



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:50 pm BST

PDB ID : 2JLG
Title : STRUCTURAL EXPLANATION FOR THE ROLE OF MN IN THE ACTIVITY OF PHI6 RNA-DEPENDENT RNA POLYMERASE
Authors : Poranen, M.M.; Salgado, P.S.; Koivunen, M.R.L.; Wright, S.; Bamford, D.H.; Stuart, D.I.; Grimes, J.M.
Deposited on : 2008-09-09
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

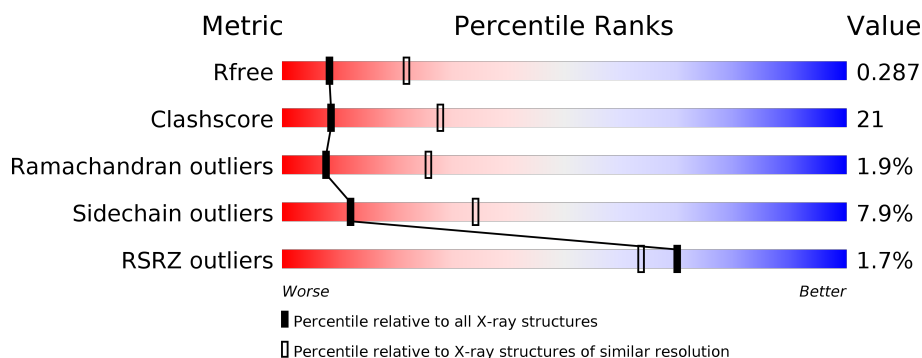
1 Overall quality at a glance

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))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$. 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	664	<div> <div>69%</div> <div>26%</div> <div>• •</div> </div>
1	B	664	<div> <div>71%</div> <div>25%</div> <div>•</div> </div>
1	C	664	<div> <div>2%</div> <div>50%</div> <div>41%</div> <div>7%</div> <div>• •</div> </div>
2	D	5	<div> <div>100%</div> <div>80%</div> <div>20%</div> </div>
2	E	5	<div> <div>20%</div> <div>60%</div> <div>40%</div> </div>
2	F	5	<div> <div>40%</div> <div>40%</div> <div>20%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16099 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 RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	0
			5265	3342	915	976	32			
1	B	664	Total	C	N	O	S	0	0	0
			5265	3342	915	976	32			
1	C	651	Total	C	N	O	S	0	0	0
			5175	3287	898	959	31			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	conflict	UNP P11124
A	491	GLN	GLU	engineered mutation	UNP P11124
B	456	MET	ILE	conflict	UNP P11124
B	491	GLN	GLU	engineered mutation	UNP P11124
C	456	MET	ILE	conflict	UNP P11124
C	491	GLN	GLU	engineered mutation	UNP P11124

- Molecule 2 is a DNA chain called 5'-D(*DT DT DT DC DCP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	5	Total	C	N	O	P	0	0	0
			95	48	12	31	4			
2	E	5	Total	C	N	O	P	0	0	0
			95	48	12	31	4			
2	F	4	Total	C	N	O	P	0	0	0
			75	38	10	24	3			

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mn	0	0
			1	1		

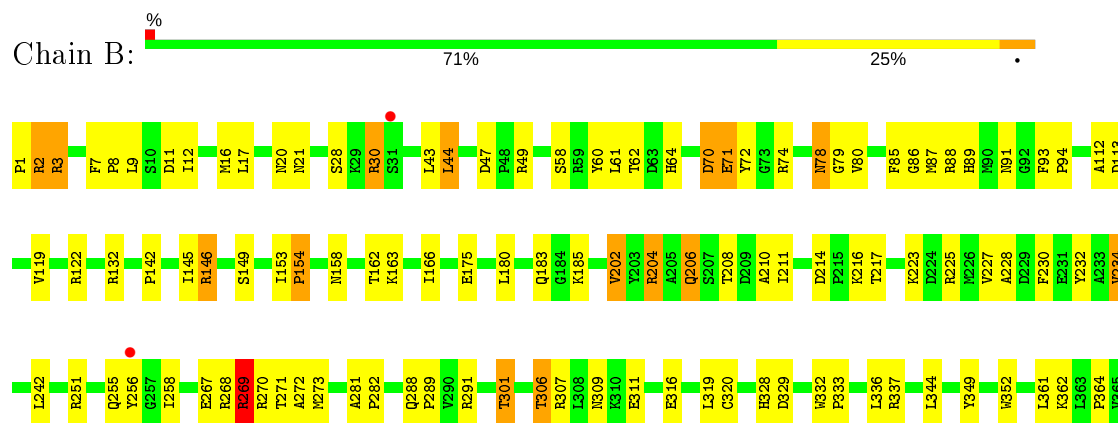
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

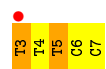
• Molecule 1: RNA-DIRECTED RNA POLYMERASE



• Molecule 1: RNA-DIRECTED RNA POLYMERASE



- Molecule 2: 5'-D(*DT DT DT DC DCP)-3'



- Molecule 2: 5'-D(*DT DT DT DC DCP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	109.03Å 109.03Å 158.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 2.80 19.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.94-2.80) 99.6 (19.94-2.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.79Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.216 , 0.295 0.206 , 0.287	Depositor DCC
R_{free} test set	2639 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.038 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16099	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, MN

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	0.44	0/5396	0.81	20/7297 (0.3%)
1	B	0.44	0/5396	0.79	19/7297 (0.3%)
1	C	0.42	0/5305	0.64	2/7173 (0.0%)
2	D	0.76	0/104	1.55	1/158 (0.6%)
2	E	0.77	0/104	1.75	3/158 (1.9%)
2	F	0.93	0/82	1.87	4/124 (3.2%)
All	All	0.44	0/16387	0.78	49/22207 (0.2%)

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	C	0	1

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ARG	NE-CZ-NH2	-14.54	113.03	120.30
1	A	307	ARG	NE-CZ-NH1	-14.22	113.19	120.30
1	A	269	ARG	NE-CZ-NH2	14.09	127.34	120.30
1	A	269	ARG	NE-CZ-NH1	-14.04	113.28	120.30
1	B	307	ARG	NE-CZ-NH2	-13.03	113.79	120.30
1	B	269	ARG	NE-CZ-NH2	-12.74	113.93	120.30
1	B	506	ARG	NE-CZ-NH2	-12.69	113.95	120.30
1	A	307	ARG	NE-CZ-NH2	12.62	126.61	120.30
1	A	204	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	B	307	ARG	NE-CZ-NH1	12.32	126.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	ARG	NE-CZ-NH1	-12.24	114.18	120.30
1	B	204	ARG	NE-CZ-NH2	12.22	126.41	120.30
1	B	269	ARG	NE-CZ-NH1	12.04	126.32	120.30
1	B	506	ARG	NE-CZ-NH1	11.99	126.29	120.30
1	A	584	ARG	NE-CZ-NH2	-11.98	114.31	120.30
1	A	584	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	B	584	ARG	NE-CZ-NH1	-11.50	114.55	120.30
1	A	506	ARG	NE-CZ-NH1	-11.29	114.66	120.30
1	A	30	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	B	584	ARG	NE-CZ-NH2	10.39	125.50	120.30
1	B	30	ARG	NE-CZ-NH1	-10.18	115.21	120.30
1	A	30	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	A	506	ARG	NE-CZ-NH2	10.12	125.36	120.30
1	B	30	ARG	NE-CZ-NH2	9.69	125.15	120.30
2	F	6	DC	O4'-C1'-N1	6.96	112.88	108.00
2	F	5	DT	N3-C4-O4	6.85	124.01	119.90
1	A	204	ARG	CD-NE-CZ	6.76	133.06	123.60
1	A	307	ARG	CD-NE-CZ	6.73	133.03	123.60
1	B	307	ARG	CD-NE-CZ	6.54	132.75	123.60
1	C	207	SER	N-CA-C	-6.34	93.88	111.00
1	B	269	ARG	CD-NE-CZ	6.33	132.46	123.60
1	B	506	ARG	CD-NE-CZ	6.23	132.32	123.60
1	B	204	ARG	CD-NE-CZ	6.19	132.26	123.60
1	A	584	ARG	CD-NE-CZ	6.16	132.22	123.60
2	F	5	DT	C1'-O4'-C4'	-5.93	104.17	110.10
1	A	506	ARG	CD-NE-CZ	5.93	131.90	123.60
1	A	71	GLU	N-CA-C	5.93	127.00	111.00
1	A	269	ARG	CD-NE-CZ	5.75	131.66	123.60
1	B	584	ARG	CD-NE-CZ	5.71	131.60	123.60
1	B	202	VAL	CB-CA-C	-5.55	100.86	111.40
2	F	4	DT	C4-C5-C7	5.52	122.31	119.00
1	C	633	THR	C-N-CA	5.52	135.50	121.70
2	D	7	DC	O4'-C1'-N1	5.35	111.75	108.00
1	B	2	ARG	C-N-CA	5.31	134.98	121.70
2	E	3	DT	O4'-C1'-N1	5.26	111.68	108.00
2	E	5	DT	C4-C5-C7	5.22	122.13	119.00
1	A	71	GLU	C-N-CA	5.20	134.71	121.70
2	E	5	DT	C6-C5-C7	-5.16	119.80	122.90
1	A	146	ARG	CB-CG-CD	5.10	124.87	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	627	LYS	Peptide

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	5265	0	5167	175	0
1	B	5265	0	5167	146	1
1	C	5175	0	5071	320	0
2	D	95	0	60	24	0
2	E	95	0	60	19	0
2	F	75	0	48	7	0
3	A	32	0	12	5	0
3	B	32	0	12	6	0
3	C	64	0	24	7	0
4	C	1	0	0	0	0
All	All	16099	0	15621	652	1

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 21.

All (652) 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:270:ARG:NH2	3:A:1665:GTP:H3'	1.56	1.20
1:C:301:THR:HG22	1:C:448:GLN:O	1.54	1.08
1:C:325:VAL:HA	1:C:326:SER:HB2	1.33	1.06
1:C:206:GLN:HA	1:C:207:SER:HB3	1.35	1.03
1:B:364:PRO:HA	1:B:387:LEU:HD22	1.40	1.00
1:C:206:GLN:HA	1:C:207:SER:CB	1.93	0.98
1:A:605:MET:HB3	1:A:606:ALA:HA	1.42	0.97
1:A:364:PRO:HA	1:A:387:LEU:HD22	1.44	0.97
1:A:150:SER:H	2:D:5:DT:H5''	1.27	0.96
1:C:628:LEU:HB2	1:C:629:GLN:HA	1.49	0.94
1:C:213:LEU:HD12	1:C:213:LEU:H	1.36	0.89
1:A:609:ALA:HB1	1:A:612:ALA:HB2	1.56	0.88
1:C:428:ASP:OD1	1:C:431:SER:OG	1.94	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ASP:HB3	1:B:72:TYR:H	1.41	0.84
1:A:270:ARG:HH21	3:A:1665:GTP:H3'	1.42	0.83
1:C:364:PRO:HA	1:C:387:LEU:CD2	2.10	0.82
1:C:502:LEU:HA	1:C:503:TYR:HB2	1.61	0.82
2:D:4:DT:H4'	2:D:5:DT:H5'	1.60	0.82
1:C:325:VAL:HA	1:C:326:SER:CB	2.09	0.82
1:A:2:ARG:HH11	1:B:64:HIS:CD2	1.97	0.81
1:C:218:GLY:HA2	1:C:219:LYS:HG2	1.62	0.81
1:A:8:PRO:HD2	1:A:11:ASP:HB2	1.61	0.81
1:C:364:PRO:HA	1:C:387:LEU:HD22	1.61	0.81
1:C:521:MET:HB2	1:C:558:TYR:CE2	2.15	0.81
1:A:214:ASP:OD1	1:A:216:LYS:HG2	1.81	0.80
1:A:2:ARG:HH11	1:B:64:HIS:HD2	1.29	0.80
1:C:505:SER:O	1:C:506:ARG:HG2	1.82	0.80
1:A:270:ARG:HH22	3:A:1665:GTP:H3'	1.44	0.79
1:C:419:ALA:HB1	1:C:422:LEU:HD12	1.62	0.79
1:C:521:MET:HB2	1:C:558:TYR:CD2	2.20	0.77
1:B:8:PRO:HD2	1:B:11:ASP:HB2	1.65	0.77
1:C:249:ALA:HB1	1:C:260:VAL:HG21	1.67	0.77
1:C:46:VAL:HB	1:C:258:ILE:HG21	1.68	0.76
1:C:57:LEU:HD21	1:C:571:ILE:HG12	1.66	0.76
1:B:281:ALA:HB3	1:B:282:PRO:HD3	1.67	0.76
1:A:281:ALA:HB3	1:A:282:PRO:HD3	1.67	0.76
1:A:605:MET:HE3	1:A:610:GLY:O	1.88	0.74
1:A:217:THR:HG21	1:A:219:LYS:HB2	1.69	0.74
1:A:603:ALA:O	1:A:606:ALA:HB2	1.86	0.73
1:C:217:THR:HB	1:C:218:GLY:HA3	1.69	0.73
1:C:175:GLU:HA	1:C:352:TRP:CE3	2.24	0.73
1:C:46:VAL:HB	1:C:258:ILE:HG12	1.69	0.72
1:C:85:PHE:HE2	1:C:220:PHE:HE1	1.34	0.72
1:B:629:GLN:HG3	2:E:7:DC:H4'	1.72	0.71
1:C:281:ALA:HB3	1:C:282:PRO:HD3	1.71	0.71
1:C:61:LEU:HD23	1:C:65:PHE:HD2	1.54	0.71
1:B:47:ASP:OD2	1:B:49:ARG:HD3	1.91	0.71
1:B:2:ARG:HG3	1:B:3:ARG:O	1.91	0.70
1:C:61:LEU:O	1:C:65:PHE:HB2	1.91	0.70
1:A:214:ASP:HB3	1:A:217:THR:HB	1.74	0.70
1:C:49:ARG:HB3	1:C:579:PHE:CE2	2.27	0.69
1:A:180:LEU:HD23	1:A:185:LYS:HE3	1.74	0.69
1:A:301:THR:HG22	1:A:440:TRP:O	1.93	0.69
1:A:217:THR:HG22	1:A:219:LYS:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:GLU:CG	2:D:7:DC:H41	2.05	0.69
1:A:2:ARG:NH1	1:B:64:HIS:HD2	1.90	0.69
1:A:217:THR:CG2	1:A:219:LYS:HB2	2.22	0.69
1:C:588:GLU:HA	1:C:591:LEU:HB3	1.73	0.69
1:B:206:GLN:HG3	3:B:1665:GTP:N2	2.08	0.69
1:B:71:GLU:H	1:B:71:GLU:CD	1.93	0.69
1:A:30:ARG:HD3	1:A:31:SER:N	2.08	0.68
1:C:55:ASN:ND2	1:C:59:ARG:HE	1.91	0.68
1:C:37:ILE:HG13	1:C:37:ILE:O	1.91	0.68
1:C:624:ASP:O	1:C:627:LYS:HG2	1.94	0.68
1:B:180:LEU:HD23	1:B:185:LYS:HE3	1.75	0.68
1:B:206:GLN:CG	3:B:1665:GTP:N2	2.57	0.68
1:A:609:ALA:CB	1:A:612:ALA:HB2	2.23	0.68
1:A:301:THR:CG2	1:A:440:TRP:O	2.42	0.68
1:B:70:ASP:CB	1:B:72:TYR:H	2.07	0.67
1:B:656:ARG:HH11	1:B:656:ARG:HG2	1.59	0.67
1:C:232:TYR:CZ	1:C:242:LEU:HD22	2.30	0.67
1:C:363:LEU:HD12	1:C:364:PRO:HD2	1.76	0.67
1:C:325:VAL:CA	1:C:326:SER:HB2	2.17	0.66
1:A:656:ARG:HG2	1:A:656:ARG:HH11	1.60	0.66
1:C:325:VAL:O	1:C:453:ASP:OD1	2.13	0.66
1:C:636:ASP:N	1:C:637:VAL:HG12	2.11	0.66
1:B:206:GLN:CG	3:B:1665:GTP:HN21	2.09	0.66
1:C:206:GLN:CA	1:C:207:SER:CB	2.74	0.65
1:B:301:THR:CG2	1:B:440:TRP:O	2.45	0.65
1:B:311:GLU:OE2	1:B:513:ILE:HG22	1.97	0.65
1:C:55:ASN:O	1:C:59:ARG:HG3	1.96	0.65
1:C:322:ALA:HB1	1:C:491:GLN:HE22	1.61	0.64
1:C:85:PHE:CE2	1:C:220:PHE:HE1	2.14	0.64
1:B:628:LEU:O	2:E:7:DC:H1'	1.97	0.64
1:C:551:TRP:CZ3	1:C:587:ARG:HG3	2.31	0.64
1:B:204:ARG:HH22	2:E:5:DT:C7	2.11	0.64
1:B:301:THR:HB	1:B:448:GLN:O	1.98	0.63
1:C:53:PHE:CZ	1:C:57:LEU:HD22	2.32	0.63
1:C:640:ASN:O	1:C:644:VAL:HG23	1.97	0.63
1:A:47:ASP:OD2	1:A:49:ARG:HD3	1.98	0.63
1:A:609:ALA:HB1	1:A:612:ALA:CB	2.26	0.63
1:C:651:VAL:O	1:C:655:GLU:HB2	1.98	0.63
1:C:404:LEU:HD12	1:C:404:LEU:O	1.97	0.63
1:A:2:ARG:HA	1:B:566:ASP:OD2	1.99	0.63
1:C:328:HIS:HE1	1:C:405:LEU:HD23	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASN:HD22	1:A:79:GLY:N	1.95	0.63
1:A:17:LEU:HB3	1:A:153:ILE:HD13	1.81	0.62
1:C:649:VAL:HG12	1:C:650:SER:N	2.14	0.62
1:C:124:ASN:O	1:C:128:ARG:HG3	1.99	0.62
1:C:234:VAL:HG23	1:C:235:THR:HG23	1.80	0.62
1:B:47:ASP:OD1	1:B:49:ARG:NH1	2.32	0.62
1:A:399:ASP:OD1	2:D:7:DC:H3'	1.99	0.62
2:D:5:DT:O4	2:D:6:DC:C5	2.52	0.62
1:A:311:GLU:OE2	1:A:513:ILE:HG22	2.00	0.62
1:C:74:ARG:CZ	1:C:507:ARG:CB	2.78	0.62
1:C:343:GLU:HA	1:C:343:GLU:OE1	2.00	0.62
1:A:150:SER:N	2:D:5:DT:H5''	2.08	0.61
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.48	0.61
1:A:634:GLU:H	2:D:7:DC:H5	1.47	0.61
1:B:251:ARG:HH11	1:B:255:GLN:HE22	1.46	0.61
1:C:17:LEU:O	1:C:153:ILE:HG23	1.99	0.61
1:C:270:ARG:NH2	3:C:1666:GTP:O1B	2.32	0.61
1:B:301:THR:HG22	1:B:440:TRP:O	1.99	0.61
1:C:249:ALA:O	1:C:260:VAL:HG11	2.01	0.61
1:C:325:VAL:CA	1:C:326:SER:CB	2.78	0.61
2:D:3:DT:H5''	2:D:4:DT:C2	2.35	0.61
1:A:656:ARG:NH1	1:A:656:ARG:HG2	2.15	0.61
1:C:322:ALA:HB1	1:C:491:GLN:NE2	2.16	0.61
1:A:301:THR:HB	1:A:448:GLN:O	2.01	0.61
1:C:453:ASP:OD2	1:C:453:ASP:C	2.39	0.61
1:C:251:ARG:O	1:C:255:GLN:HB2	2.01	0.60
1:A:605:MET:CB	1:A:606:ALA:HA	2.20	0.60
1:A:506:ARG:HD3	1:A:511:SER:OG	2.01	0.60
1:B:301:THR:HG21	1:B:440:TRP:HA	1.82	0.60
1:C:373:GLU:O	1:C:374:GLN:HB2	2.00	0.60
2:E:3:DT:H4'	2:E:4:DT:C5	2.36	0.60
1:B:575:TRP:CG	1:B:583:TYR:HB2	2.36	0.60
1:C:55:ASN:HD21	1:C:59:ARG:HE	1.50	0.59
1:B:656:ARG:HG2	1:B:656:ARG:NH1	2.14	0.59
1:C:429:MET:HB2	1:C:430:PRO:HD3	1.84	0.59
1:B:1:PRO:HB3	1:B:2:ARG:HA	1.84	0.59
1:B:629:GLN:HG2	2:E:6:DC:C2	2.36	0.59
1:C:218:GLY:HA2	1:C:219:LYS:CG	2.30	0.59
1:C:56:GLU:HG2	1:C:574:CYS:SG	2.43	0.59
1:C:29:LYS:HA	1:C:376:HIS:HE1	1.67	0.59
1:C:85:PHE:HE2	1:C:220:PHE:CE1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:VAL:HG13	1:C:326:SER:HB3	1.84	0.59
1:B:1:PRO:CB	1:B:2:ARG:HA	2.32	0.58
1:C:46:VAL:CB	1:C:258:ILE:HG12	2.33	0.58
1:C:628:LEU:CB	1:C:629:GLN:HA	2.28	0.58
1:B:204:ARG:NH1	1:B:530:TYR:OH	2.36	0.58
1:C:53:PHE:HZ	1:C:571:ILE:HG23	1.69	0.58
1:C:549:LEU:HD11	1:C:598:LEU:HD22	1.84	0.58
1:A:634:GLU:HG3	2:D:7:DC:H41	1.69	0.58
1:B:605:MET:O	1:B:606:ALA:HB3	2.03	0.58
1:C:146:ARG:HG3	1:C:147:LYS:N	2.19	0.58
1:B:9:LEU:HD11	1:B:28:SER:HB2	1.86	0.58
1:C:74:ARG:CZ	1:C:507:ARG:HB3	2.33	0.57
1:A:208:THR:HG21	1:A:523:ASN:OD1	2.03	0.57
1:A:633:THR:HG22	2:D:7:DC:C6	2.39	0.57
1:C:86:GLY:O	1:C:89:HIS:HD2	1.86	0.57
1:A:230:PHE:O	1:A:234:VAL:HG22	2.04	0.57
1:C:411:LEU:HD13	1:C:439:TYR:CZ	2.39	0.57
1:A:17:LEU:O	1:A:153:ILE:HG23	2.05	0.57
1:C:30:ARG:HH22	1:C:203:TYR:HE2	1.51	0.57
1:C:550:ALA:HB3	1:C:587:ARG:HH22	1.70	0.57
1:C:544:ARG:HG3	1:C:623:ALA:O	2.05	0.56
1:C:57:LEU:O	1:C:61:LEU:HB2	2.05	0.56
1:B:72:TYR:CE1	1:B:476:LYS:HD3	2.40	0.56
1:A:301:THR:HG21	1:A:440:TRP:HA	1.85	0.56
1:C:314:VAL:O	1:C:317:TRP:HB2	2.04	0.56
1:B:631:LYS:HE3	1:B:632:TRP:CZ2	2.41	0.56
1:B:72:TYR:HE1	1:B:476:LYS:HD3	1.70	0.56
1:C:367:VAL:CG1	1:C:370:PRO:HG3	2.35	0.56
1:C:88:ARG:O	1:C:264:PHE:HA	2.05	0.56
1:A:210:ALA:HB3	1:A:223:LYS:HB2	1.87	0.56
1:C:205:ALA:O	1:C:529:GLU:HG2	2.06	0.56
2:D:5:DT:O4	2:D:6:DC:C4	2.59	0.56
1:B:418:THR:O	1:B:464:ALA:HA	2.05	0.56
1:A:175:GLU:HG3	1:A:352:TRP:CD1	2.40	0.56
1:C:132:ARG:HA	1:C:347:MET:CE	2.36	0.56
1:C:217:THR:HB	1:C:218:GLY:CA	2.35	0.56
1:C:1:PRO:HB2	1:C:2:ARG:HH11	1.69	0.56
1:C:502:LEU:CA	1:C:503:TYR:HB2	2.36	0.56
1:A:78:ASN:ND2	1:A:80:VAL:H	2.03	0.55
1:B:78:ASN:HD22	1:B:79:GLY:N	2.02	0.55
1:C:536:VAL:HB	1:C:542:ARG:HE	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HD11	1:A:28:SER:HB2	1.88	0.55
1:A:628:LEU:O	2:D:7:DC:H1'	2.05	0.55
1:C:522:LEU:O	1:C:526:PHE:HD1	1.89	0.55
1:C:65:PHE:CD2	1:C:563:ILE:HD12	2.41	0.55
1:C:551:TRP:CD2	1:C:587:ARG:HB3	2.41	0.55
1:C:9:LEU:HD13	1:C:366:TYR:OH	2.06	0.55
1:A:629:GLN:HA	2:D:7:DC:H1'	1.87	0.55
1:A:2:ARG:N	1:B:566:ASP:OD2	2.40	0.55
1:C:38:GLU:O	1:C:532:VAL:HG22	2.07	0.55
1:C:7:PHE:CE2	1:C:13:LYS:HD2	2.42	0.55
1:B:94:PRO:HB3	1:B:269:ARG:HG3	1.88	0.55
1:B:78:ASN:ND2	1:B:80:VAL:H	2.05	0.55
1:C:74:ARG:CZ	1:C:507:ARG:HB2	2.37	0.55
1:B:306:THR:O	1:B:309:ASN:HB3	2.07	0.54
1:C:536:VAL:O	1:C:537:ARG:C	2.45	0.54
1:C:518:ILE:HD11	1:C:567:VAL:HG21	1.89	0.54
2:E:6:DC:C2'	2:E:7:DC:H5'	2.37	0.54
1:C:12:ILE:HA	1:C:15:GLN:HB2	1.89	0.54
1:B:364:PRO:HA	1:B:387:LEU:CD2	2.27	0.54
1:C:505:SER:O	1:C:506:ARG:CG	2.55	0.54
1:C:629:GLN:HG2	1:C:646:MET:CE	2.37	0.54
1:A:47:ASP:OD1	1:A:49:ARG:NH1	2.38	0.54
1:A:60:TYR:HD2	1:A:61:LEU:HD23	1.72	0.54
1:B:175:GLU:HG3	1:B:352:TRP:CD1	2.42	0.54
1:B:60:TYR:HD2	1:B:61:LEU:HD23	1.73	0.54
1:A:71:GLU:HG3	1:A:72:TYR:HD2	1.73	0.54
1:C:46:VAL:CG2	1:C:258:ILE:HG12	2.38	0.54
1:C:23:LYS:HZ2	1:C:158:ASN:HB3	1.73	0.53
1:C:168:GLU:HG2	1:C:653:LYS:HD3	1.90	0.53
1:A:232:TYR:CE1	1:A:242:LEU:HB2	2.42	0.53
1:B:551:TRP:CE3	1:B:587:ARG:HG3	2.43	0.53
1:C:328:HIS:CD2	1:C:329:ASP:H	2.26	0.53
1:B:232:TYR:CE1	1:B:242:LEU:HB2	2.43	0.53
1:B:421:HIS:HB2	1:B:463:ARG:NH2	2.23	0.53
1:B:17:LEU:HB3	1:B:153:ILE:HD13	1.91	0.53
1:C:307:ARG:HH22	1:C:557:THR:HA	1.73	0.53
1:C:328:HIS:CE1	1:C:405:LEU:HD23	2.44	0.53
1:C:87:MET:O	1:C:89:HIS:N	2.40	0.53
1:B:146:ARG:NH2	1:B:540:SER:O	2.42	0.53
1:C:632:TRP:HB2	1:C:636:ASP:OD1	2.08	0.53
1:C:150:SER:CB	2:F:5:DT:H5''	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:TRP:CE3	1:C:458:GLY:HA3	2.44	0.53
1:C:57:LEU:HG	1:C:61:LEU:HD12	1.90	0.53
1:C:143:LEU:H	1:C:654:THR:HG21	1.74	0.53
1:A:71:GLU:H	1:A:72:TYR:HB2	1.74	0.53
1:C:29:LYS:HA	1:C:376:HIS:CE1	2.44	0.53
1:A:398:THR:HG23	2:D:7:DC:OP1	2.09	0.53
1:C:638:SER:O	1:C:641:ILE:N	2.40	0.53
1:A:268:ARG:CZ	1:A:270:ARG:NH1	2.72	0.52
1:A:575:TRP:CG	1:A:583:TYR:HB2	2.43	0.52
1:C:419:ALA:HB1	1:C:422:LEU:CD1	2.35	0.52
1:C:621:VAL:HG12	1:C:645:LEU:HD12	1.90	0.52
1:B:204:ARG:HH22	2:E:5:DT:H72	1.72	0.52
1:B:214:ASP:HB3	1:B:217:THR:OG1	2.10	0.52
1:B:180:LEU:CD2	1:B:185:LYS:HE3	2.39	0.52
1:B:268:ARG:CZ	1:B:270:ARG:NH1	2.73	0.52
3:C:1665:GTP:C8	3:C:1665:GTP:O5'	2.63	0.52
1:C:112:ALA:O	1:C:113:ASP:HB2	2.09	0.52
1:B:183:GLN:OE1	1:B:185:LYS:HE2	2.09	0.52
1:C:218:GLY:CA	1:C:219:LYS:HG2	2.38	0.52
1:C:328:HIS:CD2	3:C:1666:GTP:O3'	2.63	0.52
1:C:363:LEU:CD1	1:C:364:PRO:HD2	2.39	0.52
1:C:36:ALA:HB2	1:C:46:VAL:HG22	1.92	0.52
1:C:411:LEU:HD13	1:C:439:TYR:CE1	2.45	0.52
1:C:563:ILE:O	1:C:567:VAL:HG23	2.09	0.52
1:A:74:ARG:HB3	1:A:503:TYR:CD2	2.44	0.52
1:C:16:MET:CE	1:C:16:MET:HA	2.40	0.52
1:C:22:ILE:H	1:C:22:ILE:HD12	1.75	0.52
1:C:570:ALA:O	1:C:574:CYS:HB2	2.08	0.52
1:C:57:LEU:HD22	1:C:571:ILE:HG23	1.92	0.52
1:C:300:TYR:CE2	1:C:313:LYS:HG2	2.45	0.52
1:A:30:ARG:HD3	1:A:31:SER:H	1.73	0.52
1:B:230:PHE:O	1:B:234:VAL:HG22	2.10	0.52
1:B:629:GLN:HG2	2:E:6:DC:N3	2.25	0.52
1:B:208:THR:HG21	1:B:523:ASN:OD1	2.09	0.51
1:B:419:ALA:N	1:B:420:PRO:HD3	2.24	0.51
1:C:634:GLU:O	1:C:635:ALA:C	2.48	0.51
1:A:663:PRO:O	1:A:664:ARG:CZ	2.58	0.51
1:A:2:ARG:NH1	1:B:64:HIS:CD2	2.69	0.51
1:C:626:ASN:O	1:C:630:TYR:HE2	1.92	0.51
2:F:4:DT:H6	2:F:4:DT:H3'	1.75	0.51
1:A:279:LEU:O	1:A:282:PRO:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:THR:O	1:A:464:ALA:HA	2.10	0.51
1:B:206:GLN:HG2	3:B:1665:GTP:HN21	1.75	0.51
3:C:1666:GTP:O1B	3:C:1666:GTP:H5''	2.10	0.51
1:C:81:ARG:HD2	1:C:493:GLY:HA3	1.93	0.51
1:B:210:ALA:HB3	1:B:223:LYS:HB2	1.91	0.51
1:C:99:THR:HA	1:C:227:VAL:HB	1.91	0.51
1:A:328:HIS:HD2	1:A:329:ASP:OD1	1.93	0.51
1:A:142:PRO:HB3	1:A:651:VAL:HG22	1.92	0.51
1:B:17:LEU:O	1:B:153:ILE:HG23	2.11	0.51
1:C:23:LYS:NZ	1:C:158:ASN:HB3	2.25	0.51
3:C:1666:GTP:H5''	3:C:1666:GTP:PB	2.51	0.51
1:C:620:GLU:OE1	1:C:632:TRP:CZ2	2.64	0.51
1:A:204:ARG:NH2	2:D:5:DT:O4	2.43	0.51
1:A:419:ALA:N	1:A:420:PRO:HD3	2.25	0.51
1:C:632:TRP:O	1:C:633:THR:O	2.29	0.51
1:A:306:THR:O	1:A:309:ASN:HB3	2.10	0.51
1:B:162:THR:O	1:B:166:ILE:HG13	2.11	0.51
1:B:74:ARG:HB3	1:B:503:TYR:CD2	2.45	0.51
1:C:633:THR:HB	1:C:634:GLU:CD	2.31	0.51
1:C:158:ASN:HD21	1:C:541:LYS:NZ	2.08	0.50
1:B:328:HIS:HD2	1:B:329:ASP:OD1	1.94	0.50
1:C:9:LEU:HD11	1:C:28:SER:HB2	1.93	0.50
1:C:175:GLU:HA	1:C:352:TRP:CD2	2.47	0.50
1:A:551:TRP:CE3	1:A:587:ARG:HG3	2.46	0.50
1:C:415:LEU:HA	1:C:419:ALA:HB3	1.93	0.50
1:B:288:GLN:HB3	1:B:289:PRO:HD3	1.94	0.50
1:C:232:TYR:CG	1:C:237:GLY:HA2	2.46	0.50
1:C:449:ILE:O	1:C:455:ALA:HA	2.10	0.50
1:C:629:GLN:HG2	1:C:646:MET:HE2	1.92	0.50
1:C:75:VAL:O	1:C:503:TYR:HB2	2.12	0.50
1:A:605:MET:HE3	1:A:609:ALA:HB3	1.93	0.50
1:A:634:GLU:HG2	2:D:7:DC:H41	1.74	0.50
1:C:288:GLN:HB2	1:C:289:PRO:HD3	1.94	0.50
1:C:307:ARG:HG2	1:C:499:ASP:OD2	2.12	0.50
1:C:217:THR:CB	1:C:218:GLY:HA3	2.35	0.50
1:C:395:GLN:OE1	1:C:397:ALA:N	2.44	0.50
1:A:180:LEU:CD2	1:A:185:LYS:HE3	2.39	0.50
1:A:614:LEU:HD21	1:A:641:ILE:HD11	1.93	0.50
1:C:11:ASP:OD2	1:C:12:ILE:N	2.45	0.50
1:C:13:LYS:HE3	1:C:381:ASP:OD2	2.10	0.50
1:A:217:THR:HG22	1:A:219:LYS:N	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ASN:HA	1:B:267:GLU:OE1	2.12	0.50
1:B:428:ASP:OD1	1:B:430:PRO:HD2	2.12	0.50
2:E:3:DT:H5''	2:E:4:DT:OP1	2.12	0.50
1:A:634:GLU:HG3	2:D:7:DC:N4	2.27	0.49
1:A:183:GLN:OE1	1:A:185:LYS:HE2	2.11	0.49
1:A:656:ARG:CG	1:A:656:ARG:HH11	2.25	0.49
1:C:107:LYS:HE2	1:C:238:GLU:HG2	1.93	0.49
1:A:414:GLN:HG2	1:A:459:TRP:CZ2	2.47	0.49
1:C:81:ARG:HD3	1:C:500:ILE:HD11	1.95	0.49
1:A:607:ARG:O	1:A:608:GLN:CB	2.61	0.49
1:B:420:PRO:C	1:B:422:LEU:H	2.15	0.49
1:C:71:GLU:O	1:C:476:LYS:HE2	2.13	0.49
1:C:206:GLN:OE1	1:C:270:ARG:NH1	2.46	0.49
1:C:40:TYR:HE2	1:C:525:GLN:O	1.94	0.49
1:C:631:LYS:HD2	1:C:632:TRP:CD2	2.47	0.49
1:C:618:ASP:OD1	1:C:637:VAL:HA	2.12	0.49
1:B:206:GLN:HG3	3:B:1665:GTP:HN21	1.74	0.49
1:B:86:GLY:O	1:B:89:HIS:HD2	1.94	0.49
1:B:204:ARG:CZ	2:E:5:DT:O4	2.61	0.49
1:C:328:HIS:CG	1:C:329:ASP:H	2.30	0.49
1:C:501:LEU:HD13	1:C:514:PHE:CE2	2.47	0.49
1:A:395:GLN:HB3	1:A:398:THR:HG22	1.93	0.49
1:C:230:PHE:O	1:C:234:VAL:HG22	2.12	0.49
1:C:624:ASP:HB3	1:C:627:LYS:HE3	1.95	0.49
1:B:656:ARG:CG	1:B:656:ARG:HH11	2.24	0.48
1:C:81:ARG:HG2	1:C:500:ILE:HD11	1.94	0.48
1:C:109:ARG:NH1	1:C:331:PHE:O	2.45	0.48
1:C:256:TYR:H	1:C:257:GLY:HA2	1.78	0.48
1:C:521:MET:O	1:C:525:GLN:HG3	2.14	0.48
1:A:420:PRO:C	1:A:422:LEU:H	2.16	0.48
1:C:253:LYS:HA	1:C:258:ILE:O	2.13	0.48
1:A:274:GLY:HA2	2:D:5:DT:H1'	1.94	0.48
1:B:614:LEU:HD21	1:B:641:ILE:HD11	1.94	0.48
1:C:328:HIS:HD2	3:C:1666:GTP:O3'	1.95	0.48
1:C:74:ARG:NH1	1:C:507:ARG:HB2	2.28	0.48
1:C:76:TYR:HA	1:C:502:LEU:HD13	1.95	0.48
1:A:649:VAL:O	1:A:650:SER:C	2.52	0.48
1:C:407:SER:HA	1:C:448:GLN:HE22	1.79	0.48
1:C:633:THR:OG1	1:C:634:GLU:O	2.22	0.48
1:A:288:GLN:HB3	1:A:289:PRO:HD3	1.96	0.48
1:C:363:LEU:HD12	1:C:364:PRO:CD	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:HD2	1:B:429:MET:CE	2.44	0.48
1:C:143:LEU:HD12	1:C:285:ALA:HB2	1.96	0.48
1:C:419:ALA:N	1:C:420:PRO:HD3	2.28	0.48
1:C:592:LYS:O	1:C:595:THR:HB	2.14	0.48
1:C:475:LEU:HD21	1:C:482:PRO:HG2	1.96	0.48
1:C:61:LEU:HD23	1:C:65:PHE:CD2	2.43	0.48
1:C:633:THR:HB	1:C:634:GLU:CG	2.44	0.48
1:C:7:PHE:HB2	1:C:378:LEU:HB3	1.95	0.48
1:C:53:PHE:HZ	1:C:57:LEU:HD22	1.78	0.47
1:B:175:GLU:HG3	1:B:352:TRP:NE1	2.29	0.47
1:B:364:PRO:HB3	1:B:379:LEU:O	2.13	0.47
1:B:552:ALA:HB3	1:B:619:LEU:HD13	1.95	0.47
1:A:138:LEU:HB2	1:A:662:MET:CE	2.45	0.47
1:A:149:SER:OG	1:A:163:LYS:HE3	2.14	0.47
1:A:89:HIS:CE1	1:A:211:ILE:HD11	2.49	0.47
1:B:337:ARG:HG3	1:B:361:LEU:HD12	1.97	0.47
1:B:344:LEU:O	1:B:349:TYR:HB2	2.13	0.47
1:C:620:GLU:OE1	1:C:632:TRP:CH2	2.68	0.47
1:A:112:ALA:O	1:A:113:ASP:HB2	2.14	0.47
1:B:393:SER:O	1:B:398:THR:HG21	2.15	0.47
1:C:621:VAL:CG1	1:C:645:LEU:HD12	2.44	0.47
1:A:307:ARG:HG2	1:A:499:ASP:CG	2.35	0.47
1:C:598:LEU:HD21	1:C:622:LEU:HD13	1.97	0.47
1:A:552:ALA:HB3	1:A:619:LEU:HD13	1.95	0.47
1:C:149:SER:O	1:C:163:LYS:HE2	2.15	0.47
1:C:649:VAL:HG12	1:C:650:SER:H	1.80	0.47
1:A:2:ARG:CA	1:B:566:ASP:OD2	2.62	0.47
1:C:213:LEU:HD12	1:C:213:LEU:N	2.18	0.47
1:C:217:THR:HG22	1:C:219:LYS:HG2	1.96	0.47
1:C:198:ALA:HA	1:C:363:LEU:HG	1.95	0.47
1:C:62:THR:HG21	1:C:85:PHE:HE1	1.80	0.47
1:C:99:THR:CA	1:C:227:VAL:HB	2.45	0.47
1:C:38:GLU:HG2	1:C:40:TYR:O	2.15	0.47
2:F:5:DT:H2'	2:F:5:DT:O2	2.15	0.47
1:C:32:PHE:HZ	1:C:94:PRO:HG2	1.81	0.46
1:C:626:ASN:HA	1:C:628:LEU:O	2.15	0.46
1:A:1:PRO:HB3	1:B:569:GLU:OE2	2.15	0.46
1:C:2:ARG:NE	1:C:2:ARG:N	2.63	0.46
1:C:308:LEU:H	1:C:308:LEU:HD22	1.80	0.46
1:C:508:GLU:C	1:C:510:GLY:H	2.18	0.46
1:C:567:VAL:O	1:C:571:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ARG:NH2	2:D:5:DT:C4	2.83	0.46
1:B:414:GLN:HG2	1:B:459:TRP:CZ2	2.50	0.46
1:C:217:THR:CB	1:C:218:GLY:CA	2.91	0.46
1:A:228:ALA:HB1	1:A:232:TYR:HB3	1.98	0.46
1:B:228:ALA:HB1	1:B:232:TYR:HB3	1.98	0.46
1:C:12:ILE:HG13	1:C:12:ILE:O	2.14	0.46
1:C:410:TYR:HD1	1:C:413:MET:CE	2.29	0.46
1:A:268:ARG:CZ	1:A:270:ARG:HH11	2.28	0.46
1:A:587:ARG:HA	1:A:587:ARG:HD2	1.67	0.46
1:A:86:GLY:O	1:A:89:HIS:HD2	1.98	0.46
1:A:225:ARG:HA	1:A:225:ARG:HD3	1.77	0.46
1:A:203:TYR:HB3	1:A:269:ARG:HD2	1.97	0.46
1:A:85:PHE:O	1:A:88:ARG:HG3	2.16	0.46
1:C:225:ARG:HD2	1:C:268:ARG:HG3	1.96	0.46
1:C:256:TYR:N	1:C:257:GLY:HA2	2.30	0.46
1:A:344:LEU:O	1:A:349:TYR:HB2	2.16	0.46
1:C:214:ASP:HB3	1:C:215:PRO:HA	1.98	0.46
1:C:232:TYR:CE2	1:C:237:GLY:HA3	2.51	0.46
1:C:649:VAL:CG1	1:C:650:SER:N	2.79	0.46
1:A:551:TRP:CZ3	1:A:587:ARG:HG3	2.51	0.46
1:B:316:GLU:OE1	1:B:316:GLU:HA	2.16	0.46
1:B:630:TYR:O	1:B:630:TYR:CD1	2.68	0.46
1:C:631:LYS:HD2	1:C:632:TRP:CE3	2.50	0.46
1:B:273:MET:H	1:B:393:SER:HB3	1.80	0.46
1:C:139:GLU:O	1:C:141:VAL:HG13	2.16	0.46
1:C:367:VAL:HG12	1:C:370:PRO:HG3	1.97	0.46
1:C:466:VAL:HG13	1:C:467:GLY:N	2.30	0.46
1:A:204:ARG:HH22	2:D:5:DT:H72	1.81	0.46
1:B:175:GLU:HG3	1:B:352:TRP:CE2	2.50	0.46
1:B:225:ARG:HA	1:B:225:ARG:HD3	1.77	0.46
1:B:9:LEU:HD13	1:B:366:TYR:OH	2.16	0.46
1:C:92:GLY:N	1:C:267:GLU:OE2	2.43	0.46
1:A:319:LEU:HD12	1:A:320:CYS:N	2.31	0.45
1:B:225:ARG:NH1	1:B:268:ARG:NH2	2.64	0.45
1:C:525:GLN:HB2	1:C:526:PHE:CD1	2.50	0.45
1:C:515:VAL:HG12	1:C:560:ALA:HB1	1.99	0.45
1:C:640:ASN:HD22	1:C:640:ASN:C	2.20	0.45
1:C:17:LEU:O	1:C:154:PRO:HA	2.16	0.45
1:A:310:LYS:HB3	1:A:514:PHE:CE1	2.52	0.45
1:B:649:VAL:O	1:B:650:SER:C	2.55	0.45
1:C:85:PHE:O	1:C:86:GLY:C	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:HIS:CE1	1:B:646:MET:HG3	2.51	0.45
1:A:71:GLU:CG	1:A:72:TYR:HD2	2.29	0.45
1:C:328:HIS:CG	1:C:329:ASP:N	2.84	0.45
1:C:425:ARG:NH2	1:C:444:GLU:OE2	2.44	0.45
1:A:612:ALA:HB1	1:A:613:GLU:HG2	1.98	0.45
1:C:213:LEU:H	1:C:213:LEU:CD1	2.14	0.45
1:C:546:PHE:CE1	1:C:598:LEU:HD13	2.52	0.45
2:F:4:DT:C6	2:F:4:DT:H3'	2.52	0.45
1:A:175:GLU:HG3	1:A:352:TRP:NE1	2.32	0.45
1:A:132:ARG:HD2	1:A:429:MET:CE	2.46	0.45
1:A:607:ARG:O	1:A:608:GLN:HB2	2.15	0.45
1:C:340:ILE:HG12	1:C:404:LEU:HD21	1.99	0.45
1:C:364:PRO:HA	1:C:387:LEU:HD23	1.96	0.45
1:C:546:PHE:HB2	1:C:549:LEU:HG	1.98	0.45
1:A:215:PRO:HB2	1:A:216:LYS:HE3	1.99	0.45
1:A:227:VAL:O	1:A:242:LEU:HD12	2.16	0.45
1:B:202:VAL:O	1:B:272:ALA:HB3	2.16	0.45
1:C:225:ARG:NH2	1:C:268:ARG:NH1	2.65	0.45
1:C:229:ASP:O	1:C:230:PHE:C	2.55	0.45
1:B:204:ARG:HH22	2:E:5:DT:H71	1.82	0.45
1:C:546:PHE:CB	1:C:549:LEU:HG	2.47	0.45
1:C:150:SER:HB2	2:F:5:DT:H5''	1.98	0.45
1:B:44:LEU:HD12	1:B:44:LEU:HA	1.65	0.45
2:E:7:DC:H2'	2:E:7:DC:O2	2.17	0.45
1:B:407:SER:HA	1:B:448:GLN:HE22	1.82	0.44
1:C:332:TRP:CD1	1:C:405:LEU:HD22	2.52	0.44
1:C:626:ASN:O	1:C:630:TYR:CE2	2.69	0.44
1:C:202:VAL:HG12	1:C:203:TYR:N	2.31	0.44
1:A:270:ARG:NH2	3:A:1665:GTP:C3'	2.50	0.44
1:A:445:GLU:OE1	1:A:464:ALA:N	2.38	0.44
1:A:71:GLU:N	1:A:72:TYR:HB2	2.32	0.44
1:B:630:TYR:CG	3:B:1665:GTP:N7	2.85	0.44
1:B:632:TRP:O	1:B:633:THR:HB	2.16	0.44
1:C:310:LYS:HZ2	1:C:499:ASP:HB2	1.82	0.44
1:A:153:ILE:HA	1:A:154:PRO:HA	1.61	0.44
1:A:642:HIS:CE1	1:A:646:MET:HG3	2.53	0.44
1:A:93:PHE:HA	1:A:94:PRO:HD3	1.77	0.44
1:B:488:ILE:HG22	1:B:489:SER:N	2.32	0.44
1:C:205:ALA:HB1	1:C:267:GLU:HG3	1.98	0.44
1:A:94:PRO:HB3	1:A:269:ARG:HG3	1.98	0.44
1:A:421:HIS:HB2	1:A:463:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:HIS:CE1	1:B:211:ILE:HD11	2.52	0.44
1:B:86:GLY:O	1:B:89:HIS:CD2	2.71	0.44
1:C:87:MET:C	1:C:89:HIS:H	2.21	0.44
1:B:204:ARG:NH2	2:E:5:DT:C7	2.79	0.44
1:C:410:TYR:HD1	1:C:413:MET:HE2	1.83	0.44
1:C:75:VAL:O	1:C:503:TYR:CB	2.66	0.44
1:A:33:LYS:HG3	1:A:34:GLU:H	1.82	0.44
1:C:1:PRO:HB2	1:C:2:ARG:NH1	2.33	0.44
1:C:353:TRP:HA	1:C:356:LEU:HD12	2.00	0.44
1:C:501:LEU:HD13	1:C:514:PHE:CZ	2.52	0.44
1:B:153:ILE:HA	1:B:154:PRO:HA	1.63	0.44
1:B:481:ASN:HA	1:B:482:PRO:HD3	1.74	0.44
1:B:551:TRP:CZ3	1:B:587:ARG:HG3	2.53	0.44
1:B:85:PHE:O	1:B:88:ARG:HG3	2.18	0.44
1:C:204:ARG:HH11	1:C:270:ARG:HD2	1.82	0.44
1:C:395:GLN:O	1:C:398:THR:HB	2.17	0.44
1:C:443:HIS:O	1:C:444:GLU:HG2	2.18	0.44
1:C:621:VAL:HG12	1:C:645:LEU:CD1	2.47	0.44
1:C:90:MET:HB2	1:C:90:MET:HE3	1.84	0.44
1:A:428:ASP:OD1	1:A:430:PRO:HD2	2.18	0.44
1:B:319:LEU:HD12	1:B:320:CYS:N	2.33	0.44
1:C:120:SER:O	1:C:123:ASP:N	2.51	0.44
1:C:280:ASN:HA	1:C:280:ASN:HD22	1.70	0.44
1:A:602:VAL:O	1:A:603:ALA:C	2.56	0.43
1:C:232:TYR:CZ	1:C:237:GLY:HA3	2.52	0.43
1:C:225:ARG:NH2	1:C:268:ARG:HH12	2.15	0.43
1:C:393:SER:OG	1:C:394:GLY:N	2.51	0.43
1:C:46:VAL:HB	1:C:258:ILE:CG2	2.45	0.43
1:B:564:TYR:CZ	1:B:568:LEU:HD11	2.53	0.43
1:B:62:THR:HG21	1:B:85:PHE:CZ	2.53	0.43
1:C:94:PRO:O	1:C:251:ARG:NH2	2.52	0.43
1:C:138:LEU:HB2	1:C:662:MET:SD	2.58	0.43
1:C:7:PHE:HA	1:C:8:PRO:HD3	1.78	0.43
1:C:256:TYR:H	1:C:257:GLY:CA	2.31	0.43
1:C:333:PRO:HB3	1:C:335:TRP:NE1	2.33	0.43
2:F:4:DT:C3'	2:F:4:DT:C6	3.01	0.43
1:A:364:PRO:HB3	1:A:379:LEU:O	2.18	0.43
1:A:46:VAL:HG12	1:A:90:MET:HE3	2.00	0.43
1:B:225:ARG:HG3	1:B:268:ARG:HG3	2.01	0.43
1:B:268:ARG:CZ	1:B:270:ARG:HH11	2.32	0.43
1:A:408:ILE:O	1:A:409:THR:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:MET:SD	1:A:568:LEU:HD21	2.58	0.43
1:C:217:THR:N	1:C:218:GLY:HA3	2.33	0.43
1:A:332:TRP:HA	1:A:333:PRO:HD3	1.70	0.43
1:B:145:ILE:HG21	1:B:163:LYS:HE2	2.00	0.43
1:B:227:VAL:O	1:B:242:LEU:HD12	2.18	0.43
1:B:395:GLN:HB3	1:B:398:THR:HG22	2.00	0.43
1:B:554:MET:SD	1:B:568:LEU:HD21	2.58	0.43
1:C:317:TRP:CZ2	1:C:447:ARG:HB2	2.54	0.43
1:B:628:LEU:O	2:E:7:DC:C1'	2.64	0.43
1:C:429:MET:CB	1:C:430:PRO:HD3	2.48	0.43
1:A:217:THR:HG22	1:A:219:LYS:HB2	1.99	0.43
1:B:60:TYR:CD2	1:B:61:LEU:HD23	2.53	0.43
1:B:7:PHE:HA	1:B:8:PRO:HD3	1.76	0.43
2:E:7:DC:O2	2:E:7:DC:H5"	2.18	0.43
1:C:202:VAL:CG1	1:C:203:TYR:N	2.82	0.43
1:C:138:LEU:HD12	1:C:662:MET:SD	2.59	0.43
1:A:7:PHE:HA	1:A:8:PRO:HD3	1.78	0.42
1:B:634:GLU:HB2	2:E:7:DC:N4	2.34	0.42
1:B:72:TYR:CE1	1:B:476:LYS:CD	3.02	0.42
1:C:363:LEU:HD12	1:C:363:LEU:HA	1.81	0.42
1:C:81:ARG:CG	1:C:500:ILE:HD11	2.49	0.42
1:A:91:ASN:HA	1:A:267:GLU:OE1	2.19	0.42
1:C:319:LEU:HD12	1:C:320:CYS:H	1.84	0.42
1:C:631:LYS:HD2	1:C:632:TRP:CE2	2.54	0.42
1:C:640:ASN:ND2	1:C:640:ASN:C	2.72	0.42
1:C:628:LEU:HD11	1:C:646:MET:HG3	2.00	0.42
1:A:146:ARG:NH2	1:A:540:SER:O	2.52	0.42
1:B:420:PRO:C	1:B:422:LEU:N	2.73	0.42
1:B:587:ARG:HD2	1:B:587:ARG:HA	1.65	0.42
1:C:142:PRO:HG3	1:C:651:VAL:HG22	2.02	0.42
1:C:472:PHE:HE2	1:C:476:LYS:HE3	1.84	0.42
1:C:481:ASN:HA	1:C:482:PRO:HD3	1.77	0.42
1:C:633:THR:HB	1:C:634:GLU:OE2	2.18	0.42
1:A:162:THR:O	1:A:166:ILE:HG13	2.20	0.42
1:A:633:THR:O	1:A:634:GLU:C	2.58	0.42
1:B:12:ILE:O	1:B:16:MET:HG3	2.19	0.42
1:B:208:THR:HG21	1:B:523:ASN:CG	2.40	0.42
1:B:605:MET:O	1:B:606:ALA:CB	2.67	0.42
1:C:211:ILE:HG23	1:C:265:PHE:CE1	2.54	0.42
1:C:332:TRP:CZ2	1:C:336:LEU:HD23	2.54	0.42
1:C:343:GLU:OE1	1:C:343:GLU:CA	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:LEU:HD13	1:C:439:TYR:CE2	2.55	0.42
1:C:622:LEU:HD21	1:C:641:ILE:HG23	2.01	0.42
1:A:270:ARG:HH21	3:A:1665:GTP:C3'	2.23	0.42
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.71	0.42
1:C:30:ARG:HG3	1:C:30:ARG:O	2.20	0.42
1:C:549:LEU:O	1:C:552:ALA:HB3	2.19	0.42
1:A:12:ILE:O	1:A:16:MET:HG3	2.19	0.42
1:A:605:MET:CE	1:A:607:ARG:HA	2.49	0.42
3:C:1665:GTP:HN1	2:F:7:DC:H42	1.68	0.42
1:C:622:LEU:HA	1:C:622:LEU:HD23	1.82	0.42
1:A:316:GLU:HA	1:A:316:GLU:OE1	2.19	0.42
1:A:605:MET:CB	1:A:606:ALA:CA	2.95	0.42
1:B:142:PRO:HB3	1:B:651:VAL:HG22	2.01	0.42
1:B:336:LEU:HD12	1:B:336:LEU:HA	1.83	0.42
1:B:93:PHE:HA	1:B:94:PRO:HD3	1.79	0.42
1:C:32:PHE:CZ	1:C:94:PRO:HG2	2.55	0.42
1:A:204:ARG:CZ	2:D:5:DT:O4	2.67	0.42
1:A:30:ARG:HD2	1:A:31:SER:O	2.20	0.42
1:B:437:ASP:O	1:B:441:GLN:HG3	2.19	0.42
1:C:218:GLY:CA	1:C:219:LYS:CB	2.97	0.42
1:C:56:GLU:HB3	1:C:574:CYS:SG	2.60	0.42
1:A:336:LEU:HA	1:A:336:LEU:HD12	1.80	0.42
1:B:122:ARG:HH21	1:B:412:VAL:HG13	1.85	0.42
1:C:226:MET:HA	1:C:244:ALA:HA	2.00	0.42
1:C:368:GLY:O	1:C:369:ALA:HB2	2.19	0.42
1:C:81:ARG:CD	1:C:500:ILE:HD11	2.49	0.42
1:A:481:ASN:HA	1:A:482:PRO:HD3	1.78	0.41
1:A:634:GLU:HG2	1:A:642:HIS:CE1	2.55	0.41
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.95	0.41
1:C:591:LEU:HD13	1:C:592:LYS:N	2.35	0.41
1:C:543:LYS:O	1:C:625:PRO:HD2	2.19	0.41
1:C:62:THR:HG21	1:C:85:PHE:CE1	2.55	0.41
1:A:208:THR:HG21	1:A:523:ASN:CG	2.40	0.41
1:C:206:GLN:HB3	1:C:529:GLU:HG2	2.00	0.41
1:C:555:LYS:O	1:C:559:GLY:HA3	2.20	0.41
1:C:658:LEU:HD22	1:C:658:LEU:HA	1.75	0.41
2:D:7:DC:O4'	2:D:7:DC:O2	2.36	0.41
1:B:204:ARG:NH2	2:E:5:DT:O4	2.53	0.41
1:A:521:MET:HG3	1:A:558:TYR:CD1	2.55	0.41
1:A:605:MET:HB3	1:A:606:ALA:CA	2.30	0.41
1:C:218:GLY:H	1:C:219:LYS:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:PHE:CE2	1:C:497:LEU:HD22	2.55	0.41
1:C:559:GLY:C	1:C:561:CYS:H	2.24	0.41
1:B:291:ARG:HD3	2:E:7:DC:H2'	2.00	0.41
1:A:504:ASP:OD1	1:A:506:ARG:HG3	2.20	0.41
1:B:21:ASN:OD1	1:B:21:ASN:C	2.59	0.41
1:B:256:TYR:HB2	1:B:258:ILE:HG13	2.02	0.41
1:C:141:VAL:HG11	1:C:292:ASN:ND2	2.36	0.41
1:C:141:VAL:HB	1:C:142:PRO:CD	2.50	0.41
1:C:305:THR:OG1	1:C:306:THR:N	2.52	0.41
1:C:332:TRP:HA	1:C:333:PRO:HD3	1.72	0.41
1:C:466:VAL:CG1	1:C:467:GLY:N	2.83	0.41
1:A:1:PRO:O	1:A:2:ARG:C	2.59	0.41
1:A:609:ALA:N	1:A:610:GLY:HA2	2.35	0.41
1:A:621:VAL:HG23	1:A:632:TRP:CE3	2.56	0.41
1:C:328:HIS:O	1:C:331:PHE:HB2	2.20	0.41
1:C:412:VAL:O	1:C:413:MET:C	2.57	0.41
1:C:453:ASP:OD2	1:C:454:ASP:N	2.53	0.41
1:C:74:ARG:NE	1:C:507:ARG:HB3	2.35	0.41
1:A:274:GLY:CA	2:D:5:DT:H1'	2.50	0.41
1:A:407:SER:HA	1:A:448:GLN:HE22	1.85	0.41
1:B:112:ALA:O	1:B:113:ASP:HB2	2.20	0.41
1:B:149:SER:OG	1:B:163:LYS:HE3	2.20	0.41
1:C:155:TYR:O	1:C:156:PHE:HB2	2.20	0.41
1:C:319:LEU:O	1:C:458:GLY:HA2	2.20	0.41
1:C:36:ALA:CB	1:C:46:VAL:HG22	2.50	0.41
1:C:536:VAL:O	1:C:542:ARG:NH2	2.53	0.41
1:B:430:PRO:O	1:B:434:ARG:HG3	2.19	0.41
1:B:58:SER:HB3	1:B:87:MET:SD	2.61	0.41
1:C:628:LEU:HD13	1:C:633:THR:O	2.21	0.41
1:C:55:ASN:HD21	1:C:59:ARG:HH21	1.69	0.41
2:E:4:DT:C2'	2:E:5:DT:OP2	2.69	0.41
1:A:158:ASN:ND2	2:D:3:DT:H2''	2.36	0.41
1:A:145:ILE:HG21	1:A:163:LYS:HE2	2.02	0.41
1:A:175:GLU:HG3	1:A:352:TRP:CE2	2.55	0.41
1:A:43:LEU:HA	1:A:43:LEU:HD23	1.81	0.41
1:C:419:ALA:CB	1:C:422:LEU:HD12	2.44	0.41
1:A:406:MET:HG3	1:A:453:ASP:HA	2.03	0.41
1:A:630:TYR:CD1	1:A:631:LYS:N	2.89	0.41
1:C:218:GLY:HA2	1:C:219:LYS:CB	2.50	0.41
1:C:391:LEU:HA	1:C:391:LEU:HD23	1.92	0.41
1:C:563:ILE:HG13	1:C:567:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:ILE:O	1:C:575:TRP:HB2	2.20	0.41
1:A:307:ARG:HG2	1:A:499:ASP:OD2	2.21	0.41
1:C:296:SER:O	1:C:297:LYS:C	2.57	0.41
1:C:505:SER:O	1:C:506:ARG:CB	2.69	0.41
1:A:413:MET:HE1	1:A:488:ILE:HG21	2.04	0.40
1:A:518:ILE:HD12	1:A:518:ILE:HA	1.98	0.40
1:A:96:ILE:HA	1:A:97:PRO:HA	1.85	0.40
1:C:152:CYS:O	1:C:153:ILE:C	2.59	0.40
1:B:612:ALA:HB1	1:B:613:GLU:HG2	2.02	0.40
1:C:214:ASP:HB3	1:C:215:PRO:CA	2.51	0.40
1:C:500:ILE:HG23	1:C:501:LEU:N	2.35	0.40
1:C:146:ARG:HA	1:C:646:MET:SD	2.61	0.40
1:A:319:LEU:HD12	1:A:320:CYS:H	1.86	0.40
1:A:49:ARG:HB3	1:A:578:ALA:O	2.21	0.40
1:B:461:LYS:HD3	1:B:461:LYS:HA	1.94	0.40
1:C:295:TYR:O	1:C:299:ALA:HB2	2.20	0.40
1:A:337:ARG:HG3	1:A:361:LEU:HD12	2.02	0.40
1:A:420:PRO:C	1:A:422:LEU:N	2.75	0.40
1:A:602:VAL:C	1:A:604:SER:N	2.74	0.40
1:A:60:TYR:CD2	1:A:61:LEU:HD23	2.53	0.40
1:B:332:TRP:HA	1:B:333:PRO:HD3	1.72	0.40
1:C:134:MET:HG2	1:C:294:ILE:HG21	2.03	0.40
1:A:437:ASP:O	1:A:441:GLN:HG3	2.21	0.40
1:C:640:ASN:ND2	1:C:641:ILE:N	2.70	0.40

All (1) 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:B:20:ASN:ND2	1:B:122:ARG:NH2[2_664]	2.08	0.12

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	662/664 (100%)	617 (93%)	37 (6%)	8 (1%)	13	39
1	B	662/664 (100%)	616 (93%)	38 (6%)	8 (1%)	13	39
1	C	647/664 (97%)	524 (81%)	102 (16%)	21 (3%)	4	13
All	All	1971/1992 (99%)	1757 (89%)	177 (9%)	37 (2%)	8	26

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	634	GLU
1	B	70	ASP
1	B	216	LYS
1	C	326	SER
1	C	328	HIS
1	C	329	ASP
1	C	537	ARG
1	C	633	THR
1	C	634	GLU
1	A	72	TYR
1	A	497	LEU
1	B	627	LYS
1	C	207	SER
1	C	209	ASP
1	C	374	GLN
1	C	506	ARG
1	C	639	ALA
1	A	2	ARG
1	A	608	GLN
1	B	497	LEU
1	C	83	ASN
1	C	88	ARG
1	C	373	GLU
1	C	593	ARG
1	A	650	SER
1	B	603	ALA
1	B	650	SER
1	C	58	SER
1	C	217	THR
1	C	560	ALA
1	C	635	ALA
1	C	637	VAL

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Mol	Chain	Res	Type
1	B	606	ALA
1	B	607	ARG
1	C	369	ALA
1	A	607	ARG
1	A	630	TYR

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	557/557 (100%)	520 (93%)	37 (7%)	16	44
1	B	557/557 (100%)	522 (94%)	35 (6%)	18	46
1	C	549/557 (99%)	489 (89%)	60 (11%)	6	19
All	All	1663/1671 (100%)	1531 (92%)	132 (8%)	12	34

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	23	LYS
1	A	43	LEU
1	A	44	LEU
1	A	71	GLU
1	A	75	VAL
1	A	78	ASN
1	A	119	VAL
1	A	146	ARG
1	A	154	PRO
1	A	158	ASN
1	A	202	VAL
1	A	204	ARG
1	A	206	GLN
1	A	216	LYS
1	A	234	VAL
1	A	271	THR

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Mol	Chain	Res	Type
1	A	301	THR
1	A	306	THR
1	A	362	LYS
1	A	391	LEU
1	A	398	THR
1	A	404	LEU
1	A	489	SER
1	A	497	LEU
1	A	511	SER
1	A	527	SER
1	A	576	TRP
1	A	587	ARG
1	A	591	LEU
1	A	613	GLU
1	A	630	TYR
1	A	633	THR
1	A	634	GLU
1	A	643	GLU
1	A	654	THR
1	A	656	ARG
1	B	3	ARG
1	B	30	ARG
1	B	43	LEU
1	B	44	LEU
1	B	71	GLU
1	B	78	ASN
1	B	119	VAL
1	B	146	ARG
1	B	154	PRO
1	B	158	ASN
1	B	206	GLN
1	B	234	VAL
1	B	269	ARG
1	B	271	THR
1	B	301	THR
1	B	306	THR
1	B	362	LYS
1	B	398	THR
1	B	404	LEU
1	B	497	LEU
1	B	505	SER
1	B	527	SER

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Mol	Chain	Res	Type
1	B	576	TRP
1	B	587	ARG
1	B	591	LEU
1	B	604	SER
1	B	605	MET
1	B	607	ARG
1	B	613	GLU
1	B	626	ASN
1	B	630	TYR
1	B	643	GLU
1	B	654	THR
1	B	656	ARG
1	B	664	ARG
1	C	26	GLN
1	C	43	LEU
1	C	44	LEU
1	C	55	ASN
1	C	61	LEU
1	C	69	VAL
1	C	75	VAL
1	C	91	ASN
1	C	137	ASP
1	C	158	ASN
1	C	159	ASP
1	C	206	GLN
1	C	213	LEU
1	C	216	LYS
1	C	224	ASP
1	C	243	PHE
1	C	250	SER
1	C	253	LYS
1	C	256	TYR
1	C	260	VAL
1	C	268	ARG
1	C	269	ARG
1	C	271	THR
1	C	280	ASN
1	C	304	HIS
1	C	306	THR
1	C	318	SER
1	C	365	VAL
1	C	373	GLU

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Mol	Chain	Res	Type
1	C	387	LEU
1	C	391	LEU
1	C	404	LEU
1	C	431	SER
1	C	446	ILE
1	C	453	ASP
1	C	454	ASP
1	C	463	ARG
1	C	490	TYR
1	C	491	GLN
1	C	497	LEU
1	C	500	ILE
1	C	507	ARG
1	C	532	VAL
1	C	567	VAL
1	C	574	CYS
1	C	584	ARG
1	C	587	ARG
1	C	590	MET
1	C	596	LEU
1	C	599	SER
1	C	600	ARG
1	C	624	ASP
1	C	629	GLN
1	C	631	LYS
1	C	632	TRP
1	C	633	THR
1	C	634	GLU
1	C	637	VAL
1	C	640	ASN
1	C	658	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	78	ASN
1	A	89	HIS
1	A	91	ASN
1	A	255	GLN
1	A	280	ASN
1	A	303	HIS

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Mol	Chain	Res	Type
1	A	328	HIS
1	A	384	ASN
1	A	448	GLN
1	A	525	GLN
1	A	629	GLN
1	A	642	HIS
1	B	64	HIS
1	B	78	ASN
1	B	89	HIS
1	B	255	GLN
1	B	280	ASN
1	B	328	HIS
1	B	384	ASN
1	B	448	GLN
1	B	524	ASN
1	B	525	GLN
1	B	642	HIS
1	C	15	GLN
1	C	55	ASN
1	C	158	ASN
1	C	191	GLN
1	C	255	GLN
1	C	280	ASN
1	C	303	HIS
1	C	304	HIS
1	C	328	HIS
1	C	374	GLN
1	C	448	GLN
1	C	491	GLN
1	C	524	ASN
1	C	525	GLN
1	C	629	GLN
1	C	640	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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$
3	GTP	A	1665	-	26,34,34	1.01	1 (3%)	33,54,54	2.02	9 (27%)
3	GTP	C	1666	-	26,34,34	0.97	1 (3%)	33,54,54	2.02	8 (24%)
3	GTP	C	1665	-	26,34,34	1.09	2 (7%)	33,54,54	2.04	8 (24%)
3	GTP	B	1665	-	26,34,34	0.93	1 (3%)	33,54,54	1.92	8 (24%)

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
3	GTP	A	1665	-	-	5/18/38/38	0/3/3/3
3	GTP	C	1666	-	-	3/18/38/38	0/3/3/3
3	GTP	C	1665	-	-	3/18/38/38	0/3/3/3
3	GTP	B	1665	-	-	2/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1665	GTP	C6-N1	3.74	1.39	1.33
3	A	1665	GTP	C6-N1	3.24	1.38	1.33
3	C	1666	GTP	C6-N1	3.19	1.38	1.33
3	B	1665	GTP	C6-N1	2.78	1.37	1.33
3	C	1665	GTP	C2-N1	2.21	1.39	1.35

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1665	GTP	N3-C2-N1	-5.58	119.78	127.22
3	C	1666	GTP	N3-C2-N1	-5.57	119.79	127.22
3	A	1665	GTP	N3-C2-N1	-5.35	120.08	127.22
3	B	1665	GTP	PB-O3B-PG	-4.87	116.11	132.83
3	B	1665	GTP	PA-O3A-PB	-4.87	116.12	132.83
3	B	1665	GTP	N3-C2-N1	-4.37	121.39	127.22
3	C	1666	GTP	C2-N3-C4	4.29	120.26	115.36
3	A	1665	GTP	PA-O3A-PB	-4.18	118.50	132.83
3	C	1665	GTP	PA-O3A-PB	-4.06	118.89	132.83
3	C	1666	GTP	PB-O3B-PG	-3.96	119.23	132.83
3	C	1665	GTP	C5-C6-N1	-3.90	118.09	123.43
3	A	1665	GTP	C2-N3-C4	3.83	119.73	115.36
3	C	1666	GTP	C3'-C2'-C1'	3.82	106.73	100.98
3	C	1665	GTP	C2-N3-C4	3.71	119.60	115.36
3	B	1665	GTP	C2-N3-C4	3.57	119.43	115.36
3	A	1665	GTP	C5-C6-N1	-3.55	118.58	123.43
3	A	1665	GTP	PB-O3B-PG	-3.40	121.16	132.83
3	C	1666	GTP	C5-C6-N1	-3.35	118.85	123.43
3	C	1665	GTP	N2-C2-N1	3.33	122.44	117.25
3	C	1665	GTP	C6-N1-C2	3.29	121.15	115.93
3	B	1665	GTP	C5-C6-N1	-3.15	119.12	123.43
3	A	1665	GTP	C6-N1-C2	3.14	120.91	115.93
3	C	1666	GTP	C6-N1-C2	3.02	120.72	115.93
3	C	1665	GTP	C1'-N9-C4	-2.82	121.69	126.64
3	A	1665	GTP	N2-C2-N1	2.52	121.18	117.25
3	C	1666	GTP	N2-C2-N1	2.46	121.08	117.25
3	C	1665	GTP	PB-O3B-PG	-2.30	124.92	132.83
3	B	1665	GTP	C6-N1-C2	2.30	119.59	115.93
3	C	1666	GTP	O2G-PG-O3B	2.29	112.31	104.64
3	B	1665	GTP	O3G-PG-O3B	2.28	112.27	104.64
3	B	1665	GTP	C3'-C2'-C1'	2.14	104.20	100.98
3	A	1665	GTP	C4-C5-N7	-2.09	107.22	109.40
3	A	1665	GTP	C5'-C4'-C3'	-2.07	107.41	115.18

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1665	GTP	C5'-O5'-PA-O3A
3	A	1665	GTP	C5'-O5'-PA-O1A
3	A	1665	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	C	1666	GTP	PB-O3A-PA-O5'
3	C	1666	GTP	O4'-C4'-C5'-O5'
3	C	1666	GTP	C3'-C4'-C5'-O5'
3	B	1665	GTP	C3'-C4'-C5'-O5'
3	C	1665	GTP	PB-O3A-PA-O5'
3	C	1665	GTP	C4'-C5'-O5'-PA
3	A	1665	GTP	PG-O3B-PB-O2B
3	C	1665	GTP	C5'-O5'-PA-O1A
3	B	1665	GTP	C5'-O5'-PA-O1A
3	A	1665	GTP	O4'-C4'-C5'-O5'

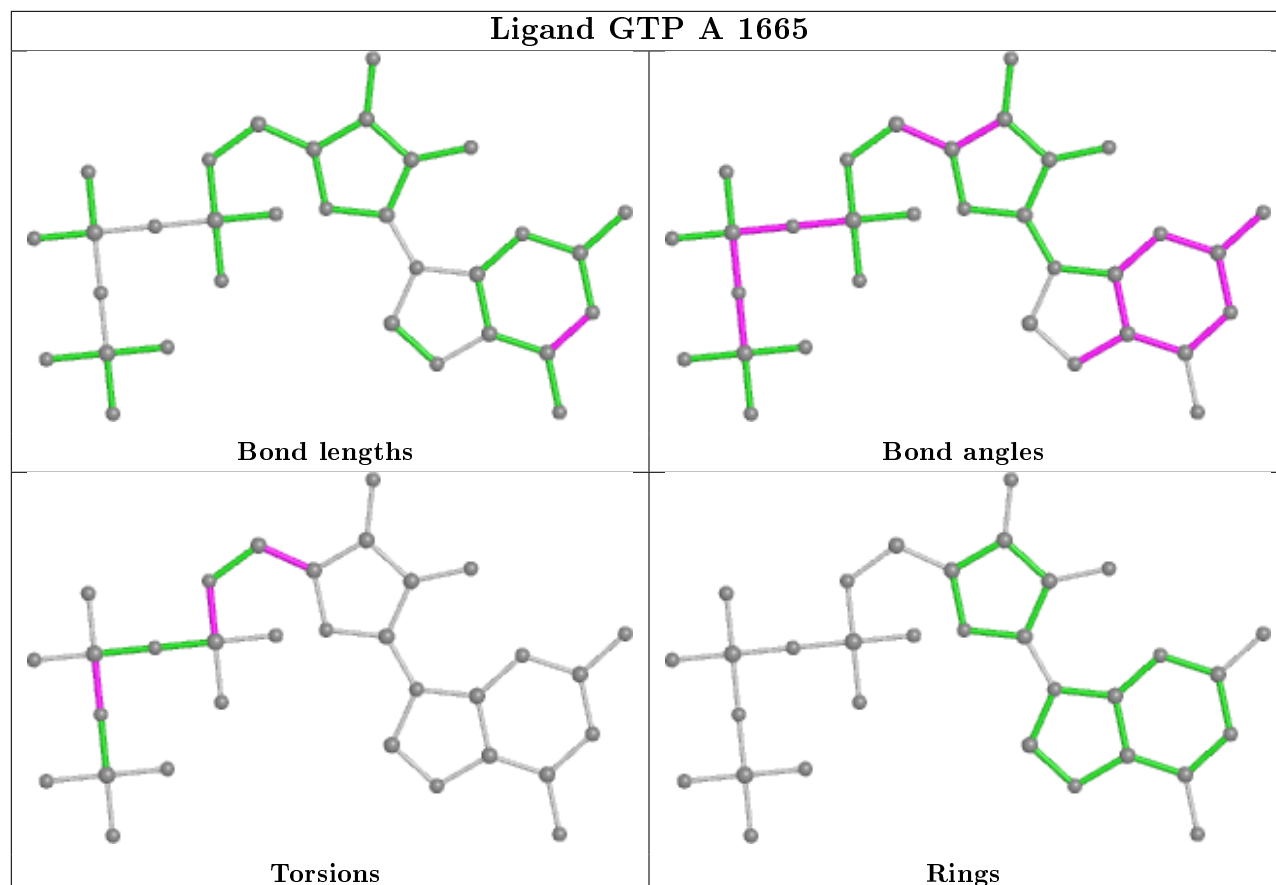
There are no ring outliers.

4 monomers are involved in 18 short contacts:

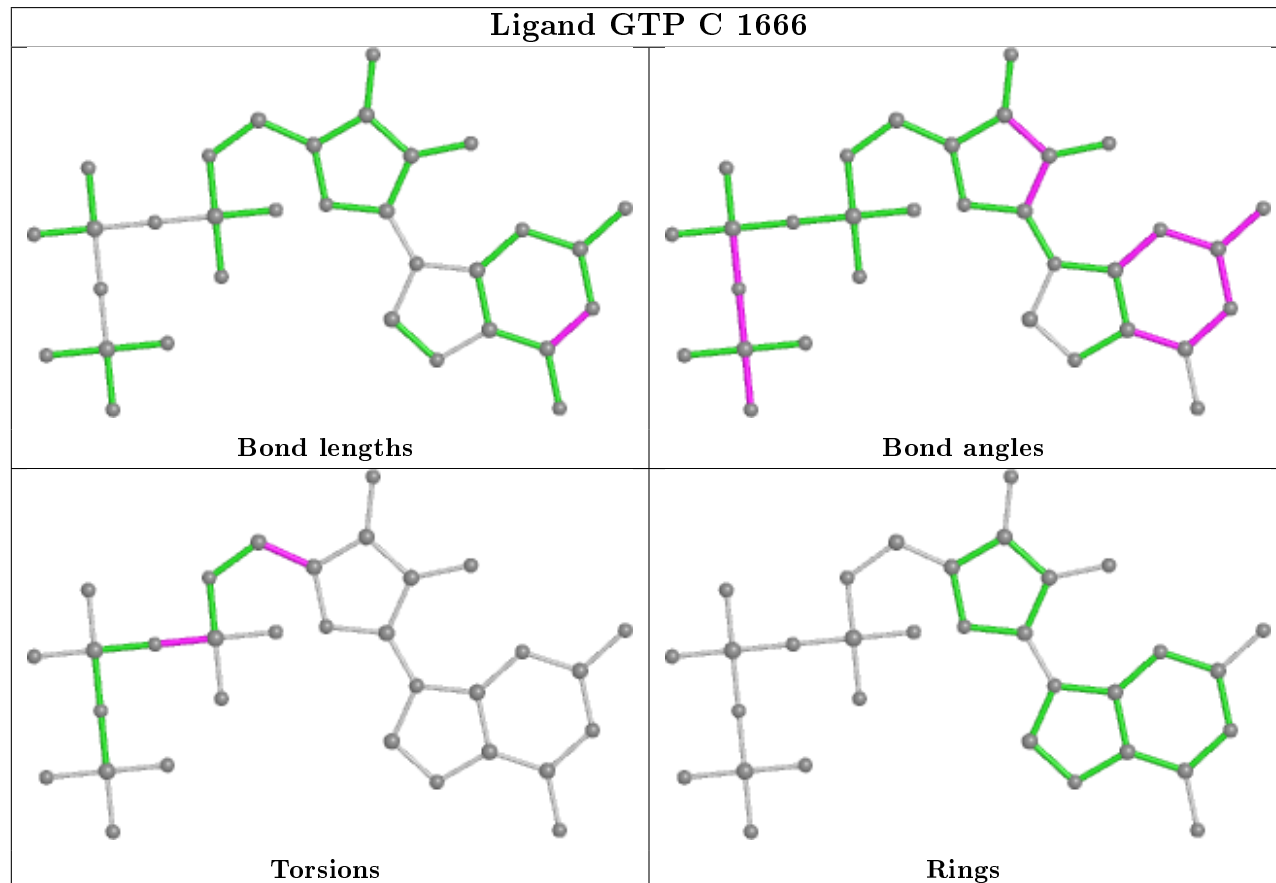
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1665	GTP	5	0
3	C	1666	GTP	5	0
3	C	1665	GTP	2	0
3	B	1665	GTP	6	0

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 than 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.

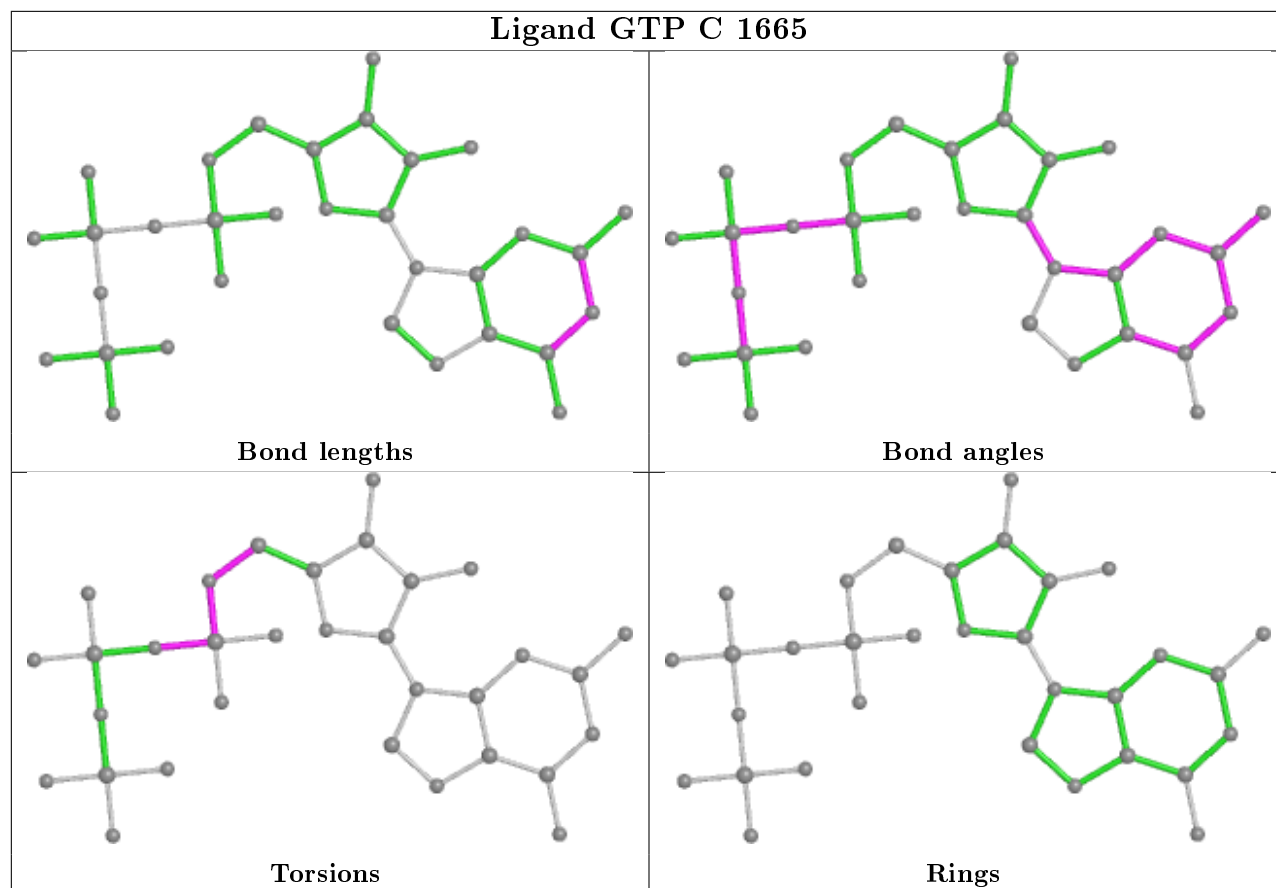
Ligand GTP A 1665



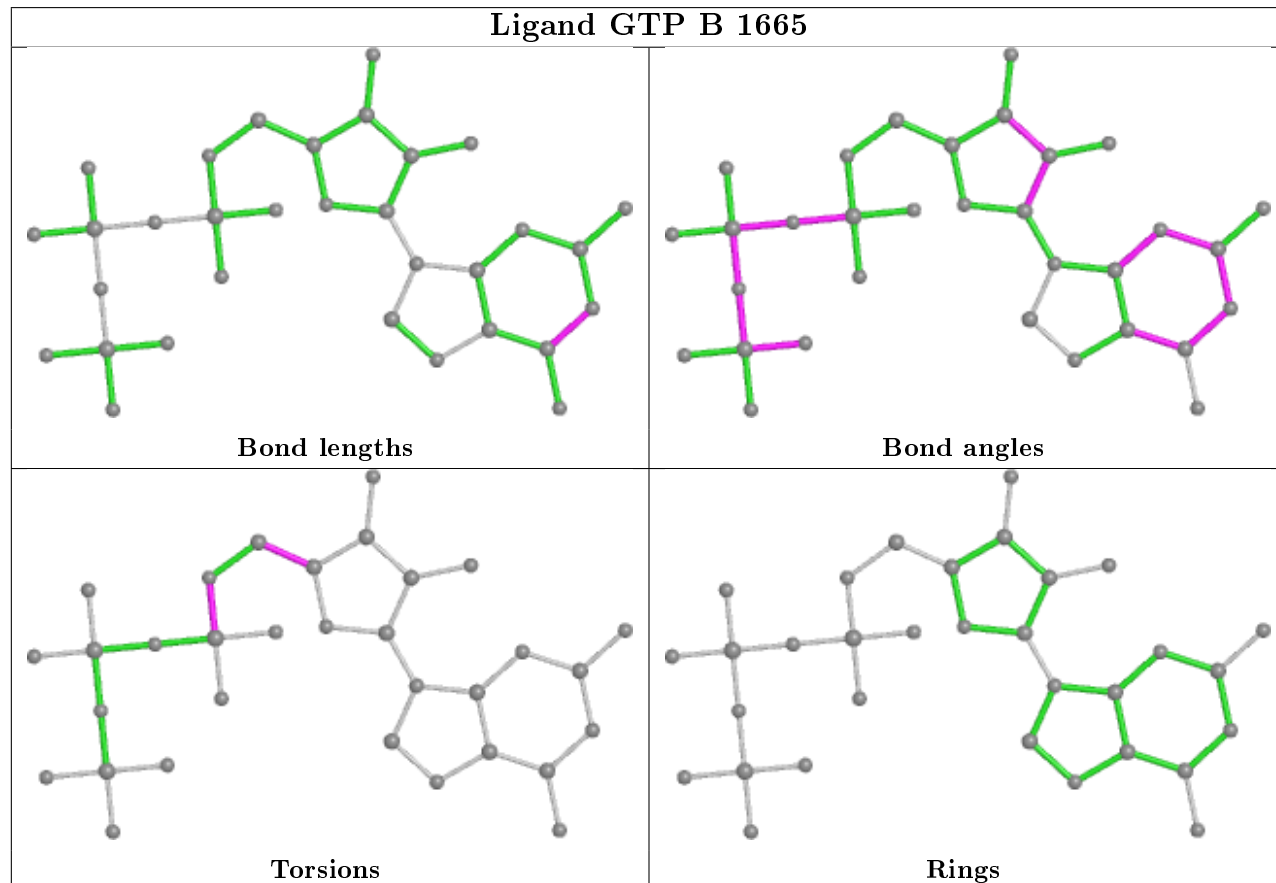
Ligand GTP C 1666



Ligand GTP C 1665



Ligand GTP B 1665



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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	664/664 (100%)	-0.47	8 (1%) 79 73	11, 24, 52, 111	0
1	B	664/664 (100%)	-0.42	4 (0%) 89 86	11, 25, 54, 84	0
1	C	651/664 (98%)	-0.20	16 (2%) 57 47	10, 39, 76, 102	0
2	D	5/5 (100%)	3.72	5 (100%) 0 0	47, 60, 63, 64	5 (100%)
2	E	5/5 (100%)	1.95	1 (20%) 1 0	23, 27, 43, 49	5 (100%)
2	F	4/5 (80%)	-0.21	0 100 100	28, 35, 54, 76	0
All	All	1993/2007 (99%)	-0.35	34 (1%) 70 63	10, 27, 69, 111	10 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	3	DT	5.8
2	E	3	DT	4.7
2	D	7	DC	3.9
2	D	6	DC	3.6
1	C	505	SER	3.5
2	D	4	DT	3.1
1	A	609	ALA	3.0
1	C	534	SER	2.9
1	C	1	PRO	2.9
1	A	603	ALA	2.8
1	A	664	ARG	2.8
1	A	607	ARG	2.8
1	B	31	SER	2.7
1	C	511	SER	2.7
1	C	576	TRP	2.6
1	C	2	ARG	2.6
1	C	253	LYS	2.5
1	C	580	GLY	2.4
1	B	664	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	250	SER	2.3
1	C	535	GLY	2.3
1	A	536	VAL	2.3
1	A	605	MET	2.3
1	A	1	PRO	2.3
1	C	259	ASP	2.2
1	C	571	ILE	2.2
1	A	608	GLN	2.2
1	B	505	SER	2.2
2	D	5	DT	2.2
1	C	241	SER	2.2
1	B	256	TYR	2.2
1	C	212	THR	2.0
1	C	71	GLU	2.0
1	C	664	ARG	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. The B-factors column lists the minimum, median, 95th 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.

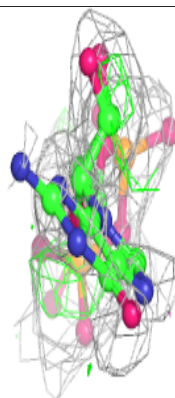
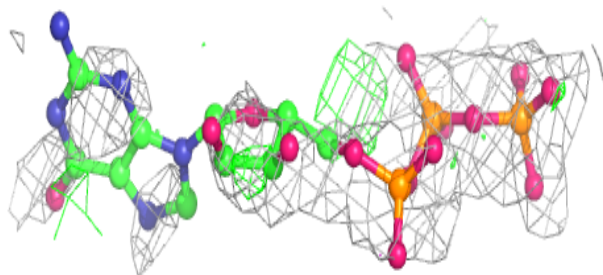
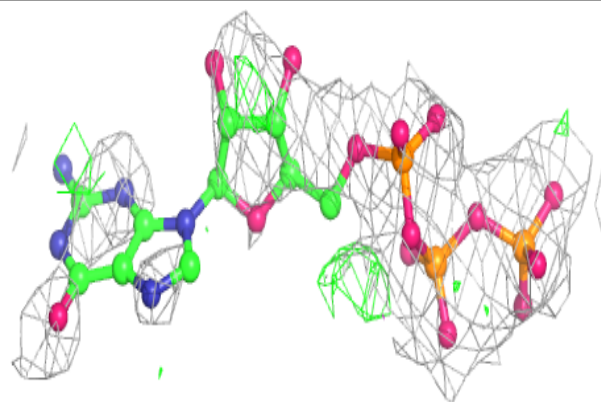
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GTP	A	1665	32/32	0.79	0.29	29,40,57,60	32
3	GTP	B	1665	32/32	0.85	0.30	13,40,63,67	32
3	GTP	C	1665	32/32	0.89	0.23	26,67,121,128	0
3	GTP	C	1666	32/32	0.96	0.18	28,40,56,59	0
4	MN	C	1667	1/1	0.97	0.04	43,43,43,43	0

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

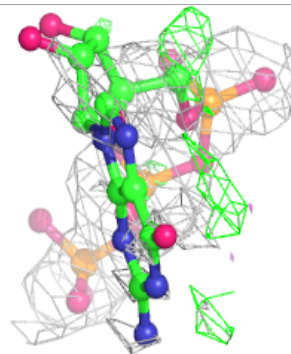
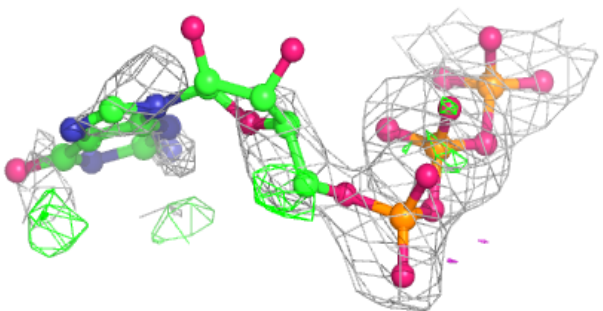
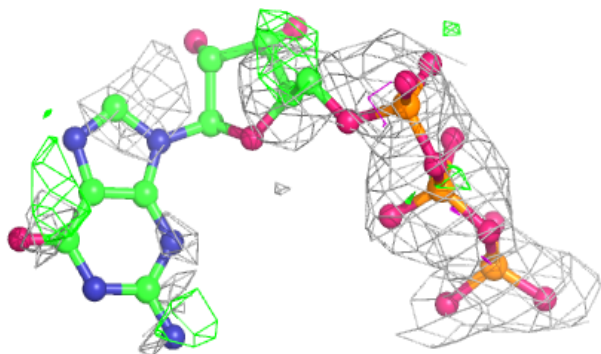
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GTP A 1665:

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

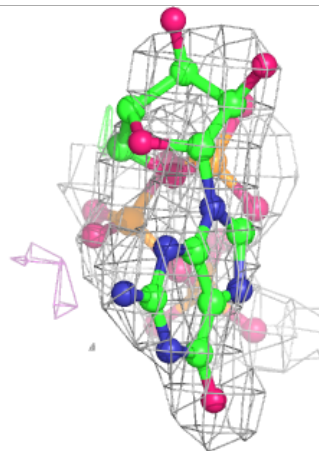
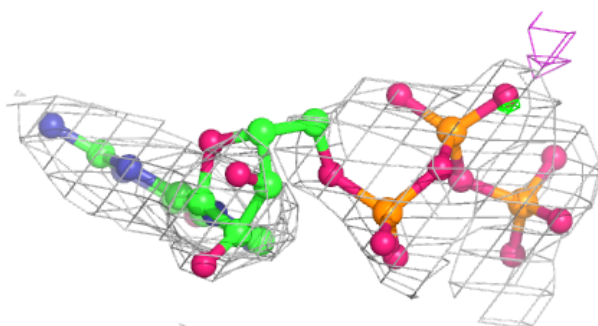
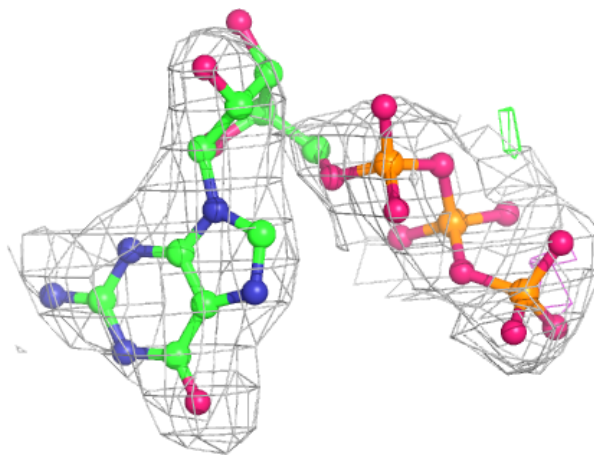
**Electron density around GTP B 1665:**

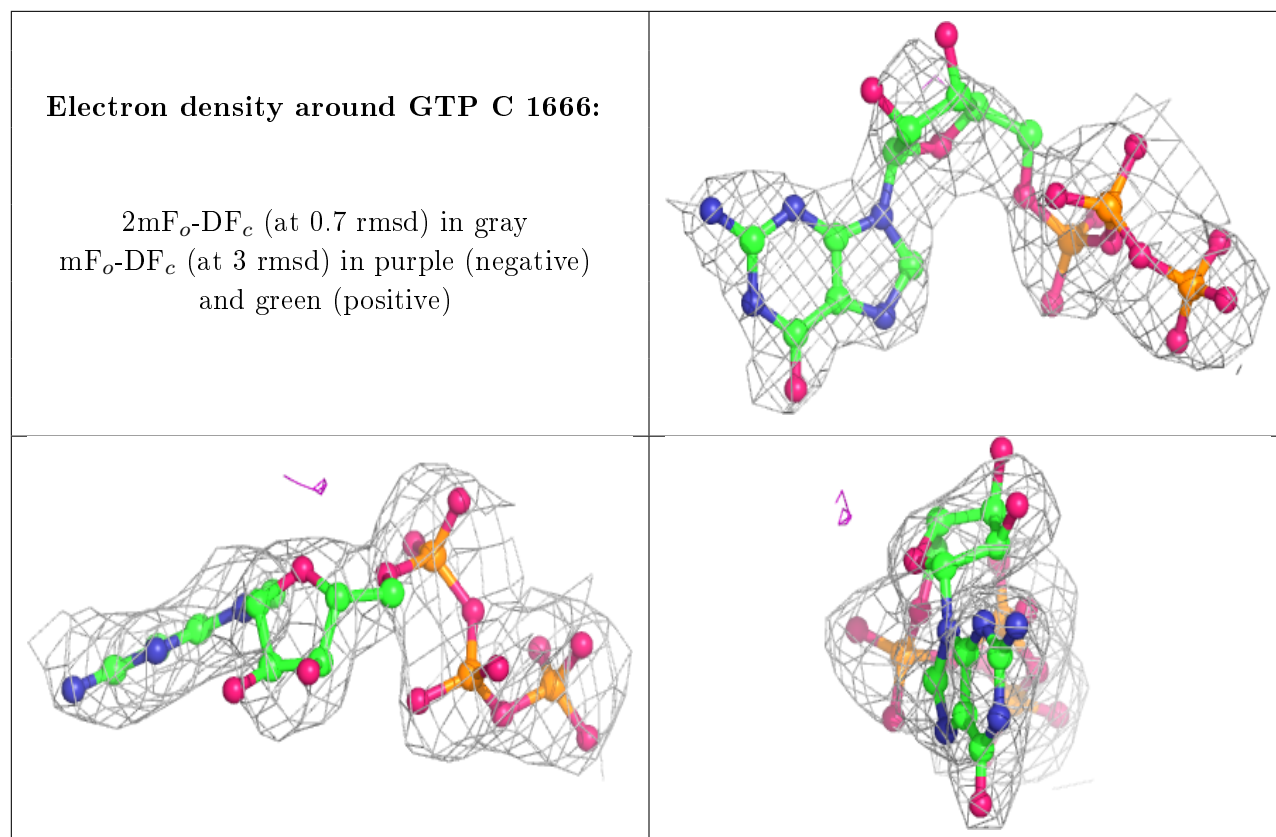
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GTP C 1665:

$2mF_o-DF_c$ (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.