:O	2.00	0.60
1:F:34:LEU:O	1:F:38:VAL:HG23	2.02	0.60
1:E:4:LEU:HD12	1:E:227:LEU:HD12	1.83	0.60
1:D:56:ASN:N	1:D:56:ASN:HD22	1.94	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:LYS:O	1:F:171:ASP:CB	2.50	0.60
1:E:174:LYS:O	1:E:175:HIS:HB2	2.02	0.60
1:E:19:MET:HE1	1:E:24:TYR:HA	1.84	0.60
1:D:108:ASN:O	1:D:109:ASP:C	2.40	0.59
1:B:212:LEU:HB2	1:B:236:VAL:HB	1.84	0.59
1:B:225:ARG:CZ	1:B:232:ILE:HD11	2.32	0.59
1:D:121:ARG:HE	1:D:125:LYS:HE3	1.67	0.59
1:C:63:LEU:CD1	3:C:2464:HOH:O	2.38	0.59
1:E:213:ARG:NE	3:E:2339:HOH:O	2.35	0.58
1:B:33:ARG:HD3	1:B:33:ARG:C	2.23	0.58
1:D:239:ARG:HH11	1:D:239:ARG:HB3	1.68	0.58
1:D:116:ARG:NH2	3:D:2089:HOH:O	2.23	0.58
1:A:228:HIS:HE1	3:A:2661:HOH:O	1.86	0.58
1:D:39:ILE:CD1	1:D:97:ALA:HB2	2.31	0.58
1:F:212:LEU:O	1:F:213:ARG:CB	2.52	0.58
1:A:90:ASP:OD2	1:A:94:LYS:HE2	2.04	0.57
1:E:187:ASP:OD1	1:E:239:ARG:HG2	2.04	0.57
1:B:100:ARG:HG3	1:B:122:HIS:CG	2.39	0.57
1:A:159:LEU:HD23	1:A:213:ARG:HG2	1.86	0.57
1:A:26:ILE:H	1:B:63:LEU:HD11	1.70	0.57
1:E:67:GLY:O	1:E:68:MET:C	2.43	0.57
1:F:115:ILE:HB	1:F:118:ARG:HB2	1.86	0.57
1:D:16:GLU:HB2	3:D:2162:HOH:O	2.04	0.57
1:A:28:PRO:CA	1:A:31:ILE:HG22	2.31	0.57
1:E:19:MET:HE3	1:E:56:ASN:HA	1.87	0.57
1:C:162:THR:HG22	3:C:2008:HOH:O	2.05	0.56
1:E:128:ILE:CD1	1:E:128:ILE:N	2.68	0.56
1:F:19:MET:SD	1:F:59:ARG:NH1	2.78	0.56
1:E:148:LEU:HD22	1:E:152:GLU:CD	2.25	0.56
1:D:149:ARG:O	1:D:153:ILE:HG12	2.06	0.56
1:A:81:THR:HG21	1:A:133:ALA:N	2.13	0.56
1:C:24:TYR:CD1	1:D:24:TYR:CD1	2.94	0.56
1:F:187:ASP:OD2	1:F:206:ARG:NH2	2.39	0.56
1:D:24:TYR:O	1:D:56:ASN:O	2.23	0.55
1:E:174:LYS:HG3	1:E:174:LYS:O	2.07	0.55
1:C:162:THR:HG23	3:C:2230:HOH:O	2.05	0.55
1:D:57:ILE:HB	1:D:80:ALA:HB1	1.89	0.55
1:A:239:ARG:N	3:A:2636:HOH:O	2.30	0.55
1:D:106:LYS:C	1:D:107:ILE:HG13	2.26	0.55
1:E:72:THR:HG22	1:E:76:MET:HE3	1.88	0.54
1:B:230:ALA:HB2	3:B:2148:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:VAL:HG12	1:F:128:ILE:HB	1.89	0.54
1:B:12:LYS:C	1:B:12:LYS:HD3	2.28	0.54
1:F:180:ARG:HB2	1:F:180:ARG:NH1	2.22	0.54
1:F:168:TYR:HB3	1:F:178:ALA:HB3	1.90	0.54
1:B:174:LYS:HG3	1:B:175:HIS:CD2	2.43	0.54
1:C:215:PHE:CE1	1:C:217:MET:HG3	2.43	0.54
1:A:228:HIS:HD2	3:A:2536:HOH:O	1.90	0.54
1:E:39:ILE:CD1	1:E:97:ALA:HB2	2.38	0.54
1:B:31:ILE:HG12	1:B:88:MET:HE2	1.90	0.53
1:A:127:ARG:NH2	2:E:2004:GTP:O1G	2.41	0.53
1:E:61:ALA:HA	1:E:65:ALA:HB2	1.90	0.53
1:E:170:LYS:O	1:E:178:ALA:HB2	2.08	0.53
1:E:10:LEU:C	1:E:10:LEU:HD23	2.29	0.53
1:F:15:GLY:O	1:F:18:LEU:N	2.41	0.53
1:B:33:ARG:HB2	3:B:2087:HOH:O	2.08	0.53
1:E:62:GLY:HA3	1:F:26:ILE:O	2.09	0.53
1:C:171:ASP:O	1:C:173:LYS:N	2.42	0.53
1:F:212:LEU:O	1:F:213:ARG:HB3	2.08	0.53
1:F:169:ASP:O	1:F:170:LYS:HB2	2.08	0.53
1:F:89:GLN:HG3	1:F:99:VAL:HG21	1.91	0.53
1:D:210:LEU:O	1:D:212:LEU:HD13	2.09	0.53
1:F:89:GLN:O	1:F:93:GLU:HG3	2.09	0.52
1:E:19:MET:CE	1:E:56:ASN:HA	2.39	0.52
1:E:120:ILE:O	1:E:124:GLU:HG3	2.10	0.52
1:E:61:ALA:O	1:E:65:ALA:HB3	2.10	0.52
1:B:185:THR:HG21	1:B:240:SER:OG	2.10	0.52
1:A:8:ARG:HE	1:A:47:GLN:HE21	1.57	0.52
1:F:18:LEU:HB3	1:F:26:ILE:HG22	1.92	0.52
1:F:160:LYS:HE2	1:F:162:THR:HG21	1.91	0.52
1:A:169:ASP:OD2	1:A:170:LYS:N	2.43	0.51
1:B:31:ILE:HG13	1:B:88:MET:HE3	1.93	0.51
1:F:86:LEU:HD11	1:F:110:VAL:CG1	2.40	0.51
1:F:157:LEU:CD1	1:F:159:LEU:HG	2.41	0.51
1:D:56:ASN:ND2	1:D:56:ASN:H	2.02	0.51
1:D:13:LEU:CD2	1:D:13:LEU:N	2.72	0.51
1:E:214:ILE:HD13	1:E:214:ILE:N	2.24	0.51
1:E:223:LEU:O	1:E:227:LEU:HD23	2.11	0.51
1:E:169:ASP:OD1	1:E:170:LYS:N	2.42	0.51
1:B:69:ASP:OD2	1:B:72:THR:HG23	2.09	0.51
1:F:88:MET:O	1:F:92:LEU:HB2	2.11	0.51
1:E:174:LYS:HB2	1:E:174:LYS:NZ	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLY:HA3	1:B:63:LEU:HD11	1.93	0.51
1:D:24:TYR:HA	1:D:59:ARG:HD3	1.93	0.51
1:B:41:ALA:HB2	1:B:223:LEU:HD13	1.92	0.51
1:A:116:ARG:HD2	1:A:152:GLU:O	2.11	0.51
1:A:81:THR:CG2	1:A:133:ALA:H	2.12	0.50
1:C:121:ARG:CG	2:E:2001:GTP:O2G	2.59	0.50
1:D:70:ARG:HG3	1:D:70:ARG:NH1	2.26	0.50
1:C:171:ASP:C	1:C:173:LYS:H	2.14	0.50
1:F:86:LEU:HD11	1:F:110:VAL:HG13	1.93	0.50
1:E:134:GLY:HA2	3:E:2427:HOH:O	2.10	0.50
1:F:72:THR:HG22	1:F:76:MET:CE	2.41	0.50
1:F:168:TYR:CZ	1:F:180:ARG:HG2	2.47	0.50
1:C:11:LEU:HG	1:C:13:LEU:HD11	1.94	0.50
1:D:106:LYS:HG2	1:D:113:ASP:OD2	2.12	0.50
1:D:222:VAL:O	1:D:226:ILE:HG13	2.11	0.50
1:A:158:LEU:HG	3:A:2668:HOH:O	2.12	0.50
1:D:13:LEU:HD13	1:D:161:ALA:HB3	1.93	0.50
1:E:7:ARG:HH11	1:E:7:ARG:CB	2.17	0.50
1:E:55:GLY:O	1:E:59:ARG:HG2	2.12	0.50
2:E:2002:GTP:O3'	1:F:117:ARG:NH1	2.45	0.49
1:C:62:GLY:HA3	1:D:26:ILE:O	2.11	0.49
1:F:168:TYR:OH	1:F:180:ARG:HD2	2.12	0.49
1:F:181:TYR:C	1:F:183:SER:H	2.15	0.49
1:B:120:ILE:HD11	1:B:153:ILE:HA	1.93	0.49
1:E:34:LEU:O	1:E:34:LEU:HD12	2.12	0.49
1:B:17:ALA:O	1:B:30:VAL:HG11	2.13	0.49
1:F:209:ASP:OD1	1:F:239:ARG:NH1	2.41	0.49
1:A:102:MET:HG2	1:A:112:GLU:HG3	1.94	0.49
1:E:186:TYR:OH	1:E:210:LEU:O	2.27	0.49
1:E:185:THR:HA	1:E:237:GLN:O	2.13	0.49
2:E:2003:GTP:O2B	2:E:2003:GTP:O2A	2.31	0.49
1:E:72:THR:HG22	1:E:76:MET:CE	2.43	0.49
1:B:28:PRO:O	1:B:31:ILE:HG22	2.12	0.49
1:C:34:LEU:HD13	1:C:88:MET:CE	2.43	0.49
1:C:34:LEU:HD13	1:C:88:MET:HE2	1.95	0.49
1:A:56:ASN:N	1:A:56:ASN:ND2	2.60	0.48
1:C:162:THR:CG2	1:C:163:LYS:H	2.24	0.48
1:B:16:GLU:OE1	1:B:16:GLU:N	2.38	0.48
1:B:89:GLN:O	1:B:93:GLU:HG3	2.13	0.48
1:B:57:ILE:HB	1:B:80:ALA:HB1	1.95	0.48
1:E:19:MET:HE2	1:E:24:TYR:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:LEU:HA	3:F:2521:HOH:O	2.13	0.48
1:F:121:ARG:HG3	1:F:125:LYS:HE3	1.94	0.48
1:C:56:ASN:HD21	1:C:84:ASN:ND2	2.01	0.48
1:E:231:GLN:HA	1:E:231:GLN:OE1	2.13	0.48
1:F:9:ILE:HD13	1:F:227:LEU:HD21	1.96	0.48
1:A:158:LEU:C	1:A:158:LEU:HD23	2.34	0.47
1:C:59:ARG:O	1:C:63:LEU:HD13	2.14	0.47
1:F:132:ALA:O	1:F:133:ALA:HB3	2.13	0.47
1:C:163:LYS:HB2	3:C:2008:HOH:O	2.14	0.47
1:B:112:GLU:OE1	1:B:122:HIS:HE1	1.96	0.47
1:B:71:VAL:HG21	1:E:116:ARG:CD	2.44	0.47
1:F:19:MET:SD	1:F:23:ASP:O	2.73	0.47
1:D:115:ILE:HD12	3:D:2072:HOH:O	2.13	0.47
1:F:19:MET:HE1	1:F:59:ARG:NH1	2.30	0.47
1:F:26:ILE:CG1	1:F:31:ILE:HD11	2.44	0.47
1:F:89:GLN:HG3	1:F:99:VAL:CG2	2.45	0.47
1:C:86:LEU:HD21	1:C:110:VAL:HG13	1.97	0.47
1:D:169:ASP:OD2	1:D:170:LYS:N	2.43	0.47
1:D:102:MET:HA	1:D:112:GLU:O	2.15	0.47
1:F:19:MET:CE	1:F:59:ARG:NH1	2.78	0.46
1:B:185:THR:HA	1:B:237:GLN:O	2.15	0.46
1:A:16:GLU:O	1:A:19:MET:HB2	2.15	0.46
1:B:187:ASP:OD1	1:B:206:ARG:NH2	2.38	0.46
1:E:12:LYS:HD3	1:E:12:LYS:C	2.35	0.46
1:F:180:ARG:CB	1:F:180:ARG:CZ	2.93	0.46
1:B:6:TYR:CD1	1:B:157:LEU:HB2	2.50	0.46
1:C:52:ILE:HD11	1:C:88:MET:HG3	1.98	0.46
1:B:71:VAL:HG21	1:E:116:ARG:NE	2.30	0.46
1:C:38:VAL:CG1	1:C:128:ILE:HD13	2.46	0.46
1:E:171:ASP:CB	3:E:2399:HOH:O	2.63	0.46
1:F:100:ARG:HG3	1:F:122:HIS:CE1	2.50	0.46
1:C:175:HIS:CD2	1:C:175:HIS:O	2.68	0.46
1:B:222:VAL:O	1:B:226:ILE:HG13	2.15	0.46
1:D:107:ILE:HG22	1:D:110:VAL:HB	1.98	0.46
1:B:56:ASN:ND2	1:B:56:ASN:H	2.05	0.46
1:E:10:LEU:HD22	1:E:158:LEU:CD1	2.46	0.46
1:E:19:MET:O	1:E:27:ASP:HB2	2.14	0.46
1:F:19:MET:HG3	1:F:56:ASN:HB2	1.97	0.45
1:D:23:ASP:OD2	1:D:23:ASP:N	2.49	0.45
1:F:7:ARG:HB3	1:F:7:ARG:CZ	2.46	0.45
1:E:42:GLN:HG3	1:E:128:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:ASN:O	1:E:109:ASP:C	2.53	0.45
1:D:67:GLY:O	1:D:68:MET:O	2.34	0.45
1:D:121:ARG:HD2	1:D:121:ARG:HA	1.46	0.45
1:D:148:LEU:HD22	1:D:152:GLU:CD	2.37	0.45
1:F:206:ARG:HH12	1:F:239:ARG:HE	1.64	0.45
1:F:72:THR:HG22	1:F:76:MET:HE2	1.97	0.45
1:C:123:LEU:HA	1:C:123:LEU:HD23	1.81	0.45
1:F:186:TYR:O	1:F:190:ILE:HD12	2.15	0.45
1:E:169:ASP:O	1:E:170:LYS:HE2	2.17	0.45
1:E:121:ARG:NH1	1:E:124:GLU:OE1	2.50	0.45
1:F:169:ASP:O	1:F:169:ASP:OD1	2.35	0.45
1:E:29:LYS:O	1:E:33:ARG:HG3	2.17	0.45
1:B:33:ARG:HD3	1:B:34:LEU:N	2.31	0.45
1:D:213:ARG:NH2	1:D:232:ILE:O	2.49	0.45
1:A:75:HIS:HB3	1:B:110:VAL:HG22	1.98	0.45
1:E:56:ASN:OD1	1:E:56:ASN:N	2.50	0.45
1:F:149:ARG:O	1:F:153:ILE:HG12	2.16	0.45
1:C:121:ARG:NE	2:E:2001:GTP:O2G	2.50	0.45
1:E:7:ARG:HG2	3:E:2035:HOH:O	2.17	0.45
1:C:121:ARG:CD	2:E:2001:GTP:O2G	2.65	0.45
1:D:70:ARG:CG	1:D:70:ARG:NH1	2.80	0.45
1:D:100:ARG:CZ	2:E:2005:GTP:H3'	2.46	0.45
1:E:206:ARG:CZ	1:E:239:ARG:HD3	2.47	0.45
1:D:168:TYR:CE2	1:D:180:ARG:HB2	2.52	0.45
1:A:170:LYS:HG3	1:A:175:HIS:CD2	2.52	0.44
1:A:175:HIS:HB3	1:A:177:ASP:OD2	2.18	0.44
1:B:160:LYS:HE2	1:B:162:THR:CG2	2.47	0.44
1:B:117:ARG:NH2	1:F:89:GLN:CG	2.80	0.44
1:F:234:THR:CG2	1:F:235:LEU:N	2.67	0.44
1:E:27:ASP:OD2	1:E:30:VAL:HG23	2.17	0.44
1:D:33:ARG:HH11	1:D:220:PRO:HD3	1.82	0.44
1:E:174:LYS:HA	1:E:174:LYS:CE	2.42	0.44
1:C:57:ILE:HB	1:C:80:ALA:HB1	1.99	0.44
1:C:106:LYS:HG3	1:C:113:ASP:OD2	2.17	0.44
1:A:170:LYS:HD2	1:A:170:LYS:HA	1.85	0.44
1:B:157:LEU:HD12	1:B:211:PRO:O	2.18	0.44
1:D:151:ILE:HD13	1:D:208:SER:OG	2.16	0.44
1:D:148:LEU:HD13	1:D:149:ARG:NH1	2.32	0.44
1:D:105:ILE:HG13	1:D:107:ILE:HD11	1.98	0.44
1:A:190:ILE:HG13	1:A:206:ARG:HH11	1.83	0.44
1:E:168:TYR:CE2	1:E:180:ARG:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:LEU:HD21	1:E:110:VAL:HG13	1.98	0.44
1:E:185:THR:O	1:E:189:VAL:HG23	2.17	0.44
1:C:195:GLU:HA	1:C:195:GLU:OE2	2.17	0.44
1:D:117:ARG:NH2	2:E:2006:GTP:O3'	2.51	0.44
1:E:170:LYS:O	1:E:171:ASP:O	2.35	0.44
1:E:15:GLY:O	1:E:18:LEU:HB2	2.18	0.44
1:D:56:ASN:N	1:D:56:ASN:ND2	2.65	0.44
1:E:180:ARG:NH2	1:E:233:GLY:H	2.16	0.43
1:F:151:ILE:HD12	1:F:208:SER:HB2	2.00	0.43
1:F:175:HIS:O	1:F:176:SER:C	2.56	0.43
1:F:57:ILE:HB	1:F:80:ALA:HB1	2.00	0.43
1:F:77:GLY:O	1:F:81:THR:HG23	2.18	0.43
1:E:182:ASP:HA	3:E:2041:HOH:O	2.17	0.43
1:B:56:ASN:N	1:B:56:ASN:ND2	2.60	0.43
1:E:121:ARG:NE	2:E:2004:GTP:O2G	2.51	0.43
1:E:89:GLN:O	1:E:93:GLU:HG3	2.17	0.43
1:C:170:LYS:HD3	1:C:175:HIS:NE2	2.33	0.43
1:E:114:PHE:C	1:E:115:ILE:HG13	2.39	0.43
1:B:3:GLU:HG3	1:B:3:GLU:H	1.53	0.43
1:E:173:LYS:HB3	3:E:2399:HOH:O	2.17	0.43
1:C:162:THR:CG2	1:C:163:LYS:N	2.82	0.43
1:D:168:TYR:CG	1:D:172:PRO:HG3	2.54	0.43
1:F:56:ASN:H	1:F:56:ASN:ND2	2.11	0.43
1:E:24:TYR:CG	1:E:25:GLY:N	2.87	0.43
1:E:12:LYS:HA	1:E:51:VAL:O	2.19	0.43
1:A:50:LEU:HA	1:A:50:LEU:HD12	1.82	0.43
1:F:95:LEU:HD11	3:F:2524:HOH:O	2.19	0.43
1:B:121:ARG:CD	2:E:2003:GTP:O2G	2.66	0.43
1:E:36:HIS:O	1:E:39:ILE:HG22	2.19	0.43
1:E:132:ALA:O	1:E:133:ALA:HB3	2.18	0.42
1:A:42:GLN:HE21	1:A:42:GLN:HB3	1.66	0.42
1:C:212:LEU:HG	1:C:214:ILE:CD1	2.49	0.42
1:F:196:VAL:HG23	1:F:197:MET:H	1.84	0.42
1:F:18:LEU:HD13	1:F:26:ILE:HG21	2.00	0.42
1:D:123:LEU:C	1:D:125:LYS:H	2.22	0.42
1:A:185:THR:OG1	1:A:188:GLU:HG3	2.18	0.42
1:F:176:SER:O	1:F:177:ASP:C	2.57	0.42
1:F:210:LEU:HD12	1:F:211:PRO:HD2	2.01	0.42
1:F:15:GLY:C	1:F:17:ALA:N	2.71	0.42
1:C:103:SER:HB2	1:C:111:CYS:SG	2.59	0.42
1:A:215:PHE:CE1	1:A:217:MET:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:PHE:HB3	3:D:2470:HOH:O	2.19	0.42
1:F:215:PHE:CE1	1:F:217:MET:HG2	2.55	0.42
1:B:63:LEU:HD12	1:B:63:LEU:N	2.34	0.42
1:E:39:ILE:HA	1:E:39:ILE:HD12	1.93	0.42
1:F:68:MET:HE1	3:F:2227:HOH:O	2.19	0.42
1:E:98:LYS:HD2	3:E:2502:HOH:O	2.20	0.42
1:A:81:THR:HG22	1:A:132:ALA:CB	2.44	0.42
1:F:222:VAL:O	1:F:226:ILE:HG13	2.20	0.42
1:D:24:TYR:CD1	1:D:25:GLY:N	2.88	0.42
1:A:100:ARG:HA	1:A:100:ARG:HD3	1.92	0.42
1:E:7:ARG:HB2	1:E:156:ASP:OD2	2.20	0.41
1:F:18:LEU:HB3	1:F:26:ILE:CG2	2.50	0.41
1:F:30:VAL:HB	3:F:2521:HOH:O	2.20	0.41
1:E:212:LEU:O	1:E:235:LEU:HD22	2.20	0.41
1:C:150:ALA:HB3	1:C:210:LEU:HD21	2.01	0.41
1:A:56:ASN:H	1:A:56:ASN:ND2	2.09	0.41
1:D:70:ARG:CG	1:D:70:ARG:HH11	2.23	0.41
1:E:121:ARG:CD	2:E:2004:GTP:O2G	2.68	0.41
1:F:226:ILE:CG1	1:F:232:ILE:HD12	2.51	0.41
1:C:74:ASP:O	1:C:78:MET:HG3	2.19	0.41
1:C:170:LYS:HD2	1:C:170:LYS:N	2.36	0.41
1:C:174:LYS:HG2	1:C:175:HIS:N	2.34	0.41
1:C:186:TYR:CD2	1:C:206:ARG:HB2	2.55	0.41
1:F:8:ARG:NH2	1:F:47:GLN:OE1	2.53	0.41
1:A:28:PRO:O	1:A:31:ILE:HG22	2.20	0.41
1:F:100:ARG:HA	1:F:100:ARG:HD3	1.83	0.41
1:E:149:ARG:HD3	1:E:152:GLU:OE2	2.21	0.41
1:F:106:LYS:HG2	1:F:113:ASP:OD1	2.21	0.41
1:D:72:THR:CG2	3:F:2632:HOH:O	2.64	0.41
1:D:160:LYS:HE2	1:D:162:THR:CG2	2.50	0.41
1:A:186:TYR:CD2	1:A:206:ARG:HB2	2.56	0.41
1:B:121:ARG:CG	1:B:125:LYS:HE3	2.44	0.41
1:E:158:LEU:HB3	1:E:212:LEU:HD23	2.02	0.41
1:C:161:ALA:HA	1:C:215:PHE:O	2.21	0.41
1:C:181:TYR:CD2	1:C:184:LEU:HD21	2.56	0.41
1:E:168:TYR:CD1	1:E:172:PRO:HG3	2.56	0.41
1:E:171:ASP:HA	1:E:172:PRO:HD3	1.94	0.41
1:E:68:MET:HE2	1:F:90:ASP:CG	2.41	0.41
1:C:68:MET:HG2	1:C:69:ASP:N	2.36	0.41
1:A:150:ALA:HB2	3:A:2668:HOH:O	2.20	0.41
1:F:180:ARG:HG2	3:F:2701:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:GLY:O	1:F:18:LEU:HB2	2.20	0.41
1:A:213:ARG:HD2	1:A:232:ILE:O	2.21	0.41
1:F:5:SER:HB2	1:F:227:LEU:O	2.21	0.41
1:D:168:TYR:CD1	1:D:172:PRO:HG3	2.56	0.41
1:F:157:LEU:CD2	1:F:211:PRO:HB2	2.51	0.41
1:A:26:ILE:H	1:B:63:LEU:CD1	2.32	0.41
1:A:117:ARG:NH2	1:D:93:GLU:OE2	2.49	0.41
1:E:70:ARG:HG2	1:E:139:PHE:CE1	2.56	0.41
1:E:149:ARG:HA	1:E:152:GLU:OE2	2.21	0.40
1:B:223:LEU:HA	1:B:223:LEU:HD23	1.89	0.40
1:E:167:VAL:HG23	1:E:234:THR:HB	2.02	0.40
1:D:115:ILE:O	1:D:116:ARG:C	2.59	0.40
1:E:39:ILE:HD11	1:E:97:ALA:HB2	2.02	0.40
1:D:38:VAL:HG13	1:D:48:VAL:HG11	2.03	0.40
1:F:56:ASN:N	1:F:56:ASN:ND2	2.68	0.40
1:F:8:ARG:NE	1:F:47:GLN:OE1	2.53	0.40
1:D:208:SER:O	1:D:209:ASP:C	2.59	0.40
1:C:171:ASP:HA	1:C:172:PRO:HD3	1.95	0.40
1:D:186:TYR:OH	1:D:210:LEU:O	2.32	0.40
1:D:186:TYR:OH	1:D:212:LEU:HD13	2.22	0.40
1:B:10:LEU:C	1:B:10:LEU:CD1	2.90	0.40

There are no symmetry-related clashes.

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	240/243 (99%)	233 (97%)	7 (3%)	0	100	100
1	B	237/243 (98%)	225 (95%)	8 (3%)	4 (2%)	11	20
1	C	237/243 (98%)	226 (95%)	9 (4%)	2 (1%)	24	43
1	D	237/243 (98%)	218 (92%)	16 (7%)	3 (1%)	15	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	237/243 (98%)	219 (92%)	13 (6%)	5 (2%)	9 15
1	F	237/243 (98%)	202 (85%)	27 (11%)	8 (3%)	5 6
All	All	1425/1458 (98%)	1323 (93%)	80 (6%)	22 (2%)	13 24

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	GLU
1	D	68	MET
1	E	66	SER
1	E	171	ASP
1	F	175	HIS
1	F	213	ARG
1	D	67	GLY
1	E	175	HIS
1	F	177	ASP
1	C	174	LYS
1	E	217	MET
1	F	212	LEU
1	F	229	GLY
1	F	171	ASP
1	F	173	LYS
1	B	61	ALA
1	D	24	TYR
1	E	173	LYS
1	B	4	LEU
1	C	172	PRO
1	B	107	ILE
1	F	107	ILE

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	184/186 (99%)	171 (93%)	13 (7%)	18 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	183/186 (98%)	164 (90%)	19 (10%)	9 14
1	C	183/186 (98%)	171 (93%)	12 (7%)	21 37
1	D	183/186 (98%)	162 (88%)	21 (12%)	7 11
1	E	183/186 (98%)	163 (89%)	20 (11%)	8 13
1	F	182/186 (98%)	164 (90%)	18 (10%)	10 16
All	All	1098/1116 (98%)	995 (91%)	103 (9%)	11 19

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	29	LYS
1	A	34	LEU
1	A	56	ASN
1	A	113	ASP
1	A	116	ARG
1	A	118	ARG
1	A	123	LEU
1	A	148	LEU
1	A	176	SER
1	A	206	ARG
1	A	219	GLU
1	A	235	LEU
1	B	2	SER
1	B	10	LEU
1	B	14	SER
1	B	16	GLU
1	B	29	LYS
1	B	32	ASN
1	B	33	ARG
1	B	56	ASN
1	B	72	THR
1	B	90	ASP
1	B	107	ILE
1	B	113	ASP
1	B	118	ARG
1	B	144	SER
1	B	148	LEU
1	B	184	LEU
1	B	212	LEU

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Mol	Chain	Res	Type
1	B	223	LEU
1	B	231	GLN
1	C	34	LEU
1	C	86	LEU
1	C	90	ASP
1	C	113	ASP
1	C	118	ARG
1	C	148	LEU
1	C	158	LEU
1	C	175	HIS
1	C	176	SER
1	C	204	LEU
1	C	227	LEU
1	C	235	LEU
1	D	3	GLU
1	D	4	LEU
1	D	11	LEU
1	D	13	LEU
1	D	19	MET
1	D	21	ASP
1	D	34	LEU
1	D	39	ILE
1	D	56	ASN
1	D	86	LEU
1	D	100	ARG
1	D	113	ASP
1	D	118	ARG
1	D	123	LEU
1	D	148	LEU
1	D	195	GLU
1	D	196	VAL
1	D	204	LEU
1	D	224	LEU
1	D	239	ARG
1	D	240	SER
1	E	3	GLU
1	E	7	ARG
1	E	13	LEU
1	E	16	GLU
1	E	42	GLN
1	E	68	MET
1	E	86	LEU

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Mol	Chain	Res	Type
1	E	90	ASP
1	E	113	ASP
1	E	123	LEU
1	E	128	ILE
1	E	137	ASN
1	E	144	SER
1	E	148	LEU
1	E	171	ASP
1	E	174	LYS
1	E	175	HIS
1	E	179	VAL
1	E	204	LEU
1	E	215	PHE
1	F	7	ARG
1	F	26	ILE
1	F	27	ASP
1	F	29	LYS
1	F	36	HIS
1	F	56	ASN
1	F	70	ARG
1	F	92	LEU
1	F	100	ARG
1	F	118	ARG
1	F	163	LYS
1	F	171	ASP
1	F	175	HIS
1	F	177	ASP
1	F	184	LEU
1	F	187	ASP
1	F	196	VAL
1	F	235	LEU

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	-1	ASN
1	A	36	HIS
1	A	42	GLN
1	A	47	GLN
1	A	56	ASN
1	A	84	ASN
1	A	122	HIS

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Mol	Chain	Res	Type
1	A	175	HIS
1	A	228	HIS
1	B	32	ASN
1	B	43	GLN
1	B	56	ASN
1	B	75	HIS
1	B	84	ASN
1	B	122	HIS
1	B	175	HIS
1	B	228	HIS
1	C	84	ASN
1	C	192	GLN
1	D	42	GLN
1	D	56	ASN
1	D	84	ASN
1	D	108	ASN
1	D	122	HIS
1	D	175	HIS
1	E	228	HIS
1	F	56	ASN
1	F	89	GLN

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

6 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	E	2001	-	25,34,34	0.89	1 (4%)	34,54,54	1.97	10 (29%)
2	GTP	E	2002	-	25,34,34	1.02	2 (8%)	34,54,54	2.22	9 (26%)
2	GTP	E	2003	-	25,34,34	0.70	1 (4%)	34,54,54	2.32	12 (35%)
2	GTP	E	2004	-	25,34,34	1.31	2 (8%)	34,54,54	2.27	12 (35%)
2	GTP	E	2005	-	25,34,34	0.67	0	34,54,54	2.24	11 (32%)
2	GTP	E	2006	-	25,34,34	0.81	1 (4%)	34,54,54	1.73	6 (17%)

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	E	2001	-	-	0/18/38/38	0/3/3/3
2	GTP	E	2002	-	-	0/18/38/38	0/3/3/3
2	GTP	E	2003	-	-	0/18/38/38	0/3/3/3
2	GTP	E	2004	-	-	0/18/38/38	0/3/3/3
2	GTP	E	2005	-	-	0/18/38/38	0/3/3/3
2	GTP	E	2006	-	-	0/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2004	GTP	PA-O5'	-5.20	1.35	1.59
2	E	2002	GTP	PB-O1B	-2.58	1.41	1.51
2	E	2006	GTP	PA-O5'	-2.02	1.49	1.59
2	E	2003	GTP	O4'-C1'	2.02	1.43	1.41
2	E	2001	GTP	O4'-C1'	2.48	1.44	1.41
2	E	2004	GTP	O4'-C1'	2.61	1.44	1.41
2	E	2002	GTP	PB-O2B	3.01	1.67	1.54

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2003	GTP	PB-O3B-PG	-7.21	108.50	132.67
2	E	2002	GTP	PB-O3B-PG	-6.19	111.93	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2005	GTP	O2B-PB-O3B	-5.69	79.26	105.09
2	E	2002	GTP	O2B-PB-O3B	-5.47	80.28	105.09
2	E	2006	GTP	N3-C2-N1	-4.74	120.23	127.44
2	E	2003	GTP	N3-C2-N1	-4.65	120.37	127.44
2	E	2005	GTP	N3-C2-N1	-4.58	120.46	127.44
2	E	2004	GTP	O5'-PA-O1A	-4.37	92.65	109.62
2	E	2001	GTP	N3-C2-N1	-4.35	120.82	127.44
2	E	2004	GTP	O2B-PB-O3B	-4.31	85.55	105.09
2	E	2002	GTP	N3-C2-N1	-4.31	120.89	127.44
2	E	2004	GTP	N3-C2-N1	-4.23	121.01	127.44
2	E	2001	GTP	PA-O3A-PB	-4.05	121.35	132.73
2	E	2005	GTP	C1'-N9-C4	-3.70	121.36	126.94
2	E	2005	GTP	PA-O3A-PB	-3.38	123.24	132.73
2	E	2005	GTP	C5-C6-N1	-3.36	118.99	123.59
2	E	2006	GTP	O5'-PA-O1A	-3.34	96.65	109.62
2	E	2004	GTP	C4-C5-N7	-3.18	106.56	109.48
2	E	2001	GTP	C5-C6-N1	-3.04	119.43	123.59
2	E	2003	GTP	O2B-PB-O3B	-2.89	91.97	105.09
2	E	2002	GTP	O3G-PG-O3B	-2.85	92.15	105.09
2	E	2003	GTP	C5-C6-N1	-2.82	119.73	123.59
2	E	2005	GTP	C4-C5-N7	-2.77	106.94	109.48
2	E	2001	GTP	O5'-PA-O1A	-2.76	98.90	109.62
2	E	2006	GTP	C5-C6-N1	-2.70	119.89	123.59
2	E	2004	GTP	PB-O3B-PG	-2.55	124.13	132.67
2	E	2004	GTP	C5-C6-N1	-2.46	120.22	123.59
2	E	2001	GTP	C4-C5-N7	-2.33	107.34	109.48
2	E	2003	GTP	C4-C5-N7	-2.29	107.37	109.48
2	E	2002	GTP	C5-C6-N1	-2.28	120.46	123.59
2	E	2005	GTP	C6-C5-C4	-2.26	118.19	120.90
2	E	2003	GTP	PA-O3A-PB	-2.19	126.57	132.73
2	E	2003	GTP	O3G-PG-O3B	-2.05	95.79	105.09
2	E	2005	GTP	C2'-C1'-N9	2.01	117.36	114.29
2	E	2003	GTP	O3A-PA-O5'	2.04	108.35	102.94
2	E	2002	GTP	O2G-PG-O3B	2.05	114.40	105.09
2	E	2004	GTP	C2'-C1'-N9	2.09	117.48	114.29
2	E	2002	GTP	O2B-PB-O1B	2.10	123.89	112.53
2	E	2005	GTP	N2-C2-N1	2.14	120.74	117.20
2	E	2004	GTP	N2-C2-N1	2.21	120.86	117.20
2	E	2004	GTP	O2A-PA-O3A	2.22	115.16	105.09
2	E	2001	GTP	O4'-C1'-N9	2.32	112.96	108.10
2	E	2004	GTP	O4'-C1'-N9	2.33	112.98	108.10
2	E	2006	GTP	O2B-PB-O3A	2.35	115.76	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2006	GTP	O2A-PA-O3A	2.52	116.53	105.09
2	E	2003	GTP	O4'-C1'-N9	2.54	113.41	108.10
2	E	2001	GTP	O2B-PB-O1B	2.73	127.30	112.53
2	E	2003	GTP	O2A-PA-O1A	2.81	127.77	112.53
2	E	2004	GTP	C6-N1-C2	2.88	119.94	115.94
2	E	2001	GTP	O2A-PA-O1A	2.89	128.19	112.53
2	E	2001	GTP	N2-C2-N1	2.97	122.12	117.20
2	E	2002	GTP	C6-N1-C2	3.06	120.19	115.94
2	E	2001	GTP	C6-N1-C2	3.25	120.45	115.94
2	E	2006	GTP	C6-N1-C2	3.45	120.73	115.94
2	E	2003	GTP	C6-N1-C2	3.60	120.93	115.94
2	E	2005	GTP	C6-N1-C2	4.11	121.64	115.94
2	E	2003	GTP	O2B-PB-O1B	4.25	135.58	112.53
2	E	2002	GTP	O2B-PB-O3A	4.72	126.49	105.09
2	E	2005	GTP	O2B-PB-O3A	4.75	126.63	105.09
2	E	2004	GTP	O2B-PB-O3A	6.15	132.98	105.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2001	GTP	4	0
2	E	2002	GTP	1	0
2	E	2003	GTP	2	0
2	E	2004	GTP	3	0
2	E	2005	GTP	2	0
2	E	2006	GTP	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	242/243 (99%)	0.15	4 (1%)	73 71	32, 50, 70, 78	0
1	B	239/243 (98%)	0.15	7 (2%)	55 53	36, 56, 73, 79	0
1	C	239/243 (98%)	-0.01	7 (2%)	55 53	33, 49, 71, 81	0
1	D	239/243 (98%)	0.04	5 (2%)	67 65	34, 51, 71, 80	0
1	E	239/243 (98%)	0.23	18 (7%)	17 15	41, 59, 76, 82	0
1	F	239/243 (98%)	0.21	20 (8%)	14 11	41, 60, 76, 81	0
All	All	1437/1458 (98%)	0.13	61 (4%)	40 37	32, 53, 74, 82	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	ALA	5.5
1	F	172	PRO	5.1
1	C	177	ASP	4.5
1	E	2	SER	4.4
1	C	170	LYS	4.1
1	C	175	HIS	3.9
1	D	66	SER	3.9
1	F	174	LYS	3.9
1	F	176	SER	3.7
1	D	179	VAL	3.7
1	F	179	VAL	3.7
1	F	170	LYS	3.7
1	F	171	ASP	3.6
1	F	177	ASP	3.5
1	F	24	TYR	3.4
1	E	66	SER	3.4
1	F	20	GLY	3.4
1	F	175	HIS	3.3
1	F	178	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	239	ARG	3.1
1	F	173	LYS	3.0
1	E	178	ALA	2.9
1	B	240	SER	2.9
1	F	2	SER	2.8
1	E	191	MET	2.8
1	F	11	LEU	2.8
1	E	61	ALA	2.8
1	E	52	ILE	2.7
1	C	176	SER	2.7
1	D	4	LEU	2.7
1	C	2	SER	2.6
1	A	159	LEU	2.6
1	B	59	ARG	2.6
1	F	10	LEU	2.6
1	F	191	MET	2.6
1	E	51	VAL	2.5
1	C	66	SER	2.5
1	E	171	ASP	2.4
1	E	49	ALA	2.4
1	E	240	SER	2.4
1	F	240	SER	2.3
1	E	130	ILE	2.3
1	C	158	LEU	2.3
1	B	60	GLY	2.3
1	D	173	LYS	2.3
1	E	176	SER	2.2
1	E	175	HIS	2.2
1	A	10	LEU	2.2
1	A	50	LEU	2.2
1	E	172	PRO	2.2
1	E	179	VAL	2.2
1	D	67	GLY	2.1
1	A	239	ARG	2.1
1	E	177	ASP	2.1
1	F	29	LYS	2.1
1	B	64	ALA	2.1
1	F	184	LEU	2.1
1	E	129	ALA	2.0
1	B	130	ILE	2.0
1	E	173	LYS	2.0
1	F	66	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GTP	E	2004	32/32	0.87	0.24	1.71	69,72,97,97	0
2	GTP	E	2001	32/32	0.88	0.21	1.33	61,66,93,93	0
2	GTP	E	2006	32/32	0.83	0.23	1.20	79,84,105,105	0
2	GTP	E	2003	32/32	0.88	0.21	1.05	65,70,94,94	0
2	GTP	E	2005	32/32	0.82	0.23	0.90	89,92,111,111	0
2	GTP	E	2002	32/32	0.90	0.16	0.19	67,70,92,92	0

6.5 Other polymers (i)

There are no such residues in this entry.