



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:41 PM UTC

PDB ID : 8CLE / pdb_00008cle
Title : Vinblastine bound to tubulin (T2R-TTL) complex
Authors : Wranik, M.; Bertrand, Q.; Kepa, M.W.; Weinert, T.; Steinmetz, M.; Standfuss, J.
Deposited on : 2023-02-16
Resolution : 3.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

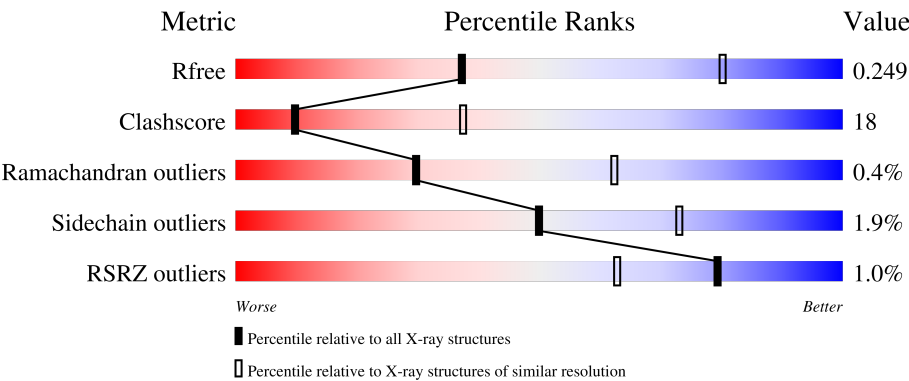
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	440	69%30%
1	C	440	% 64%32%. .
2	B	431	73%26%. .
2	D	431	% 61%36%. .
3	E	120	75%25%

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Mol	Chain	Length	Quality of chain
4	F	331	4% 63% 35% ..

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 17637 atoms, of which 58 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	5	9	0
			3465	2200	584	657	24			
1	C	440	Total	C	N	O	S	4	7	0
			3466	2197	584	662	23			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	424	Total	C	N	O	S	6	4	0
			3343	2102	567	646	28			
2	B	428	Total	C	N	O	S	6	2	0
			3370	2118	576	649	27			

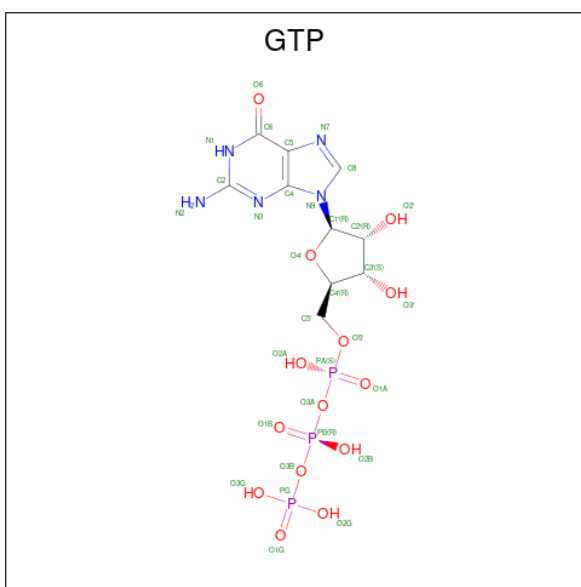
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			991	612	180	194	5			

- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	5	4	0
			2729	1762	457	496	14			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

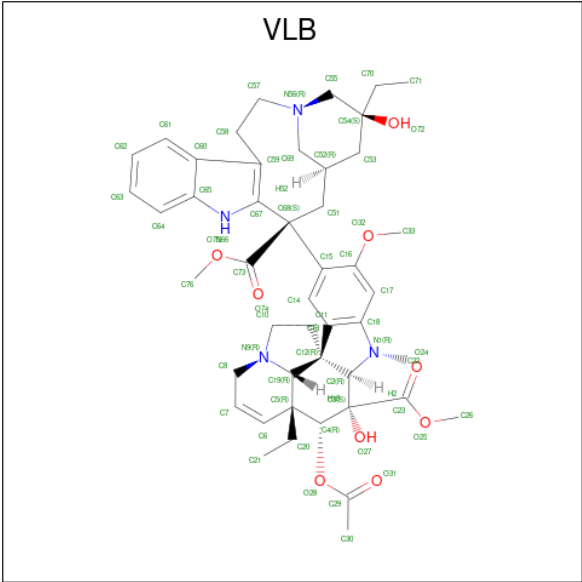
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

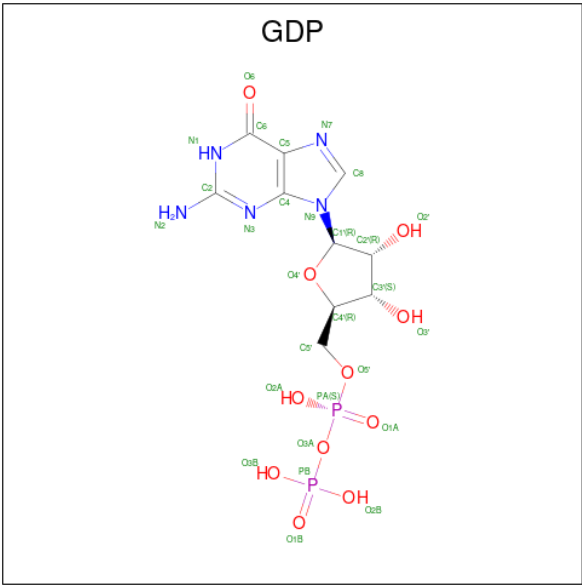
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (CCD ID: VLB) (formula: C₄₆H₅₈N₄O₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	H	N	O	0	0
			117	46	58	4	9		

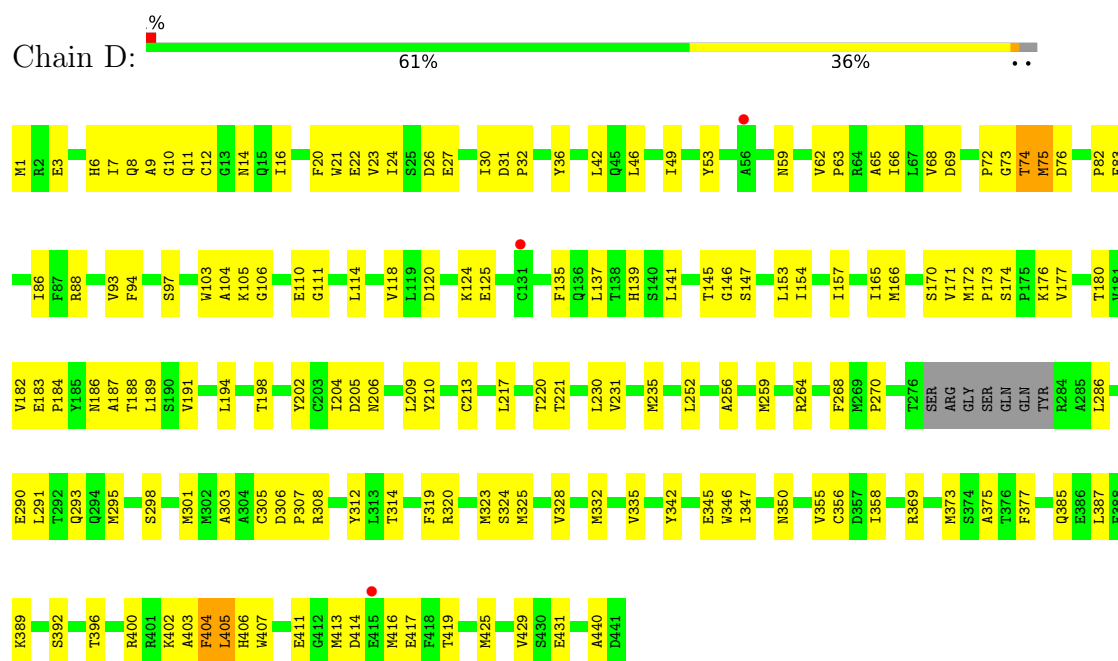
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



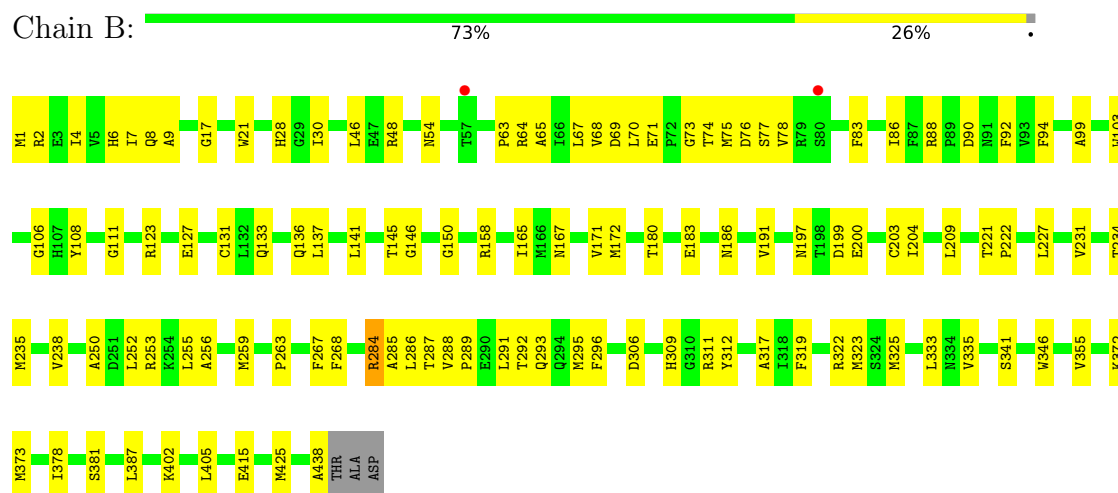
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is water.

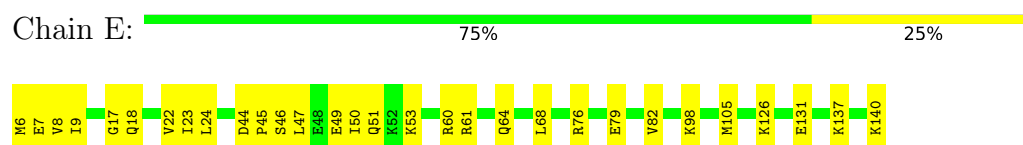
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total 2	O 2	0	0
10	C	6	Total 6	O 6	0	0
10	D	5	Total 5	O 5	0	0
10	E	1	Total 1	O 1	0	0
10	F	8	Total 8	O 8	0	0
10	B	10	Total 10	O 10	0	0



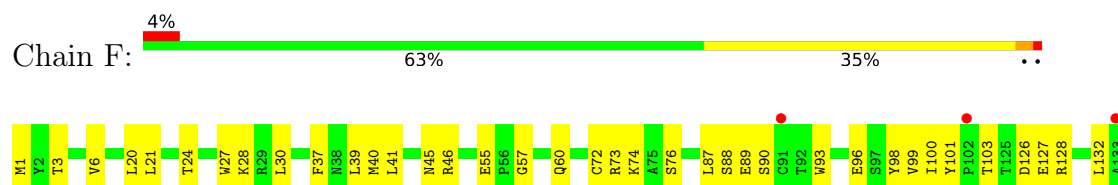
• Molecule 2: Tubulin beta-2B chain

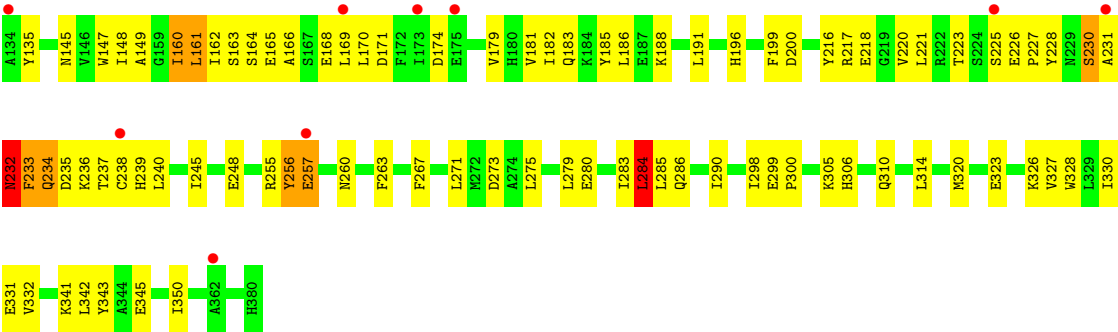


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.39Å 159.74Å 182.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.13 – 3.20 15.13 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.13-3.20) 98.8 (15.13-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20_4487	Depositor
R, R_{free}	0.200 , 0.248 0.205 , 0.249	Depositor DCC
R_{free} test set	1999 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 142.9	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	0.90	EDS
Total number of atoms	17637	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, VLB, MG, CA, GDP

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	0.27	0/3571	0.58	0/4849
1	C	0.63	0/3565	0.96	3/4842 (0.1%)
2	B	0.29	0/3451	0.62	0/4675
2	D	0.31	0/3428	0.62	2/4645 (0.0%)
3	E	0.31	0/999	0.65	0/1325
4	F	0.42	3/2802 (0.1%)	0.71	4/3789 (0.1%)
All	All	0.40	3/17816 (0.0%)	0.71	9/24125 (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
1	A	0	1
1	C	0	5
2	B	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	310	GLN	C-O	6.99	1.32	1.23
4	F	284[A]	LEU	C-O	6.31	1.31	1.24
4	F	284[B]	LEU	C-O	6.31	1.31	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	284[A]	LEU	CA-C-O	7.23	129.02	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	284[B]	LEU	CA-C-O	7.23	129.02	120.92
1	C	348	PRO	N-CA-C	-6.88	101.09	111.41
1	C	363[A]	VAL	CA-C-O	6.56	125.81	119.71
1	C	363[B]	VAL	CA-C-O	6.56	125.81	119.71
4	F	310	GLN	CA-C-O	6.55	128.56	121.16
4	F	89	GLU	N-CA-C	-6.11	105.92	113.19
2	D	74	THR	N-CA-C	-5.71	104.26	111.11
2	D	10	GLY	CA-C-O	-5.01	118.56	122.52

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	ARG	Sidechain
2	B	284	ARG	Sidechain
1	C	243	ARG	Sidechain
1	C	373	ARG	Sidechain
1	C	390	ARG	Sidechain
1	C	402	ARG	Sidechain
1	C	422	ARG	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	3465	0	3402	124	0
1	C	3466	0	3393	125	1
2	B	3370	0	3250	93	0
2	D	3343	0	3231	147	0
3	E	991	0	1012	28	1
4	F	2729	0	2715	97	0
5	A	32	0	12	0	0
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	59	58	58	16	0
9	B	28	0	12	1	0
9	D	28	0	12	3	0
10	A	2	0	0	0	0
10	B	10	0	0	0	0
10	C	6	0	0	0	0
10	D	5	0	0	1	0
10	E	1	0	0	0	0
10	F	8	0	0	1	0
All	All	17579	58	17109	607	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 18.

All (607) 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:277:SER:HB3	1:A:280:LYS:HG3	1.35	1.07
2:B:2:ARG:HD3	2:B:133:GLN:HG2	1.41	1.02
2:D:141:LEU:HD11	2:D:170:SER:HB3	1.46	0.95
2:D:319:PHE:HB3	2:D:323:MET:HE1	1.48	0.95
4:F:233:PHE:HA	4:F:239:HIS:CE1	2.02	0.95
2:D:402:LYS:HE3	2:D:405:LEU:CD1	1.97	0.94
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.50	0.94
4:F:263:PHE:HE2	4:F:341:LYS:HD3	1.34	0.93
1:C:293:ASN:HA	1:C:335:ILE:HD11	1.50	0.93
2:D:402:LYS:HG3	2:D:405:LEU:HD13	1.53	0.91
2:D:402:LYS:CG	2:D:405:LEU:HD13	2.03	0.89
4:F:320:MET:HE1	10:F:404:HOH:O	1.71	0.89
1:C:88:HIS:NE2	1:C:90:GLU:HG3	1.88	0.89
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.54	0.88
4:F:226:GLU:HG3	4:F:227:PRO:HD2	1.57	0.86
2:D:402:LYS:HE3	2:D:405:LEU:HD11	1.58	0.86
2:D:259:MET:HE2	2:D:259:MET:HA	1.58	0.86
2:D:402:LYS:CE	2:D:405:LEU:HD11	2.06	0.86
2:D:166:MET:HE3	2:D:166:MET:HA	1.58	0.84
2:D:402:LYS:CE	2:D:405:LEU:CD1	2.55	0.84
3:E:126:LYS:HE2	3:E:126:LYS:HA	1.59	0.84
8:C:501:VLB:H761	2:B:221:THR:HA	1.59	0.83
1:C:176:GLN:HE22	1:C:207:GLU:HG3	1.42	0.83
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:298:SER:HB2	2:D:307:PRO:HD2	1.60	0.82
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.61	0.82
2:B:285:ALA:HB2	2:B:372:LYS:HE3	1.60	0.82
1:A:154:MET:HE2	1:A:154:MET:HA	1.63	0.81
1:A:277:SER:HB3	1:A:280:LYS:CG	2.10	0.80
1:C:430:LYS:HE2	1:C:434:GLU:OE2	1.82	0.79
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.65	0.78
4:F:326:LYS:HE2	4:F:328:TRP:CZ2	2.18	0.78
2:D:20:PHE:HB2	2:D:235:MET:CE	2.13	0.78
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.18	0.77
4:F:257:GLU:HB3	4:F:260:ASN:HA	1.65	0.77
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.19	0.76
4:F:20:LEU:O	4:F:24:THR:HG23	1.85	0.76
1:A:317:LEU:HD21	1:A:377:MET:CE	2.16	0.75
1:A:132:LEU:O	1:A:164:LYS:HE3	1.86	0.75
1:A:154:MET:HG3	1:A:194:THR:HG23	1.68	0.74
2:D:319:PHE:HB3	2:D:323:MET:CE	2.17	0.74
1:A:209:ILE:HD11	1:A:302:MET:CE	2.18	0.74
2:D:26:ASP:OD2	2:D:369:ARG:HD2	1.88	0.74
1:A:209:ILE:HD11	1:A:302:MET:HE1	1.69	0.73
2:D:345:GLU:HG2	2:D:440:ALA:HB2	1.70	0.73
2:B:83:PHE:O	2:B:86:ILE:HG12	1.89	0.72
8:C:501:VLB:C76	2:B:221:THR:HA	2.19	0.72
1:A:277:SER:HB3	1:A:280:LYS:HE3	1.72	0.72
1:C:261:PRO:HG3	1:C:313:MET:HE2	1.71	0.72
1:C:386:GLU:O	1:C:390:ARG:HG3	1.90	0.72
1:C:329:ASN:HD21	8:C:501:VLB:H66	1.36	0.71
2:B:1:MET:HE2	2:B:1:MET:HA	1.70	0.71
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.71	0.71
2:B:83:PHE:HD2	2:B:86:ILE:HD13	1.55	0.71
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.73	0.71
1:C:271:THR:HG21	1:C:295:CYS:HA	1.72	0.70
1:A:62:VAL:HG23	1:A:86:LEU:O	1.91	0.70
4:F:305:LYS:HG2	4:F:306:HIS:CD2	2.26	0.70
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.73	0.70
1:A:332:ILE:O	1:A:335:ILE:HG13	1.91	0.70
1:A:56:THR:CG2	1:A:60:LYS:HB3	2.23	0.69
2:D:402:LYS:CE	2:D:405:LEU:HD13	2.22	0.69
2:D:406:HIS:CD2	2:D:407:TRP:HD1	2.10	0.69
1:A:317:LEU:HD21	1:A:377:MET:HE3	1.74	0.69
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:LEU:HD23	2:D:154:ILE:HD11	1.75	0.69
1:A:339:ARG:HB2	1:A:341:ILE:HD11	1.74	0.68
1:C:332:ILE:HB	8:C:501:VLB:H303	1.76	0.68
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.24	0.68
1:A:277:SER:CB	1:A:280:LYS:HG3	2.18	0.68
1:C:274:PRO:CG	1:C:371:VAL:HG11	2.24	0.67
8:C:501:VLB:C22	8:C:501:VLB:H262	2.24	0.67
2:D:105:LYS:HG2	2:D:411:GLU:OE2	1.95	0.67
1:A:270:ALA:O	1:A:302:MET:HG2	1.95	0.67
1:A:3:GLU:HG2	1:A:64:ARG:NH2	2.09	0.66
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.13	0.66
4:F:103:THR:HG22	4:F:174:ASP:OD1	1.95	0.66
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.09	0.66
1:A:22:GLU:O	1:A:26:LEU:HD13	1.95	0.66
4:F:162:ILE:HD11	4:F:234:GLN:N	2.11	0.66
1:C:252:LEU:HG	1:C:256:GLN:HE21	1.58	0.66
1:C:318:LEU:HD12	1:C:318:LEU:N	2.11	0.66
1:A:277:SER:CB	1:A:280:LYS:HE3	2.25	0.66
4:F:314:LEU:HD22	4:F:350:ILE:HD11	1.76	0.66
1:C:40:LYS:O	1:C:42:ILE:HG13	1.95	0.66
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.11	0.65
4:F:73:ARG:HB2	4:F:76:SER:HB2	1.78	0.65
2:B:136:GLN:HA	2:B:167:ASN:O	1.96	0.65
1:C:317:LEU:HG	1:C:377:MET:HG3	1.79	0.65
3:E:6:MET:HE2	3:E:23:ILE:O	1.96	0.65
1:C:322:ASP:HB3	1:C:373:ARG:HH21	1.62	0.65
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.78	0.65
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.25	0.65
1:C:301:GLN:HE22	1:C:307:PRO:HG2	1.62	0.64
1:A:336:LYS:HG2	3:E:24:LEU:HD23	1.79	0.64
2:D:286:LEU:HB2	2:D:290:GLU:OE1	1.96	0.64
1:C:431:ASP:O	1:C:435:VAL:HG13	1.98	0.64
4:F:101:TYR:CE1	4:F:126:ASP:HB3	2.33	0.64
1:C:271:THR:HG23	1:C:300:ASN:O	1.96	0.64
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.33	0.64
2:D:402:LYS:HE3	2:D:405:LEU:HD13	1.77	0.64
2:D:402:LYS:HE2	2:D:405:LEU:HD11	1.78	0.64
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.80	0.64
3:E:68:LEU:HD11	2:B:158:ARG:NH2	2.12	0.64
2:D:83:PHE:O	2:D:86:ILE:HG22	1.98	0.63
2:D:411:GLU:OE1	3:E:137:LYS:HE2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.80	0.63
2:D:20:PHE:HB2	2:D:235:MET:HE3	1.79	0.63
4:F:98:TYR:HA	4:F:127:GLU:OE2	1.99	0.63
2:B:191:VAL:HG11	2:B:425:MET:HE2	1.81	0.63
1:C:274:PRO:CB	1:C:286:LEU:HD12	2.28	0.63
2:B:2:ARG:HA	2:B:131:CYS:O	1.97	0.63
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.14	0.63
2:D:325:MET:SD	2:D:355:VAL:HG21	2.39	0.63
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.79	0.62
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.80	0.62
8:C:501:VLB:H262	8:C:501:VLB:H221	1.81	0.62
1:A:172:TYR:HE1	1:A:391:LEU:HD22	1.64	0.62
1:C:211:ASP:HB3	1:C:215:ARG:NH1	2.15	0.62
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.30	0.62
4:F:237:THR:H	4:F:240:LEU:HD12	1.65	0.62
1:C:432:TYR:O	1:C:435:VAL:HG22	2.00	0.62
3:E:46:SER:O	3:E:50:ILE:HD13	2.00	0.62
8:C:501:VLB:H511	8:C:501:VLB:H572	1.80	0.61
2:D:106:GLY:O	2:D:111:GLY:HA3	2.00	0.61
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.41	0.61
2:D:22:GLU:HG2	2:D:83:PHE:CD2	2.34	0.61
2:D:141:LEU:HA	2:D:147:SER:HB3	1.81	0.61
4:F:57:GLY:HA3	2:B:333:LEU:HD13	1.83	0.61
2:B:191:VAL:HG11	2:B:425:MET:CE	2.31	0.61
4:F:185:TYR:HE1	4:F:228:TYR:HH	1.46	0.61
1:A:155:GLU:HA	1:A:197:HIS:CD2	2.36	0.61
2:D:396:THR:O	2:D:400:ARG:HB2	2.01	0.61
4:F:3:THR:HB	4:F:30:LEU:HD11	1.83	0.61
1:C:176:GLN:NE2	1:C:207:GLU:HG3	2.14	0.60
2:B:73:GLY:O	2:B:75:MET:N	2.35	0.60
1:C:255:PHE:CE1	1:C:352:LYS:HG2	2.37	0.60
1:A:172:TYR:CE1	1:A:391:LEU:HD22	2.37	0.60
1:A:56:THR:HG22	1:A:60:LYS:HB3	1.84	0.60
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.42	0.60
8:C:501:VLB:H262	8:C:501:VLB:N1	2.16	0.60
2:D:194:LEU:HD22	2:D:198:THR:HG21	1.84	0.60
2:B:2:ARG:HD3	2:B:133:GLN:CG	2.22	0.60
1:C:165:SER:HA	1:C:199:ASP:OD2	2.02	0.59
1:C:166:LYS:HE2	1:C:197:HIS:O	2.01	0.59
1:C:274:PRO:HB3	1:C:286:LEU:HD12	1.85	0.59
2:D:103:TRP:HB2	2:D:186:ASN:OD1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ILE:CG2	1:C:341:ILE:HD11	2.32	0.59
3:E:126:LYS:HE2	3:E:126:LYS:CA	2.29	0.59
4:F:100:ILE:HG12	4:F:128:ARG:HA	1.82	0.59
8:C:501:VLB:C67	8:C:501:VLB:H691	2.33	0.59
1:A:163:LYS:O	1:A:164:LYS:HD2	2.03	0.59
2:B:171:VAL:HA	2:B:204:ILE:O	2.03	0.59
1:A:56:THR:HG21	1:A:60:LYS:HB3	1.85	0.59
2:D:12:CYS:O	2:D:16:ILE:HG12	2.03	0.59
3:E:45:PRO:HB3	3:E:49:GLU:OE1	2.03	0.59
4:F:162:ILE:C	4:F:162:ILE:HD12	2.28	0.59
1:A:317:LEU:HD21	1:A:377:MET:HE2	1.85	0.58
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.38	0.58
1:A:69:ASP:O	1:A:94:THR:HA	2.04	0.58
1:C:223:THR:O	1:C:227:LEU:HD13	2.03	0.58
2:B:200:GLU:OE2	2:B:256:ALA:HB2	2.02	0.58
1:C:311:LYS:HG2	1:C:342:GLN:HG2	1.84	0.58
1:C:405:VAL:O	1:C:409:VAL:HG23	2.03	0.58
2:D:66:ILE:HD11	2:D:125:GLU:HG3	1.86	0.58
4:F:165:GLU:O	4:F:168:GLU:HG2	2.04	0.58
1:C:261:PRO:HG3	1:C:313:MET:CE	2.33	0.58
3:E:47:LEU:O	3:E:51:GLN:HG2	2.03	0.58
4:F:186:LEU:HD21	4:F:328:TRP:CD1	2.38	0.58
2:B:69:ASP:O	2:B:94:PHE:HA	2.04	0.58
2:B:295:MET:HE1	2:B:317:ALA:HB1	1.86	0.58
1:C:88:HIS:CD2	1:C:90:GLU:HG3	2.39	0.58
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.22	0.58
4:F:326:LYS:HE2	4:F:328:TRP:CH2	2.39	0.58
2:D:104:ALA:HB2	2:D:413:MET:HE3	1.86	0.57
2:D:145:THR:N	9:D:501:GDP:O2B	2.37	0.57
2:D:20:PHE:HB2	2:D:235:MET:HE1	1.87	0.57
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.86	0.57
2:D:183:GLU:HB2	2:D:184:PRO:HD3	1.85	0.57
2:D:205:ASP:O	2:D:209:LEU:HD22	2.04	0.57
1:C:195:LEU:HD12	1:C:266:HIS:CE1	2.39	0.57
2:D:171:VAL:HA	2:D:204:ILE:O	2.05	0.57
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.39	0.57
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.87	0.57
4:F:199:PHE:HB3	4:F:223:THR:HG22	1.87	0.57
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.40	0.56
2:D:259:MET:HE1	2:D:314:THR:HB	1.87	0.56
1:C:75:ILE:HG22	1:C:79:ARG:NH1	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:O	1:A:51[B]:THR:HG23	2.05	0.56
1:A:163:LYS:HD2	1:A:163:LYS:N	2.20	0.56
1:A:285:GLN:HG3	1:A:372[B]:GLN:CD	2.30	0.56
2:D:392:SER:O	2:D:396:THR:HG22	2.05	0.56
1:C:248:LEU:HD13	8:C:501:VLB:H61	1.87	0.56
2:D:206:ASN:HA	2:D:209:LEU:HD23	1.87	0.56
1:A:180:ALA:O	1:A:183:GLU:HG3	2.06	0.56
2:D:295:MET:CE	2:D:375:ALA:HB1	2.36	0.56
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.88	0.56
1:A:277:SER:HB3	1:A:280:LYS:CE	2.36	0.56
2:D:332:MET:O	2:D:335:VAL:HG12	2.05	0.56
2:D:97:SER:HB2	2:D:110:GLU:HG2	1.87	0.56
2:D:204:ILE:HD12	2:D:204:ILE:N	2.21	0.56
4:F:46:ARG:HB3	4:F:46:ARG:CZ	2.36	0.56
1:C:311:LYS:HE3	1:C:436:GLY:O	2.05	0.55
2:D:291:LEU:HD11	2:D:373:MET:HG3	1.88	0.55
1:C:271:THR:CG2	1:C:295:CYS:HA	2.37	0.55
1:A:137:VAL:HG21	1:A:154:MET:HE1	1.89	0.55
1:C:368:LEU:HD12	1:C:369:ALA:H	1.71	0.55
1:A:137:VAL:HG21	1:A:154:MET:CE	2.36	0.55
2:D:209:LEU:HD12	2:D:230:LEU:HB2	1.88	0.55
2:D:402:LYS:HG2	2:D:405:LEU:HD22	1.87	0.55
4:F:163:SER:HB3	4:F:169:LEU:HD11	1.89	0.55
2:B:158:ARG:NH1	2:B:197:ASN:OD1	2.39	0.55
1:C:151[B]:SER:HB3	1:C:193:THR:HG21	1.88	0.55
2:D:191:VAL:CG1	2:D:425:MET:HE2	2.36	0.55
2:B:311:ARG:NH1	2:B:341:SER:O	2.38	0.55
2:D:259:MET:CE	2:D:314:THR:HB	2.36	0.54
1:C:287:SER:H	1:C:290:GLU:HG3	1.72	0.54
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.90	0.54
1:C:301:GLN:NE2	1:C:307:PRO:HG2	2.22	0.54
1:C:88:HIS:CD2	1:C:90:GLU:H	2.25	0.54
2:D:166:MET:HE3	2:D:166:MET:CA	2.35	0.54
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.90	0.54
2:D:290:GLU:O	2:D:293:GLN:HG2	2.06	0.54
4:F:162:ILE:HD11	4:F:233:PHE:C	2.33	0.54
4:F:245:ILE:HG22	4:F:245:ILE:O	2.07	0.54
1:A:56:THR:CG2	1:A:60:LYS:H	2.20	0.54
1:A:357:TYR:CD2	3:E:17:GLY:HA2	2.43	0.54
2:D:416:MET:O	2:D:417:GLU:C	2.49	0.54
2:B:30:ILE:HD12	2:B:30:ILE:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151[A]:SER:HB2	1:C:193:THR:HG21	1.90	0.54
1:C:313:MET:HE3	1:C:346:TRP:CH2	2.43	0.54
2:D:264:ARG:NE	2:D:431:GLU:OE2	2.41	0.54
2:D:286:LEU:H	2:D:286:LEU:HD23	1.72	0.54
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.23	0.54
2:D:416:MET:O	2:D:419:THR:N	2.40	0.54
1:C:414:GLU:O	1:C:417[B]:GLU:HG3	2.08	0.54
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.43	0.54
1:A:90:GLU:O	1:A:121:ARG:HD2	2.09	0.53
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.43	0.53
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.44	0.53
2:D:402:LYS:HE2	2:D:405:LEU:CD1	2.36	0.53
2:D:7:ILE:O	2:D:137:LEU:HA	2.08	0.53
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.44	0.53
1:A:339:ARG:HB2	1:A:341:ILE:CD1	2.39	0.53
1:C:332:ILE:O	1:C:336:LYS:HG3	2.08	0.53
2:D:301:MET:HA	2:D:301:MET:HE2	1.89	0.53
1:A:372[B]:GLN:OE1	1:A:373:ARG:NH1	2.42	0.53
3:E:105:MET:HE2	3:E:105:MET:HA	1.91	0.53
4:F:171:ASP:HA	4:F:174:ASP:HB2	1.91	0.53
1:C:434:GLU:HA	1:C:437:VAL:HG23	1.91	0.52
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.41	0.52
2:B:319:PHE:O	2:B:355:VAL:HA	2.09	0.52
1:A:191:THR:O	1:A:195:LEU:HB2	2.09	0.52
1:A:204:VAL:HG13	1:A:302:MET:HE3	1.90	0.52
1:C:214:ARG:HG2	1:C:219:ILE:O	2.08	0.52
1:C:401:LYS:HZ3	2:D:346:TRP:CG	2.28	0.52
8:C:501:VLB:H761	2:B:221:THR:CA	2.36	0.52
4:F:147:TRP:HB3	4:F:182:ILE:HG23	1.91	0.52
4:F:280:GLU:HA	4:F:284[A]:LEU:HB2	1.91	0.52
1:C:117:LEU:HD11	1:C:121:ARG:CZ	2.40	0.52
1:C:335:ILE:HG23	1:C:339:ARG:HD2	1.90	0.52
1:A:66[B]:VAL:HG23	1:A:125:LEU:HD12	1.92	0.52
1:C:151[B]:SER:HB3	1:C:193:THR:CG2	2.40	0.52
1:A:96:LYS:N	1:A:96:LYS:HD2	2.25	0.52
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.45	0.52
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.90	0.52
1:C:151[A]:SER:HB2	1:C:193:THR:CG2	2.40	0.52
2:D:191:VAL:HG11	2:D:425:MET:HE2	1.92	0.52
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.28	0.52
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ILE:O	2:B:64:ARG:HD2	2.09	0.52
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.92	0.51
2:D:22:GLU:HG2	2:D:83:PHE:HD2	1.75	0.51
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.90	0.51
2:D:153:LEU:O	2:D:157:ILE:HG13	2.10	0.51
2:D:320:ARG:O	2:D:373:MET:HA	2.10	0.51
4:F:87:LEU:O	4:F:90:SER:HB2	2.10	0.51
4:F:93:TRP:CZ3	4:F:290:ILE:HG23	2.46	0.51
4:F:225:SER:HB2	4:F:260:ASN:HD21	1.76	0.51
1:A:2:ARG:HB3	1:A:133:GLN:CG	2.41	0.51
1:C:27:GLU:CD	1:C:320:ARG:HH22	2.19	0.51
2:D:11:GLN:HB3	9:D:501:GDP:O2A	2.10	0.51
2:D:49:ILE:HG13	2:D:53:TYR:HD2	1.74	0.51
4:F:255:ARG:HD3	4:F:256:TYR:CZ	2.45	0.51
1:A:434:GLU:O	1:A:437:VAL:HG12	2.10	0.51
2:D:176:LYS:HD3	2:D:210:TYR:CD2	2.46	0.51
2:B:83:PHE:CD2	2:B:86:ILE:HD13	2.43	0.51
1:C:200:CYS:HA	1:C:266:HIS:HB2	1.93	0.51
1:C:227:LEU:O	1:C:231:ILE:HG13	2.10	0.51
1:A:96:LYS:HD2	1:A:96:LYS:H	1.75	0.51
1:C:313:MET:O	1:C:314:ALA:HB2	2.10	0.51
2:D:319:PHE:HB2	2:D:355:VAL:HG12	1.94	0.50
4:F:233:PHE:HA	4:F:239:HIS:NE2	2.23	0.50
1:C:335:ILE:O	1:C:336:LYS:C	2.53	0.50
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.93	0.50
2:B:75:MET:O	2:B:76:ASP:C	2.54	0.50
2:B:289:PRO:O	2:B:293:GLN:HG2	2.11	0.50
1:C:70:LEU:HD13	1:C:110:ILE:CG2	2.41	0.50
1:C:318:LEU:HD12	1:C:318:LEU:H	1.74	0.50
8:C:501:VLB:O32	8:C:501:VLB:C73	2.60	0.50
4:F:162:ILE:HD13	4:F:233:PHE:HB2	1.92	0.50
2:B:322:ARG:O	2:B:373:MET:HE2	2.11	0.50
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.41	0.50
1:A:251:ASP:OD1	1:A:253:THR:HB	2.11	0.50
2:B:48:ARG:NH2	2:B:250:ALA:O	2.41	0.50
1:C:296:PHE:HB3	1:C:339:ARG:HD3	1.93	0.50
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.92	0.50
2:D:59:ASN:O	2:D:59:ASN:ND2	2.45	0.50
2:B:83:PHE:HB3	2:B:86:ILE:CD1	2.42	0.50
1:A:277:SER:HB3	1:A:280:LYS:CD	2.41	0.49
2:D:403:ALA:O	2:D:405:LEU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:148:ILE:O	4:F:182:ILE:HG12	2.12	0.49
2:B:7:ILE:O	2:B:137:LEU:HA	2.12	0.49
1:C:320:ARG:CG	1:C:358:GLN:O	2.59	0.49
8:C:501:VLB:H211	8:C:501:VLB:H64	1.95	0.49
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.51	0.49
2:D:188:THR:HA	2:D:425:MET:HE1	1.94	0.49
1:A:123:ARG:HH22	1:A:160:ASP:HB3	1.76	0.49
1:C:287:SER:H	1:C:290:GLU:CD	2.21	0.49
1:C:295:CYS:SG	1:C:375:VAL:HG13	2.52	0.49
1:C:306:ASP:OD2	1:C:308:ARG:NH2	2.45	0.49
2:B:123:ARG:O	2:B:127:GLU:HG2	2.13	0.49
1:C:241:SER:HA	1:C:249:ASN:HD21	1.77	0.49
1:C:252:LEU:O	1:C:256:GLN:HG3	2.12	0.49
1:C:274:PRO:HB2	1:C:286:LEU:HD12	1.93	0.49
2:D:88:ARG:NH2	10:D:602:HOH:O	2.44	0.49
4:F:163:SER:HB3	4:F:169:LEU:CD1	2.43	0.49
1:A:227:LEU:O	1:A:231:ILE:HG13	2.12	0.49
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.27	0.49
3:E:131:GLU:OE1	3:E:131:GLU:HA	2.13	0.49
1:C:324:VAL:HG22	1:C:327:ASP:OD2	2.13	0.49
2:B:1:MET:HE2	2:B:1:MET:CA	2.42	0.49
1:A:71:GLU:OE2	1:A:74:VAL:HG23	2.13	0.48
1:C:40:LYS:O	1:C:42:ILE:N	2.46	0.48
1:C:383:ALA:O	1:C:386:GLU:HG3	2.13	0.48
2:D:146:GLY:N	9:D:501:GDP:O2B	2.40	0.48
2:B:312:TYR:CD1	2:B:381:SER:HB2	2.48	0.48
2:D:345:GLU:CG	2:D:440:ALA:HB2	2.40	0.48
1:A:154:MET:HG3	1:A:194:THR:CG2	2.39	0.48
4:F:320:MET:HE3	4:F:330:ILE:CD1	2.44	0.48
1:C:241:SER:HB2	1:C:250:VAL:O	2.13	0.48
2:D:135:PHE:HB2	2:D:166:MET:HE1	1.94	0.48
2:D:404:PHE:C	2:D:406:HIS:H	2.22	0.48
3:E:76:ARG:NH1	3:E:79:GLU:OE2	2.46	0.48
2:B:54:ASN:OD1	2:B:64:ARG:NH2	2.46	0.48
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.95	0.48
2:B:231:VAL:O	2:B:235:MET:HG3	2.14	0.48
4:F:135:TYR:OH	4:F:164:SER:O	2.25	0.48
4:F:99:VAL:HG23	4:F:126:ASP:HB2	1.95	0.48
4:F:299:GLU:N	4:F:300:PRO:HD2	2.28	0.48
1:A:68[A]:VAL:HG22	1:A:93:ILE:HB	1.93	0.48
1:A:141:PHE:O	1:A:147:SER:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:HB2	1:A:193:THR:CG2	2.43	0.48
2:D:104:ALA:HB2	2:D:413:MET:CE	2.43	0.48
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.49	0.48
2:B:180:THR:O	2:B:183:GLU:HG3	2.14	0.48
1:C:68[B]:VAL:HG21	1:C:118:VAL:HG21	1.95	0.48
4:F:45:ASN:C	4:F:46:ARG:HG2	2.39	0.48
2:B:284:ARG:O	2:B:284:ARG:HG3	2.14	0.48
4:F:179:VAL:HG13	4:F:179:VAL:O	2.14	0.47
2:B:74:THR:O	2:B:78:VAL:HG23	2.13	0.47
2:B:83:PHE:HB3	2:B:86:ILE:HD11	1.95	0.47
1:A:88:HIS:O	1:A:91:GLN:HG2	2.13	0.47
1:C:403:ALA:O	1:C:404:PHE:HB2	2.14	0.47
2:D:22:GLU:OE2	2:D:82:PRO:HG2	2.14	0.47
2:D:385:GLN:O	2:D:389:LYS:HG3	2.14	0.47
1:C:288:VAL:O	1:C:291:ILE:HG12	2.13	0.47
4:F:161:LEU:HD12	4:F:169:LEU:HD21	1.97	0.47
4:F:298:ILE:C	4:F:300:PRO:HD2	2.40	0.47
2:D:30:ILE:HD12	2:D:30:ILE:N	2.29	0.47
3:E:50:ILE:HD12	3:E:50:ILE:N	2.29	0.47
4:F:271:LEU:C	4:F:273:ASP:H	2.22	0.47
1:C:6:SER:O	1:C:65:ALA:HA	2.15	0.47
1:C:147:SER:HB2	1:C:190:THR:HB	1.96	0.47
1:C:283:HIS:O	1:C:284:GLU:HB2	2.14	0.47
1:C:284:GLU:OE2	1:C:286:LEU:HD21	2.14	0.47
4:F:271:LEU:HD23	4:F:275[A]:LEU:HD23	1.95	0.47
2:B:200:GLU:HB3	2:B:268:PHE:CE2	2.50	0.47
1:A:285:GLN:CG	1:A:372[B]:GLN:CD	2.88	0.47
1:C:328:VAL:O	1:C:332:ILE:HG13	2.15	0.47
2:D:308:ARG:HG3	2:D:342:TYR:CZ	2.50	0.47
3:E:53:LYS:HE3	3:E:53:LYS:HB2	1.72	0.47
4:F:267:PHE:O	4:F:271:LEU:HG	2.15	0.47
2:D:411:GLU:OE1	3:E:137:LYS:CE	2.63	0.47
4:F:326:LYS:HE2	4:F:328:TRP:CE2	2.48	0.47
1:A:7:ILE:HG21	1:A:153:LEU:HD21	1.96	0.47
1:A:79:ARG:HG2	1:A:92:LEU:HD13	1.95	0.47
1:A:241:SER:HB2	1:A:248:LEU:O	2.15	0.47
1:C:83:TYR:HD2	1:C:86:LEU:HD22	1.79	0.47
1:A:3:GLU:HG2	1:A:64:ARG:HH21	1.79	0.47
1:A:296:PHE:CZ	1:A:377:MET:HE1	2.49	0.47
2:D:286:LEU:HD23	2:D:286:LEU:N	2.30	0.47
2:D:355:VAL:HG23	2:D:355:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:LEU:C	2:B:387:LEU:HD23	2.40	0.47
2:D:49:ILE:HG13	2:D:53:TYR:CD2	2.49	0.46
2:B:296:PHE:CE1	2:B:335:VAL:HG11	2.50	0.46
2:B:323:MET:HB3	2:B:373:MET:HE2	1.97	0.46
1:C:313:MET:HE3	1:C:346:TRP:CZ2	2.50	0.46
2:D:9:ALA:HA	2:D:68:VAL:O	2.15	0.46
4:F:98:TYR:O	4:F:181:VAL:HG23	2.15	0.46
4:F:148:ILE:HG12	4:F:149:ALA:N	2.30	0.46
4:F:196:HIS:O	4:F:228:TYR:N	2.48	0.46
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.97	0.46
2:B:291:LEU:HD11	2:B:373:MET:HB3	1.96	0.46
2:D:62:VAL:HG11	2:D:88:ARG:HG3	1.97	0.46
4:F:221:LEU:HD12	4:F:221:LEU:N	2.30	0.46
4:F:283:ILE:HG23	4:F:327:VAL:CG2	2.45	0.46
2:D:174:SER:O	2:D:177:VAL:HG12	2.15	0.46
2:D:320:ARG:HA	2:D:356:CYS:O	2.16	0.46
4:F:283:ILE:HG23	4:F:327:VAL:HG21	1.97	0.46
2:B:141:LEU:HD12	2:B:172:MET:CE	2.45	0.46
2:B:346:TRP:HE1	2:B:438:ALA:HB3	1.81	0.46
2:B:402:LYS:HE2	2:B:415:GLU:OE1	2.16	0.46
2:D:220:THR:HG22	2:D:221:THR:HG23	1.97	0.46
2:D:406:HIS:CD2	2:D:407:TRP:CD1	2.98	0.46
4:F:132:LEU:HD21	4:F:170:LEU:CD1	2.34	0.46
4:F:162:ILE:CD1	4:F:233:PHE:HB2	2.44	0.46
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.51	0.46
2:B:292:THR:HG22	2:B:335:VAL:CG2	2.44	0.46
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.98	0.46
1:A:258:ASN:OD1	1:A:352:LYS:HE2	2.16	0.46
2:D:135:PHE:HB2	2:D:166:MET:CE	2.46	0.46
1:C:287:SER:H	1:C:290:GLU:CG	2.29	0.46
1:C:333:ALA:O	1:C:334:THR:C	2.57	0.46
2:D:20:PHE:CE2	2:D:24:ILE:HD13	2.51	0.46
2:D:406:HIS:NE2	2:D:407:TRP:CD1	2.83	0.46
1:A:2:ARG:O	1:A:133:GLN:NE2	2.42	0.46
4:F:72:CYS:HA	4:F:332:VAL:O	2.15	0.46
2:B:141:LEU:HD12	2:B:172:MET:HE1	1.98	0.46
2:B:145:THR:N	9:B:501:GDP:O2B	2.49	0.46
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.51	0.45
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.46	0.45
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.98	0.45
4:F:200:ASP:O	4:F:221:LEU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:MET:HE3	2:B:325:MET:HB3	1.78	0.45
2:B:405:LEU:HD12	2:B:405:LEU:HA	1.80	0.45
2:D:69:ASP:HA	2:D:145:THR:HG21	1.98	0.45
1:A:155:GLU:HA	1:A:197:HIS:HD2	1.81	0.45
2:D:141:LEU:HB3	2:D:187:ALA:HA	1.98	0.45
4:F:235:ASP:O	4:F:236:LYS:HB2	2.15	0.45
1:A:341:ILE:N	1:A:341:ILE:HD12	2.30	0.45
1:C:88:HIS:HD2	1:C:90:GLU:HB2	1.82	0.45
1:C:308:ARG:C	1:C:310:GLY:H	2.25	0.45
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.51	0.45
3:E:44:ASP:HA	3:E:45:PRO:HD3	1.76	0.45
1:A:275:VAL:HG13	1:A:368:LEU:CD2	2.46	0.45
1:C:328:VAL:CG1	1:C:353:VAL:HG11	2.40	0.45
4:F:286:GLN:O	4:F:290:ILE:HG13	2.16	0.45
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.52	0.45
2:D:404:PHE:C	2:D:406:HIS:N	2.74	0.45
3:E:126:LYS:CA	3:E:126:LYS:CE	2.95	0.45
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.45
2:B:287:THR:O	2:B:288:VAL:C	2.57	0.45
2:D:73:GLY:O	2:D:74:THR:C	2.60	0.45
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.52	0.45
1:A:2:ARG:HB3	1:A:131:GLY:O	2.17	0.45
1:A:357:TYR:OH	3:E:18:GLN:HG3	2.16	0.45
1:C:287:SER:N	1:C:290:GLU:HG3	2.32	0.45
2:B:209:LEU:HB3	2:B:227:LEU:HG	1.98	0.45
2:D:166:MET:HA	2:D:166:MET:CE	2.40	0.44
3:E:82:VAL:HG11	2:B:108:TYR:CG	2.52	0.44
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.53	0.44
4:F:191:LEU:HD13	4:F:196:HIS:CE1	2.53	0.44
2:B:9:ALA:HA	2:B:68:VAL:O	2.17	0.44
8:C:501:VLB:H762	2:B:222:PRO:HD2	1.99	0.44
2:D:319:PHE:CB	2:D:323:MET:HE1	2.33	0.44
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.98	0.44
1:A:258:ASN:HB2	1:A:259:LEU:HD22	1.99	0.44
2:B:165:ILE:HA	2:B:199:ASP:OD2	2.17	0.44
2:D:36:TYR:CD1	2:D:46:LEU:HD11	2.53	0.44
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.99	0.44
2:D:191:VAL:HB	2:D:425:MET:HE2	1.99	0.44
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.44
2:D:137:LEU:HG	2:D:139:HIS:ND1	2.32	0.44
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASP:HB3	1:A:373:ARG:HH21	1.83	0.44
2:B:28:HIS:C	2:B:30:ILE:HD12	2.43	0.44
2:D:402:LYS:HG2	2:D:402:LYS:O	2.18	0.44
3:E:7:GLU:O	3:E:22:VAL:HA	2.17	0.44
4:F:135:TYR:HE1	4:F:145:ASN:HB3	1.83	0.44
1:A:52:PHE:O	1:A:64:ARG:HG3	2.17	0.43
1:A:413:MET:CE	1:A:418:PHE:CE1	3.01	0.43
1:C:219:ILE:HD13	1:C:226:ASN:ND2	2.33	0.43
4:F:284[A]:LEU:HD12	4:F:284[A]:LEU:HA	1.76	0.43
2:B:106:GLY:O	2:B:111:GLY:HA3	2.18	0.43
2:B:319:PHE:HB2	2:B:355:VAL:HG22	2.01	0.43
1:C:18:ASN:OD1	1:C:78:VAL:HG22	2.18	0.43
1:C:330:ALA:O	1:C:333:ALA:HB3	2.18	0.43
2:D:23:VAL:O	2:D:27:GLU:HG3	2.18	0.43
1:A:101:ASN:ND2	1:A:180:ALA:HB2	2.34	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.18	0.43
1:C:407:TRP:CH2	2:D:256:ALA:HB1	2.53	0.43
8:C:501:VLB:H762	8:C:501:VLB:H512	1.99	0.43
2:D:69:ASP:O	2:D:94:PHE:HA	2.18	0.43
2:D:194:LEU:CD2	2:D:198:THR:HG21	2.48	0.43
2:D:26:ASP:CG	2:D:369:ARG:HD2	2.42	0.43
2:D:73:GLY:HA2	2:D:76:ASP:HB2	1.99	0.43
2:D:180:THR:O	2:D:182:VAL:N	2.46	0.43
4:F:88:SER:C	4:F:90:SER:N	2.76	0.43
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.01	0.43
1:C:154:MET:HE2	1:C:194[A]:THR:CG2	2.49	0.43
1:C:335:ILE:HG22	1:C:341:ILE:HD11	2.00	0.43
1:A:56:THR:HG22	1:A:60:LYS:N	2.34	0.43
1:C:250:VAL:HG11	1:C:352:LYS:HE2	2.00	0.43
4:F:21:LEU:HD22	4:F:27:TRP:NE1	2.34	0.43
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.53	0.43
4:F:342:LEU:O	4:F:343:TYR:C	2.61	0.43
2:D:75:MET:HB3	2:D:75:MET:HE3	1.70	0.43
4:F:231:ALA:O	4:F:232:ASN:HB3	2.17	0.43
4:F:286:GLN:OE1	4:F:327:VAL:HG23	2.18	0.43
1:A:346:TRP:H	1:A:346:TRP:CD1	2.36	0.43
2:D:21:TRP:CZ2	2:D:65:ALA:HB2	2.53	0.43
2:D:93:VAL:HG12	2:D:114:LEU:HD11	2.01	0.43
2:D:295:MET:HE2	2:D:377:PHE:HB2	2.01	0.43
4:F:88:SER:C	4:F:90:SER:H	2.27	0.43
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.01	0.42
4:F:257:GLU:HB3	4:F:260:ASN:CA	2.43	0.42
2:B:146:GLY:O	2:B:150:GLY:HA3	2.17	0.42
2:B:285:ALA:HB2	2:B:372:LYS:CE	2.42	0.42
2:D:204:ILE:HG21	2:D:231:VAL:HG22	2.01	0.42
2:D:268:PHE:O	2:D:270:PRO:HD3	2.19	0.42
4:F:234:GLN:O	4:F:235:ASP:C	2.62	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.42
1:C:377:MET:HE3	1:C:377:MET:HB3	1.76	0.42
1:C:399:TYR:O	1:C:402:ARG:HD3	2.19	0.42
1:C:413:MET:HB3	1:C:413:MET:HE2	1.65	0.42
1:C:422:ARG:HD2	1:C:422:ARG:HA	1.74	0.42
2:D:172:MET:HA	2:D:173:PRO:HD3	1.91	0.42
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.48	0.42
1:C:1:MET:O	1:C:2:ARG:HB2	2.20	0.42
1:C:415:GLU:O	1:C:418:PHE:HB2	2.19	0.42
2:D:120:ASP:O	2:D:124:LYS:HG3	2.19	0.42
2:D:298:SER:HB2	2:D:306:ASP:OD1	2.18	0.42
2:D:298:SER:CB	2:D:307:PRO:HD2	2.42	0.42
2:D:414:ASP:OD1	2:D:414:ASP:N	2.43	0.42
4:F:248:GLU:O	4:F:248:GLU:HG2	2.19	0.42
2:B:103:TRP:HB2	2:B:186:ASN:OD1	2.18	0.42
2:B:30:ILE:HD12	2:B:30:ILE:H	1.84	0.42
1:A:2:ARG:CB	1:A:133:GLN:HG2	2.47	0.42
1:A:70:LEU:HB2	1:A:98:ASP:HA	2.01	0.42
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.54	0.42
2:D:303:ALA:O	2:D:305:CYS:N	2.51	0.42
3:E:137:LYS:NZ	3:E:140:LYS:NZ	2.67	0.42
1:A:75:ILE:O	1:A:79:ARG:HG3	2.20	0.42
1:A:344:VAL:HG23	1:A:347:CYS:HB2	2.02	0.42
3:E:60:ARG:O	3:E:64:GLN:HG2	2.20	0.42
4:F:1:MET:CE	4:F:28:LYS:HB2	2.50	0.42
2:B:141:LEU:HD12	2:B:172:MET:SD	2.59	0.42
2:B:158:ARG:NH1	2:B:197:ASN:HA	2.34	0.42
1:A:406:HIS:CD2	2:B:263:PRO:HD3	2.55	0.42
4:F:188:LYS:O	4:F:323:GLU:HG3	2.20	0.42
1:A:238:ILE:HG12	1:A:378:LEU:HD21	2.02	0.42
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.02	0.42
2:D:205:ASP:O	2:D:209:LEU:CD2	2.68	0.42
4:F:6:VAL:HG22	4:F:41:LEU:HD12	2.02	0.42
4:F:279:LEU:HG	4:F:284[A]:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:279:LEU:HG	4:F:284[B]:LEU:HG	2.01	0.42
2:B:46:LEU:HD23	2:B:46:LEU:HA	1.90	0.42
2:B:234:THR:O	2:B:238:VAL:HG13	2.20	0.42
1:C:104:ALA:HB2	1:C:413:MET:HG3	2.02	0.41
1:A:28:HIS:O	1:A:36:MET:HE3	2.20	0.41
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.34	0.41
1:C:98:ASP:HB2	5:C:502:GTP:O3G	2.20	0.41
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.56	0.41
4:F:160:ILE:HG13	4:F:240:LEU:HD21	2.01	0.41
2:B:259:MET:HE2	2:B:378:ILE:HG22	2.02	0.41
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.44	0.41
1:C:296:PHE:CB	1:C:339:ARG:HD3	2.49	0.41
2:D:42:LEU:HB3	2:D:358:ILE:HD11	2.02	0.41
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.01	0.41
4:F:217:ARG:HH21	4:F:345:GLU:CD	2.28	0.41
1:C:430:LYS:O	1:C:434:GLU:HG3	2.19	0.41
4:F:55:GLU:HB2	4:F:60:GLN:HE21	1.85	0.41
1:A:100:ALA:HB2	2:B:253:ARG:HD2	2.03	0.41
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.55	0.41
1:A:213:CYS:O	1:A:217:LEU:HB2	2.20	0.41
1:C:90:GLU:HB3	1:C:121:ARG:HD2	2.03	0.41
4:F:98:TYR:HB3	4:F:127:GLU:HG3	2.02	0.41
1:A:372[B]:GLN:HG3	1:A:373:ARG:CZ	2.50	0.41
1:A:255:PHE:O	1:A:259:LEU:HD23	2.20	0.41
4:F:96:GLU:O	4:F:183:GLN:HA	2.21	0.41
1:A:296:PHE:CE1	1:A:377:MET:HE1	2.56	0.41
1:C:328:VAL:HG11	8:C:501:VLB:H63	2.02	0.41
3:E:46:SER:O	3:E:50:ILE:CD1	2.68	0.41
1:A:56:THR:HG22	1:A:60:LYS:H	1.86	0.41
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.57	0.41
1:C:399:TYR:C	1:C:402:ARG:H	2.29	0.41
3:E:24:LEU:HD12	3:E:24:LEU:N	2.36	0.41
1:C:285:GLN:HE21	1:C:373:ARG:HH12	1.68	0.40
1:C:398:MET:HE3	2:D:347:ILE:HG23	2.02	0.40
2:D:36:TYR:CE1	2:D:46:LEU:CD1	3.04	0.40
2:D:202:TYR:O	2:D:204:ILE:HD12	2.21	0.40
2:D:324:SER:O	2:D:328:VAL:HG23	2.21	0.40
4:F:216:TYR:OH	4:F:342:LEU:HD22	2.21	0.40
2:B:191:VAL:CG1	2:B:425:MET:CE	2.97	0.40
1:A:335:ILE:HD12	1:A:336:LYS:N	2.37	0.40
4:F:39:LEU:HD21	4:F:41:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.56	0.40
2:B:199:ASP:C	2:B:200:GLU:HG3	2.47	0.40
2:B:255:LEU:HD12	2:B:259:MET:HG2	2.03	0.40
2:D:1:MET:HG3	2:D:3:GLU:OE2	2.21	0.40
3:E:8:VAL:O	3:E:9:ILE:HD13	2.22	0.40
2:B:28:HIS:HB2	2:B:30:ILE:CD1	2.52	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:C:322:ASP:OD2	3:E:98:LYS:NZ[4_455]	1.92	0.28

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/440 (101%)	426 (96%)	18 (4%)	2 (0%)	30	62
1	C	445/440 (101%)	415 (93%)	27 (6%)	3 (1%)	18	52
2	B	428/431 (99%)	415 (97%)	13 (3%)	0	100	100
2	D	424/431 (98%)	402 (95%)	20 (5%)	2 (0%)	24	59
3	E	116/120 (97%)	113 (97%)	3 (3%)	0	100	100
4	F	323/331 (98%)	295 (91%)	26 (8%)	2 (1%)	21	56
All	All	2182/2193 (100%)	2066 (95%)	107 (5%)	9 (0%)	30	62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	41	THR
1	C	284	GLU

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Mol	Chain	Res	Type
2	D	404	PHE
4	F	230	SER
1	A	284	GLU
1	C	314	ALA
1	A	282	TYR
2	D	72	PRO
4	F	232	ASN

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	378/371 (102%)	377 (100%)	1 (0%)	86	88
1	C	378/371 (102%)	358 (95%)	20 (5%)	20	53
2	B	369/372 (99%)	366 (99%)	3 (1%)	73	82
2	D	369/372 (99%)	367 (100%)	2 (0%)	81	85
3	E	108/108 (100%)	107 (99%)	1 (1%)	70	81
4	F	303/299 (101%)	292 (96%)	11 (4%)	31	63
All	All	1905/1893 (101%)	1867 (98%)	38 (2%)	50	72

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	C	242	LEU
1	C	280	LYS
1	C	290	GLU
1	C	302	MET
1	C	307	PRO
1	C	311	LYS
1	C	317	LEU
1	C	318	LEU
1	C	325	PRO
1	C	332	ILE

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Mol	Chain	Res	Type
1	C	349	THR
1	C	352	LYS
1	C	363[A]	VAL
1	C	363[B]	VAL
1	C	368	LEU
1	C	370	LYS
1	C	377	MET
1	C	391	LEU
1	C	413	MET
1	C	439	SER
2	D	75	MET
2	D	405	LEU
3	E	61	ARG
4	F	160	ILE
4	F	161	LEU
4	F	230	SER
4	F	232	ASN
4	F	233	PHE
4	F	234	GLN
4	F	238	CYS
4	F	256	TYR
4	F	257	GLU
4	F	284[A]	LEU
4	F	284[B]	LEU
2	B	71	GLU
2	B	77	SER
2	B	286	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	101	ASN
1	A	128	GLN
1	A	300	ASN
1	A	356	ASN
1	C	88	HIS
1	C	256	GLN
1	C	266	HIS
1	C	283	HIS
1	C	285	GLN
1	C	329	ASN

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Mol	Chain	Res	Type
1	C	342	GLN
1	C	372	GLN
2	D	37	HIS
2	D	45	GLN
4	F	60	GLN
4	F	229	ASN
4	F	260	ASN
4	F	333	ASN
4	F	379	HIS
2	B	8	GLN
2	B	167	ASN
2	B	229	HIS
2	B	339	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z > 2$
5	GTP	A	501	6	33,34,34	0.56	0	50,54,54	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	C	502	6	33,34,34	0.58	0	50,54,54	0.50	0
8	VLB	C	501	-	66,67,67	3.20	23 (34%)	82,108,108	2.77	35 (42%)
9	GDP	B	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.64	5 (11%)
9	GDP	D	501	-	29,30,30	1.19	5 (17%)	45,47,47	1.71	7 (15%)

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
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
5	GTP	C	502	6	-	7/22/38/38	0/3/3/3
8	VLB	C	501	-	-	15/40/131/131	0/7/9/9
9	GDP	B	501	-	-	2/16/32/32	0/3/3/3
9	GDP	D	501	-	-	3/16/32/32	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	501	VLB	C68-C73	15.80	1.74	1.53
8	C	501	VLB	C58-C59	-8.95	1.37	1.51
8	C	501	VLB	C57-N56	6.52	1.62	1.47
8	C	501	VLB	O75-C76	-5.81	1.32	1.45
8	C	501	VLB	O32-C33	-5.55	1.27	1.42
8	C	501	VLB	C68-C15	-4.69	1.40	1.54
8	C	501	VLB	C5-C6	-3.99	1.44	1.51
8	C	501	VLB	O25-C26	-3.97	1.36	1.45
8	C	501	VLB	C57-C58	-3.86	1.44	1.52
8	C	501	VLB	C60-C65	-3.46	1.37	1.41
8	C	501	VLB	C67-N66	3.27	1.43	1.38
8	C	501	VLB	C20-C5	-3.17	1.50	1.55
8	C	501	VLB	C69-N56	3.15	1.52	1.46
9	B	501	GDP	C5-C4	3.15	1.47	1.38
8	C	501	VLB	C70-C54	3.05	1.58	1.53
9	D	501	GDP	C5-C4	3.00	1.47	1.38
8	C	501	VLB	C69-C52	2.89	1.56	1.52
8	C	501	VLB	O28-C4	-2.83	1.38	1.44
8	C	501	VLB	C21-C20	2.82	1.63	1.51
8	C	501	VLB	O74-C73	2.77	1.26	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	501	VLB	C19-N9	2.65	1.51	1.47
9	B	501	GDP	C6-N1	-2.63	1.33	1.38
8	C	501	VLB	O75-C73	2.47	1.37	1.33
8	C	501	VLB	C14-C13	-2.46	1.36	1.39
9	D	501	GDP	PA-O3A	2.41	1.62	1.59
8	C	501	VLB	C55-C54	2.36	1.56	1.54
8	C	501	VLB	O27-C3	-2.34	1.38	1.42
9	D	501	GDP	C6-N1	-2.33	1.34	1.38
9	B	501	GDP	C4-N9	-2.05	1.32	1.38
9	D	501	GDP	C5-N7	-2.03	1.35	1.39
9	D	501	GDP	C4-N9	-2.00	1.33	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	501	VLB	O32-C16-C15	7.39	123.91	116.59
8	C	501	VLB	O25-C23-C3	7.23	124.10	112.21
8	C	501	VLB	O72-C54-C70	-5.70	99.11	108.74
8	C	501	VLB	C3-C2-N1	-5.58	105.13	112.81
8	C	501	VLB	C57-C58-C59	5.57	122.65	113.65
9	D	501	GDP	C5-C4-N3	-5.54	119.58	128.39
9	B	501	GDP	C5-C4-N3	-5.52	119.60	128.39
8	C	501	VLB	C33-O32-C16	-5.39	109.60	117.51
8	C	501	VLB	O75-C73-C68	5.16	119.54	111.21
8	C	501	VLB	C58-C59-C60	-5.11	110.07	123.91
8	C	501	VLB	C22-N1-C18	-5.04	105.32	120.94
8	C	501	VLB	C22-N1-C2	-4.87	107.35	119.14
9	D	501	GDP	C2-N3-C4	4.74	120.47	112.30
8	C	501	VLB	O32-C16-C17	-4.73	115.93	124.08
8	C	501	VLB	O75-C73-O74	-4.43	116.33	123.95
9	B	501	GDP	C2-N3-C4	4.31	119.73	112.30
9	D	501	GDP	N9-C4-N3	4.29	134.53	125.95
8	C	501	VLB	C13-C18-N1	4.03	115.33	110.93
8	C	501	VLB	C19-C5-C6	3.94	112.21	108.27
8	C	501	VLB	O24-C23-C3	-3.92	117.91	123.92
9	B	501	GDP	N9-C4-N3	3.88	133.71	125.95
8	C	501	VLB	O28-C29-C30	3.64	117.58	111.09
8	C	501	VLB	C17-C18-N1	-3.57	122.69	127.59
9	B	501	GDP	C6-C5-N7	3.48	136.62	130.29
8	C	501	VLB	O25-C23-O24	-3.46	117.99	123.95
9	D	501	GDP	C6-C5-N7	3.24	136.19	130.29
8	C	501	VLB	C18-N1-C2	-3.21	104.57	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	501	VLB	C52-C69-N56	3.12	116.42	111.20
8	C	501	VLB	C65-N66-C67	-3.08	104.79	109.06
8	C	501	VLB	C60-C65-N66	2.97	111.57	108.23
8	C	501	VLB	C8-N9-C19	-2.96	104.99	112.48
8	C	501	VLB	C14-C15-C16	2.90	120.91	116.80
9	B	501	GDP	C4-C5-N7	-2.84	106.17	110.67
8	C	501	VLB	C64-C65-N66	-2.82	125.13	130.83
8	C	501	VLB	C4-C3-C2	-2.62	103.84	109.23
8	C	501	VLB	C76-O75-C73	-2.60	111.65	115.91
8	C	501	VLB	C4-O28-C29	-2.42	113.98	117.65
8	C	501	VLB	C54-C53-C52	2.35	116.37	109.98
9	D	501	GDP	O6-C6-C5	-2.29	120.48	126.53
8	C	501	VLB	C7-C8-N9	-2.28	105.47	110.94
9	D	501	GDP	C4-C5-N7	-2.28	107.06	110.67
8	C	501	VLB	C53-C52-C69	2.21	111.15	108.67
9	D	501	GDP	O3B-PB-O3A	2.21	112.05	104.64
8	C	501	VLB	O28-C29-O31	-2.17	118.80	122.99
8	C	501	VLB	C61-C60-C65	2.13	121.05	118.84
8	C	501	VLB	C69-N56-C55	-2.07	108.06	110.87
8	C	501	VLB	C4-C3-C23	2.01	115.98	110.85

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O1A
8	C	501	VLB	C57-C58-C59-C60
8	C	501	VLB	C57-C58-C59-C67
8	C	501	VLB	C68-C73-O75-C76
8	C	501	VLB	C3-C23-O25-C26
8	C	501	VLB	O24-C23-O25-C26
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O2A
8	C	501	VLB	O74-C73-O75-C76
8	C	501	VLB	C30-C29-O28-C4

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Mol	Chain	Res	Type	Atoms
8	C	501	VLB	C17-C16-O32-C33
8	C	501	VLB	O31-C29-O28-C4
8	C	501	VLB	C15-C16-O32-C33
5	C	502	GTP	PB-O3A-PA-O1A
8	C	501	VLB	C58-C57-N56-C55
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	502	GTP	C5'-O5'-PA-O2A
8	C	501	VLB	C15-C68-C73-O75
5	C	502	GTP	C4'-C5'-O5'-PA
8	C	501	VLB	C15-C68-C73-O74
5	A	501	GTP	PB-O3B-PG-O3G
5	C	502	GTP	C3'-C4'-C5'-O5'
5	C	502	GTP	PB-O3A-PA-O2A
8	C	501	VLB	C21-C20-C5-C4
8	C	501	VLB	O25-C23-C3-O27
5	A	501	GTP	PG-O3B-PB-O2B

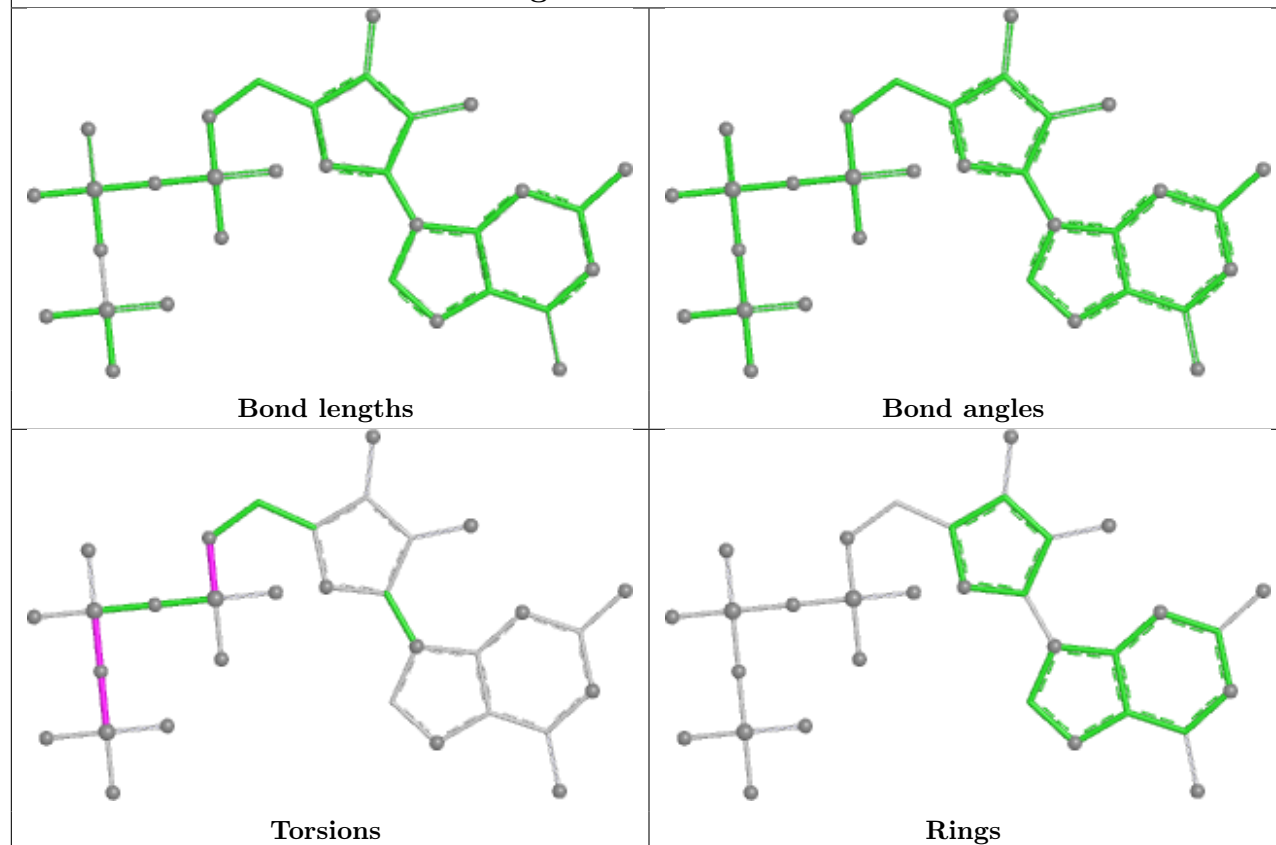
There are no ring outliers.

4 monomers are involved in 21 short contacts:

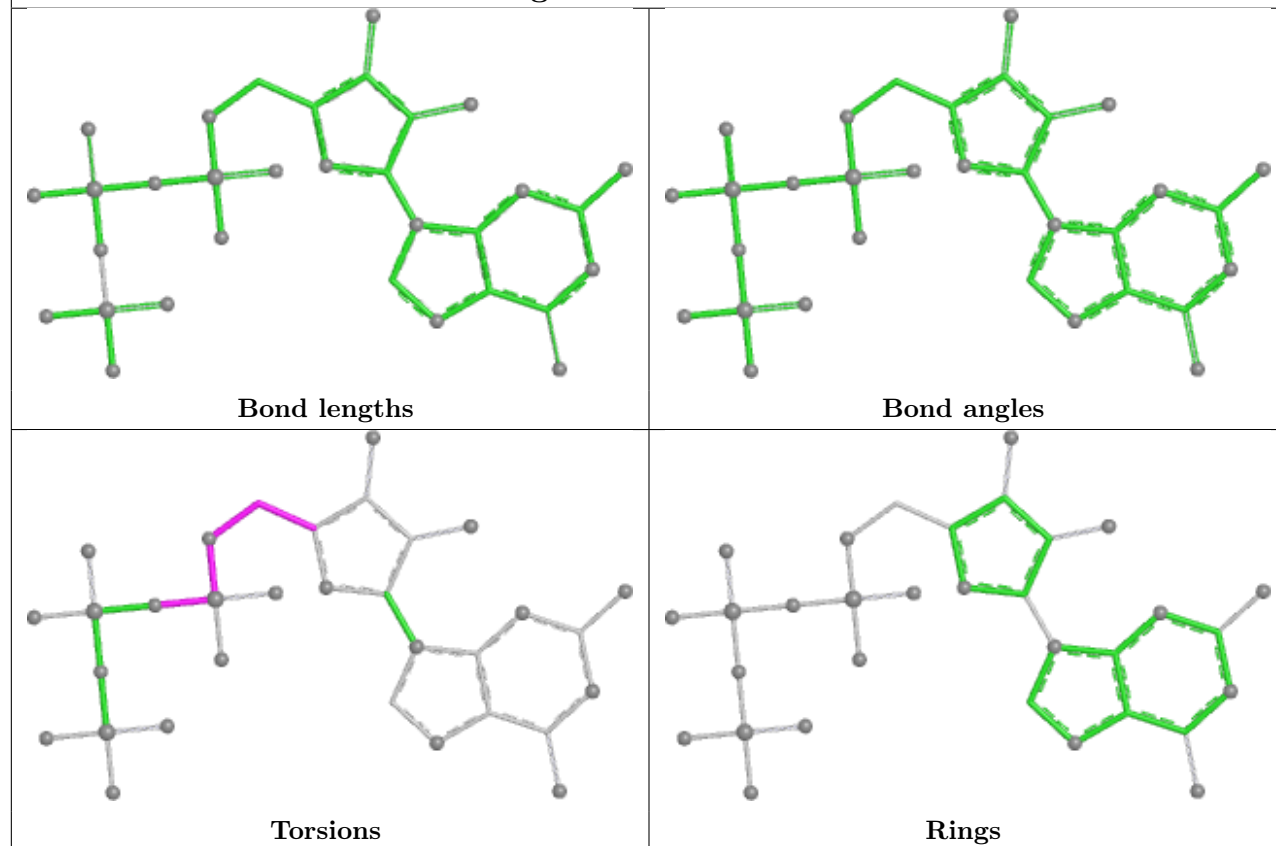
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	502	GTP	1	0
8	C	501	VLB	16	0
9	B	501	GDP	1	0
9	D	501	GDP	3	0

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.

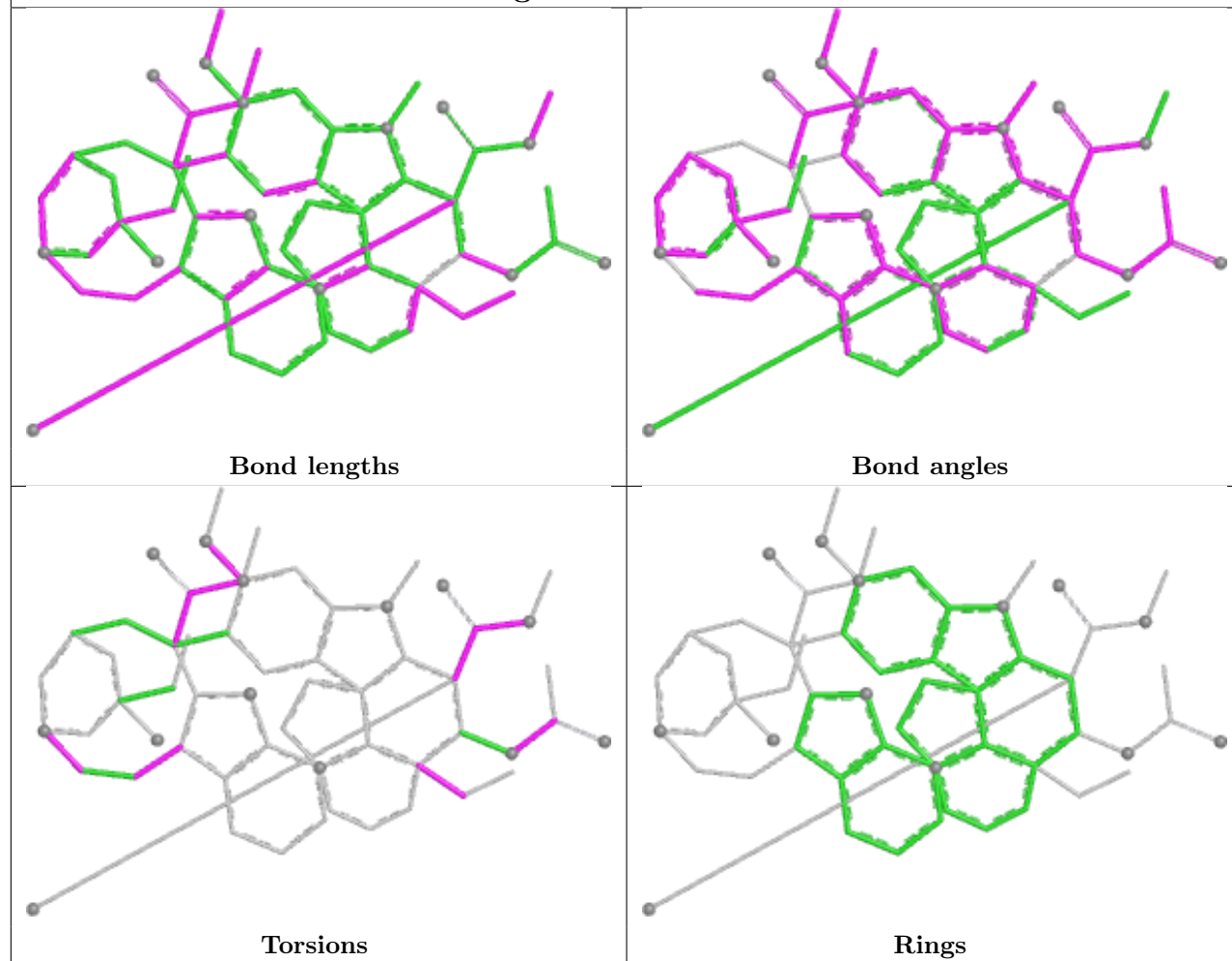
Ligand GTP A 501



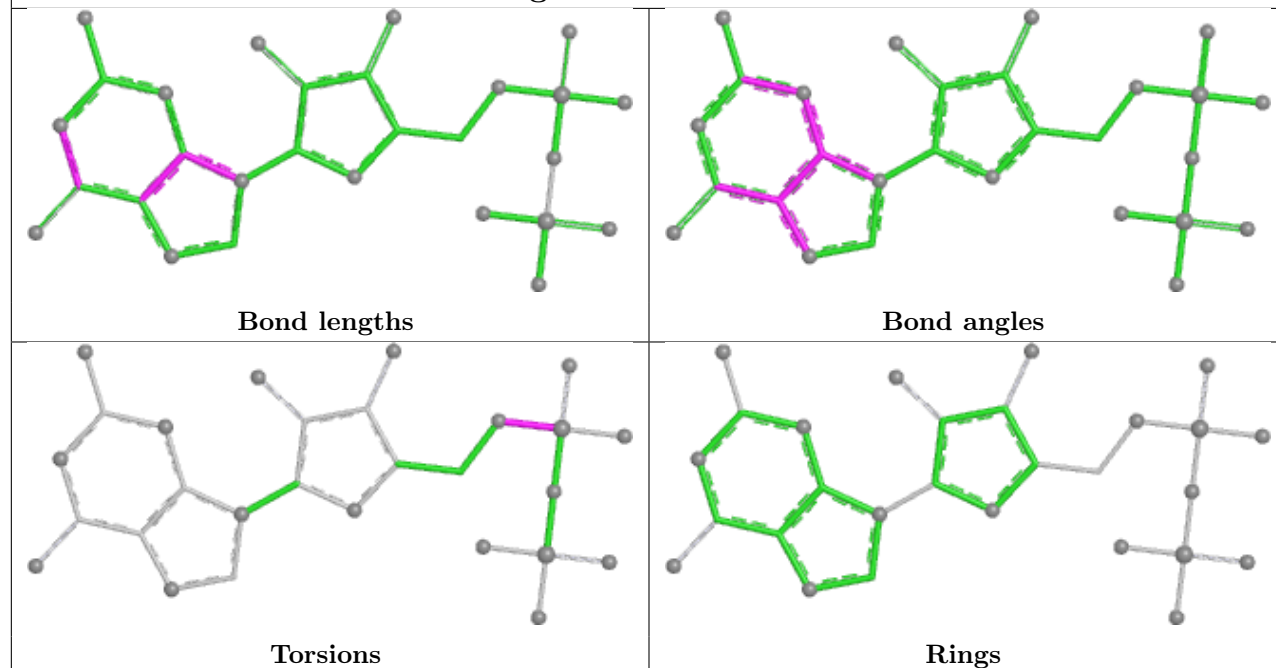
Ligand GTP C 502

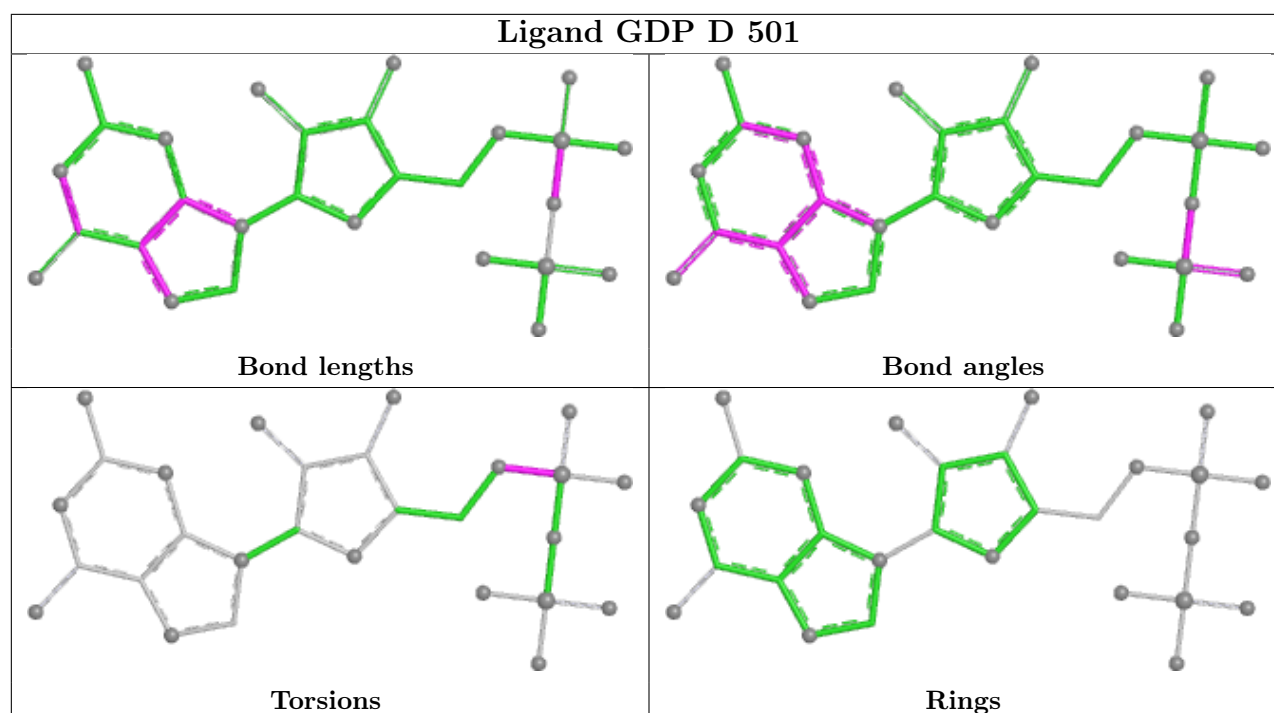


Ligand VLB C 501



Ligand GDP B 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	F	5
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	32.56
1	F	362:ALA	C	372:THR	N	20.09
1	F	103:THR	C	125:THR	N	13.23
1	F	250:SER	C	255:ARG	N	9.11
1	F	149:ALA	C	159:GLY	N	8.13
1	F	137:ARG	C	144:GLY	N	7.47

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	439/440 (99%)	-0.23	0 100 100	30, 65, 112, 259	9 (2%)
1	C	440/440 (100%)	-0.17	5 (1%) 78 61	24, 50, 88, 226	7 (1%)
2	B	428/431 (99%)	-0.36	2 (0%) 87 76	17, 54, 97, 150	6 (1%)
2	D	424/431 (98%)	-0.07	3 (0%) 84 69	31, 82, 130, 180	5 (1%)
3	E	120/120 (100%)	0.09	0 100 100	47, 82, 130, 153	0
4	F	331/331 (100%)	0.19	12 (3%) 46 28	40, 97, 172, 212	4 (1%)
All	All	2182/2193 (99%)	-0.13	22 (1%) 79 63	17, 68, 134, 259	31 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	THR	4.0
4	F	238	CYS	3.7
4	F	175	GLU	3.1
4	F	231	ALA	3.1
4	F	257	GLU	3.1
2	B	57	THR	2.9
1	C	284	GLU	2.8
4	F	173	ILE	2.6
1	C	283	HIS	2.5
4	F	102	PRO	2.4
2	B	80	SER	2.4
2	D	131	CYS	2.4
4	F	169	LEU	2.3
1	C	249	ASN	2.3
4	F	134	ALA	2.2
4	F	133	ALA	2.2
4	F	91	CYS	2.1
4	F	362	ALA	2.1
2	D	415	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	293	ASN	2.1
2	D	56	ALA	2.1
4	F	225	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

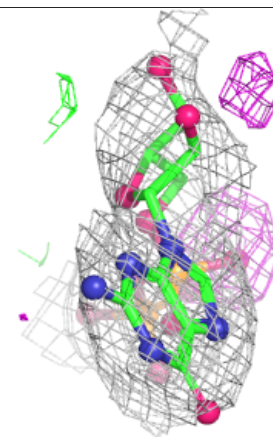
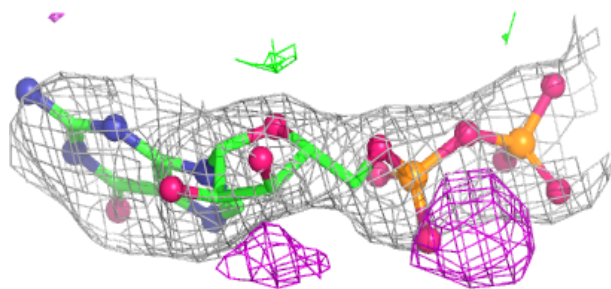
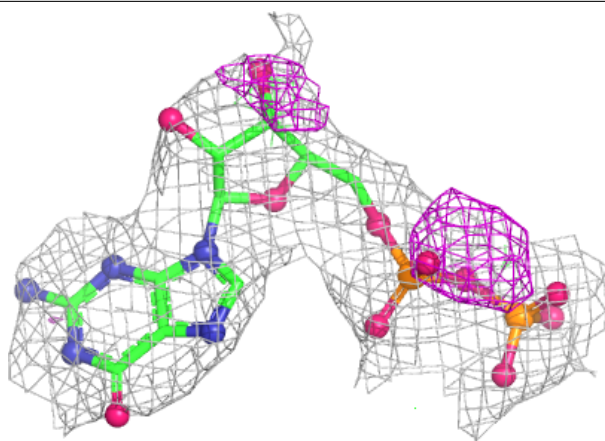
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	GDP	D	501	28/28	0.84	0.12	74,78,89,101	0
6	MG	C	503	1/1	0.89	0.35	41,41,41,41	0
6	MG	A	502	1/1	0.92	0.27	45,45,45,45	0
5	GTP	C	502	32/32	0.94	0.09	41,45,48,48	0
8	VLB	C	501	59/59	0.94	0.09	38,47,55,59	0
5	GTP	A	501	32/32	0.94	0.09	49,51,55,55	0
7	CA	A	503	1/1	0.96	0.05	91,91,91,91	0
9	GDP	B	501	28/28	0.96	0.07	36,41,43,44	0
7	CA	C	504	1/1	0.98	0.15	30,30,30,30	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.

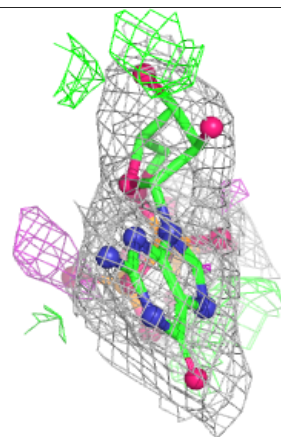
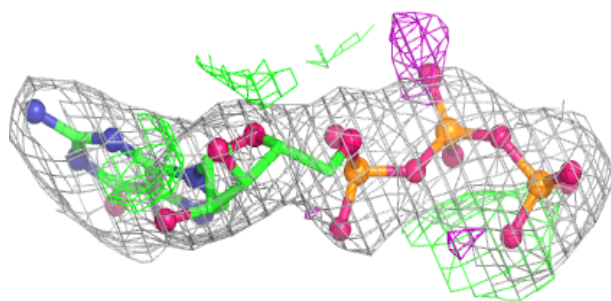
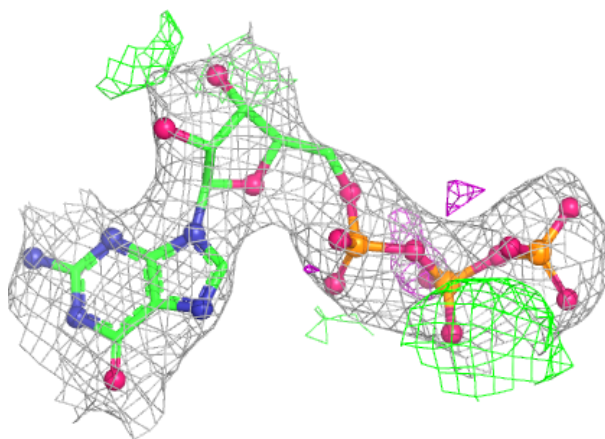
Electron density around GDP D 501:

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



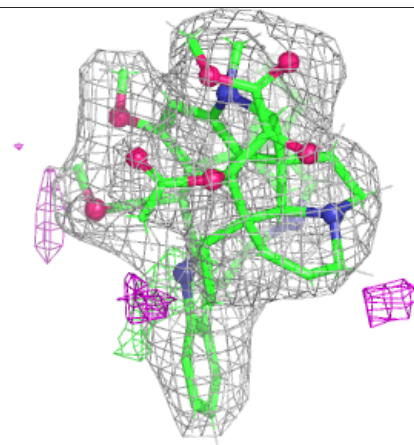
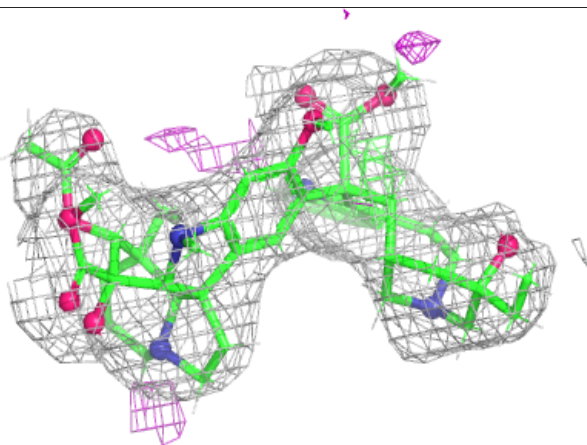
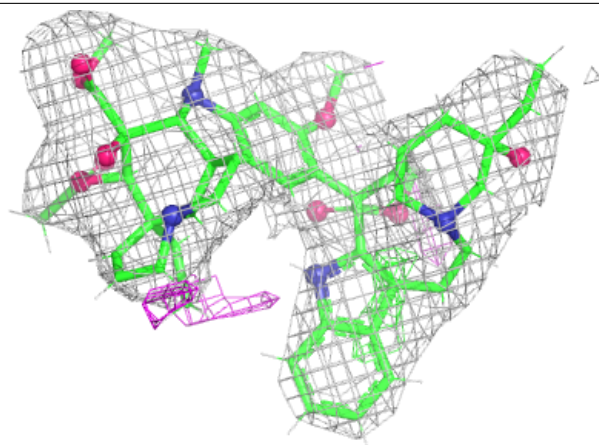
Electron density around GTP C 502:

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



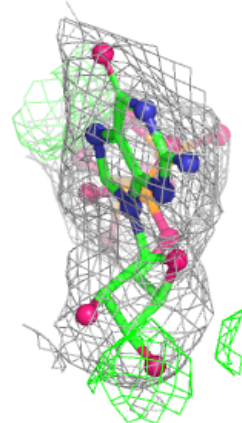
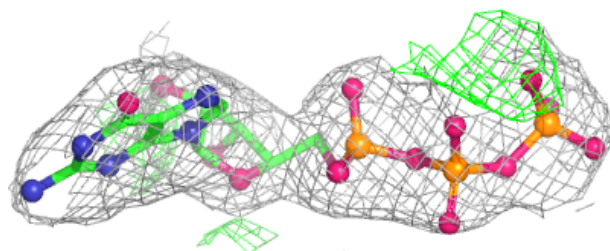
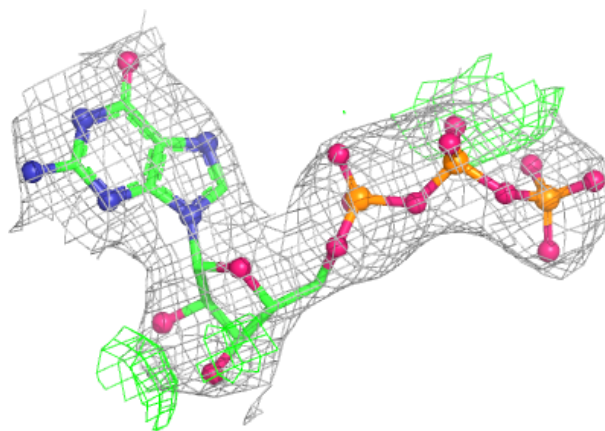
Electron density around VLB C 501:

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



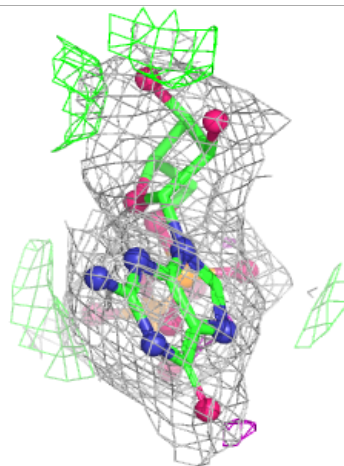
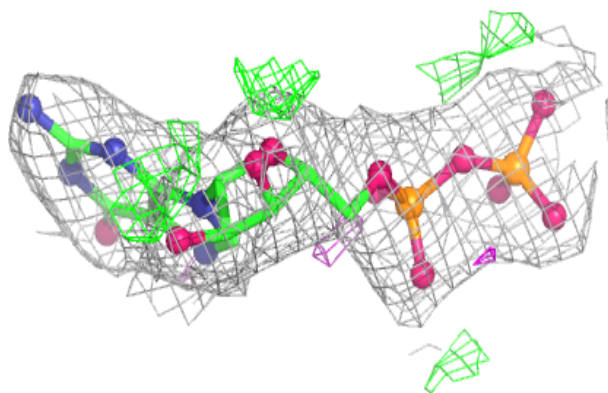
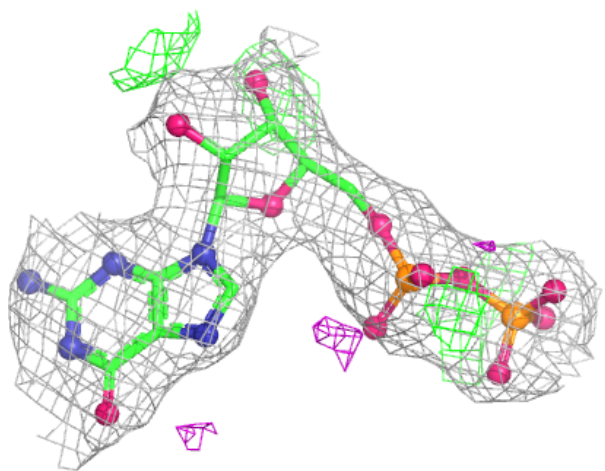
Electron density around GTP A 501:

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



Electron density around GDP B 501:

$2mF_o-DF_c$ (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.