



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2020 – 08:56 pm BST

PDB ID : 5CJP
Title : The Structural Basis for Cdc42-Induced Dimerization of IQGAPs
Authors : WorthyLake, D.K.; Boyapati, V.K.; LeCour Jr, L.
Deposited on : 2015-07-14
Resolution : 2.60 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

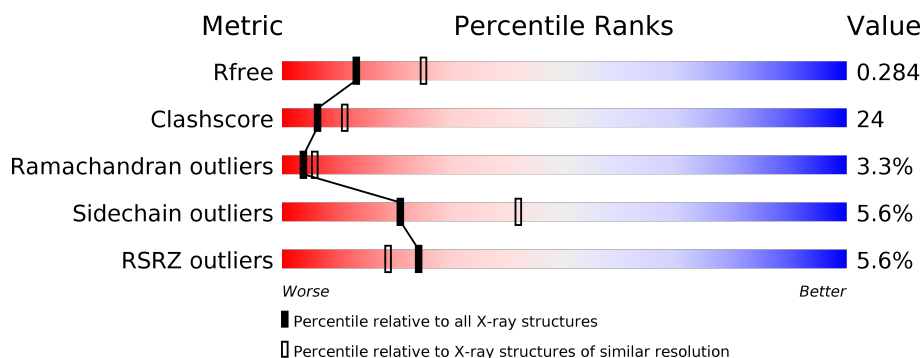
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	179	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>..</div> </div> </div>
1	B	179	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>31%</div> <div>..</div> </div> </div>
1	C	179	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>42%</div> <div>..</div> </div> </div>
1	D	179	<div> <div>17%</div> <div> <div></div> <div>47%</div> <div>49%</div> <div>..</div> </div> </div>
2	E	387	<div> <div>5%</div> <div> <div></div> <div>57%</div> <div>31%</div> <div>7%</div> <div>..</div> </div> </div>
2	F	387	<div> <div>5%</div> <div> <div></div> <div>50%</div> <div>39%</div> <div>7%</div> <div>..</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11762 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 Cell division cycle 42 (GTP binding protein, 25kDa), isoform CRA_a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1379	889	219	264	7			
1	B	177	Total	C	N	O	S	0	0	0
			1379	889	219	264	7			
1	C	177	Total	C	N	O	S	0	0	0
			1379	889	219	264	7			
1	D	177	Total	C	N	O	S	0	0	0
			1379	889	219	264	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A024RAE4
A	0	ALA	-	expression tag	UNP A0A024RAE4
A	61	LEU	GLN	engineered mutation	UNP A0A024RAE4
B	-1	GLY	-	expression tag	UNP A0A024RAE4
B	0	ALA	-	expression tag	UNP A0A024RAE4
B	61	LEU	GLN	engineered mutation	UNP A0A024RAE4
C	-1	GLY	-	expression tag	UNP A0A024RAE4
C	0	ALA	-	expression tag	UNP A0A024RAE4
C	61	LEU	GLN	engineered mutation	UNP A0A024RAE4
D	-1	GLY	-	expression tag	UNP A0A024RAE4
D	0	ALA	-	expression tag	UNP A0A024RAE4
D	61	LEU	GLN	engineered mutation	UNP A0A024RAE4

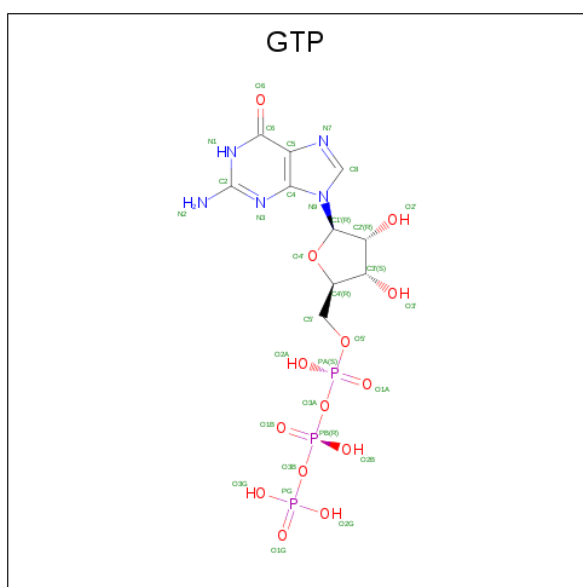
- Molecule 2 is a protein called Ras GTPase-activating-like protein IQGAP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	372	Total	C	N	O	S	0	0	0
			2998	1913	494	583	8			
2	F	372	Total	C	N	O	S	0	0	0
			2998	1913	494	583	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	872	GLY	-	expression tag	UNP Q13576
E	873	ALA	-	expression tag	UNP Q13576
E	874	MET	-	expression tag	UNP Q13576
F	872	GLY	-	expression tag	UNP Q13576
F	873	ALA	-	expression tag	UNP Q13576
F	874	MET	-	expression tag	UNP Q13576

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

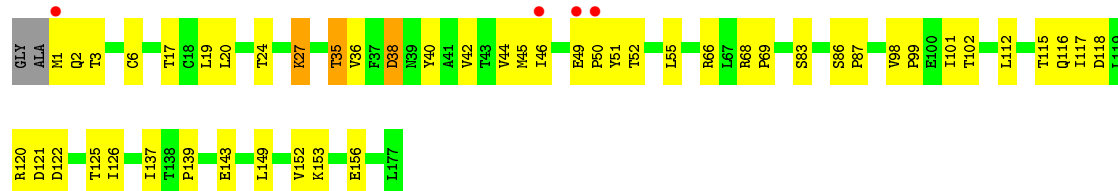
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total 30	O 30	0	0
5	B	21	Total 21	O 21	0	0
5	C	10	Total 10	O 10	0	0
5	D	3	Total 3	O 3	0	0
5	E	32	Total 32	O 32	0	0
5	F	22	Total 22	O 22	0	0

3 Residue-property plots [i](#)

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

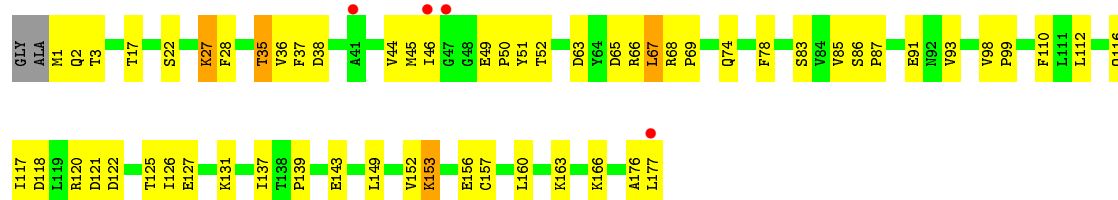
- Molecule 1: Cell division cycle 42 (GTP binding protein, 25kDa), isoform CRA_a

Chain A: 



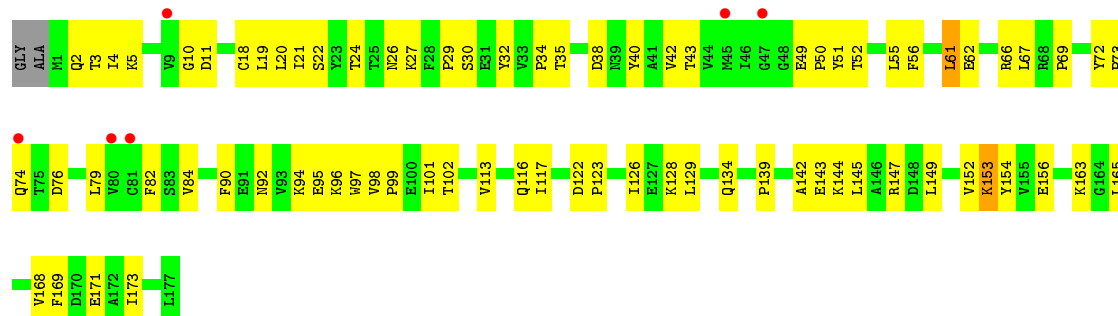
- Molecule 1: Cell division cycle 42 (GTP binding protein, 25kDa), isoform CRA_a

Chain B: 

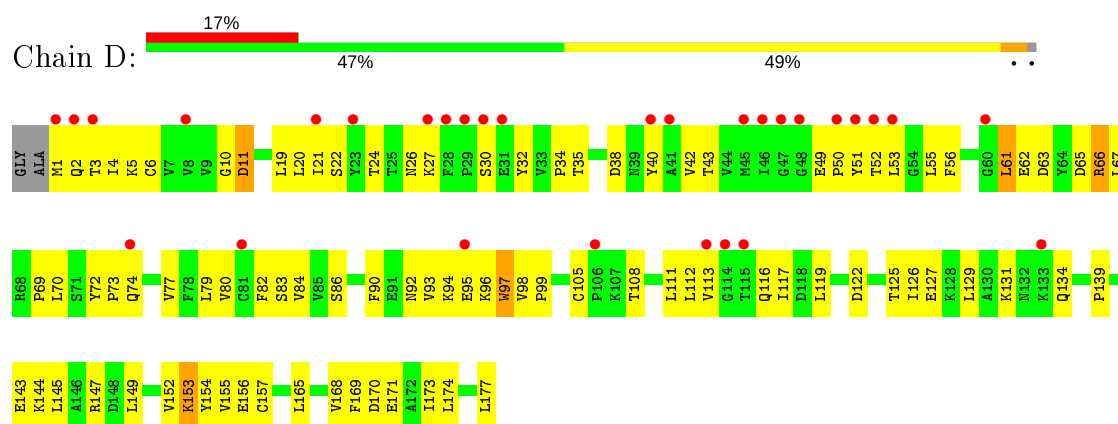


- Molecule 1: Cell division cycle 42 (GTP binding protein, 25kDa), isoform CRA_a

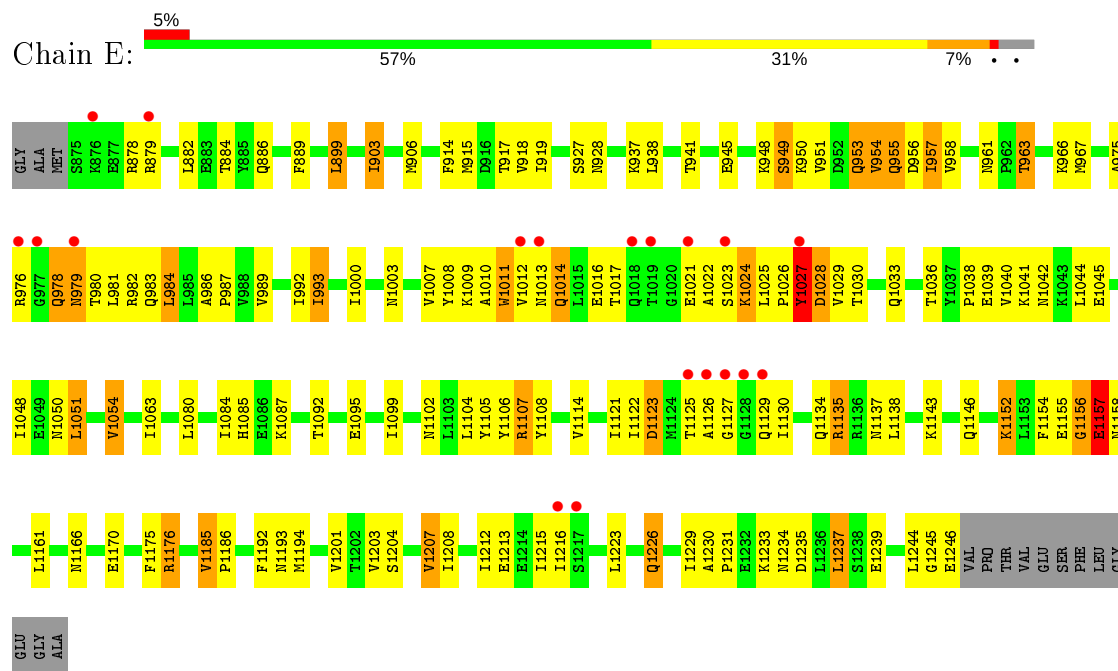
Chain C: 



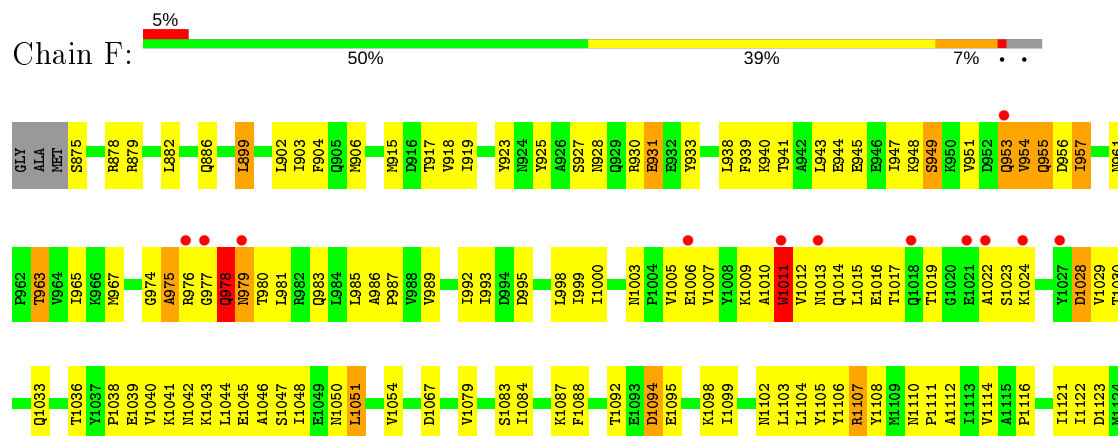
- Molecule 1: Cell division cycle 42 (GTP binding protein, 25kDa), isoform CRA_a

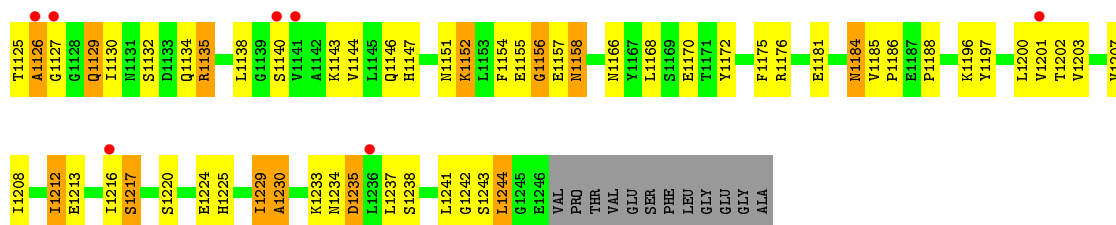


• Molecule 2: Ras GTPase-activating-like protein IQGAP2



• Molecule 2: Ras GTPase-activating-like protein IQGAP2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.63Å 120.17Å 157.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.97 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.60) 99.8 (19.97-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.56Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.287 0.245 , 0.284	Depositor DCC
R_{free} test set	3112 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11762	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, 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	0.45	0/1409	0.67	0/1917
1	B	0.43	0/1409	0.68	0/1917
1	C	0.36	0/1409	0.59	0/1917
1	D	0.32	0/1409	0.57	0/1917
2	E	0.42	0/3050	0.61	0/4131
2	F	0.41	0/3050	0.64	1/4131 (0.0%)
All	All	0.40	0/11736	0.63	1/15930 (0.0%)

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
2	E	0	1
2	F	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	977	GLY	N-CA-C	-7.17	95.16	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	1105	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	F	1105	TYR	Sidechain

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	1379	0	1402	38	0
1	B	1379	0	1402	61	0
1	C	1379	0	1402	64	0
1	D	1379	0	1402	74	0
2	E	2998	0	3032	163	0
2	F	2998	0	3032	198	0
3	A	32	0	12	3	0
3	B	32	0	12	3	0
3	C	32	0	12	4	0
3	D	32	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	30	0	0	1	0
5	B	21	0	0	5	0
5	C	10	0	0	1	0
5	D	3	0	0	3	0
5	E	32	0	0	8	0
5	F	22	0	0	3	0
All	All	11762	0	11720	568	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 24.

All (568) 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)
2:F:957:ILE:HD11	2:F:1084:ILE:HD11	1.29	1.07
2:E:1107:ARG:HH11	2:E:1107:ARG:HG3	1.23	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:951:VAL:HG21	2:F:957:ILE:HD13	1.48	0.96
2:E:1000:ILE:H	2:E:1137:ASN:HD21	1.14	0.93
2:F:927:SER:O	2:F:976:ARG:NH2	2.03	0.92
1:B:160:LEU:HD11	2:F:1200:LEU:HD11	1.56	0.88
2:F:927:SER:HA	2:F:976:ARG:NH1	1.89	0.87
2:F:1094:ASP:O	2:F:1098:LYS:HG3	1.75	0.86
1:B:35:THR:HG23	3:B:201:GTP:O3G	1.76	0.86
2:F:993:ILE:HD11	2:F:1138:LEU:HD11	1.56	0.85
2:F:957:ILE:CD1	2:F:1084:ILE:HD11	2.07	0.84
2:F:1044:LEU:O	2:F:1048:ILE:HG12	1.77	0.84
2:E:954:VAL:HG12	2:E:955:GLN:H	1.40	0.83
1:B:1:MET:HG3	1:B:50:PRO:O	1.79	0.82
2:F:951:VAL:O	2:F:1087:LYS:HE2	1.80	0.82
2:E:1041:LYS:O	2:E:1045:GLU:HG2	1.80	0.82
2:F:1029:VAL:HG22	2:F:1033:GLN:HG3	1.59	0.82
2:F:919:ILE:HD11	2:F:967:MET:HG3	1.62	0.82
2:F:1041:LYS:O	2:F:1045:GLU:HG2	1.81	0.81
1:B:98:VAL:HG21	1:B:149:LEU:HD13	1.62	0.81
2:E:963:THR:HG21	5:E:1304:HOH:O	1.79	0.81
2:F:1107:ARG:HH11	2:F:1107:ARG:HG3	1.46	0.81
1:B:120:ARG:O	1:B:126:ILE:HD11	1.80	0.81
2:F:927:SER:HA	2:F:976:ARG:HH12	1.45	0.80
2:E:1000:ILE:HG21	2:E:1051:LEU:HG	1.63	0.80
2:E:1029:VAL:HG22	2:E:1033:GLN:HG3	1.63	0.79
2:E:1130:ILE:HG23	2:E:1134:GLN:HB2	1.64	0.79
2:F:957:ILE:HD11	2:F:1084:ILE:CD1	2.12	0.79
2:F:1130:ILE:HG23	2:F:1134:GLN:HB2	1.64	0.78
2:F:1029:VAL:CG2	2:F:1033:GLN:HE21	1.97	0.78
2:F:1012:VAL:HB	2:F:1016:GLU:HG2	1.64	0.78
5:D:301:HOH:O	2:F:1107:ARG:HD3	1.82	0.77
1:D:84:VAL:HG11	5:D:302:HOH:O	1.84	0.77
2:E:919:ILE:HD11	2:E:967:MET:HG3	1.67	0.77
2:F:1229:ILE:N	2:F:1229:ILE:HD12	2.00	0.77
2:F:954:VAL:HG12	2:F:955:GLN:H	1.47	0.76
1:B:74:GLN:HG2	1:C:95:GLU:OE1	1.85	0.76
1:B:116:GLN:HB2	5:B:302:HOH:O	1.86	0.75
1:B:122:ASP:OD2	1:B:125:THR:HG23	1.86	0.75
2:E:1216:ILE:H	2:E:1216:ILE:HD12	1.51	0.75
2:F:976:ARG:NH1	2:F:976:ARG:HG2	2.02	0.74
2:F:976:ARG:HH11	2:F:976:ARG:HG2	1.51	0.74
2:F:1029:VAL:HG22	2:F:1033:GLN:HE21	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:OD2	1:A:125:THR:HG23	1.89	0.72
1:A:98:VAL:HG21	1:A:149:LEU:HD13	1.69	0.72
1:D:98:VAL:HG21	1:D:149:LEU:HD13	1.70	0.72
2:E:1244:LEU:HD23	2:E:1245:GLY:N	2.03	0.72
1:D:32:TYR:CD1	3:D:201:GTP:H5"	2.24	0.72
2:E:954:VAL:O	2:E:956:ASP:N	2.22	0.72
2:E:993:ILE:HD11	2:E:1138:LEU:HD11	1.71	0.72
2:F:954:VAL:C	2:F:956:ASP:H	1.94	0.71
1:A:35:THR:HG23	3:A:201:GTP:O2G	1.91	0.71
1:B:117:ILE:HD12	1:B:117:ILE:C	2.12	0.70
2:E:1107:ARG:HG3	2:E:1107:ARG:NH1	2.01	0.70
2:F:1156:GLY:O	2:F:1157:GLU:HB2	1.90	0.70
2:E:954:VAL:HG12	2:E:955:GLN:N	2.06	0.70
2:F:1229:ILE:O	2:F:1230:ALA:HB3	1.90	0.70
2:F:954:VAL:O	2:F:956:ASP:N	2.25	0.70
1:D:40:TYR:HB2	1:D:55:LEU:HB2	1.72	0.69
2:F:1000:ILE:HG21	2:F:1051:LEU:HG	1.72	0.69
2:E:951:VAL:HG13	2:E:956:ASP:HB2	1.74	0.69
2:E:1027:TYR:O	2:E:1028:ASP:HB3	1.92	0.69
2:F:1212:ILE:HD12	2:F:1213:GLU:N	2.08	0.69
1:C:5:LYS:HG3	1:C:56:PHE:CE1	2.27	0.69
2:E:957:ILE:HD12	2:E:957:ILE:H	1.58	0.69
1:B:139:PRO:O	1:B:143:GLU:HG3	1.93	0.68
2:E:1029:VAL:HG22	2:E:1030:THR:H	1.58	0.68
2:E:954:VAL:C	2:E:956:ASP:H	1.97	0.68
2:F:944:GLU:HA	2:F:947:ILE:HD12	1.76	0.68
2:F:1122:ILE:O	2:F:1122:ILE:HG13	1.94	0.68
2:F:965:ILE:HD12	2:F:1103:LEU:HD13	1.76	0.68
2:E:1030:THR:OG1	2:E:1033:GLN:HG2	1.96	0.66
1:B:93:VAL:HG11	1:B:112:LEU:HD11	1.76	0.66
2:E:882:LEU:O	2:E:886:GLN:HG3	1.95	0.66
2:E:1000:ILE:H	2:E:1137:ASN:ND2	1.89	0.66
2:F:1030:THR:OG1	2:F:1033:GLN:HG2	1.96	0.66
2:F:1003:ASN:O	2:F:1007:VAL:HG23	1.95	0.66
2:F:951:VAL:CG2	2:F:957:ILE:HD13	2.25	0.65
2:E:1029:VAL:CG2	2:E:1033:GLN:HE21	2.08	0.65
1:D:34:PRO:HB2	2:F:1106:TYR:CZ	2.31	0.65
1:D:92:ASN:HA	1:D:95:GLU:HB2	1.78	0.65
1:C:5:LYS:HE3	1:C:56:PHE:CZ	2.31	0.65
2:E:1027:TYR:O	2:E:1028:ASP:CB	2.45	0.65
2:F:923:TYR:CD1	2:F:975:ALA:HA	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:HG21	2:E:1208:ILE:HG22	1.79	0.65
2:E:1229:ILE:HG22	2:E:1229:ILE:O	1.95	0.65
2:F:1216:ILE:O	2:F:1217:SER:HB2	1.97	0.65
2:F:951:VAL:HG13	2:F:956:ASP:HB2	1.79	0.65
2:E:937:LYS:O	2:E:941:THR:HG23	1.97	0.65
2:E:1003:ASN:O	2:E:1007:VAL:HG23	1.97	0.64
2:F:1011:TRP:CE3	2:F:1012:VAL:HG13	2.32	0.64
1:C:4:ILE:HD12	1:C:4:ILE:N	2.11	0.64
1:C:92:ASN:HA	1:C:95:GLU:HB2	1.77	0.64
1:A:3:THR:HG22	1:A:52:THR:HB	1.79	0.64
2:F:1009:LYS:O	2:F:1013:ASN:HB2	1.98	0.64
2:F:1220:SER:O	2:F:1224:GLU:HG2	1.98	0.64
2:E:879:ARG:HH11	2:E:879:ARG:HG3	1.63	0.64
2:F:1197:TYR:HA	2:F:1200:LEU:HD12	1.80	0.64
1:D:98:VAL:HB	1:D:99:PRO:HD3	1.79	0.63
2:E:915:MET:O	2:E:919:ILE:HG12	1.97	0.63
1:A:120:ARG:O	1:A:126:ILE:HD11	1.98	0.63
1:A:139:PRO:O	1:A:143:GLU:HG3	1.98	0.63
2:E:1152:LYS:HB3	2:E:1152:LYS:NZ	2.14	0.62
2:F:928:ASN:HB2	5:F:1302:HOH:O	2.00	0.62
1:B:117:ILE:HD12	1:B:118:ASP:N	2.14	0.62
1:D:5:LYS:HD3	1:D:74:GLN:O	1.99	0.62
2:F:961:ASN:ND2	2:F:1107:ARG:HH22	1.97	0.62
2:E:1012:VAL:O	2:E:1016:GLU:HG2	1.99	0.62
2:E:1208:ILE:HG23	2:F:1212:ILE:HD13	1.81	0.62
2:F:980:THR:HG23	2:F:981:LEU:N	2.14	0.62
1:D:5:LYS:HE3	1:D:56:PHE:CZ	2.35	0.61
1:B:83:SER:HB3	1:B:86:SER:HB3	1.80	0.61
2:E:1009:LYS:O	2:E:1013:ASN:HB2	1.99	0.61
1:C:116:GLN:HG2	3:C:201:GTP:C5	2.35	0.61
1:D:2:GLN:HB3	1:D:51:TYR:HD1	1.65	0.61
2:F:919:ILE:CD1	2:F:967:MET:HG3	2.30	0.61
1:B:37:PHE:HD2	1:B:67:LEU:HD21	1.66	0.61
1:C:40:TYR:HB2	1:C:55:LEU:HB2	1.82	0.61
1:D:35:THR:HG23	5:D:303:HOH:O	2.01	0.61
2:E:1063:ILE:HG23	5:E:1332:HOH:O	2.01	0.61
1:B:3:THR:HG22	1:B:52:THR:HB	1.82	0.60
2:E:1244:LEU:HD23	2:E:1244:LEU:C	2.22	0.60
1:D:70:LEU:HD22	2:F:1135:ARG:HB3	1.84	0.60
2:F:1229:ILE:O	2:F:1230:ALA:CB	2.49	0.60
2:E:1185:VAL:HG22	2:E:1186:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1011:TRP:NE1	2:E:1039:GLU:HG3	2.17	0.59
2:F:1011:TRP:HE3	2:F:1012:VAL:HG22	1.67	0.59
2:F:961:ASN:HD22	2:F:1107:ARG:HH22	1.49	0.59
2:F:979:ASN:HB3	2:F:983:GLN:HB2	1.84	0.59
1:D:117:ILE:HG12	1:D:157:CYS:O	2.03	0.59
1:D:143:GLU:O	1:D:147:ARG:HD3	2.02	0.59
1:A:45:MET:HG2	1:A:49:GLU:O	2.03	0.59
2:E:1011:TRP:CG	2:E:1012:VAL:N	2.67	0.59
2:E:992:ILE:HG12	2:E:1054:VAL:CG1	2.32	0.59
1:D:43:THR:HG22	1:D:52:THR:OG1	2.03	0.58
2:E:1029:VAL:HG22	2:E:1033:GLN:HE21	1.67	0.58
2:E:986:ALA:HB3	2:E:987:PRO:HD3	1.84	0.58
2:F:1010:ALA:O	2:F:1014:GLN:HB2	2.02	0.58
2:F:1235:ASP:C	2:F:1237:LEU:H	2.05	0.58
1:A:87:PRO:HA	1:A:137:ILE:HD11	1.85	0.58
1:B:35:THR:CG2	5:B:301:HOH:O	2.51	0.58
2:E:1092:THR:OG1	2:E:1095:GLU:HG3	2.04	0.58
1:B:35:THR:HG22	5:B:301:HOH:O	2.03	0.58
1:B:44:VAL:HG12	1:B:45:MET:H	1.68	0.58
2:E:1156:GLY:O	2:E:1157:GLU:CB	2.51	0.58
2:F:941:THR:O	2:F:945:GLU:HB2	2.04	0.58
2:F:954:VAL:HG12	2:F:955:GLN:N	2.17	0.58
2:E:1014:GLN:NE2	2:E:1014:GLN:HA	2.19	0.58
2:E:1000:ILE:N	2:E:1137:ASN:HD21	1.94	0.58
2:F:1009:LYS:O	2:F:1014:GLN:HG2	2.04	0.58
1:A:83:SER:HB3	1:A:86:SER:HB3	1.84	0.57
1:D:83:SER:HB3	1:D:86:SER:HB3	1.85	0.57
2:E:1135:ARG:HH11	2:E:1135:ARG:HG3	1.68	0.57
2:E:992:ILE:HG12	2:E:1054:VAL:HG11	1.86	0.57
2:F:961:ASN:ND2	2:F:1107:ARG:NH2	2.51	0.57
2:E:1208:ILE:HG23	2:F:1212:ILE:CD1	2.34	0.57
2:F:1030:THR:HG1	2:F:1033:GLN:HG2	1.68	0.57
1:B:2:GLN:HB2	1:B:51:TYR:CD1	2.38	0.57
1:C:152:VAL:O	1:C:153:LYS:HB3	2.04	0.57
1:D:152:VAL:O	1:D:153:LYS:HB3	2.04	0.57
2:F:875:SER:O	2:F:879:ARG:HB2	2.04	0.57
2:E:928:ASN:HB2	5:E:1311:HOH:O	2.05	0.57
2:E:980:THR:HG23	2:E:981:LEU:N	2.19	0.57
2:E:1135:ARG:HH11	2:E:1135:ARG:CG	2.17	0.57
2:F:1107:ARG:HG3	2:F:1107:ARG:NH1	2.19	0.57
1:D:10:GLY:HA2	1:D:97:TRP:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:LEU:HD22	1:D:55:LEU:HD13	1.86	0.56
2:E:1036:THR:O	2:E:1038:PRO:HD3	2.04	0.56
2:E:1234:ASN:HD22	2:E:1234:ASN:N	2.03	0.56
2:F:1046:ALA:HB3	5:F:1308:HOH:O	2.03	0.56
1:A:44:VAL:HG12	1:A:45:MET:H	1.71	0.56
1:D:90:PHE:CZ	1:D:145:LEU:HD22	2.41	0.56
2:F:878:ARG:HG3	2:F:878:ARG:HH11	1.70	0.56
1:D:2:GLN:HB3	1:D:51:TYR:CD1	2.41	0.56
1:D:5:LYS:HG3	1:D:56:PHE:CE1	2.41	0.56
1:A:117:ILE:C	1:A:117:ILE:HD12	2.25	0.56
2:F:1009:LYS:HE3	2:F:1028:ASP:OD1	2.05	0.56
2:F:986:ALA:HB3	2:F:987:PRO:HD3	1.88	0.56
2:E:919:ILE:CD1	2:E:967:MET:HG3	2.35	0.56
2:F:947:ILE:HD13	2:F:1083:SER:OG	2.06	0.55
3:B:201:GTP:O2'	2:F:931:GLU:OE2	2.20	0.55
2:E:1080:LEU:O	2:E:1084:ILE:HD13	2.06	0.55
2:E:1176:ARG:HH11	2:E:1176:ARG:HG3	1.71	0.55
1:C:43:THR:HG22	1:C:52:THR:OG1	2.07	0.55
2:E:980:THR:HG23	2:E:981:LEU:H	1.71	0.55
2:E:1122:ILE:O	2:E:1122:ILE:HG13	2.06	0.55
2:F:1029:VAL:CG2	2:F:1033:GLN:HG3	2.35	0.55
2:E:1050:ASN:O	2:E:1054:VAL:HG22	2.06	0.55
2:E:1223:LEU:O	2:E:1226:GLN:HG2	2.07	0.55
1:C:35:THR:HG23	5:C:302:HOH:O	2.06	0.55
1:D:67:LEU:HD22	2:F:1114:VAL:HG11	1.89	0.55
1:B:122:ASP:OD1	2:F:1196:LYS:NZ	2.40	0.54
1:C:2:GLN:HB3	1:C:51:TYR:HD1	1.73	0.54
2:F:1229:ILE:N	2:F:1229:ILE:CD1	2.71	0.54
1:A:17:THR:OG1	1:A:35:THR:HG21	2.06	0.54
1:C:32:TYR:CD1	3:C:201:GTP:H5''	2.43	0.54
2:E:1012:VAL:HA	2:E:1016:GLU:HG2	1.90	0.54
2:F:1011:TRP:O	2:F:1014:GLN:N	2.35	0.54
2:E:1107:ARG:CG	2:E:1107:ARG:HH11	2.07	0.54
2:F:998:LEU:HD11	2:F:1000:ILE:HG13	1.89	0.54
2:F:1003:ASN:HD22	2:F:1006:GLU:CG	2.21	0.54
2:F:1130:ILE:N	2:F:1130:ILE:HD12	2.23	0.54
2:F:947:ILE:HD13	2:F:1083:SER:CB	2.37	0.54
1:B:127:GLU:O	1:B:131:LYS:HG3	2.07	0.54
1:C:62:GLU:HG2	1:C:96:LYS:NZ	2.22	0.54
1:D:153:LYS:HD2	1:D:171:GLU:OE1	2.08	0.54
2:F:1185:VAL:HG22	2:F:1186:PRO:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:SER:O	1:D:26:ASN:HA	2.07	0.53
2:F:915:MET:O	2:F:919:ILE:HG12	2.07	0.53
2:E:1193:ASN:N	5:E:1301:HOH:O	2.41	0.53
2:E:1084:ILE:HD12	2:E:1084:ILE:N	2.23	0.53
2:F:1212:ILE:HD12	2:F:1212:ILE:C	2.28	0.53
2:F:999:ILE:HG22	2:F:999:ILE:O	2.07	0.53
1:B:87:PRO:HA	1:B:137:ILE:HD11	1.91	0.53
2:E:957:ILE:CD1	2:E:957:ILE:H	2.19	0.53
1:B:166:LYS:HE2	5:B:316:HOH:O	2.09	0.53
2:F:1233:LYS:HE2	2:F:1235:ASP:OD1	2.09	0.53
2:F:904:PHE:HZ	2:F:967:MET:HE2	1.73	0.53
1:D:65:ASP:O	1:D:69:PRO:HD3	2.09	0.53
1:D:122:ASP:O	1:D:126:ILE:HG13	2.09	0.52
2:F:947:ILE:HA	2:F:951:VAL:CG2	2.38	0.52
2:F:954:VAL:C	2:F:956:ASP:N	2.60	0.52
1:B:17:THR:OG1	1:B:35:THR:HG21	2.09	0.52
1:C:10:GLY:HA2	1:C:97:TRP:CE2	2.45	0.52
2:E:1012:VAL:CA	2:E:1016:GLU:HG2	2.38	0.52
2:E:957:ILE:N	2:E:957:ILE:HD12	2.23	0.52
2:F:980:THR:HG23	2:F:981:LEU:H	1.74	0.52
1:C:153:LYS:HD2	1:C:171:GLU:OE1	2.09	0.52
2:E:1152:LYS:HB3	2:E:1152:LYS:HZ3	1.74	0.52
2:F:989:VAL:O	2:F:993:ILE:HG12	2.10	0.52
1:B:117:ILE:HD11	1:B:163:LYS:HE2	1.91	0.52
1:C:22:SER:HA	1:C:27:LYS:H	1.74	0.52
2:E:989:VAL:O	2:E:993:ILE:HD13	2.09	0.52
2:F:983:GLN:HG2	2:F:983:GLN:O	2.09	0.52
1:A:122:ASP:O	1:A:126:ILE:HG12	2.09	0.52
1:D:43:THR:HA	1:D:51:TYR:O	2.09	0.52
2:F:992:ILE:HG12	2:F:1054:VAL:CG1	2.40	0.52
2:F:1015:LEU:C	2:F:1017:THR:H	2.13	0.52
2:F:1130:ILE:HD12	2:F:1130:ILE:H	1.74	0.52
2:F:985:LEU:O	2:F:989:VAL:HG23	2.09	0.52
2:F:947:ILE:HD13	2:F:1083:SER:HB3	1.92	0.52
1:C:143:GLU:O	1:C:147:ARG:HD3	2.10	0.52
1:D:94:LYS:HB3	1:D:149:LEU:HD11	1.92	0.52
2:E:1011:TRP:CD1	2:E:1012:VAL:HG22	2.45	0.52
2:E:954:VAL:C	2:E:956:ASP:N	2.63	0.52
1:C:169:PHE:O	1:C:173:ILE:HG13	2.10	0.52
2:E:1203:VAL:HG22	2:E:1204:SER:N	2.25	0.52
2:F:1135:ARG:CG	2:F:1135:ARG:HH11	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1225:HIS:O	2:F:1229:ILE:HD13	2.10	0.51
1:A:116:GLN:HG2	3:A:201:GTP:C5	2.45	0.51
2:F:963:THR:HG22	5:F:1316:HOH:O	2.10	0.51
1:B:44:VAL:HG12	1:B:45:MET:N	2.25	0.51
2:E:1216:ILE:HD12	2:E:1216:ILE:N	2.22	0.51
2:F:1135:ARG:HG3	2:F:1135:ARG:HH11	1.75	0.51
1:D:119:LEU:O	1:D:122:ASP:HB3	2.10	0.51
2:E:914:PHE:HZ	2:F:1244:LEU:HD12	1.74	0.51
1:D:94:LYS:HD3	1:D:145:LEU:HD11	1.92	0.51
1:D:169:PHE:O	1:D:173:ILE:HG13	2.11	0.51
1:D:21:ILE:HG22	1:D:27:LYS:O	2.10	0.51
2:F:974:GLY:O	2:F:975:ALA:O	2.28	0.51
1:D:3:THR:HA	1:D:52:THR:O	2.10	0.51
2:E:1185:VAL:CG2	5:E:1315:HOH:O	2.58	0.51
1:A:38:ASP:OD2	2:F:878:ARG:NH2	2.44	0.51
1:D:24:THR:HG22	1:D:42:VAL:HG21	1.93	0.51
2:E:1156:GLY:O	2:E:1157:GLU:HB2	2.10	0.51
2:F:1092:THR:OG1	2:F:1095:GLU:HG3	2.10	0.51
1:D:1:MET:O	1:D:2:GLN:HG2	2.12	0.50
2:F:902:LEU:O	2:F:906:MET:HG3	2.11	0.50
1:B:67:LEU:O	1:B:67:LEU:HD23	2.10	0.50
2:E:1166:ASN:O	2:E:1170:GLU:HG3	2.11	0.50
2:E:1192:PHE:O	2:E:1194:MET:N	2.44	0.50
1:C:96:LYS:C	1:C:99:PRO:HD2	2.32	0.50
1:D:93:VAL:HG11	1:D:112:LEU:HD11	1.92	0.50
1:C:61:LEU:HD23	1:C:62:GLU:H	1.76	0.50
1:D:22:SER:HA	1:D:27:LYS:H	1.77	0.50
2:E:1215:ILE:CG2	2:F:1207:VAL:HG22	2.42	0.50
1:C:90:PHE:CZ	1:C:145:LEU:HD22	2.46	0.50
2:F:978:GLN:O	2:F:980:THR:N	2.44	0.50
1:C:43:THR:HA	1:C:51:TYR:O	2.11	0.50
2:F:965:ILE:CG2	2:F:1107:ARG:NH1	2.75	0.50
2:F:1011:TRP:CZ3	2:F:1012:VAL:HG13	2.47	0.50
2:E:889:PHE:CE2	2:E:1212:ILE:HG13	2.47	0.50
2:F:933:TYR:HD1	2:F:1188:PRO:HB2	1.76	0.50
2:F:1229:ILE:HD12	2:F:1229:ILE:H	1.76	0.50
1:A:27:LYS:HG2	2:E:1203:VAL:HB	1.92	0.49
1:B:176:ALA:O	1:B:177:LEU:HD23	2.12	0.49
1:D:165:LEU:O	1:D:168:VAL:HG23	2.12	0.49
1:C:117:ILE:HD11	1:C:163:LYS:HD3	1.95	0.49
2:E:978:GLN:O	2:E:980:THR:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:PHE:CD2	1:B:67:LEU:HD21	2.47	0.49
2:F:992:ILE:HG12	2:F:1054:VAL:HG13	1.93	0.49
1:B:28:PHE:O	2:F:1202:THR:HA	2.13	0.49
2:E:1235:ASP:O	2:E:1239:GLU:HG2	2.12	0.49
1:C:2:GLN:HB3	1:C:51:TYR:CD1	2.48	0.49
1:C:98:VAL:HG21	1:C:149:LEU:HD13	1.94	0.49
2:F:1157:GLU:OE1	2:F:1157:GLU:HA	2.12	0.49
1:A:2:GLN:HB2	1:A:51:TYR:CD1	2.48	0.49
1:C:116:GLN:HG2	3:C:201:GTP:C6	2.48	0.49
2:F:1112:ALA:HB1	2:F:1121:ILE:HD11	1.94	0.49
1:C:94:LYS:HB3	1:C:149:LEU:HD11	1.94	0.48
2:F:1104:LEU:O	2:F:1108:TYR:HB3	2.13	0.48
2:F:1154:PHE:CD1	2:F:1168:LEU:HD11	2.48	0.48
1:B:85:VAL:HG22	5:B:302:HOH:O	2.11	0.48
2:E:1226:GLN:HB3	2:E:1231:PRO:HG3	1.96	0.48
2:F:918:VAL:HG23	2:F:919:ILE:N	2.28	0.48
2:E:1135:ARG:NH1	2:E:1135:ARG:CG	2.73	0.48
2:E:984:LEU:O	2:E:984:LEU:HD23	2.14	0.48
2:E:1154:PHE:CD1	2:E:1161:LEU:HB3	2.48	0.48
2:E:1216:ILE:CD1	2:E:1216:ILE:H	2.22	0.48
1:A:19:LEU:HD12	1:A:20:LEU:N	2.28	0.48
2:E:979:ASN:HB3	2:E:983:GLN:HB2	1.94	0.48
1:B:27:LYS:CB	2:F:1203:VAL:HG13	2.44	0.48
2:F:882:LEU:O	2:F:886:GLN:HG3	2.13	0.48
1:B:67:LEU:C	1:B:67:LEU:HD23	2.34	0.48
2:F:1039:GLU:HG2	2:F:1040:VAL:H	1.78	0.48
1:C:18:CYS:SG	3:C:201:GTP:H2'	2.53	0.48
2:F:1029:VAL:HG22	2:F:1033:GLN:NE2	2.25	0.48
1:A:1:MET:HG3	1:A:50:PRO:O	2.14	0.48
1:C:24:THR:HG22	1:C:42:VAL:HG21	1.96	0.48
2:F:1012:VAL:CB	2:F:1016:GLU:HG2	2.38	0.48
2:F:1087:LYS:HD3	2:F:1088:PHE:HE1	1.79	0.48
2:F:1216:ILE:O	2:F:1217:SER:CB	2.61	0.48
1:D:105:CYS:HB3	1:D:108:THR:OG1	2.14	0.47
1:B:45:MET:HG2	1:B:50:PRO:HA	1.96	0.47
2:E:1107:ARG:CG	2:E:1107:ARG:NH1	2.73	0.47
2:F:1003:ASN:HD22	2:F:1006:GLU:HG3	1.79	0.47
1:A:98:VAL:HB	1:A:99:PRO:HD3	1.96	0.47
1:A:117:ILE:HD12	1:A:118:ASP:N	2.29	0.47
1:A:44:VAL:HG12	1:A:45:MET:N	2.28	0.47
1:C:32:TYR:HE2	2:E:958:VAL:HG12	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:TYR:OH	1:D:156:GLU:HB3	2.14	0.47
2:F:1116:PRO:HA	2:F:1121:ILE:HD13	1.96	0.47
2:F:953:GLN:C	2:F:954:VAL:O	2.50	0.47
1:B:78:PHE:HB2	1:B:110:PHE:HB3	1.97	0.47
2:E:1185:VAL:HG23	5:E:1315:HOH:O	2.15	0.47
2:F:957:ILE:CG1	2:F:1084:ILE:HD11	2.45	0.47
2:E:961:ASN:ND2	2:E:1107:ARG:NH2	2.63	0.47
2:F:1234:ASN:O	2:F:1237:LEU:HB3	2.15	0.47
2:F:933:TYR:CD1	2:F:1188:PRO:HB2	2.49	0.47
1:D:125:THR:O	1:D:129:LEU:HD13	2.15	0.47
1:D:69:PRO:O	1:D:73:PRO:HD3	2.14	0.47
2:E:879:ARG:HH11	2:E:879:ARG:CG	2.28	0.47
1:A:46:ILE:O	1:A:46:ILE:HG22	2.15	0.47
1:D:170:ASP:O	1:D:174:LEU:HG	2.15	0.47
2:E:1011:TRP:HE1	2:E:1039:GLU:HG3	1.79	0.47
2:E:953:GLN:C	2:E:954:VAL:O	2.49	0.47
1:C:21:ILE:HD12	1:C:29:PRO:HG2	1.96	0.46
1:D:116:GLN:HG2	3:D:201:GTP:C5	2.50	0.46
2:E:906:MET:HG2	2:F:1238:SER:O	2.15	0.46
2:E:982:ARG:HA	2:E:1121:ILE:HG23	1.95	0.46
1:B:117:ILE:HG23	1:B:157:CYS:O	2.15	0.46
2:E:945:GLU:O	2:E:949:SER:HB3	2.15	0.46
2:E:953:GLN:O	2:E:953:GLN:CG	2.63	0.46
2:F:1029:VAL:HG22	2:F:1030:THR:H	1.79	0.46
2:F:925:TYR:CE2	2:F:931:GLU:HB3	2.51	0.46
1:B:68:ARG:HB3	1:B:69:PRO:HD3	1.97	0.46
1:D:96:LYS:O	1:D:99:PRO:HD2	2.15	0.46
1:A:6:CYS:HB3	1:A:55:LEU:HD23	1.97	0.46
1:C:3:THR:HA	1:C:52:THR:O	2.14	0.46
1:B:116:GLN:HG2	3:B:201:GTP:C5	2.50	0.46
1:C:19:LEU:HD12	1:C:20:LEU:N	2.31	0.46
2:F:1047:SER:HA	2:F:1050:ASN:HD22	1.80	0.46
1:D:173:ILE:O	1:D:177:LEU:HG	2.16	0.46
1:D:4:ILE:HB	1:D:53:LEU:HD12	1.97	0.46
2:E:1023:SER:C	2:E:1025:LEU:H	2.18	0.46
1:A:101:ILE:HG13	1:A:102:THR:N	2.31	0.46
1:C:5:LYS:HD3	1:C:74:GLN:O	2.16	0.46
2:E:1154:PHE:O	2:E:1155:GLU:HB3	2.16	0.46
2:F:878:ARG:HG3	2:F:878:ARG:NH1	2.28	0.46
1:D:117:ILE:HG12	1:D:157:CYS:C	2.36	0.46
2:E:1009:LYS:C	2:E:1013:ASN:HB2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:882:LEU:HD11	2:E:1212:ILE:HG22	1.98	0.46
2:F:1029:VAL:HG23	2:F:1033:GLN:HE21	1.77	0.46
2:F:953:GLN:O	2:F:953:GLN:CG	2.64	0.46
2:F:1140:SER:O	2:F:1144:VAL:HG23	2.16	0.45
2:E:1014:GLN:HE21	2:E:1014:GLN:HA	1.80	0.45
2:F:1197:TYR:HA	2:F:1200:LEU:CD1	2.46	0.45
1:A:116:GLN:HG2	3:A:201:GTP:C6	2.51	0.45
1:C:142:ALA:O	1:C:145:LEU:N	2.50	0.45
1:C:67:LEU:HB2	2:E:1114:VAL:CG1	2.46	0.45
1:C:98:VAL:HB	1:C:99:PRO:HD3	1.99	0.45
1:D:129:LEU:O	1:D:134:GLN:N	2.47	0.45
2:E:1029:VAL:CG2	2:E:1033:GLN:HG3	2.40	0.45
2:F:1012:VAL:HA	2:F:1015:LEU:HB2	1.99	0.45
1:B:22:SER:HA	1:B:27:LYS:O	2.17	0.45
1:D:79:LEU:HD22	1:D:113:VAL:HG21	1.98	0.45
2:F:1099:ILE:O	2:F:1102:ASN:HB3	2.16	0.45
2:F:1135:ARG:CG	2:F:1135:ARG:NH1	2.79	0.45
2:E:1012:VAL:O	2:E:1016:GLU:CG	2.64	0.45
2:E:1212:ILE:HG22	2:E:1213:GLU:N	2.31	0.45
2:E:927:SER:CB	2:E:976:ARG:NH2	2.79	0.45
1:C:154:TYR:OH	1:C:156:GLU:HB3	2.17	0.45
1:D:19:LEU:HD12	1:D:19:LEU:C	2.36	0.45
2:F:954:VAL:HG23	2:F:1088:PHE:CD2	2.52	0.45
2:E:1008:TYR:HA	2:E:1040:VAL:HG21	1.99	0.45
2:E:1044:LEU:O	2:E:1048:ILE:HG13	2.16	0.45
2:E:927:SER:HB3	2:E:976:ARG:CZ	2.47	0.45
2:F:1067:ASP:OD1	2:F:1067:ASP:N	2.46	0.45
2:F:943:LEU:HG	2:F:947:ILE:HD11	1.99	0.45
1:A:115:THR:O	1:A:116:GLN:HB2	2.17	0.45
1:D:49:GLU:CD	1:D:50:PRO:HD2	2.37	0.45
1:D:62:GLU:HG2	1:D:96:LYS:HZ1	1.82	0.45
2:E:878:ARG:NH2	2:F:1208:ILE:HD11	2.32	0.45
1:C:128:LYS:NZ	2:E:950:LYS:HA	2.31	0.45
2:F:993:ILE:HG23	2:F:1134:GLN:NE2	2.31	0.45
1:C:165:LEU:O	1:C:168:VAL:HG23	2.17	0.44
1:C:84:VAL:HG21	1:C:117:ILE:HA	1.99	0.44
1:B:98:VAL:HB	1:B:99:PRO:HD3	1.99	0.44
1:D:62:GLU:HG2	1:D:96:LYS:NZ	2.32	0.44
2:E:1233:LYS:O	2:E:1237:LEU:HB2	2.18	0.44
2:E:983:GLN:HG2	2:E:983:GLN:O	2.17	0.44
2:E:1017:THR:HG22	2:E:1017:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:LYS:C	1:D:99:PRO:HD2	2.37	0.44
2:E:948:LYS:HA	2:E:1087:LYS:HZ2	1.82	0.44
2:F:1011:TRP:CZ3	2:F:1039:GLU:HG3	2.52	0.44
2:F:1110:ASN:N	2:F:1111:PRO:CD	2.81	0.44
2:F:1143:LYS:O	2:F:1147:HIS:HD2	2.01	0.44
1:A:45:MET:HG2	1:A:50:PRO:HA	1.98	0.44
1:B:74:GLN:HG2	1:C:95:GLU:CD	2.38	0.44
2:F:1155:GLU:O	2:F:1156:GLY:O	2.35	0.44
1:C:62:GLU:HG2	1:C:96:LYS:HZ2	1.83	0.44
1:D:97:TRP:O	1:D:98:VAL:C	2.55	0.44
2:E:899:LEU:O	2:E:903:ILE:HD13	2.18	0.44
1:A:49:GLU:HB2	1:A:51:TYR:CE2	2.53	0.44
1:C:122:ASP:O	1:C:126:ILE:HG13	2.18	0.44
1:C:129:LEU:O	1:C:134:GLN:N	2.45	0.44
1:D:49:GLU:OE2	1:D:50:PRO:HD2	2.18	0.44
2:E:1244:LEU:CD2	2:E:1244:LEU:C	2.86	0.44
2:F:980:THR:CG2	2:F:981:LEU:N	2.79	0.44
1:A:36:VAL:CG2	2:E:1208:ILE:HG22	2.45	0.44
1:B:46:ILE:O	1:B:46:ILE:HG22	2.18	0.43
1:C:69:PRO:O	1:C:73:PRO:HD3	2.18	0.43
1:D:66:ARG:HH11	1:D:66:ARG:HG3	1.83	0.43
2:E:1084:ILE:N	2:E:1084:ILE:CD1	2.81	0.43
2:F:965:ILE:HA	2:F:965:ILE:HD13	1.78	0.43
1:D:6:CYS:HA	1:D:77:VAL:O	2.18	0.43
2:F:1016:GLU:OE1	2:F:1019:THR:HG21	2.18	0.43
1:B:27:LYS:CG	2:F:1201:VAL:HG12	2.49	0.43
1:B:2:GLN:HB2	1:B:51:TYR:CE1	2.53	0.43
2:E:1010:ALA:O	2:E:1014:GLN:HB3	2.18	0.43
1:C:49:GLU:OE2	1:C:50:PRO:HD2	2.18	0.43
2:E:1207:VAL:C	2:E:1208:ILE:HD12	2.39	0.43
2:E:984:LEU:C	2:E:984:LEU:HD23	2.39	0.43
2:F:1155:GLU:O	2:F:1156:GLY:C	2.57	0.43
2:F:904:PHE:CZ	2:F:967:MET:HE2	2.52	0.43
1:C:61:LEU:HD23	1:C:62:GLU:N	2.34	0.43
1:D:10:GLY:O	1:D:11:ASP:C	2.56	0.43
2:E:1029:VAL:HG13	2:E:1030:THR:N	2.34	0.43
1:B:112:LEU:HA	1:B:112:LEU:HD12	1.83	0.43
1:D:84:VAL:HG21	1:D:117:ILE:HA	2.00	0.43
1:B:44:VAL:C	1:B:45:MET:HG3	2.39	0.43
1:C:79:LEU:HD22	1:C:113:VAL:HG21	2.00	0.43
2:E:1042:ASN:O	2:E:1045:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1123:ASP:OD1	2:E:1125:THR:HG23	2.19	0.43
2:E:1234:ASN:N	2:E:1234:ASN:ND2	2.65	0.43
1:B:36:VAL:O	1:B:37:PHE:HB3	2.19	0.43
1:C:3:THR:C	1:C:4:ILE:HD12	2.39	0.43
1:D:152:VAL:O	1:D:153:LYS:CB	2.67	0.43
2:F:1036:THR:O	2:F:1038:PRO:HD3	2.19	0.43
2:F:1152:LYS:NZ	2:F:1152:LYS:HB3	2.34	0.43
2:F:965:ILE:HG22	2:F:1107:ARG:NH1	2.34	0.43
2:E:918:VAL:HG23	2:E:919:ILE:N	2.33	0.43
1:A:152:VAL:O	1:A:153:LYS:HB3	2.19	0.42
1:B:27:LYS:HG3	2:F:1201:VAL:HG12	2.01	0.42
1:B:91:GLU:HA	1:B:91:GLU:OE1	2.19	0.42
1:D:80:VAL:HG11	1:D:93:VAL:HG13	2.00	0.42
2:E:954:VAL:CG1	2:E:955:GLN:H	2.19	0.42
2:F:919:ILE:HG22	2:F:923:TYR:CZ	2.53	0.42
2:E:1104:LEU:O	2:E:1108:TYR:HB3	2.19	0.42
2:E:1208:ILE:N	2:E:1208:ILE:HD12	2.34	0.42
2:F:1012:VAL:HG12	2:F:1016:GLU:OE2	2.19	0.42
2:F:1129:GLN:HB3	2:F:1129:GLN:HE21	1.61	0.42
1:D:127:GLU:O	1:D:131:LYS:HG3	2.19	0.42
2:F:947:ILE:HA	2:F:951:VAL:HG21	2.00	0.42
1:A:112:LEU:HA	1:A:112:LEU:HD12	1.87	0.42
1:B:152:VAL:O	1:B:153:LYS:HB3	2.20	0.42
2:E:1023:SER:C	2:E:1025:LEU:N	2.73	0.42
2:E:993:ILE:CD1	2:E:993:ILE:N	2.83	0.42
2:F:1012:VAL:C	2:F:1014:GLN:N	2.72	0.42
1:B:2:GLN:HB2	1:B:51:TYR:HD1	1.85	0.42
1:B:49:GLU:HB2	1:B:51:TYR:CE2	2.54	0.42
1:C:34:PRO:HB2	2:E:1106:TYR:CZ	2.54	0.42
1:D:69:PRO:HA	1:D:72:TYR:CD2	2.55	0.42
2:F:1166:ASN:O	2:F:1170:GLU:HG3	2.18	0.42
1:C:139:PRO:O	1:C:143:GLU:HG3	2.18	0.42
2:F:1012:VAL:C	2:F:1014:GLN:H	2.23	0.42
1:B:45:MET:HG2	1:B:49:GLU:O	2.20	0.42
1:D:82:PHE:CD1	1:D:82:PHE:C	2.93	0.42
2:E:1012:VAL:C	2:E:1014:GLN:H	2.22	0.42
2:E:914:PHE:O	2:E:918:VAL:HG13	2.19	0.42
2:E:953:GLN:HE21	2:E:953:GLN:HB3	1.55	0.42
2:E:978:GLN:O	2:E:980:THR:HG22	2.19	0.42
2:F:976:ARG:HH11	2:F:976:ARG:CG	2.21	0.42
1:D:19:LEU:HD12	1:D:20:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LEU:HD23	1:D:62:GLU:H	1.85	0.42
2:F:940:LYS:HG3	2:F:1079:VAL:HG11	2.02	0.42
2:E:1229:ILE:CG2	2:E:1229:ILE:O	2.64	0.42
2:F:978:GLN:HE21	2:F:978:GLN:HB2	1.56	0.42
1:A:35:THR:CG2	5:A:301:HOH:O	2.68	0.41
2:F:965:ILE:HG21	2:F:1107:ARG:NH1	2.35	0.41
1:B:27:LYS:HB3	2:F:1203:VAL:HG13	2.01	0.41
1:C:82:PHE:C	1:C:82:PHE:CD1	2.92	0.41
2:E:1246:GLU:HA	2:E:1246:GLU:OE1	2.19	0.41
2:F:1087:LYS:HD3	2:F:1088:PHE:CE1	2.55	0.41
2:F:1130:ILE:H	2:F:1130:ILE:CD1	2.32	0.41
1:A:44:VAL:C	1:A:45:MET:HG3	2.40	0.41
1:B:117:ILE:CD1	1:B:163:LYS:HE2	2.50	0.41
1:C:5:LYS:HE3	1:C:56:PHE:CE1	2.55	0.41
2:E:1237:LEU:HA	2:E:1237:LEU:HD12	1.90	0.41
1:C:19:LEU:HD12	1:C:19:LEU:C	2.40	0.41
1:C:67:LEU:HB2	2:E:1114:VAL:HG11	2.02	0.41
2:F:1107:ARG:NH1	2:F:1107:ARG:CG	2.82	0.41
2:F:1158:ASN:HD22	2:F:1158:ASN:HA	1.60	0.41
1:B:137:ILE:N	1:B:137:ILE:HD12	2.35	0.41
1:C:98:VAL:N	1:C:99:PRO:CD	2.83	0.41
2:E:889:PHE:HE2	2:E:1212:ILE:HG13	1.84	0.41
2:E:884:THR:CG2	2:F:1244:LEU:HD21	2.50	0.41
1:C:122:ASP:HA	1:C:123:PRO:HD3	1.90	0.41
2:E:884:THR:HG22	2:F:1244:LEU:HD21	2.01	0.41
2:F:1011:TRP:CE3	2:F:1012:VAL:HG22	2.52	0.41
2:F:939:PHE:HE2	2:F:967:MET:HE2	1.86	0.41
1:A:24:THR:HG22	1:A:42:VAL:HG21	2.02	0.41
1:D:61:LEU:HD23	1:D:62:GLU:N	2.36	0.41
2:E:1099:ILE:O	2:E:1102:ASN:HB3	2.21	0.41
2:E:889:PHE:N	2:E:889:PHE:CD1	2.88	0.41
2:F:1185:VAL:HA	2:F:1186:PRO:HD3	1.90	0.41
2:F:998:LEU:HD12	2:F:999:ILE:N	2.36	0.41
2:F:1151:ASN:HB2	2:F:1172:TYR:CE1	2.56	0.41
2:F:899:LEU:O	2:F:903:ILE:HG12	2.20	0.41
2:F:953:GLN:HB3	2:F:953:GLN:HE21	1.54	0.41
1:B:65:ASP:OD1	1:B:68:ARG:NH1	2.47	0.41
1:C:21:ILE:HG22	1:C:27:LYS:O	2.20	0.41
1:C:49:GLU:CD	1:C:50:PRO:HD2	2.42	0.41
2:E:1021:GLU:O	2:E:1024:LYS:HG2	2.20	0.41
2:E:1085:HIS:CD2	5:E:1310:HOH:O	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1215:ILE:HA	2:E:1215:ILE:HD12	1.82	0.41
2:F:1154:PHE:CE1	2:F:1168:LEU:HD11	2.56	0.41
1:A:68:ARG:HB3	1:A:69:PRO:HD3	2.03	0.41
1:B:117:ILE:HD13	1:B:163:LYS:NZ	2.36	0.41
2:E:1012:VAL:HG21	2:E:1025:LEU:HD12	2.02	0.41
2:E:966:LYS:HE3	2:E:966:LYS:HB2	1.79	0.41
2:F:1235:ASP:C	2:F:1237:LEU:N	2.71	0.41
2:F:948:LYS:O	2:F:949:SER:HB2	2.20	0.41
2:F:1181:GLU:O	2:F:1184:ASN:HB2	2.21	0.41
2:F:1241:LEU:C	2:F:1243:SER:H	2.24	0.41
2:F:918:VAL:CG2	2:F:919:ILE:N	2.84	0.41
2:F:1042:ASN:O	2:F:1045:GLU:HB2	2.21	0.40
1:C:101:ILE:HG13	1:C:102:THR:N	2.36	0.40
1:D:139:PRO:O	1:D:143:GLU:HG3	2.20	0.40
1:D:61:LEU:HD22	1:D:63:ASP:H	1.86	0.40
2:E:1143:LYS:NZ	5:E:1305:HOH:O	2.51	0.40
2:E:992:ILE:HG12	2:E:1054:VAL:HG12	2.03	0.40
1:A:120:ARG:HH12	1:A:156:GLU:CD	2.25	0.40
1:B:37:PHE:C	1:B:37:PHE:CD1	2.95	0.40
1:B:46:ILE:HD12	1:B:46:ILE:N	2.37	0.40
1:C:4:ILE:HA	1:C:76:ASP:OD1	2.21	0.40
1:D:154:TYR:CG	1:D:155:VAL:N	2.90	0.40
2:E:1011:TRP:O	2:E:1014:GLN:N	2.55	0.40
2:E:878:ARG:HH22	2:F:1208:ILE:HD11	1.87	0.40
1:B:117:ILE:HG21	1:B:156:GLU:HB2	2.04	0.40
1:C:22:SER:O	1:C:26:ASN:HA	2.20	0.40
1:C:69:PRO:HA	1:C:72:TYR:CD2	2.57	0.40
1:D:111:LEU:N	1:D:111:LEU:HD12	2.36	0.40
2:E:1011:TRP:C	2:E:1013:ASN:N	2.73	0.40
2:E:1176:ARG:HG3	2:E:1176:ARG:NH1	2.34	0.40
2:F:953:GLN:O	2:F:953:GLN:CD	2.59	0.40
2:F:1125:THR:O	2:F:1126:ALA:C	2.59	0.40
2:F:930:ARG:O	2:F:933:TYR:HB3	2.21	0.40

There are no symmetry-related clashes.

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	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
1	B	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	25	47
1	C	175/179 (98%)	153 (87%)	19 (11%)	3 (2%)	9	18
1	D	175/179 (98%)	152 (87%)	19 (11%)	4 (2%)	6	11
2	E	370/387 (96%)	329 (89%)	22 (6%)	19 (5%)	2	2
2	F	370/387 (96%)	314 (85%)	36 (10%)	20 (5%)	2	2
All	All	1440/1490 (97%)	1282 (89%)	111 (8%)	47 (3%)	4	6

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	153	LYS
1	D	153	LYS
2	E	949	SER
2	E	954	VAL
2	E	975	ALA
2	E	978	GLN
2	E	979	ASN
2	E	1011	TRP
2	E	1028	ASP
2	F	949	SER
2	F	954	VAL
2	F	975	ALA
2	F	979	ASN
2	F	1011	TRP
1	D	11	ASP
2	E	955	GLN
2	E	1022	ALA
2	E	1027	TYR
2	E	1156	GLY
2	F	955	GLN

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Mol	Chain	Res	Type
2	F	978	GLN
2	F	1156	GLY
2	F	1230	ALA
2	F	1244	LEU
1	C	11	ASP
1	D	97	TRP
2	E	984	LEU
2	E	1014	GLN
2	F	1022	ALA
2	F	1028	ASP
2	F	1217	SER
1	C	30	SER
1	D	30	SER
2	E	1026	PRO
2	E	1126	ALA
2	E	1230	ALA
2	F	995	ASP
2	F	1024	LYS
2	F	1126	ALA
2	F	1229	ILE
2	F	1242	GLY
1	B	153	LYS
2	E	1024	LYS
2	E	1157	GLU
2	F	1023	SER
2	F	1127	GLY
2	E	1127	GLY

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	157/157 (100%)	151 (96%)	6 (4%)	33	59
1	B	157/157 (100%)	150 (96%)	7 (4%)	27	52
1	C	157/157 (100%)	153 (98%)	4 (2%)	47	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	157/157 (100%)	153 (98%)	4 (2%)	47	73
2	E	339/349 (97%)	313 (92%)	26 (8%)	13	25
2	F	339/349 (97%)	313 (92%)	26 (8%)	13	25
All	All	1306/1326 (98%)	1233 (94%)	73 (6%)	21	42

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	35	THR
1	A	38	ASP
1	A	40	TYR
1	A	66	ARG
1	A	121	ASP
1	B	27	LYS
1	B	35	THR
1	B	38	ASP
1	B	63	ASP
1	B	66	ARG
1	B	67	LEU
1	B	121	ASP
1	C	38	ASP
1	C	61	LEU
1	C	66	ARG
1	C	144	LYS
1	D	38	ASP
1	D	61	LEU
1	D	66	ARG
1	D	144	LYS
2	E	899	LEU
2	E	903	ILE
2	E	917	THR
2	E	938	LEU
2	E	953	GLN
2	E	957	ILE
2	E	963	THR
2	E	993	ILE
2	E	1027	TYR
2	E	1051	LEU
2	E	1054	VAL
2	E	1107	ARG

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Mol	Chain	Res	Type
2	E	1123	ASP
2	E	1129	GLN
2	E	1135	ARG
2	E	1146	GLN
2	E	1152	LYS
2	E	1157	GLU
2	E	1158	ASN
2	E	1175	PHE
2	E	1176	ARG
2	E	1185	VAL
2	E	1201	VAL
2	E	1207	VAL
2	E	1226	GLN
2	E	1237	LEU
2	F	899	LEU
2	F	917	THR
2	F	931	GLU
2	F	938	LEU
2	F	953	GLN
2	F	957	ILE
2	F	963	THR
2	F	978	GLN
2	F	1005	VAL
2	F	1011	TRP
2	F	1043	LYS
2	F	1051	LEU
2	F	1094	ASP
2	F	1107	ARG
2	F	1123	ASP
2	F	1129	GLN
2	F	1132	SER
2	F	1135	ARG
2	F	1146	GLN
2	F	1152	LYS
2	F	1158	ASN
2	F	1175	PHE
2	F	1176	ARG
2	F	1184	ASN
2	F	1212	ILE
2	F	1235	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	103	HIS
1	B	74	GLN
1	C	132	ASN
1	D	132	ASN
2	E	905	GLN
2	E	953	GLN
2	E	961	ASN
2	E	983	GLN
2	E	1014	GLN
2	E	1033	GLN
2	E	1042	ASN
2	E	1060	ASN
2	E	1085	HIS
2	E	1131	ASN
2	E	1137	ASN
2	E	1147	HIS
2	E	1158	ASN
2	E	1226	GLN
2	E	1234	ASN
2	F	929	GLN
2	F	953	GLN
2	F	961	ASN
2	F	978	GLN
2	F	1003	ASN
2	F	1018	GLN
2	F	1033	GLN
2	F	1050	ASN
2	F	1060	ASN
2	F	1131	ASN
2	F	1137	ASN
2	F	1147	HIS
2	F	1158	ASN
2	F	1184	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 8 ligands modelled in this entry, 4 are 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	D	201	4	26,34,34	1.34	3 (11%)	33,54,54	2.06	8 (24%)
3	GTP	B	201	4	26,34,34	1.50	4 (15%)	33,54,54	2.00	9 (27%)
3	GTP	C	201	4	26,34,34	1.33	3 (11%)	33,54,54	1.97	8 (24%)
3	GTP	A	201	4	26,34,34	1.50	4 (15%)	33,54,54	2.01	9 (27%)

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	D	201	4	-	1/18/38/38	0/3/3/3
3	GTP	B	201	4	-	2/18/38/38	0/3/3/3
3	GTP	C	201	4	-	1/18/38/38	0/3/3/3
3	GTP	A	201	4	-	2/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	GTP	C6-N1	4.40	1.40	1.33
3	B	201	GTP	C6-N1	4.34	1.40	1.33
3	C	201	GTP	C6-N1	4.18	1.40	1.33
3	D	201	GTP	C6-N1	4.16	1.40	1.33
3	B	201	GTP	PG-O1G	3.40	1.61	1.50
3	A	201	GTP	PG-O1G	3.37	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	GTP	C2-N1	2.99	1.40	1.35
3	B	201	GTP	C2-N1	2.83	1.40	1.35
3	C	201	GTP	C2-N1	2.82	1.40	1.35
3	A	201	GTP	C2-N1	2.74	1.40	1.35
3	A	201	GTP	O4'-C1'	2.33	1.44	1.41
3	D	201	GTP	O4'-C1'	2.29	1.44	1.41
3	C	201	GTP	O4'-C1'	2.23	1.44	1.41
3	B	201	GTP	O4'-C1'	2.23	1.44	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	GTP	C2-N3-C4	5.51	121.66	115.36
3	C	201	GTP	C2-N3-C4	5.48	121.61	115.36
3	D	201	GTP	N3-C2-N1	-5.41	120.01	127.22
3	C	201	GTP	N3-C2-N1	-5.27	120.19	127.22
3	A	201	GTP	N3-C2-N1	-5.26	120.20	127.22
3	B	201	GTP	N3-C2-N1	-5.21	120.27	127.22
3	B	201	GTP	C2-N3-C4	5.13	121.21	115.36
3	A	201	GTP	C2-N3-C4	5.00	121.07	115.36
3	D	201	GTP	PA-O3A-PB	-3.73	120.02	132.83
3	A	201	GTP	C5-C6-N1	-3.71	118.35	123.43
3	B	201	GTP	C5-C6-N1	-3.57	118.55	123.43
3	B	201	GTP	PA-O3A-PB	-3.51	120.80	132.83
3	D	201	GTP	PB-O3B-PG	-3.49	120.84	132.83
3	A	201	GTP	PA-O3A-PB	-3.47	120.91	132.83
3	D	201	GTP	C5-C6-N1	-3.28	118.94	123.43
3	C	201	GTP	C5-C6-N1	-3.28	118.95	123.43
3	B	201	GTP	PB-O3B-PG	-3.11	122.16	132.83
3	A	201	GTP	O2G-PG-O3B	3.02	114.77	104.64
3	C	201	GTP	PA-O3A-PB	-3.02	122.47	132.83
3	A	201	GTP	PB-O3B-PG	-2.99	122.56	132.83
3	C	201	GTP	C3'-C2'-C1'	-2.98	96.49	100.98
3	B	201	GTP	O3G-PG-O3B	2.96	114.58	104.64
3	D	201	GTP	O4'-C1'-C2'	-2.95	102.62	106.93
3	D	201	GTP	C3'-C2'-C1'	-2.90	96.61	100.98
3	C	201	GTP	O4'-C1'-C2'	-2.77	102.88	106.93
3	C	201	GTP	PB-O3B-PG	-2.65	123.73	132.83
3	A	201	GTP	C4-C5-N7	-2.56	106.73	109.40
3	A	201	GTP	C6-N1-C2	2.36	119.69	115.93
3	B	201	GTP	C6-N1-C2	2.20	119.43	115.93
3	B	201	GTP	C4-C5-N7	-2.19	107.12	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	GTP	C2'-C3'-C4'	-2.16	98.45	102.64
3	D	201	GTP	C6-N1-C2	2.09	119.25	115.93
3	C	201	GTP	C6-N1-C2	2.05	119.18	115.93
3	B	201	GTP	C2'-C3'-C4'	-2.02	98.71	102.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

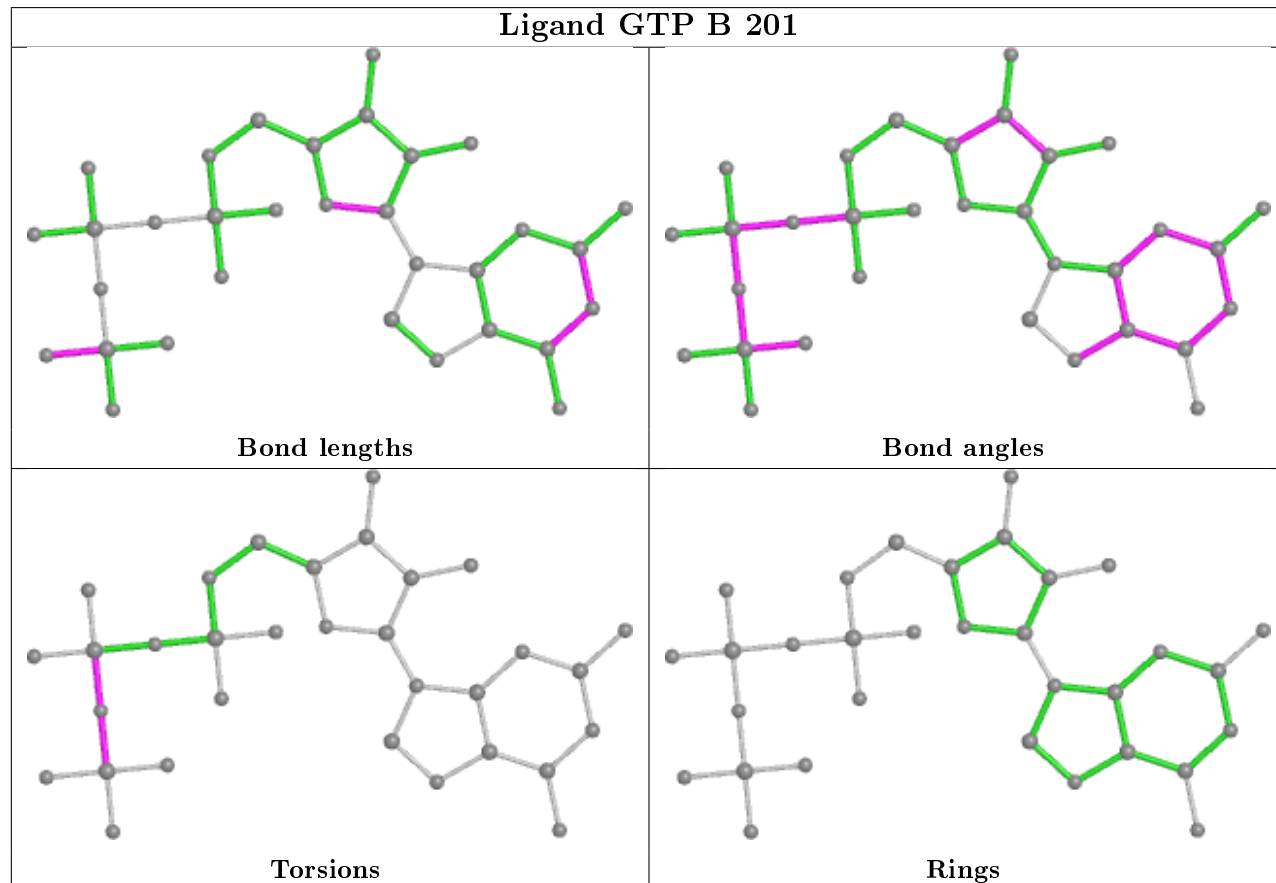
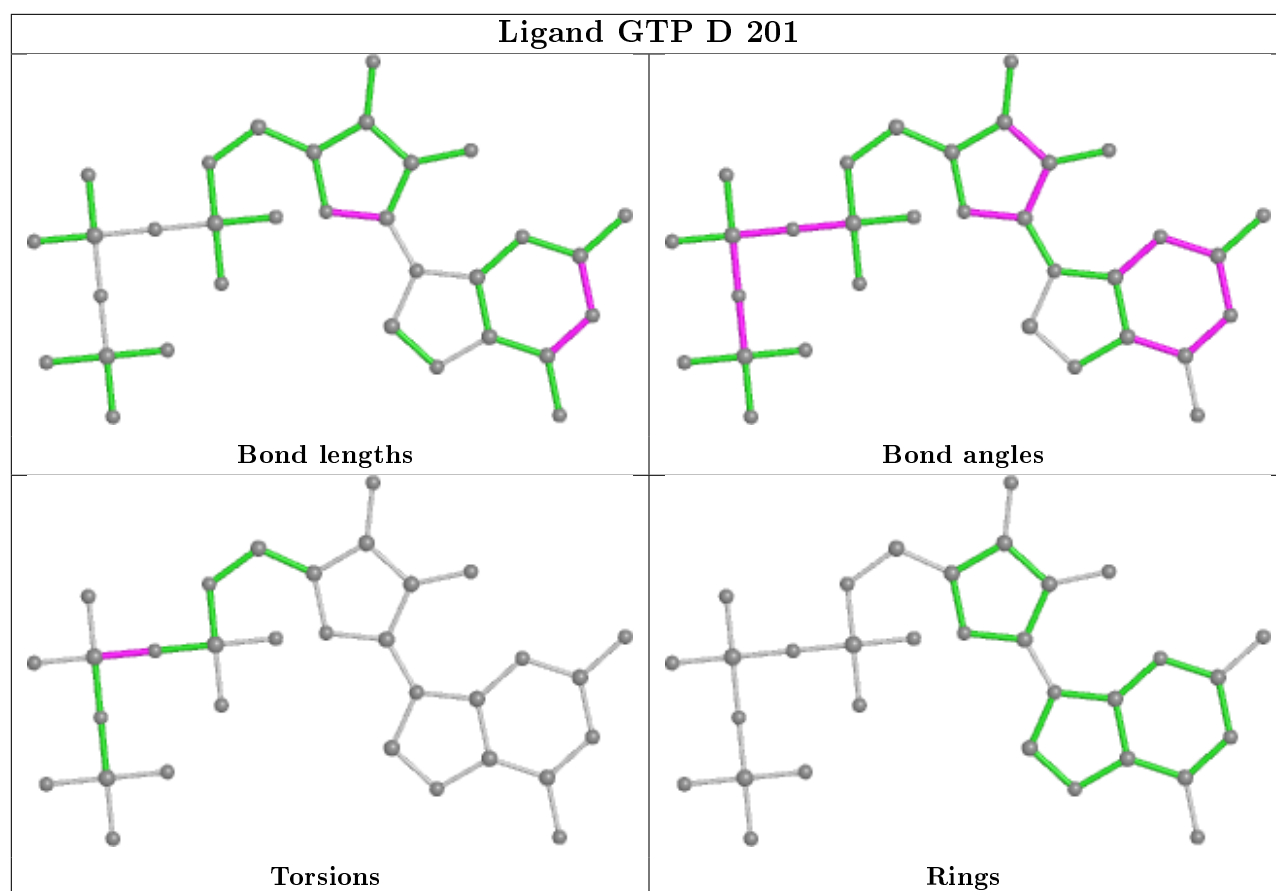
Mol	Chain	Res	Type	Atoms
3	A	201	GTP	PB-O3B-PG-O2G
3	B	201	GTP	PG-O3B-PB-O2B
3	A	201	GTP	PG-O3B-PB-O2B
3	B	201	GTP	PB-O3B-PG-O1G
3	D	201	GTP	PA-O3A-PB-O1B
3	C	201	GTP	PA-O3A-PB-O2B

There are no ring outliers.

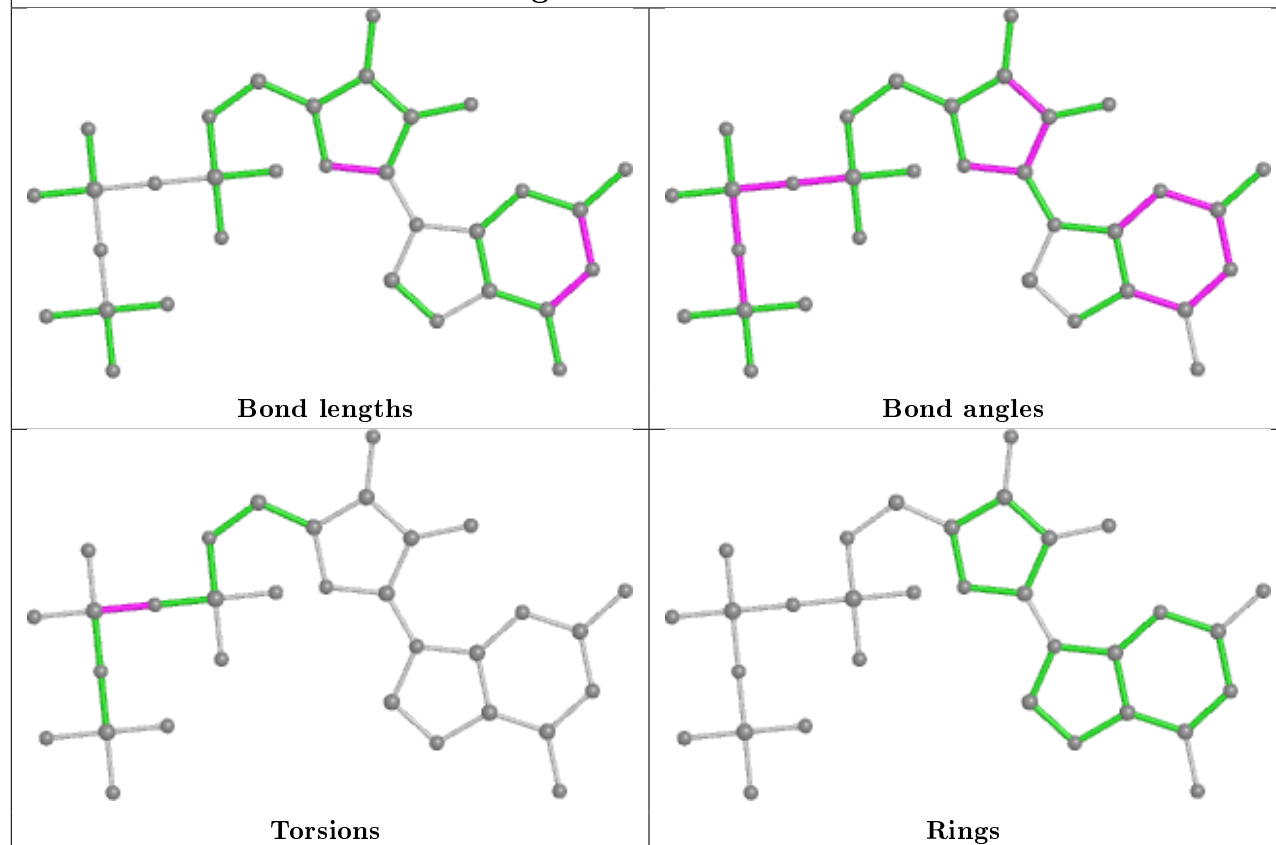
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	201	GTP	2	0
3	B	201	GTP	3	0
3	C	201	GTP	4	0
3	A	201	GTP	3	0

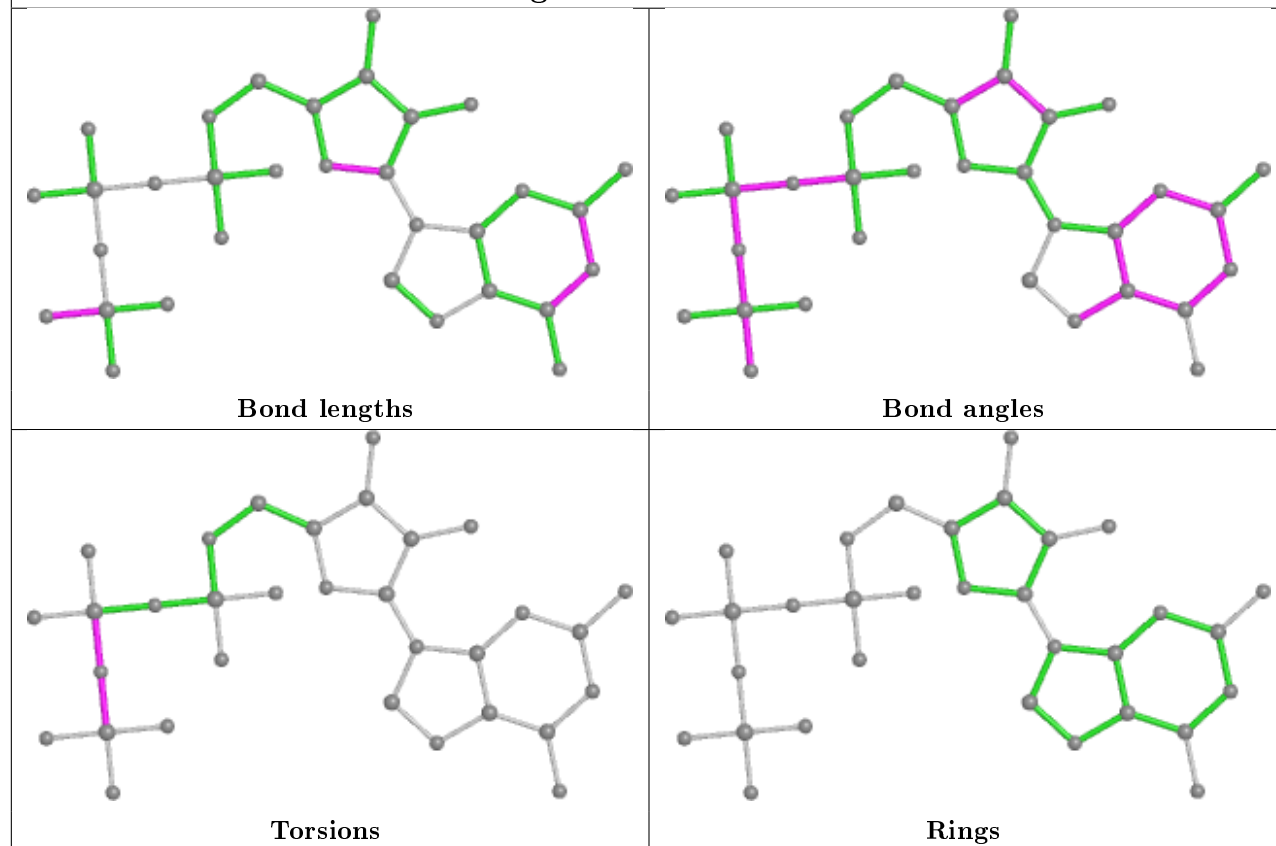
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 C 201



Ligand GTP A 201



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	177/179 (98%)	-0.43	4 (2%) 60 54	25, 48, 102, 156	0
1	B	177/179 (98%)	-0.21	4 (2%) 60 54	35, 58, 111, 149	0
1	C	177/179 (98%)	0.06	6 (3%) 45 38	45, 73, 114, 147	0
1	D	177/179 (98%)	1.06	30 (16%) 1 1	62, 105, 146, 174	0
2	E	372/387 (96%)	-0.03	19 (5%) 28 22	26, 57, 124, 171	0
2	F	372/387 (96%)	0.10	19 (5%) 28 22	27, 70, 136, 165	0
All	All	1452/1490 (97%)	0.08	82 (5%) 24 19	25, 66, 134, 174	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	41	ALA	10.1
2	E	1126	ALA	9.2
1	D	46	ILE	8.2
2	E	1012	VAL	8.0
1	D	2	GLN	6.3
2	E	1018	GLN	6.1
2	F	1027	TYR	6.0
2	F	1126	ALA	5.8
2	F	979	ASN	5.6
2	F	1018	GLN	5.3
1	B	46	ILE	5.2
1	D	47	GLY	5.1
1	D	1	MET	4.8
2	E	1021	GLU	4.7
2	E	1127	GLY	4.6
2	E	1128	GLY	4.4
2	F	1022	ALA	4.2
1	A	46	ILE	4.1
2	F	1216	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
2	E	1125	THR	3.9
2	E	1216	ILE	3.9
1	D	81	CYS	3.8
1	D	3	THR	3.8
1	D	29	PRO	3.7
1	D	51	TYR	3.6
2	E	976	ARG	3.6
1	D	23	TYR	3.5
1	D	74	GLN	3.5
1	D	45	MET	3.4
2	F	1013	ASN	3.3
2	E	977	GLY	3.2
1	A	49	GLU	3.2
1	D	113	VAL	3.2
1	A	1	MET	3.1
2	F	953	GLN	3.1
1	D	40	TYR	3.1
2	F	1024	LYS	3.1
1	D	28	PHE	3.0
2	F	1127	GLY	3.0
1	D	50	PRO	3.0
2	F	977	GLY	2.9
1	C	47	GLY	2.9
2	E	1027	TYR	2.9
2	F	1006	GLU	2.9
2	F	976	ARG	2.8
2	E	876	LYS	2.8
1	D	114	GLY	2.7
2	F	1011	TRP	2.6
2	E	979	ASN	2.6
1	A	50	PRO	2.6
1	D	48	GLY	2.6
1	D	53	LEU	2.6
1	B	177	LEU	2.5
1	D	60	GLY	2.5
1	C	9	VAL	2.5
1	D	30	SER	2.5
1	C	81	CYS	2.5
1	B	47	GLY	2.4
2	F	1021	GLU	2.4
1	B	41	ALA	2.4
2	E	1013	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	52	THR	2.4
1	D	27	LYS	2.4
2	E	1019	THR	2.4
2	E	1023	SER	2.4
1	D	8	VAL	2.4
1	D	31	GLU	2.3
2	E	1129	GLN	2.3
2	F	1201	VAL	2.3
2	F	1236	LEU	2.3
1	C	45	MET	2.2
1	D	133	LYS	2.2
2	E	879	ARG	2.2
1	D	95	GLU	2.2
2	E	1217	SER	2.2
1	D	21	ILE	2.2
1	C	80	VAL	2.1
1	D	115	THR	2.1
2	F	1140	SER	2.1
1	D	106	PRO	2.1
1	C	74	GLN	2.1
2	F	1141	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

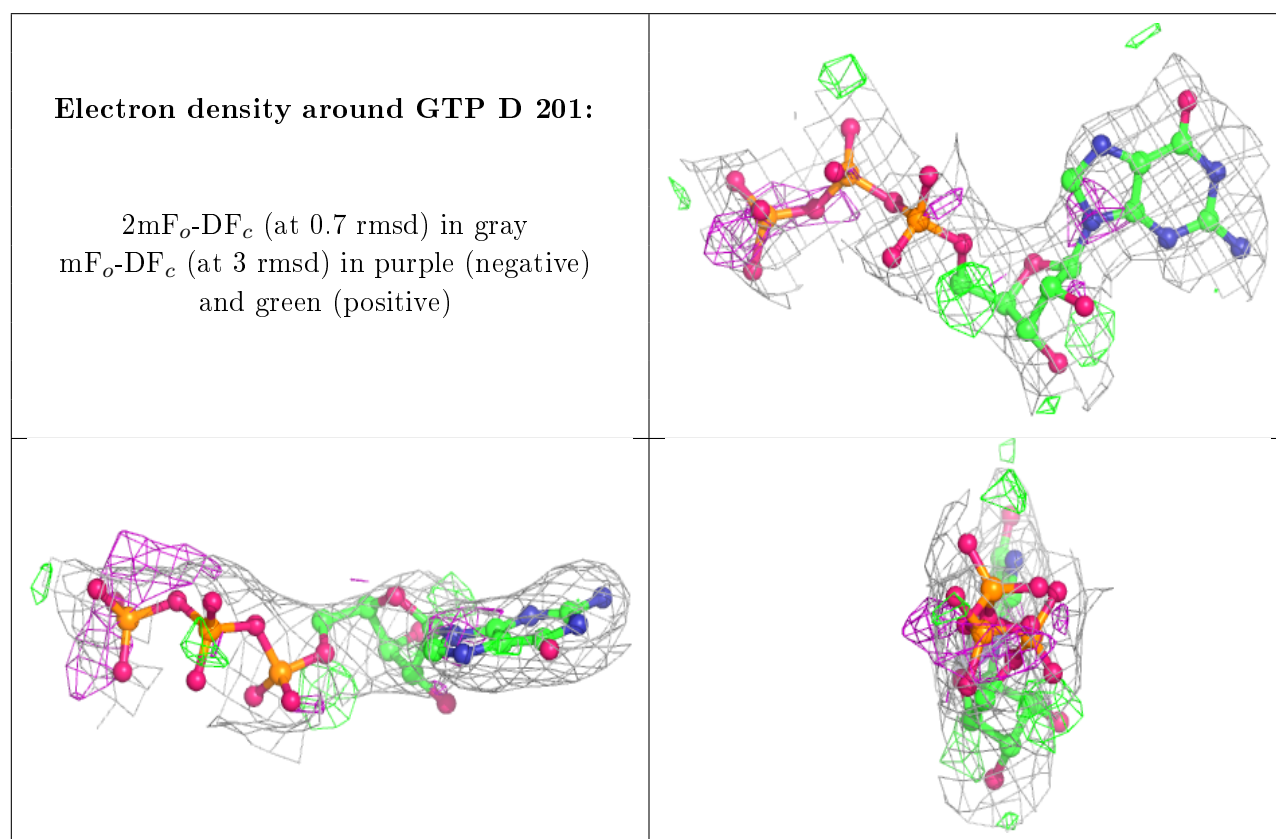
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	A	202	1/1	0.77	0.26	39,39,39,39	0
4	MG	D	202	1/1	0.82	0.17	56,56,56,56	0

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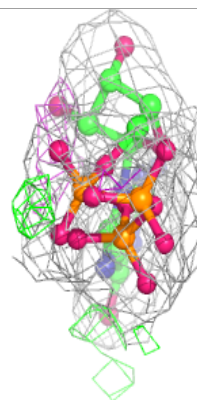
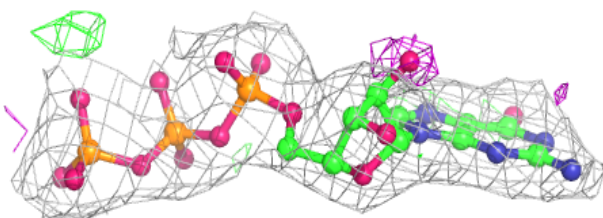
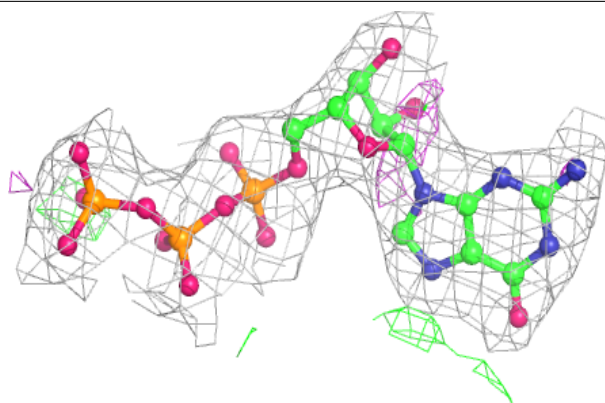
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GTP	D	201	32/32	0.88	0.18	62,65,68,71	0
4	MG	B	202	1/1	0.92	0.13	38,38,38,38	0
4	MG	C	202	1/1	0.94	0.20	51,51,51,51	0
3	GTP	C	201	32/32	0.95	0.15	47,59,64,68	0
3	GTP	B	201	32/32	0.98	0.10	26,35,39,41	0
3	GTP	A	201	32/32	0.98	0.13	21,32,35,39	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.

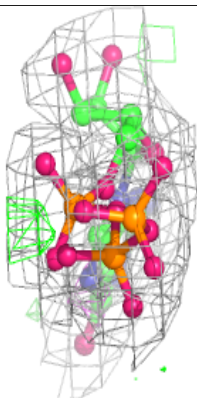
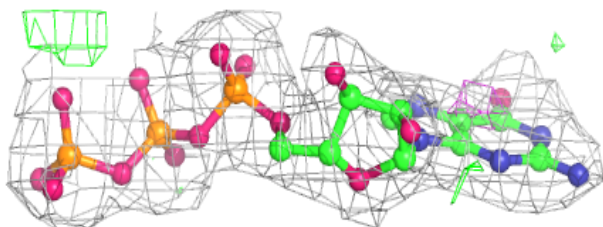
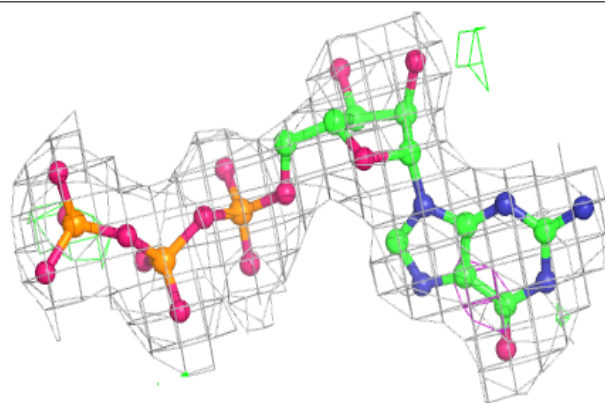


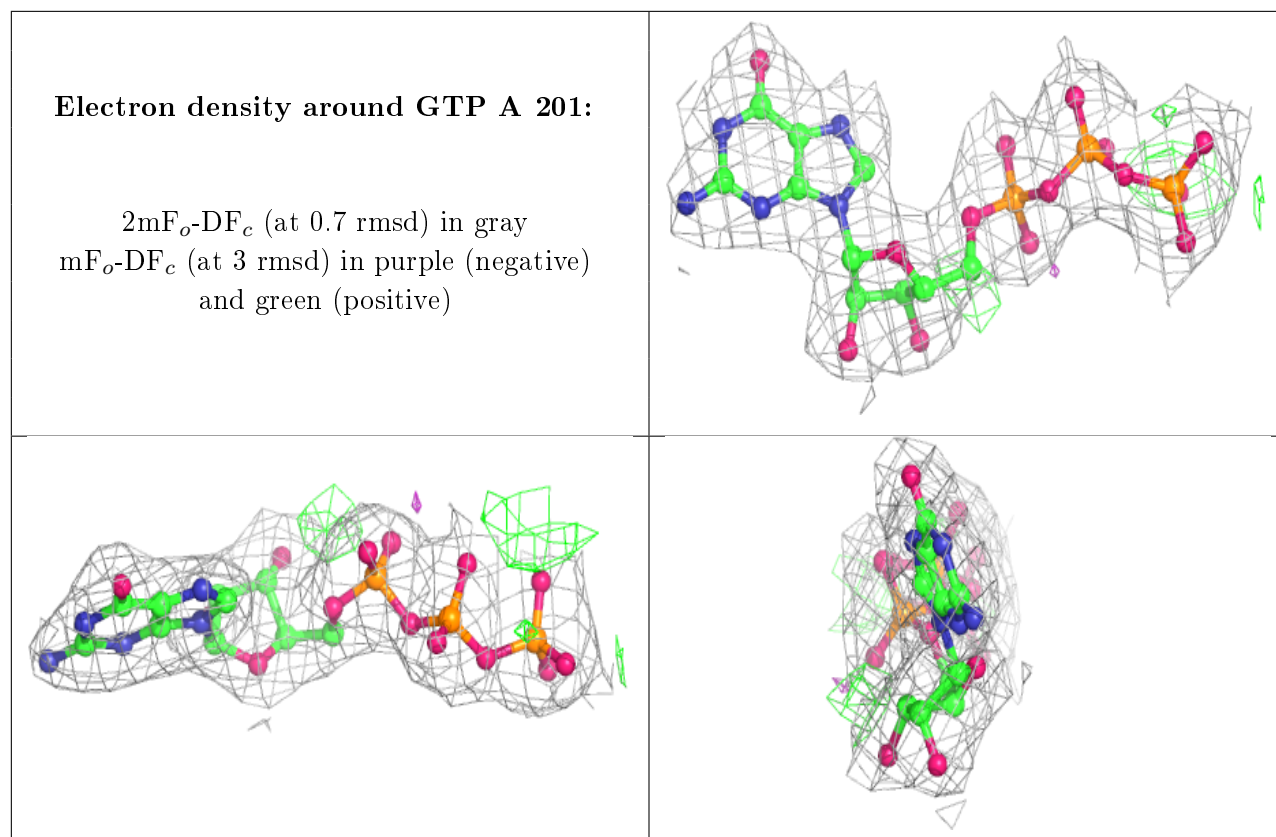
Electron density around GTP C 201:

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

**Electron density around GTP B 201:**

$2mF_o-DF_c$ (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.