



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:53 AM GMT

PDB ID : 2V4Y  
Title : THE STRUCTURE OF E. COLI UMP KINASE IN COMPLEX WITH ITS ALLOSTERIC REGULATOR GTP  
Authors : Meyer, P.; Evrin, C.; Briozzo, P.; Joly, N.; Barzu, O.; Gilles, A.M.  
Deposited on : 2008-09-30  
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](mailto: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.

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

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

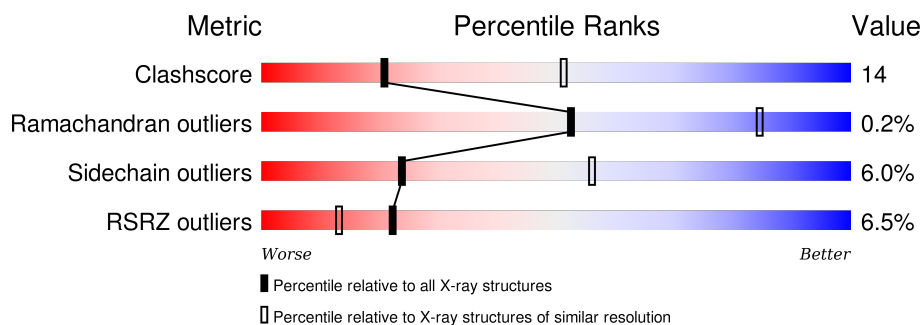
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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)
RSRZ outliers	91569	2404 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	241	<div> <div>5%</div> <div>71% 24% ..</div> </div>
1	B	241	<div> <div>3%</div> <div>71% 20% . .</div> </div>
1	C	241	<div> <div>5%</div> <div>73% 23% ..</div> </div>
1	D	241	<div> <div>11%</div> <div>73% 20% . .</div> </div>
1	E	241	<div> <div>6%</div> <div>75% 19% . .</div> </div>
1	F	241	<div> <div>8%</div> <div>75% 20% . .</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10907 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.

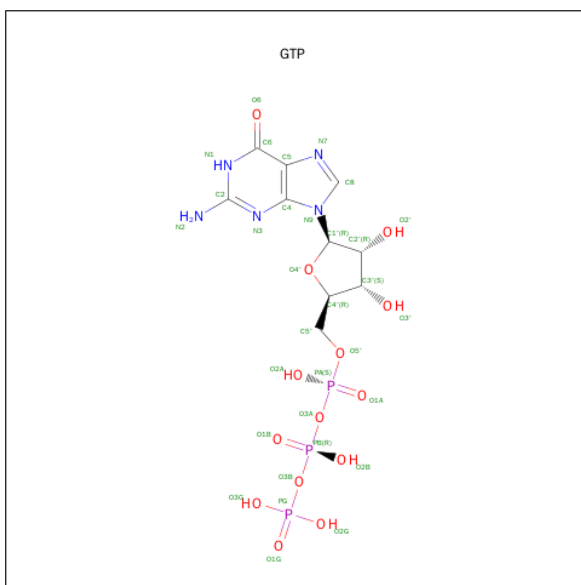
- Molecule 1 is a protein called URIDYLATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1788	1129	314	332	13			
1	B	231	Total	C	N	O	S	0	0	0
			1746	1104	307	322	13			
1	C	237	Total	C	N	O	S	0	0	0
			1788	1129	314	332	13			
1	D	233	Total	C	N	O	S	0	0	0
			1761	1113	310	325	13			
1	E	236	Total	C	N	O	S	0	0	0
			1779	1123	312	331	13			
1	F	233	Total	C	N	O	S	0	0	0
			1763	1114	310	326	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	ASN	ASP	ENGINEERED MUTATION	UNP P0A7E9
B	159	ASN	ASP	ENGINEERED MUTATION	UNP P0A7E9
C	159	ASN	ASP	ENGINEERED MUTATION	UNP P0A7E9
D	159	ASN	ASP	ENGINEERED MUTATION	UNP P0A7E9
E	159	ASN	ASP	ENGINEERED MUTATION	UNP P0A7E9
F	159	ASN	ASP	ENGINEERED MUTATION	UNP P0A7E9

- 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	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	A	1	Total 13	O 10	P 3			0	0
2	B	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	B	1	Total 13	O 10	P 3			0	0
2	C	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	C	1	Total 13	O 10	P 3			0	0
2	D	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	D	1	Total 13	O 10	P 3			0	0
2	E	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	E	1	Total 13	O 10	P 3			0	0
2	F	1	Total 32	C 10	N 5	O 14	P 3	0	0
2	F	1	Total 13	O 10	P 3			0	0

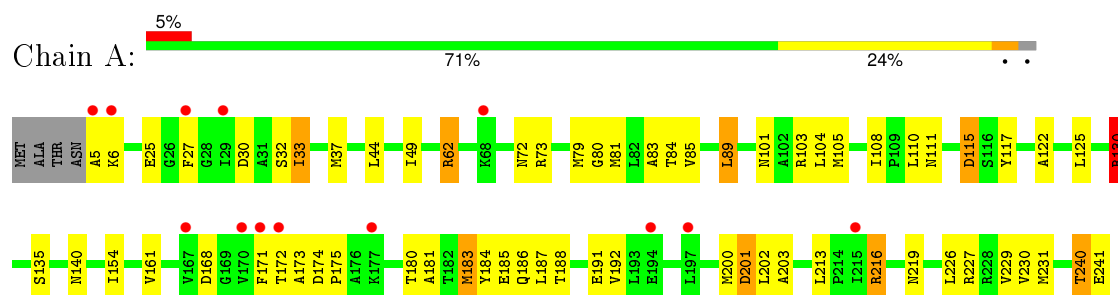
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	B	3	Total 3	O 3	0	0
3	C	3	Total 3	O 3	0	0
3	D	3	Total 3	O 3	0	0
3	E	2	Total 2	O 2	0	0

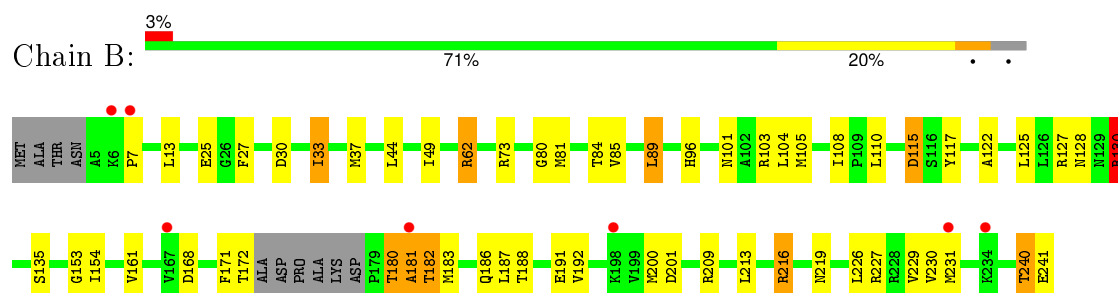
### 3 Residue-property plots

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.

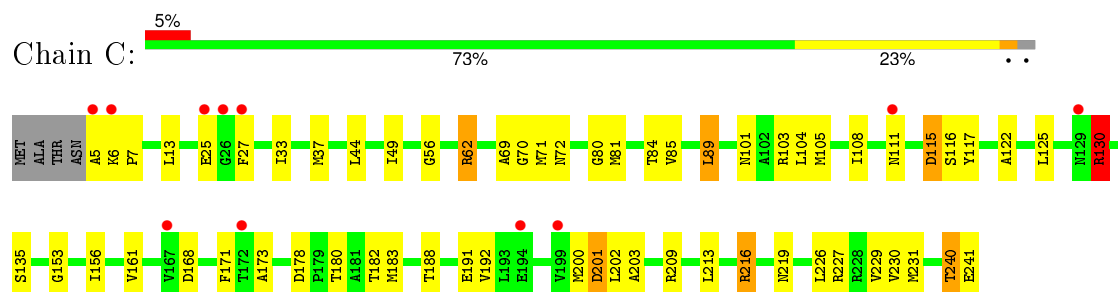
#### • Molecule 1: URIDYLATE KINASE



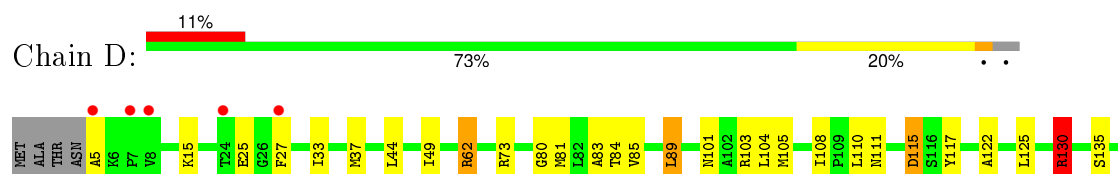
#### • Molecule 1: URIDYLATE KINASE

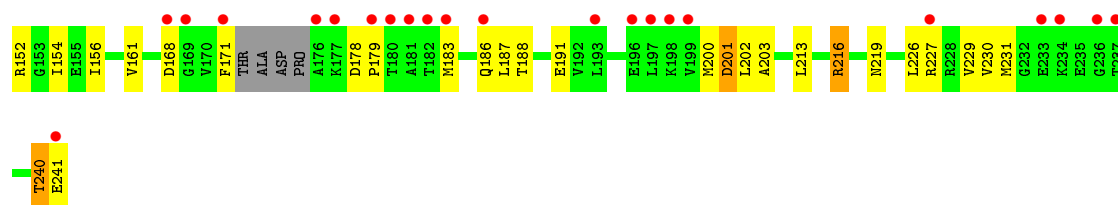


#### • Molecule 1: URIDYLATE KINASE

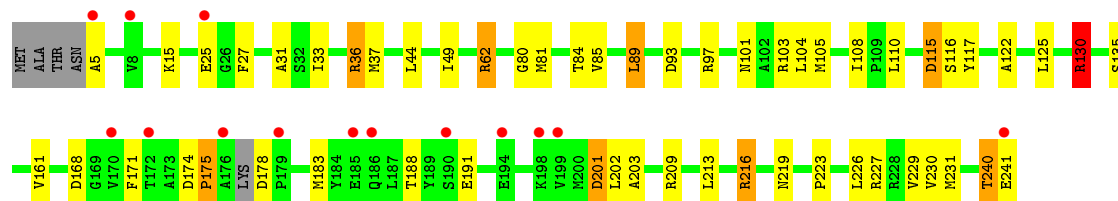
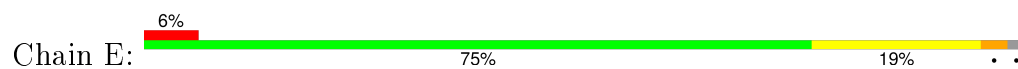


#### • Molecule 1: URIDYLATE KINASE

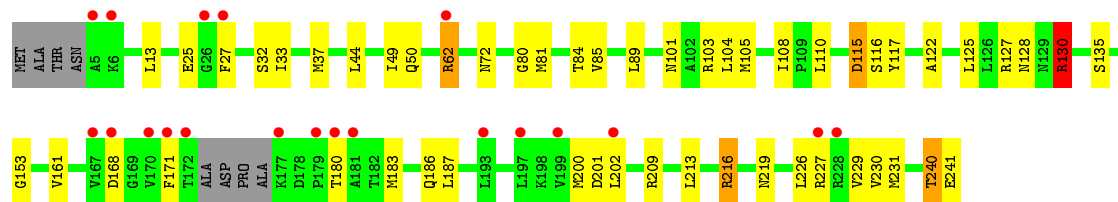
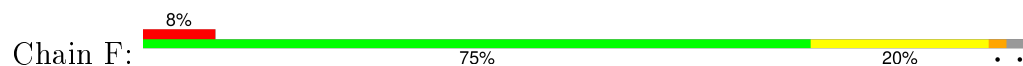




• Molecule 1: URIDYLATE KINASE



• Molecule 1: URIDYLATE KINASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.28 Å 145.78 Å 146.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.80 49.04 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.04-2.80) 95.0 (49.04-2.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.81 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.207 , 0.239 0.199 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	68.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.8	EDS
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 33999 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10907	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 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	0.35	0/1811	0.56	2/2442 (0.1%)
1	B	0.33	0/1767	0.71	3/2379 (0.1%)
1	C	0.34	0/1811	0.54	2/2442 (0.1%)
1	D	0.32	0/1782	0.53	2/2399 (0.1%)
1	E	0.34	0/1801	0.55	2/2428 (0.1%)
1	F	0.34	0/1784	0.70	3/2402 (0.1%)
All	All	0.34	0/10756	0.61	14/14492 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ARG	NE-CZ-NH1	-16.77	111.91	120.30
1	F	130	ARG	NE-CZ-NH1	-16.76	111.92	120.30
1	B	130	ARG	NE-CZ-NH2	16.42	128.51	120.30
1	F	130	ARG	NE-CZ-NH2	15.73	128.17	120.30
1	E	130	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	130	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	C	130	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	B	130	ARG	CD-NE-CZ	8.09	134.92	123.60
1	D	130	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	F	130	ARG	CD-NE-CZ	7.80	134.52	123.60
1	E	130	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	130	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	D	130	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	C	130	ARG	NE-CZ-NH1	6.85	123.72	120.30

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	1788	0	1848	59	2
1	B	1746	0	1810	61	0
1	C	1788	0	1848	57	0
1	D	1761	0	1824	48	0
1	E	1779	0	1834	50	2
1	F	1763	0	1826	48	0
2	A	45	0	12	1	0
2	B	45	0	12	2	0
2	C	45	0	12	2	0
2	D	45	0	12	0	0
2	E	45	0	12	2	0
2	F	45	0	12	2	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0
All	All	10907	0	11062	315	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 14.

All (315) 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:62:ARG:HG3	1:D:62:ARG:HH21	1.17	1.09
1:A:62:ARG:HH21	1:A:62:ARG:HG3	1.17	1.09
1:B:62:ARG:HH21	1:B:62:ARG:HG3	1.17	1.08
1:C:62:ARG:HG3	1:C:62:ARG:HH21	1.17	1.04
1:E:62:ARG:HH21	1:E:62:ARG:HG3	1.18	1.03
1:F:62:ARG:HG3	1:F:62:ARG:HH21	1.17	1.03
1:B:172:THR:OG1	1:B:181:ALA:HB1	1.69	0.91
1:E:216:ARG:HG2	1:E:216:ARG:HH11	1.37	0.89
1:F:216:ARG:HG2	1:F:216:ARG:HH11	1.40	0.87
1:D:216:ARG:HH11	1:D:216:ARG:HG2	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ARG:HG2	1:B:216:ARG:HH11	1.40	0.86
1:D:62:ARG:HG3	1:D:62:ARG:NH2	1.90	0.85
1:A:62:ARG:NH2	1:A:62:ARG:HG3	1.90	0.84
1:C:62:ARG:HG3	1:C:62:ARG:NH2	1.91	0.84
1:A:216:ARG:HH11	1:A:216:ARG:HG2	1.42	0.83
1:E:36:ARG:HH11	1:E:36:ARG:HG3	1.44	0.82
1:B:62:ARG:NH2	1:B:62:ARG:HG3	1.90	0.82
1:C:216:ARG:HH11	1:C:216:ARG:HG2	1.43	0.80
1:E:36:ARG:NH1	1:E:36:ARG:HG3	1.96	0.80
1:D:49:ILE:HD11	1:D:230:VAL:HG11	1.64	0.79
1:B:181:ALA:O	1:B:182:THR:HB	1.81	0.79
1:F:62:ARG:HG3	1:F:62:ARG:NH2	1.89	0.77
1:E:36:ARG:HH11	1:E:36:ARG:CG	1.96	0.77
1:F:49:ILE:HD11	1:F:230:VAL:HG11	1.67	0.77
1:E:62:ARG:NH2	1:E:62:ARG:HG3	1.91	0.76
1:E:49:ILE:HD11	1:E:230:VAL:HG11	1.67	0.76
1:C:49:ILE:HD11	1:C:230:VAL:HG11	1.66	0.76
1:A:49:ILE:HD11	1:A:230:VAL:HG11	1.67	0.76
1:B:49:ILE:HD11	1:B:230:VAL:HG11	1.66	0.76
1:C:240:THR:O	1:C:241:GLU:HB2	1.86	0.75
1:E:216:ARG:NH1	1:E:216:ARG:HG2	1.99	0.75
1:B:180:THR:O	1:B:181:ALA:CB	2.35	0.74
1:D:216:ARG:NH1	1:D:216:ARG:HG2	2.00	0.74
1:E:240:THR:O	1:E:241:GLU:HB2	1.86	0.73
1:F:216:ARG:NH1	1:F:216:ARG:HG2	2.01	0.73
1:A:240:THR:O	1:A:241:GLU:HB2	1.89	0.73
1:B:216:ARG:HG2	1:B:216:ARG:NH1	2.01	0.72
1:C:216:ARG:HG2	1:C:216:ARG:NH1	2.04	0.72
1:B:240:THR:O	1:B:241:GLU:HB2	1.89	0.72
1:C:201:ASP:OD1	1:C:202:LEU:N	2.23	0.71
1:B:172:THR:OG1	1:B:181:ALA:CB	2.38	0.71
1:D:240:THR:O	1:D:241:GLU:HB2	1.89	0.71
1:F:240:THR:O	1:F:241:GLU:HB2	1.90	0.71
1:D:201:ASP:OD1	1:D:201:ASP:C	2.30	0.70
1:D:201:ASP:OD1	1:D:203:ALA:N	2.24	0.70
1:C:201:ASP:OD1	1:C:201:ASP:C	2.30	0.70
1:E:105:MET:HE3	1:E:117:TYR:HD1	1.57	0.69
1:A:216:ARG:NH1	1:A:216:ARG:HG2	2.02	0.67
1:F:105:MET:HE3	1:F:117:TYR:HD1	1.60	0.67
1:E:201:ASP:C	1:E:201:ASP:OD1	2.33	0.66
1:A:201:ASP:OD1	1:A:203:ALA:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:ASP:OD1	1:E:202:LEU:N	2.28	0.66
1:A:201:ASP:OD1	1:A:201:ASP:C	2.31	0.66
1:F:81:MET:SD	1:F:108:ILE:HD11	2.35	0.66
1:E:104:LEU:HD11	1:E:135:SER:OG	1.96	0.66
2:A:1242:GTP:N2	1:F:72:ASN:HB2	2.11	0.65
1:A:105:MET:HE3	1:A:117:TYR:HD1	1.61	0.65
1:D:105:MET:HE3	1:D:117:TYR:HD1	1.60	0.65
1:C:81:MET:SD	1:C:108:ILE:HD11	2.37	0.65
1:B:81:MET:SD	1:B:108:ILE:HD11	2.37	0.65
1:C:201:ASP:OD1	1:C:203:ALA:N	2.30	0.65
1:A:201:ASP:OD1	1:A:202:LEU:N	2.29	0.64
1:E:81:MET:SD	1:E:108:ILE:HD11	2.37	0.64
1:A:183:MET:HG2	1:A:183:MET:O	1.94	0.64
1:D:81:MET:SD	1:D:108:ILE:HD11	2.37	0.63
1:A:171:PHE:CD2	1:A:175:PRO:HG3	2.34	0.62
1:C:105:MET:HE3	1:C:117:TYR:HD1	1.64	0.62
1:C:125:LEU:O	1:C:130:ARG:HB2	2.00	0.62
1:A:183:MET:O	1:A:183:MET:CG	2.47	0.61
1:A:81:MET:SD	1:A:108:ILE:HD11	2.41	0.61
1:B:105:MET:HE3	1:B:117:TYR:HD1	1.66	0.61
1:E:216:ARG:HD3	1:E:229:VAL:HG13	1.81	0.61
1:A:104:LEU:HD11	1:A:135:SER:OG	2.01	0.61
1:B:180:THR:OG1	1:B:181:ALA:N	2.34	0.60
1:A:72:ASN:HB2	2:F:1242:GTP:N2	2.16	0.60
1:B:104:LEU:HD11	1:B:135:SER:OG	2.02	0.60
1:B:216:ARG:HD3	1:B:229:VAL:HG13	1.84	0.60
1:C:44:LEU:HD11	1:C:226:LEU:HD21	1.84	0.59
1:A:216:ARG:HD3	1:A:229:VAL:HG13	1.84	0.59
1:F:105:MET:HE3	1:F:117:TYR:CD1	2.37	0.59
1:D:104:LEU:HD11	1:D:135:SER:OG	2.02	0.59
1:B:171:PHE:CE2	1:B:183:MET:HB2	2.38	0.59
1:D:171:PHE:CE2	1:D:183:MET:HB2	2.38	0.58
1:B:7:PRO:HB3	1:B:230:VAL:HG13	1.84	0.58
1:C:104:LEU:HD11	1:C:135:SER:OG	2.04	0.58
1:C:178:ASP:OD1	1:C:180:THR:HG22	2.04	0.57
1:A:105:MET:HE3	1:A:117:TYR:CD1	2.38	0.57
1:C:171:PHE:CE2	1:C:183:MET:HB2	2.38	0.57
1:F:216:ARG:HD3	1:F:229:VAL:HG13	1.86	0.57
1:F:128:ASN:HB3	1:F:130:ARG:HH11	1.69	0.57
1:E:171:PHE:CE2	1:E:183:MET:HB2	2.40	0.56
1:B:44:LEU:HD11	1:B:226:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:MET:HE3	1:D:117:TYR:CD1	2.40	0.56
1:F:171:PHE:CE2	1:F:183:MET:HB2	2.40	0.56
1:C:105:MET:HE3	1:C:117:TYR:CD1	2.40	0.56
1:E:105:MET:HE3	1:E:117:TYR:CD1	2.38	0.56
1:E:201:ASP:OD1	1:E:203:ALA:N	2.37	0.56
2:C:1242:GTP:O3B	2:C:1242:GTP:H5"	2.05	0.56
1:F:101:ASN:HB3	1:F:130:ARG:CD	2.36	0.56
1:B:128:ASN:HB3	1:B:130:ARG:HH11	1.70	0.56
1:B:180:THR:O	1:B:181:ALA:HB3	2.06	0.55
1:C:216:ARG:HD3	1:C:229:VAL:HG13	1.88	0.55
1:D:216:ARG:HH11	1:D:216:ARG:CG	2.16	0.55
1:F:104:LEU:HD11	1:F:135:SER:OG	2.06	0.55
1:A:111:ASN:HD21	1:E:116:SER:HB3	1.71	0.55
1:B:101:ASN:HB3	1:B:130:ARG:CD	2.37	0.55
1:A:183:MET:HG3	1:A:184:TYR:O	2.07	0.55
1:D:216:ARG:HD3	1:D:229:VAL:HG13	1.87	0.55
1:D:44:LEU:HD11	1:D:226:LEU:HD21	1.89	0.54
1:A:44:LEU:HD11	1:A:226:LEU:HD21	1.90	0.54
1:C:62:ARG:CG	1:C:62:ARG:NH2	2.68	0.54
1:E:227:ARG:O	1:E:231:MET:HG2	2.08	0.54
1:C:89:LEU:HD13	1:C:104:LEU:HD23	1.89	0.53
1:B:227:ARG:O	1:B:231:MET:HG2	2.09	0.53
1:B:101:ASN:CB	1:B:130:ARG:HD3	2.39	0.53
1:B:105:MET:HE3	1:B:117:TYR:CD1	2.43	0.53
1:F:101:ASN:CB	1:F:130:ARG:HD3	2.39	0.53
1:A:227:ARG:O	1:A:231:MET:HG2	2.09	0.53
1:F:44:LEU:HD11	1:F:226:LEU:HD21	1.91	0.52
1:C:70:GLY:O	1:E:97:ARG:HD3	2.09	0.52
1:D:227:ARG:O	1:D:231:MET:HG2	2.09	0.52
1:C:216:ARG:HH11	1:C:216:ARG:CG	2.19	0.52
1:F:227:ARG:O	1:F:231:MET:HG2	2.10	0.52
1:D:125:LEU:O	1:D:130:ARG:HB2	2.10	0.52
1:D:80:GLY:O	1:D:84:THR:HG23	2.08	0.52
1:C:116:SER:HB3	1:D:111:ASN:HD21	1.74	0.51
1:C:171:PHE:CB	1:C:173:ALA:O	2.59	0.51
1:F:62:ARG:CG	1:F:62:ARG:NH2	2.67	0.50
1:B:180:THR:O	1:B:181:ALA:HB2	2.08	0.50
1:D:49:ILE:HD11	1:D:230:VAL:CG1	2.40	0.50
1:B:105:MET:CE	1:B:122:ALA:HB2	2.41	0.50
1:D:62:ARG:CG	1:D:62:ARG:NH2	2.68	0.50
1:B:125:LEU:O	1:B:130:ARG:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:LEU:HD11	1:E:226:LEU:HD21	1.94	0.50
1:E:105:MET:CE	1:E:117:TYR:CD1	2.95	0.49
1:F:44:LEU:HD22	1:F:230:VAL:HG21	1.94	0.49
1:D:105:MET:CE	1:D:117:TYR:CD1	2.95	0.49
1:B:85:VAL:O	1:B:89:LEU:HB2	2.12	0.49
1:B:101:ASN:HB3	1:B:130:ARG:HD3	1.93	0.49
1:F:85:VAL:O	1:F:89:LEU:HB2	2.12	0.49
1:C:5:ALA:HB3	1:C:231:MET:SD	2.52	0.49
1:D:25:GLU:HB2	1:D:27:PHE:CE2	2.47	0.49
1:A:105:MET:CE	1:A:122:ALA:HB2	2.42	0.49
1:B:80:GLY:O	1:B:84:THR:HG23	2.12	0.49
1:F:168:ASP:HA	1:F:219:ASN:HB2	1.95	0.49
1:F:101:ASN:HB3	1:F:130:ARG:HD3	1.95	0.49
1:A:80:GLY:O	1:A:84:THR:HG23	2.11	0.49
1:E:216:ARG:CG	1:E:216:ARG:HH11	2.15	0.49
1:E:49:ILE:CD1	1:E:230:VAL:HG11	2.41	0.49
1:F:89:LEU:HD13	1:F:104:LEU:HD23	1.94	0.49
1:C:56:GLY:HA3	2:C:1243:GTP:O2B	2.13	0.48
1:B:25:GLU:HB2	1:B:27:PHE:CE2	2.48	0.48
1:C:80:GLY:O	1:C:84:THR:HG23	2.12	0.48
1:C:227:ARG:O	1:C:231:MET:HG2	2.13	0.48
1:C:168:ASP:HA	1:C:219:ASN:HB2	1.96	0.48
1:D:5:ALA:HB3	1:D:231:MET:SD	2.54	0.48
1:B:7:PRO:HB3	1:B:230:VAL:CG1	2.42	0.48
1:D:201:ASP:OD1	1:D:202:LEU:N	2.47	0.48
1:E:80:GLY:O	1:E:84:THR:HG23	2.14	0.48
1:C:105:MET:CE	1:C:117:TYR:CD1	2.96	0.48
1:E:115:ASP:N	1:E:115:ASP:OD1	2.46	0.48
1:E:25:GLU:HB2	1:E:27:PHE:CE2	2.49	0.48
1:C:25:GLU:HB2	1:C:27:PHE:CE2	2.48	0.48
1:A:25:GLU:HB2	1:A:27:PHE:CE2	2.49	0.47
1:B:49:ILE:CD1	1:B:230:VAL:HG11	2.42	0.47
1:F:101:ASN:HB3	1:F:130:ARG:HD2	1.96	0.47
1:F:105:MET:CE	1:F:117:TYR:CD1	2.97	0.47
1:A:105:MET:CE	1:A:117:TYR:CD1	2.97	0.47
1:F:25:GLU:HB2	1:F:27:PHE:CE2	2.50	0.47
1:A:168:ASP:HA	1:A:219:ASN:HB2	1.95	0.47
1:A:101:ASN:CB	1:A:130:ARG:HD2	2.45	0.47
1:B:168:ASP:HA	1:B:219:ASN:HB2	1.96	0.47
1:F:161:VAL:CG2	1:F:213:LEU:HD21	2.44	0.47
1:E:49:ILE:HD11	1:E:230:VAL:CG1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ASN:CB	1:C:130:ARG:HD2	2.45	0.47
1:B:89:LEU:HD13	1:B:104:LEU:HD23	1.96	0.47
1:A:125:LEU:O	1:A:130:ARG:HB2	2.15	0.47
1:E:168:ASP:HA	1:E:219:ASN:HB2	1.96	0.47
1:D:168:ASP:HA	1:D:219:ASN:HB2	1.97	0.47
1:A:5:ALA:HB3	1:A:231:MET:SD	2.55	0.47
1:F:80:GLY:O	1:F:84:THR:HG23	2.15	0.47
1:B:105:MET:CE	1:B:117:TYR:CD1	2.99	0.47
1:D:115:ASP:OD1	1:D:115:ASP:N	2.48	0.47
1:E:101:ASN:CB	1:E:130:ARG:HD2	2.45	0.46
1:D:101:ASN:CB	1:D:130:ARG:HD2	2.45	0.46
1:E:125:LEU:O	1:E:130:ARG:HB2	2.15	0.46
1:A:188:THR:O	1:A:192:VAL:HG23	2.15	0.46
1:F:101:ASN:ND2	2:F:1242:GTP:O3G	2.49	0.46
1:C:111:ASN:HD21	1:F:116:SER:HB3	1.79	0.46
1:A:89:LEU:HD13	1:A:104:LEU:HD23	1.96	0.46
1:E:161:VAL:CG2	1:E:213:LEU:HD21	2.45	0.46
1:B:49:ILE:HD11	1:B:230:VAL:CG1	2.43	0.46
1:C:171:PHE:HB2	1:C:173:ALA:O	2.16	0.46
1:F:115:ASP:N	1:F:115:ASP:OD1	2.47	0.46
1:D:49:ILE:CD1	1:D:230:VAL:HG11	2.41	0.46
1:A:85:VAL:O	1:A:89:LEU:HB2	2.15	0.46
1:F:49:ILE:CD1	1:F:230:VAL:HG11	2.43	0.46
1:B:62:ARG:HH21	1:B:62:ARG:CG	2.04	0.46
1:E:85:VAL:O	1:E:89:LEU:HB2	2.16	0.45
1:D:85:VAL:O	1:D:89:LEU:HB2	2.16	0.45
1:B:101:ASN:HB3	1:B:130:ARG:HD2	1.98	0.45
1:C:105:MET:CE	1:C:122:ALA:HB2	2.46	0.45
1:C:115:ASP:OD1	1:C:115:ASP:N	2.47	0.45
1:C:161:VAL:CG2	1:C:213:LEU:HD21	2.47	0.45
1:C:171:PHE:HB3	1:C:173:ALA:O	2.17	0.45
1:C:72:ASN:HB2	2:E:1242:GTP:N2	2.31	0.45
1:B:115:ASP:N	1:B:115:ASP:OD1	2.48	0.45
1:D:178:ASP:HA	1:D:179:PRO:HD2	1.87	0.45
1:A:115:ASP:N	1:A:115:ASP:OD1	2.50	0.45
1:A:216:ARG:HH11	1:A:216:ARG:CG	2.18	0.44
1:F:180:THR:O	1:F:180:THR:HG23	2.17	0.44
1:C:69:ALA:HB2	1:E:31:ALA:HB1	2.00	0.44
1:A:186:GLN:HG3	1:A:187:LEU:N	2.31	0.44
1:E:89:LEU:HD13	1:E:104:LEU:HD23	1.99	0.44
1:F:49:ILE:HD11	1:F:230:VAL:CG1	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:HD13	1:B:153:GLY:N	2.32	0.44
1:C:49:ILE:HD11	1:C:230:VAL:CG1	2.43	0.44
1:D:44:LEU:HD22	1:D:230:VAL:HG21	1.99	0.44
1:A:111:ASN:HD21	1:E:116:SER:CB	2.30	0.44
1:D:73:ARG:HD2	1:D:73:ARG:HA	1.85	0.44
1:F:105:MET:CE	1:F:122:ALA:HB2	2.48	0.44
1:C:188:THR:OG1	1:C:191:GLU:HB2	2.17	0.44
1:B:172:THR:HG23	1:B:182:THR:O	2.18	0.43
1:F:125:LEU:O	1:F:130:ARG:HB2	2.18	0.43
1:D:161:VAL:CG2	1:D:213:LEU:HD21	2.48	0.43
1:A:154:ILE:HG13	1:A:213:LEU:HD22	2.00	0.43
1:E:85:VAL:HG11	1:E:110:LEU:CD1	2.48	0.43
1:E:216:ARG:HD3	1:E:229:VAL:CG1	2.48	0.43
1:C:200:MET:O	1:C:201:ASP:C	2.57	0.43
1:A:85:VAL:HG11	1:A:110:LEU:CD1	2.48	0.43
1:E:5:ALA:HB3	1:E:231:MET:SD	2.58	0.43
1:A:80:GLY:O	1:A:83:ALA:HB3	2.18	0.43
1:E:44:LEU:HD22	1:E:230:VAL:HG21	2.01	0.43
1:B:105:MET:HE2	1:B:122:ALA:HB2	2.00	0.43
1:D:25:GLU:H	1:D:25:GLU:CD	2.21	0.43
1:B:127:ARG:NH1	2:E:1242:GTP:O3'	2.41	0.43
1:B:154:ILE:HG13	1:B:213:LEU:HD22	2.01	0.43
1:C:111:ASN:HD21	1:F:116:SER:CB	2.31	0.43
1:F:50:GLN:NE2	1:F:127:ARG:HA	2.33	0.43
1:B:188:THR:O	1:B:192:VAL:HG23	2.19	0.43
1:A:172:THR:OG1	1:A:173:ALA:N	2.52	0.43
1:A:49:ILE:HD11	1:A:230:VAL:CG1	2.44	0.43
1:F:101:ASN:HB2	1:F:130:ARG:HD3	2.00	0.43
1:D:89:LEU:HD13	1:D:104:LEU:HD23	2.00	0.43
1:F:25:GLU:CD	1:F:25:GLU:H	2.22	0.43
1:F:200:MET:O	1:F:201:ASP:C	2.57	0.43
1:A:175:PRO:HA	1:A:181:ALA:HB3	1.99	0.43
1:B:161:VAL:CG2	1:B:213:LEU:HD21	2.49	0.43
1:E:174:ASP:HA	1:E:175:PRO:HD2	1.86	0.43
1:C:49:ILE:CD1	1:C:230:VAL:HG11	2.43	0.42
1:A:188:THR:OG1	1:A:191:GLU:HB2	2.19	0.42
1:A:6:LYS:HA	1:A:6:LYS:HD3	1.85	0.42
1:B:25:GLU:CD	1:B:25:GLU:H	2.23	0.42
1:A:161:VAL:CG2	1:A:213:LEU:HD21	2.50	0.42
1:D:188:THR:OG1	1:D:191:GLU:HB2	2.19	0.42
1:B:62:ARG:CG	1:B:62:ARG:NH2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:PHE:HD2	1:C:182:THR:C	2.23	0.42
1:B:101:ASN:HB2	1:B:130:ARG:HD3	2.01	0.42
1:E:101:ASN:HB2	1:E:130:ARG:HD2	2.02	0.42
1:A:79:MET:HB3	1:A:79:MET:HE2	1.94	0.42
1:A:30:ASP:O	1:A:33:ILE:HG22	2.20	0.42
1:D:152:ARG:O	1:D:156:ILE:HG12	2.19	0.42
1:D:105:MET:CE	1:D:122:ALA:HB2	2.50	0.42
1:A:171:PHE:CE2	1:A:183:MET:HB2	2.55	0.42
1:F:85:VAL:HG11	1:F:110:LEU:CD1	2.49	0.42
1:B:186:GLN:HG3	1:B:187:LEU:N	2.34	0.42
1:E:174:ASP:O	1:E:178:ASP:HB3	2.19	0.42
1:E:15:LYS:HD3	1:E:15:LYS:C	2.41	0.42
1:C:101:ASN:HB3	1:C:130:ARG:HD2	2.01	0.42
1:B:73:ARG:HD2	1:B:73:ARG:HA	1.84	0.42
1:E:188:THR:OG1	1:E:191:GLU:HB2	2.20	0.42
1:D:15:LYS:HD3	1:D:15:LYS:C	2.41	0.41
1:B:181:ALA:O	1:B:182:THR:CB	2.58	0.41
1:C:25:GLU:CD	1:C:25:GLU:H	2.22	0.41
1:A:101:ASN:HB2	1:A:130:ARG:HD2	2.02	0.41
1:F:13:LEU:HD13	1:F:153:GLY:N	2.35	0.41
1:A:200:MET:O	1:A:201:ASP:C	2.57	0.41
1:C:116:SER:CB	1:D:111:ASN:HD21	2.33	0.41
1:C:188:THR:O	1:C:192:VAL:HG23	2.21	0.41
1:D:154:ILE:HG13	1:D:213:LEU:HD22	2.02	0.41
1:A:105:MET:HE1	1:A:122:ALA:HB2	2.02	0.41
1:A:174:ASP:HA	1:A:175:PRO:HD3	1.65	0.41
1:D:80:GLY:O	1:D:83:ALA:HB3	2.20	0.41
1:F:216:ARG:CG	1:F:216:ARG:HH11	2.16	0.41
1:F:105:MET:HE1	1:F:122:ALA:HB2	2.03	0.41
1:B:44:LEU:HD22	1:B:230:VAL:HG21	2.02	0.41
1:E:105:MET:CE	1:E:122:ALA:HB2	2.50	0.41
1:C:85:VAL:O	1:C:89:LEU:HB2	2.21	0.41
1:D:101:ASN:HB3	1:D:130:ARG:HD2	2.03	0.41
1:A:25:GLU:CD	1:A:25:GLU:H	2.24	0.41
1:B:188:THR:OG1	1:B:191:GLU:HB2	2.20	0.41
1:D:186:GLN:HG3	1:D:187:LEU:N	2.36	0.41
1:A:73:ARG:HD2	1:A:73:ARG:HA	1.85	0.41
1:A:44:LEU:HD22	1:A:230:VAL:HG21	2.01	0.41
1:C:6:LYS:HA	1:C:7:PRO:HD3	1.87	0.41
1:C:13:LEU:HD12	1:C:156:ILE:HD11	2.03	0.41
1:B:33:ILE:O	1:B:33:ILE:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:MET:HE2	1:C:122:ALA:HB2	2.02	0.41
1:D:85:VAL:HG11	1:D:110:LEU:CD1	2.51	0.41
1:E:25:GLU:CD	1:E:25:GLU:H	2.23	0.41
1:F:186:GLN:HG3	1:F:187:LEU:N	2.36	0.41
1:B:200:MET:O	1:B:201:ASP:C	2.60	0.41
1:B:85:VAL:HG11	1:B:110:LEU:CD1	2.51	0.40
1:B:101:ASN:HB3	2:B:1242:GTP:O3G	2.21	0.40
1:B:30:ASP:O	1:B:33:ILE:HG22	2.21	0.40
1:A:101:ASN:HB3	1:A:130:ARG:HD2	2.03	0.40
1:C:71:MET:HA	1:E:93:ASP:OD2	2.21	0.40
1:D:200:MET:O	1:D:201:ASP:C	2.59	0.40
1:B:96:HIS:NE2	2:B:1242:GTP:O2G	2.52	0.40
1:C:6:LYS:HD3	1:C:6:LYS:HA	1.84	0.40
1:C:13:LEU:HD13	1:C:153:GLY:N	2.36	0.40
1:E:62:ARG:NH2	1:E:62:ARG:CG	2.68	0.40
1:A:105:MET:HE2	1:A:122:ALA:HB2	2.03	0.40
1:A:81:MET:HE1	1:A:140:ASN:O	2.22	0.40
1:F:201:ASP:OD1	1:F:202:LEU:N	2.54	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)
1:A:186:GLN:OE1	1:E:223:PRO:O[3_545]	2.07	0.13
1:A:185:GLU:OE1	1:E:36:ARG:NH1[3_545]	2.15	0.05

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/241 (98%)	225 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	227/241 (94%)	219 (96%)	6 (3%)	2 (1%)	21	55
1	C	235/241 (98%)	227 (97%)	8 (3%)	0	100	100
1	D	229/241 (95%)	220 (96%)	9 (4%)	0	100	100
1	E	232/241 (96%)	224 (97%)	7 (3%)	1 (0%)	39	74
1	F	229/241 (95%)	223 (97%)	6 (3%)	0	100	100
All	All	1387/1446 (96%)	1338 (96%)	46 (3%)	3 (0%)	52	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	181	ALA
1	B	182	THR
1	E	175	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	187/190 (98%)	174 (93%)	13 (7%)	19	47
1	B	183/190 (96%)	172 (94%)	11 (6%)	24	56
1	C	187/190 (98%)	176 (94%)	11 (6%)	24	57
1	D	184/190 (97%)	174 (95%)	10 (5%)	27	60
1	E	186/190 (98%)	174 (94%)	12 (6%)	21	52
1	F	185/190 (97%)	175 (95%)	10 (5%)	27	60
All	All	1112/1140 (98%)	1045 (94%)	67 (6%)	24	56

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	33	ILE
1	A	37	MET

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Mol	Chain	Res	Type
1	A	62	ARG
1	A	89	LEU
1	A	103	ARG
1	A	115	ASP
1	A	130	ARG
1	A	180	THR
1	A	183	MET
1	A	201	ASP
1	A	216	ARG
1	A	240	THR
1	B	33	ILE
1	B	37	MET
1	B	62	ARG
1	B	89	LEU
1	B	103	ARG
1	B	115	ASP
1	B	130	ARG
1	B	180	THR
1	B	209	ARG
1	B	216	ARG
1	B	240	THR
1	C	33	ILE
1	C	37	MET
1	C	62	ARG
1	C	89	LEU
1	C	103	ARG
1	C	115	ASP
1	C	130	ARG
1	C	201	ASP
1	C	209	ARG
1	C	216	ARG
1	C	240	THR
1	D	33	ILE
1	D	37	MET
1	D	62	ARG
1	D	89	LEU
1	D	103	ARG
1	D	115	ASP
1	D	130	ARG
1	D	201	ASP
1	D	216	ARG
1	D	240	THR

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Mol	Chain	Res	Type
1	E	33	ILE
1	E	36	ARG
1	E	37	MET
1	E	62	ARG
1	E	89	LEU
1	E	103	ARG
1	E	115	ASP
1	E	130	ARG
1	E	201	ASP
1	E	209	ARG
1	E	216	ARG
1	E	240	THR
1	F	32	SER
1	F	33	ILE
1	F	37	MET
1	F	62	ARG
1	F	103	ARG
1	F	115	ASP
1	F	130	ARG
1	F	209	ARG
1	F	216	ARG
1	F	240	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	B	111	ASN
1	C	111	ASN
1	D	111	ASN
1	E	22	GLN
1	E	111	ASN
1	F	111	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 ⓘ

12 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	1242	-	25,34,34	0.90	1 (4%)	34,54,54	1.79	8 (23%)
2	GTP	A	1243	-	8,12,34	1.29	1 (12%)	15,20,54	1.56	2 (13%)
2	GTP	B	1242	-	25,34,34	0.94	1 (4%)	34,54,54	1.73	5 (14%)
2	GTP	B	1243	-	8,12,34	1.31	1 (12%)	15,20,54	1.68	1 (6%)
2	GTP	C	1242	-	25,34,34	0.97	1 (4%)	34,54,54	1.63	7 (20%)
2	GTP	C	1243	-	8,12,34	1.29	1 (12%)	15,20,54	1.64	2 (13%)
2	GTP	D	1242	-	25,34,34	0.88	1 (4%)	34,54,54	1.55	7 (20%)
2	GTP	D	1243	-	8,12,34	1.41	1 (12%)	15,20,54	1.54	2 (13%)
2	GTP	E	1242	-	25,34,34	0.81	1 (4%)	34,54,54	1.88	7 (20%)
2	GTP	E	1243	-	8,12,34	1.32	1 (12%)	15,20,54	1.54	2 (13%)
2	GTP	F	1242	-	25,34,34	0.96	2 (8%)	34,54,54	2.01	7 (20%)
2	GTP	F	1243	-	8,12,34	1.28	1 (12%)	15,20,54	1.45	2 (13%)

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	1242	-	-	0/18/38/38	0/3/3/3
2	GTP	A	1243	-	-	0/12/12/38	0/0/0/3
2	GTP	B	1242	-	-	0/18/38/38	0/3/3/3
2	GTP	B	1243	-	-	0/12/12/38	0/0/0/3
2	GTP	C	1242	-	-	0/18/38/38	0/3/3/3
2	GTP	C	1243	-	-	0/12/12/38	0/0/0/3
2	GTP	D	1242	-	-	0/18/38/38	0/3/3/3
2	GTP	D	1243	-	-	0/12/12/38	0/0/0/3
2	GTP	E	1242	-	-	0/18/38/38	0/3/3/3
2	GTP	E	1243	-	-	0/12/12/38	0/0/0/3
2	GTP	F	1242	-	-	0/18/38/38	0/3/3/3
2	GTP	F	1243	-	-	0/12/12/38	0/0/0/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1242	GTP	C2-N1	2.05	1.39	1.35
2	E	1242	GTP	C6-N1	2.37	1.37	1.33
2	D	1242	GTP	C6-N1	2.44	1.37	1.33
2	A	1242	GTP	C6-N1	2.86	1.38	1.33
2	C	1242	GTP	C6-N1	3.04	1.38	1.33
2	B	1242	GTP	C6-N1	3.08	1.38	1.33
2	F	1243	GTP	PG-O1G	3.10	1.61	1.51
2	A	1243	GTP	PG-O1G	3.12	1.61	1.51
2	F	1242	GTP	C6-N1	3.16	1.39	1.33
2	C	1243	GTP	PG-O1G	3.20	1.61	1.51
2	B	1243	GTP	PG-O1G	3.27	1.61	1.51
2	E	1243	GTP	PG-O1G	3.28	1.62	1.51
2	D	1243	GTP	PG-O1G	3.44	1.62	1.51

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1242	GTP	C2'-C1'-N9	-7.04	103.54	114.29
2	B	1243	GTP	PB-O3A-PA	-5.63	113.80	132.67
2	C	1243	GTP	PB-O3A-PA	-5.23	115.12	132.67
2	E	1242	GTP	N3-C2-N1	-4.95	119.90	127.44
2	F	1242	GTP	N3-C2-N1	-4.85	120.06	127.44
2	A	1242	GTP	N3-C2-N1	-4.77	120.18	127.44
2	B	1242	GTP	N3-C2-N1	-4.74	120.22	127.44
2	C	1242	GTP	N3-C2-N1	-4.64	120.38	127.44
2	B	1242	GTP	C2'-C1'-N9	-4.50	107.42	114.29
2	E	1242	GTP	C2'-C1'-N9	-4.44	107.51	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1242	GTP	PB-O3B-PG	-4.30	118.25	132.67
2	D	1242	GTP	PB-O3B-PG	-4.27	118.34	132.67
2	D	1243	GTP	PB-O3A-PA	-4.18	118.64	132.67
2	D	1242	GTP	N3-C2-N1	-4.16	121.11	127.44
2	A	1242	GTP	PA-O3A-PB	-4.16	121.05	132.73
2	C	1242	GTP	C2'-C1'-N9	-4.08	108.06	114.29
2	E	1243	GTP	PB-O3A-PA	-4.08	119.00	132.67
2	B	1242	GTP	PB-O3B-PG	-4.00	119.25	132.67
2	A	1242	GTP	PB-O3B-PG	-3.80	119.94	132.67
2	F	1242	GTP	C5-C6-N1	-3.58	118.69	123.59
2	A	1242	GTP	C2'-C1'-N9	-3.56	108.85	114.29
2	F	1243	GTP	PB-O3B-PG	-3.50	120.94	132.67
2	A	1243	GTP	PB-O3B-PG	-3.39	121.30	132.67
2	C	1242	GTP	PB-O3B-PG	-3.24	121.82	132.67
2	B	1242	GTP	C5-C6-N1	-3.13	119.31	123.59
2	E	1243	GTP	PB-O3B-PG	-3.11	122.25	132.67
2	A	1243	GTP	PB-O3A-PA	-3.08	122.33	132.67
2	A	1242	GTP	C5-C6-N1	-3.08	119.38	123.59
2	C	1242	GTP	C5-C6-N1	-3.02	119.46	123.59
2	F	1242	GTP	PA-O3A-PB	-2.97	124.38	132.73
2	E	1242	GTP	C5-C6-N1	-2.89	119.64	123.59
2	F	1243	GTP	PB-O3A-PA	-2.88	123.02	132.67
2	F	1242	GTP	PB-O3B-PG	-2.73	123.50	132.67
2	D	1242	GTP	C5-C6-N1	-2.73	119.86	123.59
2	D	1243	GTP	PB-O3B-PG	-2.70	123.61	132.67
2	D	1242	GTP	PA-O3A-PB	-2.67	125.24	132.73
2	C	1242	GTP	PA-O3A-PB	-2.54	125.60	132.73
2	D	1242	GTP	C4-C5-N7	-2.44	107.23	109.48
2	D	1242	GTP	C2'-C1'-N9	-2.27	110.83	114.29
2	A	1242	GTP	C4-C5-N7	-2.25	107.41	109.48
2	C	1243	GTP	PB-O3B-PG	-2.07	125.73	132.67
2	C	1242	GTP	C4'-O4'-C1'	2.03	111.94	109.72
2	F	1242	GTP	N2-C2-N1	2.17	120.80	117.20
2	D	1242	GTP	C6-N1-C2	2.26	119.08	115.94
2	E	1242	GTP	C4'-O4'-C1'	2.34	112.29	109.72
2	A	1242	GTP	C4'-O4'-C1'	2.36	112.31	109.72
2	C	1242	GTP	C6-N1-C2	2.58	119.52	115.94
2	A	1242	GTP	C6-N1-C2	2.75	119.76	115.94
2	E	1242	GTP	O3A-PA-O5'	2.84	110.48	102.94
2	B	1242	GTP	C6-N1-C2	2.87	119.93	115.94
2	E	1242	GTP	C6-N1-C2	3.23	120.43	115.94
2	F	1242	GTP	C6-N1-C2	3.36	120.61	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1242	GTP	1	0
2	B	1242	GTP	2	0
2	C	1242	GTP	1	0
2	C	1243	GTP	1	0
2	E	1242	GTP	2	0
2	F	1242	GTP	2	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	237/241 (98%)	0.26	13 (5%) 29 18	42, 66, 110, 128	0
1	B	231/241 (95%)	0.14	7 (3%) 54 41	42, 64, 111, 143	0
1	C	237/241 (98%)	0.21	11 (4%) 36 25	40, 66, 110, 130	0
1	D	233/241 (96%)	0.44	27 (11%) 6 3	38, 67, 117, 170	0
1	E	236/241 (97%)	0.31	14 (5%) 26 16	39, 66, 121, 150	0
1	F	233/241 (96%)	0.35	20 (8%) 13 6	43, 69, 114, 147	0
All	All	1407/1446 (97%)	0.29	92 (6%) 22 13	38, 66, 113, 170	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	177	LYS	7.4
1	F	171	PHE	5.9
1	B	6	LYS	5.4
1	A	171	PHE	5.1
1	F	179	PRO	4.9
1	E	5	ALA	4.6
1	C	26	GLY	4.6
1	D	176	ALA	4.5
1	D	8	VAL	4.4
1	D	180	THR	4.3
1	F	168	ASP	4.3
1	D	179	PRO	4.2
1	D	182	THR	4.2
1	B	181	ALA	4.1
1	F	180	THR	4.1
1	C	5	ALA	3.9
1	D	177	LYS	3.9
1	F	197	LEU	3.9
1	C	25	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	6	LYS	3.5
1	E	199	VAL	3.5
1	A	197	LEU	3.4
1	C	27	PHE	3.3
1	D	181	ALA	3.3
1	A	172	THR	3.3
1	E	241	GLU	3.3
1	A	194	GLU	3.3
1	F	181	ALA	3.2
1	F	6	LYS	3.2
1	D	5	ALA	3.2
1	D	171	PHE	3.1
1	A	170	VAL	3.0
1	E	179	PRO	3.0
1	F	170	VAL	3.0
1	D	7	PRO	3.0
1	A	6	LYS	2.9
1	E	25	GLU	2.9
1	E	198	LYS	2.9
1	F	193	LEU	2.9
1	D	197	LEU	2.9
1	C	129	ASN	2.9
1	D	198	LYS	2.8
1	E	176	ALA	2.8
1	E	172	THR	2.8
1	A	177	LYS	2.8
1	D	193	LEU	2.8
1	F	27	PHE	2.8
1	D	241	GLU	2.7
1	D	196	GLU	2.7
1	C	199	VAL	2.7
1	F	26	GLY	2.7
1	A	68	LYS	2.7
1	D	24	THR	2.7
1	C	172	THR	2.7
1	E	194	GLU	2.7
1	B	234	LYS	2.6
1	F	62	ARG	2.6
1	E	186	GLN	2.6
1	B	167	VAL	2.6
1	A	167	VAL	2.5
1	A	29	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	169	GLY	2.4
1	B	198	LYS	2.4
1	E	190	SER	2.4
1	A	5	ALA	2.4
1	C	167	VAL	2.3
1	D	234	LYS	2.3
1	E	170	VAL	2.3
1	D	236	GLY	2.3
1	A	27	PHE	2.3
1	F	199	VAL	2.2
1	F	228	ARG	2.2
1	D	183	MET	2.2
1	D	186	GLN	2.2
1	D	233	GLU	2.2
1	F	167	VAL	2.2
1	B	231	MET	2.2
1	F	172	THR	2.1
1	E	8	VAL	2.1
1	A	215	ILE	2.1
1	C	194	GLU	2.1
1	D	27	PHE	2.1
1	D	168	ASP	2.1
1	D	227	ARG	2.1
1	E	185	GLU	2.0
1	D	237	THR	2.0
1	B	7	PRO	2.0
1	C	111	ASN	2.0
1	F	202	LEU	2.0
1	F	5	ALA	2.0
1	F	227	ARG	2.0
1	D	199	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	GTP	F	1242	32/32	0.94	0.19	0.11	65,88,135,153	0
2	GTP	E	1242	32/32	0.95	0.16	-0.53	37,62,103,139	0
2	GTP	C	1242	32/32	0.94	0.15	-0.54	40,69,120,153	0
2	GTP	C	1243	13/32	0.95	0.15	-0.66	41,90,109,118	0
2	GTP	A	1242	32/32	0.94	0.16	-0.78	33,67,106,128	0
2	GTP	E	1243	13/32	0.94	0.15	-0.96	53,92,121,122	0
2	GTP	D	1243	13/32	0.96	0.13	-0.97	60,75,98,104	0
2	GTP	A	1243	13/32	0.95	0.12	-1.19	60,78,116,124	0
2	GTP	F	1243	13/32	0.95	0.10	-1.34	52,91,121,128	0
2	GTP	B	1243	13/32	0.96	0.10	-2.75	60,83,99,105	0
2	GTP	D	1242	32/32	0.95	0.12	-2.77	38,75,108,138	0
2	GTP	B	1242	32/32	0.96	0.13	-3.27	38,63,103,126	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.