Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 01:49 AM JST

PDB ID	:	5YU6
Title	:	CRYSTAL STRUCTURE OF EXPORTIN-5:RANGTP COMPLEX
Authors	:	Yamazawa, R.; Jiko, C.; Lee, S.J.; Yamashita, E.
Deposited on	:	2017-11-20
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

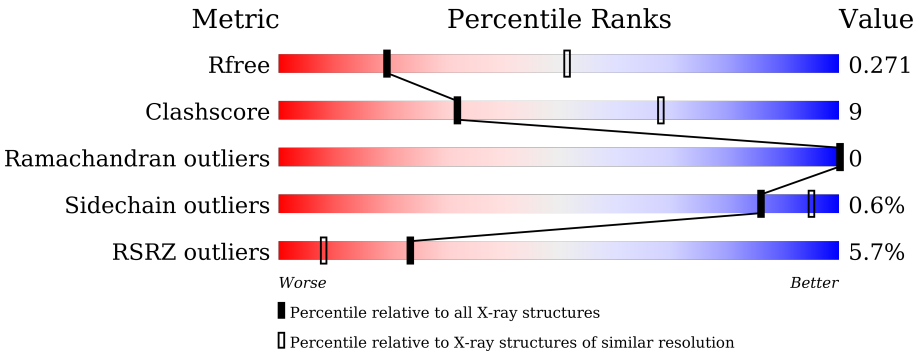
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	1204	4% 71% 18% 11%
1	C	1204	8% 69% 20% 11%
2	E	13	100%
2	F	13	100%
3	B	216	% 53% 26% 21%
3	D	216	% 59% 19% 21%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20096 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 Exportin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1069	Total	C	N	O	S	0	0	0
			8549	5468	1439	1569	73			
1	C	1073	Total	C	N	O	S	0	0	0
			8577	5486	1443	1574	74			

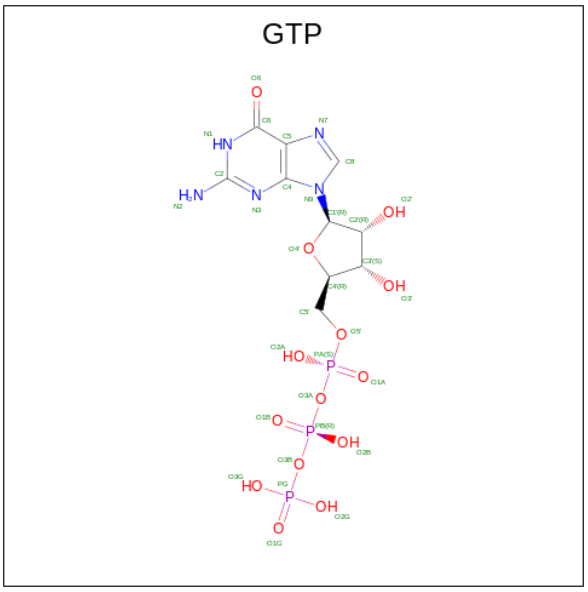
- Molecule 2 is a protein called 13-mer peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	0	0	0
			66	39	13	14			
2	F	13	Total	C	N	O	0	0	0
			66	39	13	14			

- Molecule 3 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	170	Total	C	N	O	S	0	0	0
			1386	900	244	238	4			
3	D	170	Total	C	N	O	S	0	0	0
			1386	900	244	238	4			

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

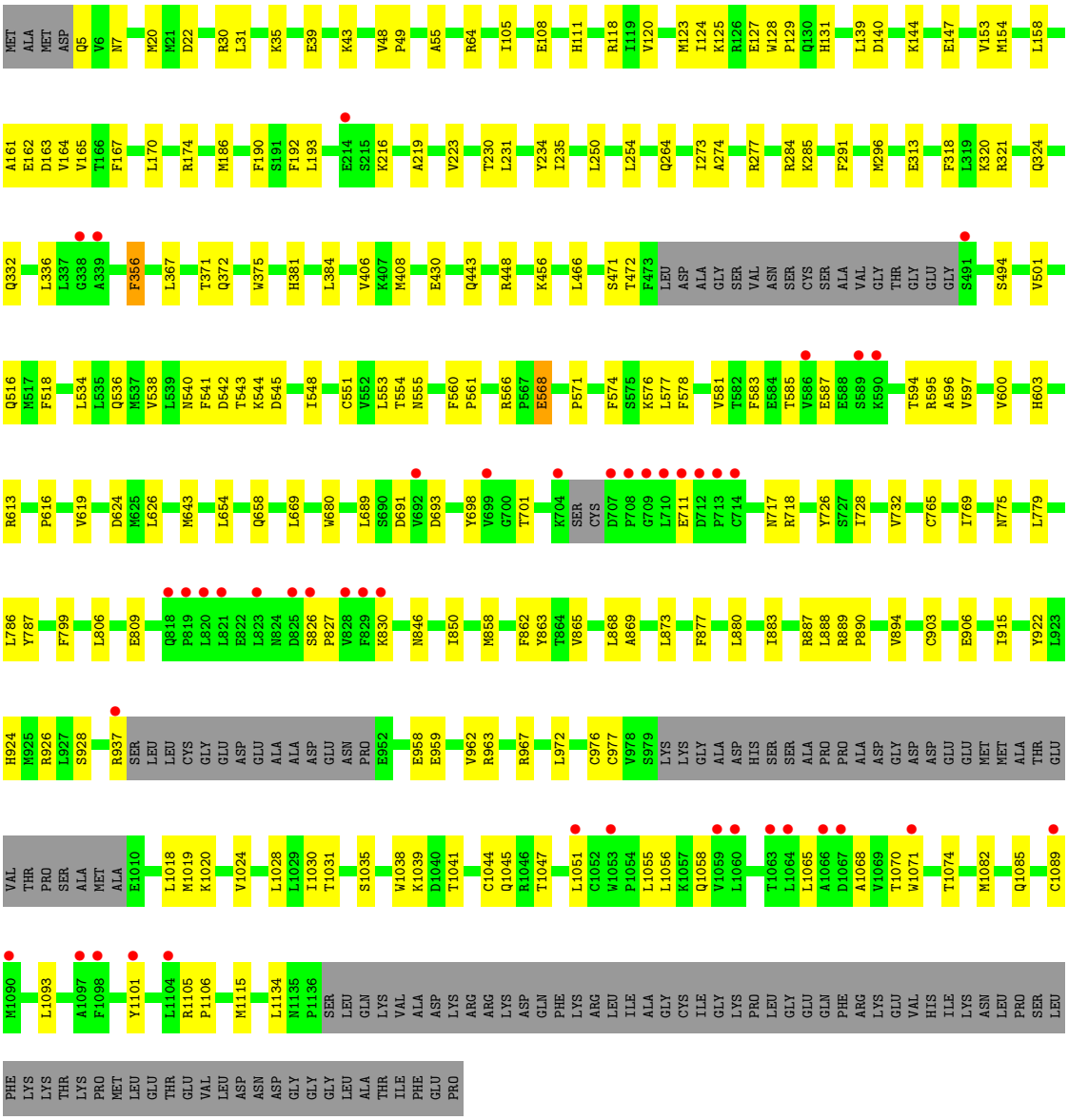
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

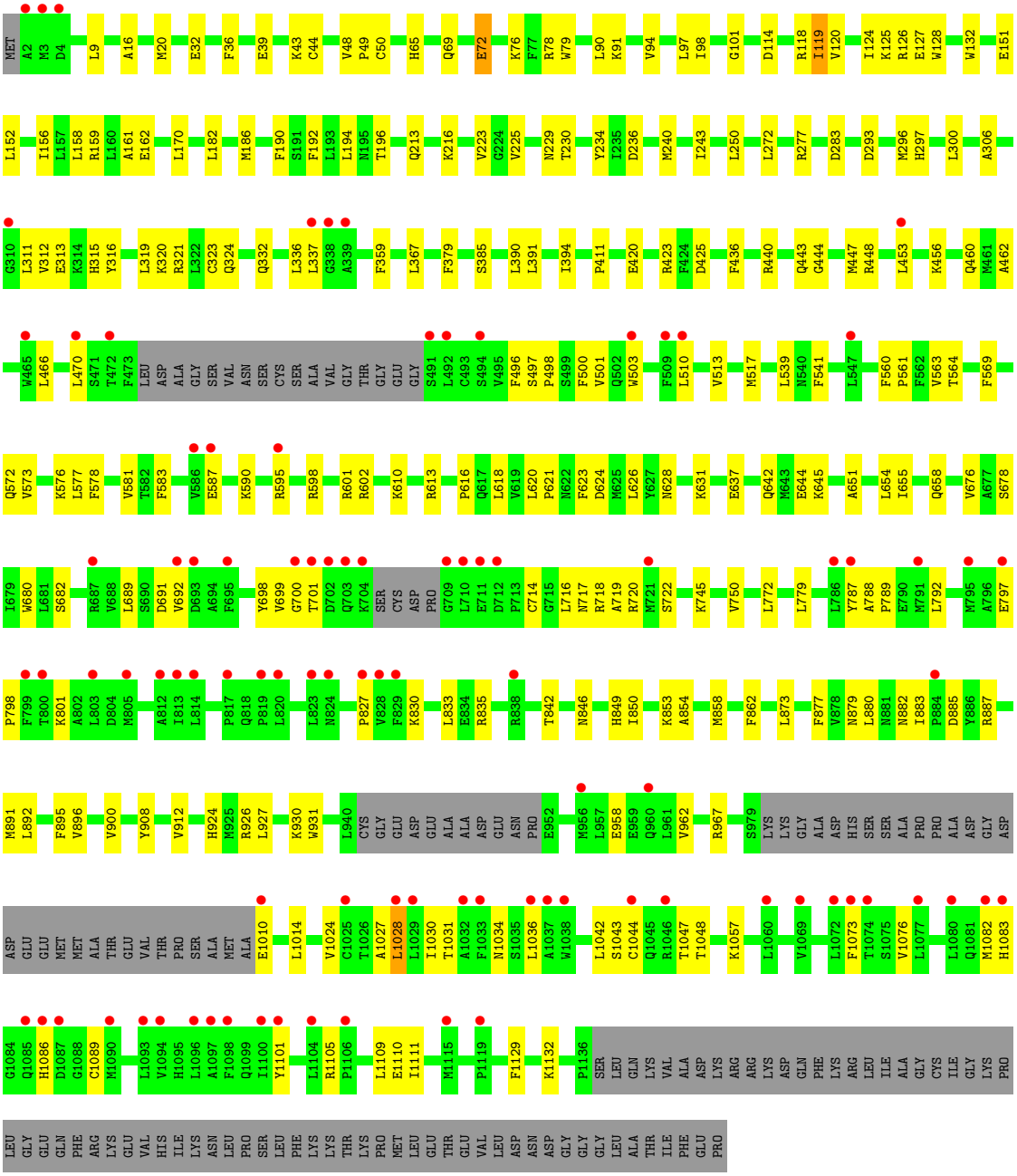
- Molecule 1: Exportin-5

Chain A:



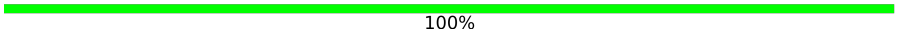
• Molecule 1: Exportin-5

Chain C:



• Molecule 2: 13-mer peptide

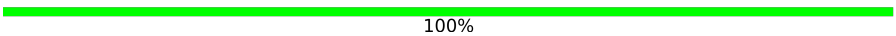
Chain E:



There are no outlier residues recorded for this chain.

• Molecule 2: 13-mer peptide

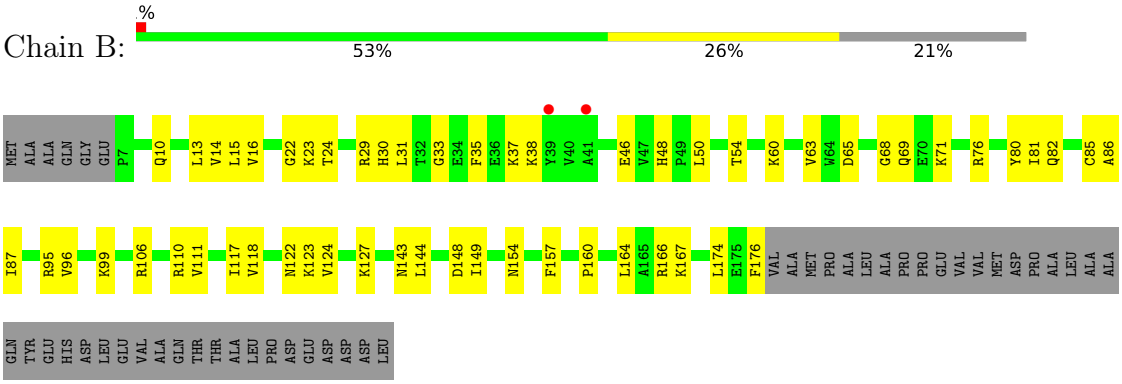
Chain F:



There are no outlier residues recorded for this chain.

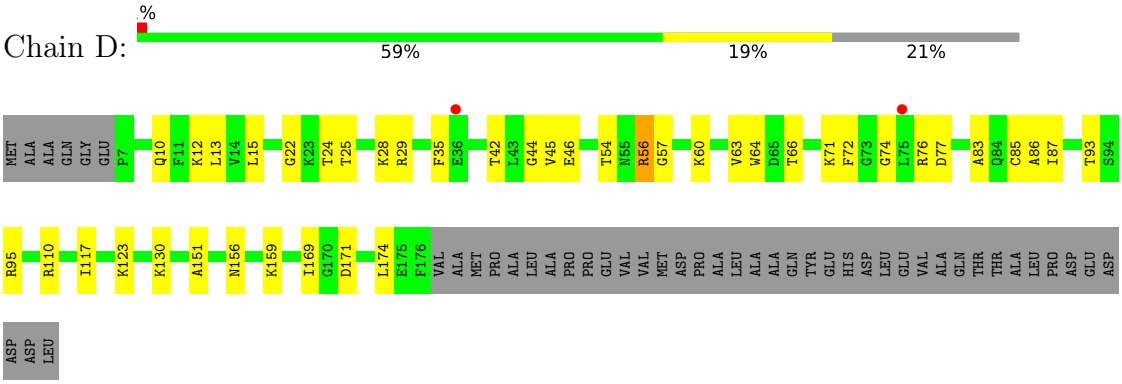
• Molecule 3: GTP-binding nuclear protein Ran

Chain B:



• Molecule 3: GTP-binding nuclear protein Ran

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.56Å 302.68Å 88.26Å 90.00° 109.24° 90.00°	Depositor
Resolution (Å)	48.98 – 3.00 50.45 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.9 (48.98-3.00) 82.0 (50.45-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.218 , 0.269 0.221 , 0.271	Depositor DCC
R_{free} test set	2875 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	20096	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, MG

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	0.25	0/8717	0.39	0/11803
1	C	0.24	0/8744	0.39	0/11838
3	B	0.25	0/1421	0.42	0/1918
3	D	0.25	0/1421	0.42	0/1918
All	All	0.25	0/20303	0.40	0/27477

There are no bond length outliers.

There are no bond angle outliers.

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	8549	0	8646	146	0
1	C	8577	0	8680	153	0
2	E	66	0	15	0	0
2	F	66	0	15	0	0
3	B	1386	0	1409	44	0
3	D	1386	0	1407	30	0
4	B	32	0	12	5	0
4	D	32	0	12	3	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
All	All	20096	0	20196	360	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 9.

All (360) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLU:O	1:C:43:LYS:HB2	1.69	0.92
1:A:890:PRO:O	1:A:894:VAL:HB	1.76	0.85
1:C:125:LYS:HB3	1:C:170:LEU:HD21	1.63	0.79
1:A:732:VAL:HG22	1:A:769:ILE:HD13	1.65	0.78
3:D:13:LEU:HD11	3:D:87:ILE:HG13	1.64	0.78
1:A:595:ARG:H	1:A:827:PRO:HB2	1.50	0.76
1:A:543:THR:HG22	1:A:545:ASP:H	1.52	0.75
1:C:927:LEU:O	1:C:931:TRP:HB2	1.87	0.75
1:A:39:GLU:HG3	1:A:43:LYS:HE3	1.70	0.74
3:B:29:ARG:HH21	3:B:35:PHE:HB2	1.53	0.72
1:A:1089:CYS:O	1:A:1093:LEU:HB2	1.90	0.71
1:C:642:GLN:HE22	1:C:722:SER:HB2	1.56	0.71
3:D:15:LEU:O	3:D:66:THR:HB	1.90	0.70
1:C:182:LEU:O	1:C:186:MET:HB2	1.92	0.70
1:A:163:ASP:OD1	3:B:106:ARG:NH1	2.25	0.70
1:A:858:MET:O	1:A:862:PHE:HB3	1.92	0.69
1:A:147:GLU:HB3	1:A:223:VAL:HG21	1.74	0.69
1:C:158:LEU:HD13	1:C:230:THR:HA	1.75	0.67
1:C:1105:ARG:HH12	1:C:1109:LEU:HD12	1.59	0.67
1:C:616:PRO:HB2	1:C:658:GLN:HG2	1.76	0.67
3:B:13:LEU:HD11	3:B:87:ILE:HG13	1.77	0.66
1:C:564:THR:HA	1:C:618:LEU:HD21	1.77	0.66
1:C:842:THR:O	1:C:846:ASN:HB2	1.96	0.66
1:C:1043:SER:O	1:C:1047:THR:HB	1.96	0.65
1:A:372:GLN:NE2	1:A:443:GLN:OE1	2.29	0.65
1:C:158:LEU:HB2	1:C:230:THR:HG22	1.78	0.65
1:A:5:GLN:OE1	1:A:7:ASN:N	2.29	0.64
1:C:1086:HIS:HB3	1:C:1089:CYS:HB3	1.80	0.64
1:A:551:CYS:O	1:A:555:ASN:ND2	2.31	0.64
1:C:642:GLN:NE2	1:C:719:ALA:O	2.31	0.64
1:A:937:ARG:HD3	3:B:127:LYS:HE3	1.80	0.63
1:C:924:HIS:HE1	1:C:1030:ILE:HG22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1010:GLU:OE2	1:C:1057:LYS:NZ	2.28	0.63
1:A:880:LEU:HD23	1:A:883:ILE:HD12	1.80	0.63
1:A:536:GLN:NE2	1:A:540:ASN:OD1	2.32	0.62
1:A:291:PHE:HA	1:A:296:MET:HG2	1.81	0.61
1:C:541:PHE:O	1:C:576:LYS:NZ	2.33	0.61
1:A:787:TYR:OH	1:A:887:ARG:NH1	2.32	0.61
1:C:1024:VAL:O	1:C:1028:LEU:HB2	2.00	0.61
1:C:120:VAL:HB	1:C:156:ILE:HD12	1.83	0.60
1:C:312:VAL:HG23	1:C:315:HIS:HB2	1.83	0.60
1:A:313:GLU:OE1	3:B:167:LYS:NZ	2.34	0.60
3:B:81:ILE:HG22	3:B:82:GLN:HG2	1.84	0.60
1:C:1036:LEU:HD21	1:C:1044:CYS:HA	1.83	0.60
1:A:1018:LEU:HD22	1:A:1024:VAL:HG11	1.83	0.60
1:C:236:ASP:O	1:C:277:ARG:NH1	2.34	0.60
1:C:850:ILE:O	1:C:854:ALA:HB2	2.01	0.59
1:C:637:GLU:OE1	1:C:645:LYS:NZ	2.36	0.59
1:A:858:MET:O	1:A:862:PHE:CB	2.50	0.59
3:D:42:THR:HG23	3:D:46:GLU:HG3	1.86	0.58
1:C:128:TRP:HA	1:C:132:TRP:HB3	1.85	0.58
1:A:158:LEU:HB2	1:A:230:THR:HG22	1.86	0.58
1:C:98:ILE:HD11	1:C:120:VAL:HG21	1.85	0.58
1:C:293:ASP:O	1:C:297:HIS:HB2	2.03	0.58
1:A:124:ILE:HG23	1:A:128:TRP:HB2	1.86	0.58
1:C:120:VAL:O	1:C:124:ILE:HG12	2.02	0.58
1:A:541:PHE:O	1:A:576:LYS:NZ	2.29	0.57
1:A:883:ILE:O	1:A:926:ARG:NH2	2.32	0.57
1:A:958:GLU:O	1:A:962:VAL:HG23	2.05	0.57
1:A:1051:LEU:O	1:A:1055:LEU:HG	2.04	0.57
1:A:128:TRP:H	1:A:174:ARG:HH22	1.52	0.57
1:C:225:VAL:O	1:C:229:ASN:ND2	2.32	0.57
1:C:1044:CYS:O	1:C:1048:THR:HB	2.05	0.57
1:A:111:HIS:HB3	3:B:111:VAL:HG13	1.87	0.56
1:A:698:TYR:CZ	1:A:717:ASN:HB3	2.40	0.56
1:A:250:LEU:O	1:A:254:LEU:HB2	2.05	0.56
3:B:29:ARG:NH2	3:B:35:PHE:HB2	2.20	0.56
1:A:906:GLU:OE2	1:A:906:GLU:N	2.36	0.56
1:A:1101:TYR:CZ	1:A:1105:ARG:HG3	2.40	0.56
1:C:620:LEU:HD22	1:C:658:GLN:HB3	1.87	0.56
1:A:321:ARG:NH1	3:B:143:ASN:OD1	2.36	0.56
1:C:924:HIS:CE1	1:C:1030:ILE:HG22	2.40	0.56
1:A:868:LEU:HD12	1:A:869:ALA:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:HD13	1:A:153:VAL:HG13	1.88	0.55
1:C:1044:CYS:O	1:C:1048:THR:CB	2.54	0.55
1:A:154:MET:HB3	1:A:230:THR:HG21	1.89	0.55
3:B:124:VAL:HG21	3:B:148:ASP:HB3	1.89	0.55
3:B:24:THR:HG23	4:B:301:GTP:O2B	2.06	0.55
1:A:1065:LEU:HB2	1:A:1068:ALA:HB3	1.89	0.55
1:C:624:ASP:O	1:C:628:ASN:ND2	2.31	0.54
1:A:701:THR:HG22	1:A:799:PHE:HD2	1.72	0.54
1:C:72:GLU:HB3	1:C:119:ILE:HD13	1.89	0.54
1:C:830:LYS:HB2	1:C:835:ARG:HG3	1.88	0.54
3:B:166:ARG:HG2	3:B:174:LEU:HB3	1.89	0.54
1:C:496:PHE:HA	1:C:500:PHE:HD2	1.73	0.54
3:D:13:LEU:O	3:D:63:VAL:HA	2.07	0.54
1:A:125:LYS:HB3	1:A:170:LEU:HD21	1.90	0.54
1:A:164:VAL:HG13	1:A:165:VAL:HG23	1.90	0.54
3:B:22:GLY:N	4:B:301:GTP:O1B	2.32	0.54
1:A:877:PHE:HB3	1:A:880:LEU:HD11	1.90	0.53
1:C:152:LEU:O	1:C:156:ILE:HG12	2.08	0.53
1:A:616:PRO:HB2	1:A:658:GLN:HG2	1.89	0.53
1:C:587:GLU:HG3	1:C:590:LYS:HD2	1.89	0.53
1:C:162:GLU:OE2	3:D:110:ARG:NH1	2.42	0.53
1:A:140:ASP:OD1	1:A:144:LYS:NZ	2.42	0.53
1:C:789:PRO:HD3	1:C:882:ASN:HD21	1.74	0.53
1:A:566:ARG:NH1	1:A:568:GLU:OE1	2.40	0.53
3:B:24:THR:HG22	3:B:65:ASP:OD2	2.08	0.53
1:A:1047:THR:HG23	1:A:1051:LEU:HD23	1.91	0.53
1:A:321:ARG:NH2	1:A:324:GLN:OE1	2.41	0.53
1:C:79:TRP:NE1	1:C:127:GLU:OE2	2.27	0.53
1:C:908:TYR:CZ	1:C:1014:LEU:HB2	2.45	0.52
1:A:162:GLU:OE2	3:B:110:ARG:NH2	2.43	0.52
1:A:977:CYS:SG	1:A:1028:LEU:HD21	2.50	0.52
3:B:29:ARG:HG3	3:B:157:PHE:CZ	2.45	0.52
3:D:171:ASP:HB3	3:D:174:LEU:HD13	1.91	0.52
1:A:689:LEU:HD22	1:A:779:LEU:HB2	1.89	0.52
1:A:1024:VAL:O	1:A:1028:LEU:HB2	2.10	0.52
1:C:443:GLN:HE21	1:C:447:MET:HB2	1.74	0.52
1:A:1020:LYS:NZ	1:A:1058:GLN:OE1	2.42	0.52
1:A:235:ILE:O	1:A:277:ARG:NH1	2.43	0.52
3:D:10:GLN:HG2	3:D:60:LYS:HD2	1.92	0.52
1:C:332:GLN:O	1:C:336:LEU:HB2	2.11	0.51
1:A:125:LYS:HD2	1:A:170:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:MET:HE1	1:A:1055:LEU:HD22	1.92	0.51
1:A:128:TRP:H	1:A:174:ARG:NH2	2.09	0.51
1:A:583:PHE:HD2	1:A:597:VAL:HG23	1.74	0.51
1:C:787:TYR:OH	1:C:887:ARG:NE	2.43	0.51
3:D:29:ARG:NH1	3:D:151:ALA:O	2.43	0.51
1:A:192:PHE:HD2	1:A:193:LEU:HD12	1.74	0.51
1:C:16:ALA:O	1:C:20:MET:HG3	2.10	0.51
1:C:885:ASP:OD1	1:C:926:ARG:NH2	2.37	0.51
1:A:105:ILE:HD11	1:A:147:GLU:HB2	1.92	0.51
1:C:311:LEU:HD22	1:C:420:GLU:HG3	1.93	0.51
1:A:406:VAL:HG22	1:A:408:MET:HG2	1.93	0.51
1:C:578:PHE:HE2	1:C:626:LEU:HD22	1.75	0.51
1:C:700:GLY:HA3	1:C:714:CYS:SG	2.51	0.51
1:A:284:ARG:HD2	1:A:332:GLN:HE22	1.75	0.51
1:A:120:VAL:HA	1:A:123:MET:HE2	1.92	0.50
3:B:117:ILE:HB	3:B:144:LEU:HD22	1.94	0.50
3:B:14:VAL:HG12	3:B:16:VAL:HG13	1.94	0.50
3:B:86:ALA:HB3	3:B:117:ILE:HG12	1.94	0.50
1:A:118:ARG:HH22	3:B:76:ARG:HH22	1.59	0.50
1:A:129:PRO:HD2	1:A:174:ARG:HH12	1.77	0.50
1:A:728:ILE:O	1:A:732:VAL:HG23	2.11	0.50
3:D:13:LEU:HA	3:D:85:CYS:O	2.12	0.50
1:A:167:PHE:HE2	3:B:106:ARG:HD3	1.77	0.49
3:B:10:GLN:HG2	3:B:60:LYS:HD3	1.93	0.49
1:C:391:LEU:HA	1:C:394:ILE:HD12	1.94	0.49
1:C:1027:ALA:O	1:C:1031:THR:OG1	2.24	0.49
1:C:892:LEU:HA	1:C:896:VAL:HG22	1.95	0.49
1:C:1110:GLU:N	1:C:1110:GLU:OE2	2.45	0.49
3:D:54:THR:HG22	3:D:56:ARG:H	1.76	0.49
3:B:31:LEU:HD21	3:B:48:HIS:HB3	1.94	0.49
1:C:161:ALA:HB2	1:C:234:TYR:CZ	2.47	0.49
1:C:698:TYR:CZ	1:C:717:ASN:HB3	2.48	0.49
1:C:243:ILE:HG23	1:C:250:LEU:HD23	1.93	0.49
1:C:9:LEU:HD23	1:C:50:CYS:SG	2.52	0.49
3:D:12:LYS:HD2	3:D:83:ALA:HA	1.95	0.49
1:C:385:SER:HB3	1:C:453:LEU:HD21	1.94	0.48
3:D:25:THR:HG21	4:D:301:GTP:H3'	1.95	0.48
1:A:64:ARG:NH2	1:A:108:GLU:OE2	2.46	0.48
1:C:879:ASN:O	1:C:883:ILE:HG12	2.14	0.48
1:C:456:LYS:O	1:C:460:GLN:HG2	2.13	0.48
3:D:71:LYS:HE2	3:D:72:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1105:ARG:HA	1:C:1111:ILE:HD11	1.95	0.48
3:D:86:ALA:HB3	3:D:117:ILE:HD13	1.95	0.48
1:A:613:ARG:HB2	1:A:654:LEU:HD13	1.95	0.48
3:B:118:VAL:HG11	3:B:160:PRO:HB3	1.95	0.48
1:A:880:LEU:O	1:A:922:TYR:OH	2.29	0.48
1:A:20:MET:O	1:A:30:ARG:NH1	2.46	0.48
1:A:865:VAL:N	1:A:868:LEU:HD23	2.28	0.48
1:C:151:GLU:HB2	1:C:223:VAL:HG12	1.96	0.48
1:C:858:MET:O	1:C:862:PHE:HB3	2.14	0.48
3:B:37:LYS:HB3	3:B:38:LYS:HZ2	1.78	0.48
1:C:958:GLU:O	1:C:962:VAL:HG23	2.12	0.48
1:A:430:GLU:OE1	1:A:430:GLU:N	2.43	0.47
1:A:1030:ILE:HA	1:A:1071:TRP:HH2	1.79	0.47
1:A:583:PHE:CD2	1:A:597:VAL:HG23	2.50	0.47
1:C:379:PHE:O	1:C:385:SER:OG	2.32	0.47
1:C:967:ARG:HE	1:C:1042:LEU:HD12	1.79	0.47
1:A:448:ARG:HG2	1:A:516:GLN:HE21	1.78	0.47
3:B:29:ARG:HH11	3:B:154:ASN:HD21	1.61	0.47
1:A:863:TYR:CE2	1:A:903:CYS:HA	2.49	0.47
1:C:698:TYR:CE2	1:C:717:ASN:HB3	2.50	0.47
1:C:1129:PHE:HA	1:C:1132:LYS:HB3	1.97	0.47
1:A:1041:THR:HA	1:A:1044:CYS:SG	2.55	0.47
1:C:44:CYS:O	1:C:78:ARG:NH1	2.36	0.47
3:D:169:ILE:HD12	3:D:174:LEU:HD21	1.97	0.47
1:C:72:GLU:O	1:C:76:LYS:HB2	2.14	0.47
1:C:443:GLN:O	1:C:443:GLN:NE2	2.48	0.47
3:B:123:LYS:HG2	4:B:301:GTP:C5	2.50	0.47
1:C:79:TRP:CD1	1:C:126:ARG:HD3	2.50	0.47
3:D:24:THR:O	3:D:28:LYS:HB2	2.14	0.47
3:D:156:ASN:HA	3:D:159:LYS:HD3	1.96	0.46
1:A:371:THR:HG22	1:A:375:TRP:CD1	2.51	0.46
1:C:194:LEU:HD11	1:C:250:LEU:HA	1.97	0.46
1:C:598:ARG:NH1	1:C:602:ARG:HH12	2.12	0.46
1:C:316:TYR:OH	1:C:425:ASP:OD2	2.32	0.46
1:C:470:LEU:HD23	1:C:503:TRP:HH2	1.81	0.46
1:C:846:ASN:O	1:C:850:ILE:HG13	2.16	0.46
1:A:534:LEU:O	1:A:538:VAL:HG23	2.15	0.46
1:A:553:LEU:HD22	1:A:577:LEU:HD23	1.98	0.46
1:A:574:PHE:CE1	1:A:626:LEU:HD21	2.50	0.46
3:D:45:VAL:HG21	3:D:64:TRP:HB3	1.98	0.46
1:A:161:ALA:HB2	1:A:234:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:14:VAL:HG11	3:B:80:TYR:CD1	2.51	0.46
1:C:296:MET:O	1:C:300:LEU:HG	2.16	0.46
1:A:596:ALA:O	1:A:600:VAL:HG23	2.15	0.46
3:B:29:ARG:HD3	3:B:33:GLY:HA2	1.98	0.46
1:C:32:GLU:O	1:C:36:PHE:HB3	2.14	0.46
1:C:213:GLN:HB3	1:C:216:LYS:HB3	1.98	0.46
1:C:873:LEU:HA	1:C:877:PHE:HB2	1.97	0.46
1:C:689:LEU:HD22	1:C:779:LEU:HB2	1.98	0.45
1:A:643:MET:HG3	1:A:726:TYR:CZ	2.51	0.45
1:A:826:SER:N	1:A:827:PRO:HD3	2.31	0.45
3:B:123:LYS:HG2	4:B:301:GTP:C6	2.52	0.45
3:D:76:ARG:HG3	3:D:77:ASP:H	1.82	0.45
1:A:167:PHE:CE2	3:B:106:ARG:HD3	2.51	0.45
1:C:190:PHE:HZ	1:C:250:LEU:HB2	1.82	0.45
1:C:390:LEU:O	1:C:394:ILE:HG13	2.16	0.45
1:C:699:VAL:O	1:C:718:ARG:NH2	2.49	0.45
1:A:471:SER:O	1:A:472:THR:OG1	2.29	0.45
1:A:560:PHE:N	1:A:561:PRO:HD2	2.30	0.45
3:B:54:THR:HG22	3:B:176:PHE:HD1	1.82	0.45
3:D:93:THR:O	3:D:130:LYS:HE2	2.16	0.45
1:C:32:GLU:O	1:C:36:PHE:CB	2.65	0.45
1:A:231:LEU:O	1:A:235:ILE:HG13	2.17	0.45
1:A:963:ARG:O	1:A:967:ARG:HG2	2.17	0.45
1:C:891:MET:O	1:C:895:PHE:HB3	2.17	0.45
3:B:13:LEU:HD23	3:B:63:VAL:HG12	1.99	0.45
1:C:444:GLY:O	1:C:448:ARG:HG3	2.17	0.45
1:C:678:SER:O	1:C:682:SER:OG	2.26	0.45
1:A:669:LEU:HD13	1:A:765:CYS:HB3	1.98	0.45
1:A:158:LEU:HD13	1:A:230:THR:HA	1.99	0.44
1:A:972:LEU:O	1:A:976:CYS:HB2	2.17	0.44
1:C:788:ALA:HA	1:C:882:ASN:HD22	1.83	0.44
1:A:711:GLU:HG3	1:A:718:ARG:HH12	1.82	0.44
1:A:888:LEU:HD22	1:A:926:ARG:NH1	2.32	0.44
1:C:272:LEU:HD11	1:C:324:GLN:HB2	2.00	0.44
1:C:676:VAL:O	1:C:680:TRP:HB2	2.18	0.44
1:A:127:GLU:HB2	1:A:131:HIS:HB2	1.99	0.44
1:A:1045:GLN:HG3	1:A:1089:CYS:SG	2.56	0.44
3:B:15:LEU:HD21	3:B:23:LYS:HB2	1.99	0.44
3:B:29:ARG:NH1	3:B:154:ASN:OD1	2.51	0.44
1:C:443:GLN:NE2	1:C:447:MET:HB2	2.33	0.44
1:C:691:ASP:OD1	1:C:692:VAL:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:VAL:H	1:A:868:LEU:HD23	1.82	0.44
3:B:96:VAL:HA	3:B:99:LYS:HD2	2.00	0.44
1:C:48:VAL:HG13	1:C:90:LEU:HD13	2.00	0.44
1:C:513:VAL:O	1:C:517:MET:HB2	2.17	0.44
1:C:94:VAL:HG11	1:C:119:ILE:HG21	1.98	0.44
1:C:560:PHE:N	1:C:561:PRO:HD2	2.32	0.44
1:C:788:ALA:O	1:C:792:LEU:N	2.51	0.44
1:A:594:THR:OG1	1:A:597:VAL:HG12	2.17	0.44
1:A:616:PRO:HB2	1:A:658:GLN:CG	2.46	0.44
1:A:1035:SER:HA	1:A:1038:TRP:CE2	2.52	0.44
3:B:46:GLU:O	3:B:65:ASP:HB3	2.18	0.44
1:C:306:ALA:HB3	1:C:319:LEU:HD13	1.99	0.44
1:A:494:SER:HB3	1:A:545:ASP:OD2	2.18	0.44
1:A:873:LEU:HD11	1:A:915:ILE:HA	2.00	0.44
1:C:613:ARG:HB2	1:C:654:LEU:HD13	1.98	0.44
1:C:849:HIS:O	1:C:853:LYS:HB2	2.18	0.44
1:A:846:ASN:O	1:A:850:ILE:HG13	2.18	0.43
1:C:1082:MET:HG3	1:C:1083:HIS:CD2	2.53	0.43
1:A:466:LEU:HD23	1:A:534:LEU:HD22	1.99	0.43
1:A:806:LEU:HB3	1:A:809:GLU:HG3	2.00	0.43
1:C:240:MET:HG2	1:C:283:ASP:O	2.17	0.43
1:A:285:LYS:HA	1:A:336:LEU:HD13	2.00	0.43
1:A:518:PHE:CE2	1:A:561:PRO:HB2	2.52	0.43
1:A:554:THR:OG1	1:A:603:HIS:NE2	2.41	0.43
1:A:680:TRP:NE1	1:A:775:ASN:HB2	2.33	0.43
1:C:595:ARG:HB3	1:C:827:PRO:HD2	2.00	0.43
1:A:830:LYS:HD2	1:A:830:LYS:HA	1.78	0.43
1:A:865:VAL:HB	1:A:868:LEU:HB3	2.01	0.43
1:C:316:TYR:CE2	1:C:320:LYS:HD2	2.53	0.43
1:C:498:PRO:HA	1:C:501:VAL:HG22	2.01	0.43
3:D:44:GLY:HA2	3:D:74:GLY:H	1.83	0.43
1:C:97:LEU:HA	1:C:101:GLY:HA3	2.01	0.43
1:C:192:PHE:O	1:C:196:THR:HG22	2.18	0.43
1:C:651:ALA:O	1:C:655:ILE:HG13	2.19	0.43
1:C:323:CYS:HB2	1:C:359:PHE:CE1	2.53	0.43
3:B:30:HIS:HB3	3:B:50:LEU:HD21	2.01	0.43
1:A:321:ARG:HA	1:A:321:ARG:HH21	1.84	0.43
1:C:797:GLU:HG3	1:C:798:PRO:HD3	2.00	0.43
3:D:12:LYS:HE3	3:D:64:TRP:CD1	2.54	0.43
1:C:411:PRO:O	1:C:423:ARG:NH1	2.50	0.43
1:C:676:VAL:O	1:C:680:TRP:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1044:CYS:O	1:C:1048:THR:OG1	2.35	0.43
1:A:264:GLN:HB2	1:A:318:PHE:CE1	2.53	0.43
1:A:1039:LYS:NZ	1:A:1082:MET:SD	2.88	0.43
1:A:216:LYS:O	1:A:219:ALA:HB3	2.19	0.42
3:B:69:GLN:NE2	3:B:71:LYS:HE2	2.34	0.42
1:C:48:VAL:HB	1:C:49:PRO:HD3	2.01	0.42
1:A:959:GLU:O	1:A:963:ARG:HG3	2.20	0.42
1:C:539:LEU:HD21	1:C:573:VAL:HG12	2.01	0.42
1:C:563:VAL:HG23	1:C:569:PHE:HB2	2.01	0.42
1:C:789:PRO:HD3	1:C:882:ASN:ND2	2.34	0.42
3:D:22:GLY:HA2	4:D:301:GTP:H5'	2.00	0.42
1:A:406:VAL:HG23	1:A:501:VAL:HG12	2.00	0.42
1:A:574:PHE:HZ	1:A:619:VAL:HG13	1.84	0.42
1:A:924:HIS:HB2	1:A:1031:THR:OG1	2.18	0.42
1:A:1056:LEU:HD23	1:A:1056:LEU:HA	1.91	0.42
1:A:48:VAL:HB	1:A:49:PRO:HD3	2.01	0.42
1:C:1043:SER:O	1:C:1047:THR:CB	2.66	0.42
1:A:356:PHE:CZ	1:A:371:THR:HG23	2.54	0.42
1:C:159:ARG:HH21	3:D:110:ARG:HG3	1.85	0.42
1:A:542:ASP:OD2	1:A:544:LYS:NZ	2.46	0.42
1:C:436:PHE:O	1:C:440:ARG:HB2	2.19	0.42
1:C:497:SER:HB3	1:C:498:PRO:HD2	2.02	0.42
1:C:631:LYS:HA	1:C:631:LYS:HD2	1.80	0.42
1:A:55:ALA:HA	1:A:64:ARG:HA	2.01	0.42
1:A:235:ILE:HG21	1:A:274:ALA:HB2	2.01	0.42
1:A:928:SER:HA	1:A:1038:TRP:CH2	2.55	0.42
1:A:1070:THR:O	1:A:1074:THR:OG1	2.26	0.42
1:C:618:LEU:O	1:C:621:PRO:HD2	2.20	0.42
1:A:456:LYS:HA	1:A:456:LYS:HD2	1.85	0.41
1:A:624:ASP:N	1:A:624:ASP:OD1	2.53	0.41
1:A:691:ASP:OD1	1:A:693:ASP:N	2.53	0.41
1:C:65:HIS:O	1:C:69:GLN:HB2	2.19	0.41
1:C:114:ASP:O	1:C:118:ARG:HG3	2.20	0.41
3:D:54:THR:HB	3:D:57:GLY:O	2.20	0.41
1:A:585:THR:OG1	1:A:587:GLU:O	2.35	0.41
1:A:1085:GLN:OE1	3:B:95:ARG:NH1	2.53	0.41
3:B:68:GLY:N	4:B:301:GTP:O2G	2.38	0.41
1:C:680:TRP:CD1	1:C:772:LEU:HD22	2.55	0.41
1:C:716:LEU:O	1:C:720:ARG:HG3	2.21	0.41
1:C:930:LYS:HD3	1:C:962:VAL:HG22	2.02	0.41
1:C:1030:ILE:O	1:C:1034:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:ARG:HB3	1:A:890:PRO:HD3	2.02	0.41
1:C:91:LYS:HE2	1:C:132:TRP:CZ2	2.55	0.41
1:C:337:LEU:HD23	1:C:337:LEU:HA	1.94	0.41
1:C:801:LYS:HB2	1:C:833:LEU:HD21	2.02	0.41
1:A:22:ASP:O	1:A:30:ARG:NH2	2.53	0.41
1:A:381:HIS:HB3	1:A:384:LEU:HB2	2.02	0.41
1:C:379:PHE:CE1	1:C:390:LEU:HD21	2.56	0.41
1:C:601:ARG:NE	1:C:644:GLU:OE1	2.53	0.41
1:C:900:VAL:HG22	1:C:912:VAL:HG23	2.03	0.41
3:B:85:CYS:HB2	3:B:164:LEU:HD22	2.03	0.41
1:C:272:LEU:HD13	1:C:321:ARG:NH2	2.35	0.41
1:C:359:PHE:HD1	1:C:367:LEU:HD13	1.86	0.41
3:D:13:LEU:HB2	3:D:85:CYS:SG	2.61	0.41
3:D:123:LYS:HG2	4:D:301:GTP:C5	2.56	0.41
1:A:320:LYS:HG2	1:A:367:LEU:HD21	2.03	0.41
1:A:578:PHE:O	1:A:581:VAL:HB	2.20	0.41
1:A:1035:SER:HA	1:A:1038:TRP:NE1	2.36	0.41
1:A:1105:ARG:N	1:A:1106:PRO:HD2	2.36	0.41
1:C:124:ILE:HD13	1:C:132:TRP:CZ3	2.56	0.41
1:C:462:ALA:HB1	1:C:510:LEU:HD12	2.03	0.41
1:C:583:PHE:O	1:C:601:ARG:HD3	2.20	0.41
1:C:850:ILE:O	1:C:854:ALA:CB	2.68	0.41
1:C:1073:PHE:HA	1:C:1076:VAL:HG12	2.02	0.41
3:D:29:ARG:NH1	3:D:35:PHE:HB2	2.36	0.41
1:A:31:LEU:O	1:A:35:LYS:HB2	2.20	0.41
1:A:786:LEU:HD12	1:A:786:LEU:HA	1.97	0.40
3:B:48:HIS:O	3:B:63:VAL:HG22	2.21	0.40
3:B:122:ASN:HA	3:B:149:ILE:HG13	2.02	0.40
1:C:1082:MET:HG3	1:C:1083:HIS:HD2	1.86	0.40
1:A:595:ARG:H	1:A:827:PRO:CB	2.27	0.40
1:C:577:LEU:O	1:C:581:VAL:HG23	2.22	0.40
3:D:95:ARG:CZ	3:D:130:LYS:HB3	2.51	0.40
1:C:877:PHE:HB3	1:C:880:LEU:HD11	2.03	0.40
1:A:273:ILE:HD12	1:A:273:ILE:HA	2.00	0.40
1:A:545:ASP:OD2	1:A:548:ILE:HG12	2.22	0.40
1:A:1065:LEU:HD22	1:A:1065:LEU:H	1.86	0.40
1:C:699:VAL:HG23	1:C:701:THR:HG23	2.03	0.40
1:C:745:LYS:HA	1:C:750:VAL:HG22	2.04	0.40
1:C:1101:TYR:CZ	1:C:1105:ARG:HD3	2.56	0.40
1:A:571:PRO:HG2	1:C:572:GLN:HA	2.04	0.40
3:D:86:ALA:O	3:D:117:ILE:HA	2.22	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	1059/1204 (88%)	1036 (98%)	23 (2%)	0	100	100
1	C	1063/1204 (88%)	1036 (98%)	27 (2%)	0	100	100
3	B	168/216 (78%)	166 (99%)	2 (1%)	0	100	100
3	D	168/216 (78%)	160 (95%)	8 (5%)	0	100	100
All	All	2458/2840 (86%)	2398 (98%)	60 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	965/1073 (90%)	959 (99%)	6 (1%)	86	95
1	C	968/1073 (90%)	961 (99%)	7 (1%)	84	94
3	B	150/185 (81%)	150 (100%)	0	100	100
3	D	150/185 (81%)	149 (99%)	1 (1%)	84	94
All	All	2233/2516 (89%)	2219 (99%)	14 (1%)	86	95

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	MET
1	A	190	PHE
1	A	356	PHE
1	A	568	GLU
1	A	1115	MET
1	A	1134	LEU
1	C	72	GLU
1	C	119	ILE
1	C	313	GLU
1	C	466	LEU
1	C	610	LYS
1	C	623	PHE
1	C	1028	LEU
3	D	56	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	GLN
1	A	443	GLN
1	A	516	GLN
1	C	642	GLN
1	C	882	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GTP	B	301	5	26,34,34	1.13	2 (7%)	32,54,54	1.59	7 (21%)
4	GTP	D	301	5	26,34,34	1.12	2 (7%)	32,54,54	1.66	7 (21%)

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
4	GTP	B	301	5	-	4/18/38/38	0/3/3/3
4	GTP	D	301	5	-	1/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	GTP	C5-C6	-4.01	1.39	1.47
4	D	301	GTP	C5-C6	-3.94	1.39	1.47
4	B	301	GTP	C2-N3	2.28	1.38	1.33
4	D	301	GTP	C2-N3	2.24	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	301	GTP	PB-O3B-PG	-3.97	119.20	132.83
4	B	301	GTP	PA-O3A-PB	-3.66	120.26	132.83
4	B	301	GTP	C5-C6-N1	3.23	119.65	113.95
4	D	301	GTP	C3'-C2'-C1'	3.21	105.81	100.98
4	D	301	GTP	C5-C6-N1	3.20	119.61	113.95
4	B	301	GTP	PB-O3B-PG	-3.17	121.96	132.83
4	B	301	GTP	C3'-C2'-C1'	3.03	105.54	100.98
4	B	301	GTP	C8-N7-C5	3.01	108.73	102.99
4	D	301	GTP	C8-N7-C5	2.97	108.65	102.99
4	D	301	GTP	PA-O3A-PB	-2.94	122.75	132.83
4	D	301	GTP	C2-N1-C6	-2.87	119.81	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	301	GTP	C2-N1-C6	-2.80	119.94	125.10
4	D	301	GTP	O6-C6-C5	-2.14	120.19	124.37
4	B	301	GTP	O6-C6-C5	-2.14	120.20	124.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	GTP	O4'-C4'-C5'-O5'
4	B	301	GTP	C3'-C4'-C5'-O5'
4	B	301	GTP	PB-O3B-PG-O2G
4	D	301	GTP	O4'-C4'-C5'-O5'
4	B	301	GTP	C5'-O5'-PA-O1A

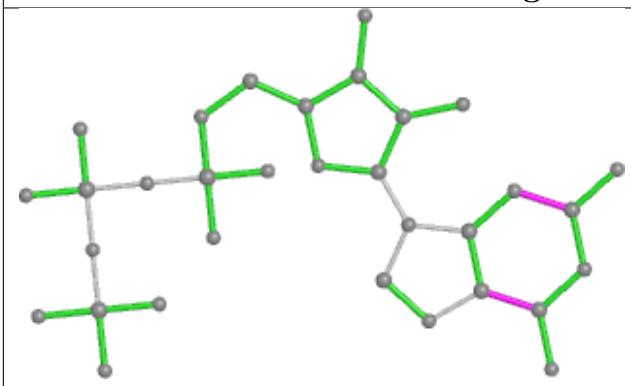
There are no ring outliers.

2 monomers are involved in 8 short contacts:

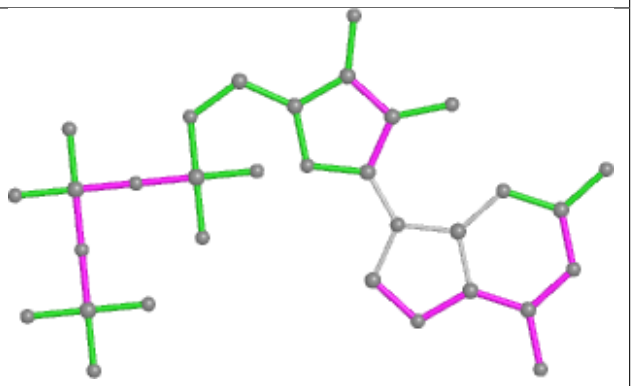
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	GTP	5	0
4	D	301	GTP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

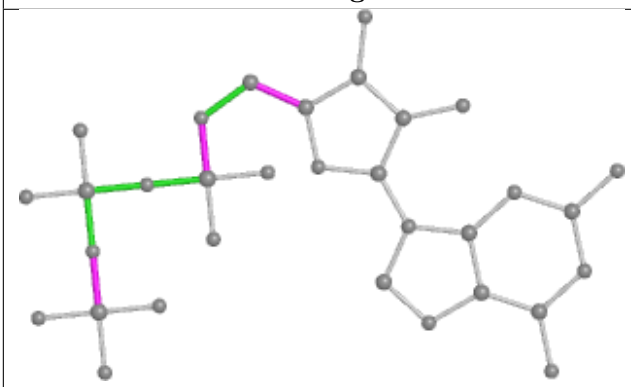
Ligand GTP B 301



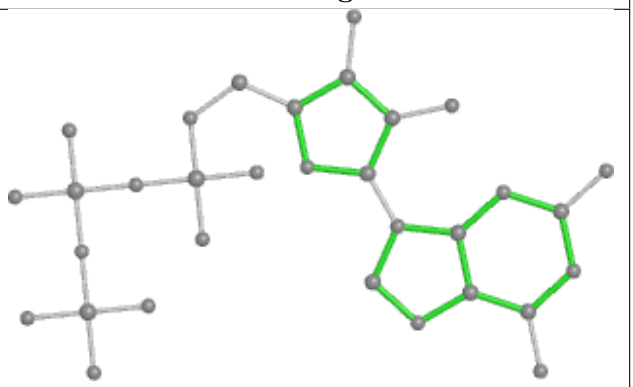
Bond lengths



Bond angles

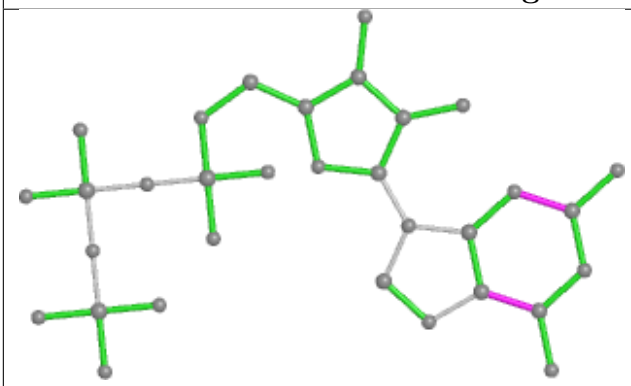


Torsions

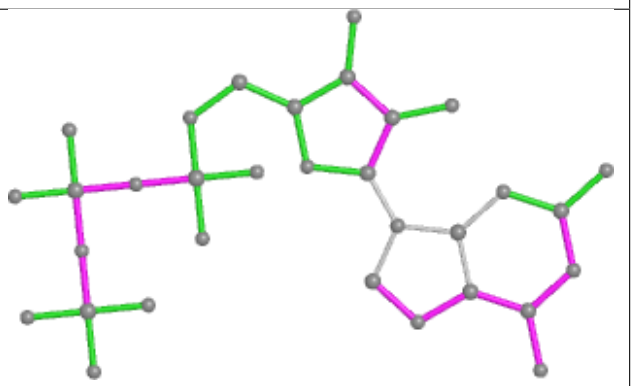


Rings

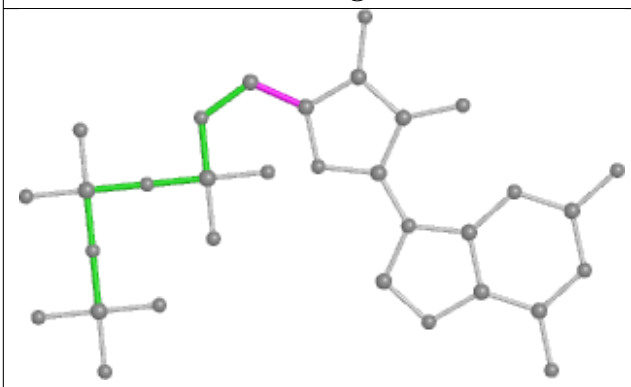
Ligand GTP D 301



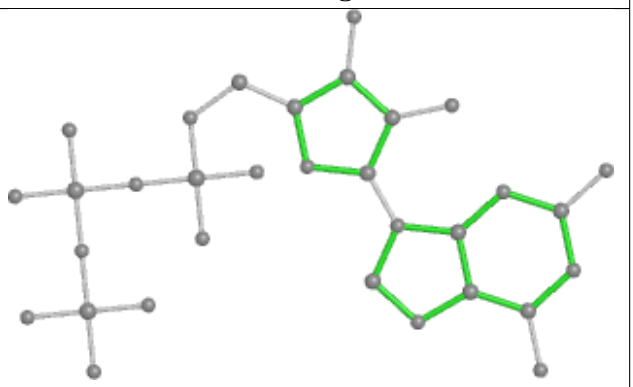
Bond lengths



Bond angles



Torsions



Rings

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	1069/1204 (88%)	0.16	44 (4%) 37 14	23, 57, 121, 215	0
1	C	1073/1204 (89%)	0.42	94 (8%) 10 3	27, 74, 139, 249	0
2	E	0/13	-	-	-	-
2	F	0/13	-	-	-	-
3	B	170/216 (78%)	0.01	2 (1%) 79 54	28, 49, 80, 109	0
3	D	170/216 (78%)	0.01	2 (1%) 79 54	27, 52, 91, 122	0
All	All	2482/2866 (86%)	0.25	142 (5%) 23 8	23, 63, 129, 249	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	338	GLY	12.2
1	C	1073	PHE	7.4
1	A	708	PRO	6.3
1	C	829	PHE	6.1
1	A	339	ALA	5.8
1	A	586	VAL	5.8
1	A	825	ASP	5.8
1	A	826	SER	5.8
1	C	703	GLN	5.6
1	A	819	PRO	5.5
1	C	712	ASP	5.3
1	A	818	GLN	5.2
1	A	712	ASP	5.1
1	C	1100	ILE	5.1
1	C	4	ASP	5.0
1	C	709	GLY	4.9
1	C	1080	LEU	4.6
1	A	1067	ASP	4.5
1	A	829	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	1101	TYR	4.4
1	C	823	LEU	4.3
1	C	795	MET	4.2
1	C	453	LEU	4.1
1	C	828	VAL	4.1
1	C	1069	VAL	4.1
1	C	3	MET	3.9
1	C	1106	PRO	3.9
1	A	821	LEU	3.8
1	C	702	ASP	3.8
1	C	1037	ALA	3.7
1	C	491	SER	3.7
1	C	803	LEU	3.7
1	C	1085	GLN	3.6
1	C	827	PRO	3.6
1	C	813	ILE	3.5
1	A	711	GLU	3.5
1	C	710	LEU	3.5
1	C	339	ALA	3.5
1	C	1104	LEU	3.4
1	C	812	ALA	3.4
1	A	1063	THR	3.4
1	A	1104	LEU	3.4
1	C	787	TYR	3.3
1	C	1083	HIS	3.2
1	A	830	LYS	3.2
1	C	1032	ALA	3.2
1	A	709	GLY	3.2
1	A	589	SER	3.1
1	C	1046	ARG	3.1
1	C	1029	LEU	3.1
1	C	797	GLU	3.1
1	C	817	PRO	3.1
1	C	1033	PHE	3.0
1	A	937	ARG	3.0
1	C	587	GLU	3.0
1	A	1060	LEU	3.0
1	C	509	PHE	3.0
1	A	704	LYS	3.0
1	C	704	LYS	3.0
1	C	1082	MET	3.0
1	C	1036	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	711	GLU	3.0
1	A	1089	CYS	3.0
1	C	510	LEU	2.9
1	C	692	VAL	2.9
1	A	699	VAL	2.9
1	C	2	ALA	2.9
1	C	1115	MET	2.9
1	A	491	SER	2.8
3	D	36	GLU	2.8
1	C	1096	LEU	2.8
1	C	310	GLY	2.8
1	A	1097	ALA	2.8
1	C	687	ARG	2.8
1	C	791	MET	2.8
1	A	590	LYS	2.8
1	A	707	ASP	2.8
1	C	1060	LEU	2.8
1	A	1053	TRP	2.8
1	A	1051	LEU	2.7
1	C	819	PRO	2.7
1	C	1077	LEU	2.7
1	C	1044	CYS	2.7
1	C	1086	HIS	2.7
1	C	586	VAL	2.7
1	A	1090	MET	2.6
1	C	799	PHE	2.6
1	C	956	MET	2.6
1	C	884	PRO	2.6
1	A	713	PRO	2.6
1	C	494	SER	2.6
1	A	820	LEU	2.5
1	C	800	THR	2.5
1	A	214	GLU	2.5
1	A	714	CYS	2.5
1	C	824	ASN	2.5
1	C	814	LEU	2.4
1	C	1038	TRP	2.4
1	C	805	MET	2.4
1	A	1059	VAL	2.4
1	C	1119	PRO	2.3
1	C	547	LEU	2.3
1	C	1072	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	338	GLY	2.3
1	C	1094	VAL	2.3
1	C	721	MET	2.3
1	C	1025	CYS	2.3
1	C	1010	GLU	2.3
1	C	465	TRP	2.3
3	B	41	ALA	2.2
1	C	960	GLN	2.2
1	A	1064	LEU	2.2
1	C	820	LEU	2.2
1	A	692	VAL	2.2
1	C	700	GLY	2.2
1	C	470	LEU	2.2
1	C	1097	ALA	2.2
1	A	1066	ALA	2.2
1	C	595	ARG	2.2
1	C	693	ASP	2.2
1	C	695	PHE	2.2
1	C	1098	PHE	2.2
1	C	503	TRP	2.2
1	A	1098	PHE	2.2
1	C	701	THR	2.2
1	C	337	LEU	2.1
1	C	1087	ASP	2.1
1	C	1090	MET	2.1
1	C	1093	LEU	2.1
1	C	786	LEU	2.1
1	C	1074	THR	2.1
1	C	838	ARG	2.1
1	A	823	LEU	2.1
3	D	75	LEU	2.0
1	A	1071	TRP	2.0
1	C	472	THR	2.0
3	B	39	TYR	2.0
1	A	1101	TYR	2.0
1	A	828	VAL	2.0
1	C	492	LEU	2.0
1	C	1028	LEU	2.0
1	A	710	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

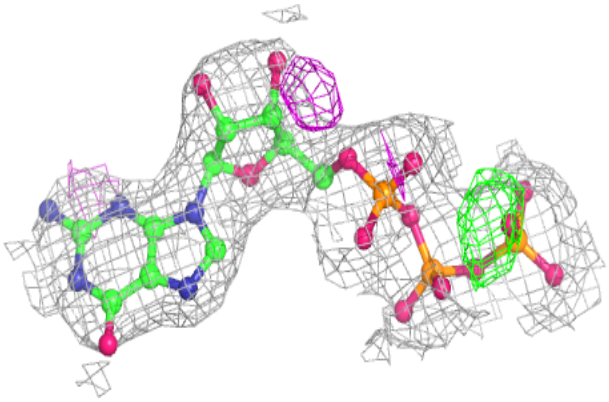
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

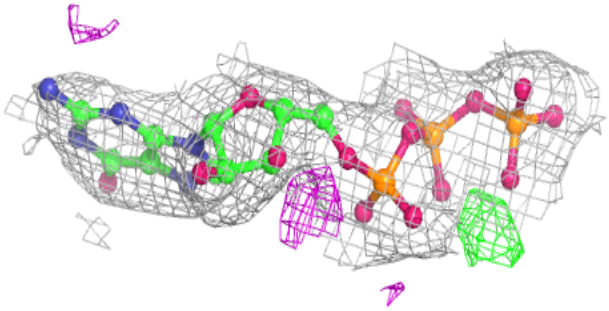
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	D	302	1/1	0.91	0.26	54,54,54,54	0
5	MG	B	302	1/1	0.95	0.18	41,41,41,41	0
4	GTP	B	301	32/32	0.96	0.18	33,55,63,71	0
4	GTP	D	301	32/32	0.97	0.17	38,61,81,85	0

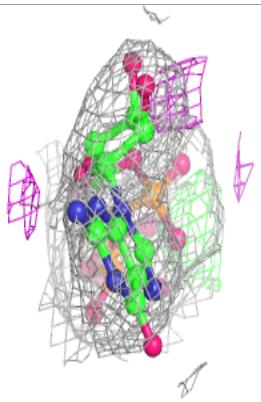
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GTP B 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

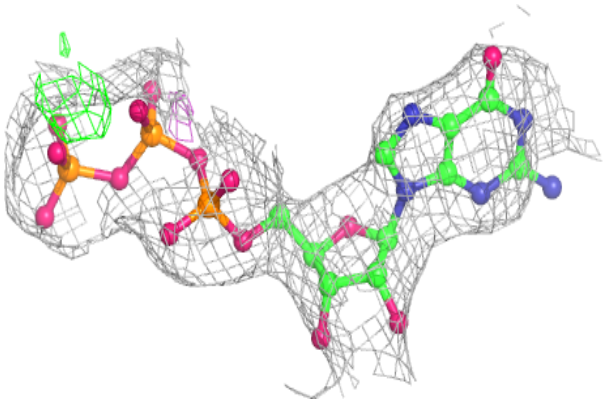


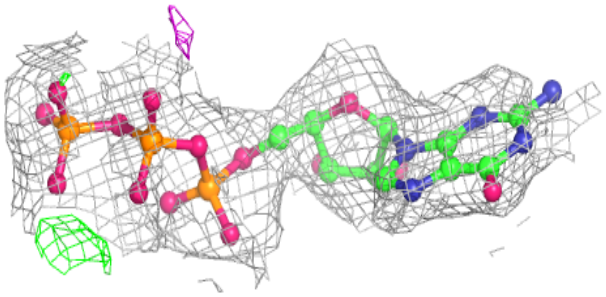


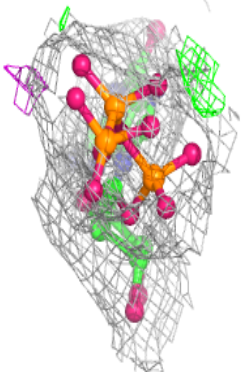


Electron density around GTP D 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.