



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 04:18 pm GMT

PDB ID : 8CLE
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

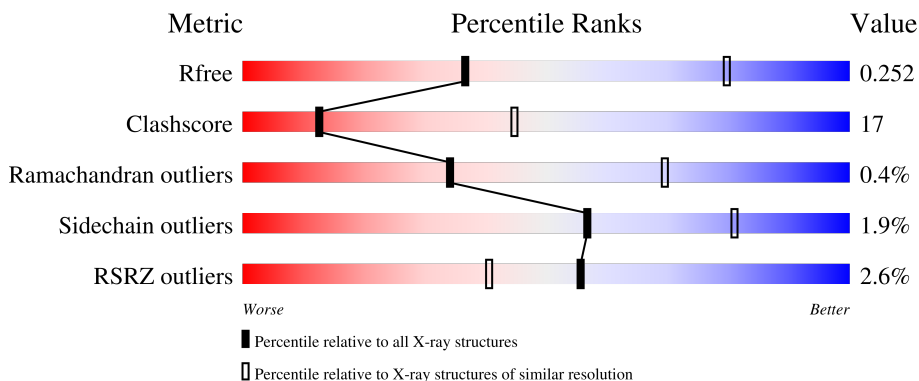
1 Overall quality at a glance

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.



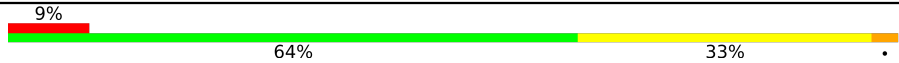
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	
1	C	440	
2	B	431	
2	D	431	
3	E	120	

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Mol	Chain	Length	Quality of chain
4	F	331	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '9%', a green segment in the middle labeled '64%', and a yellow segment on the right labeled '33%'. A small black dot is visible at the far right end of the bar.</p>

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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
4	F	331	Total	C	N	O	S	5	4	0
			2729	1762	457	496	14			

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



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

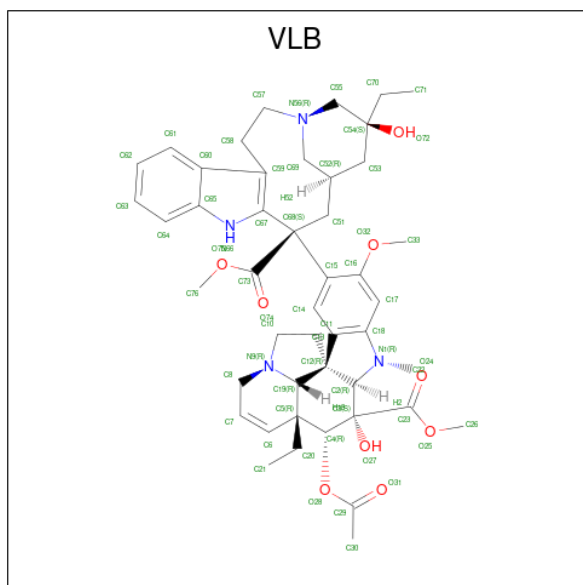
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

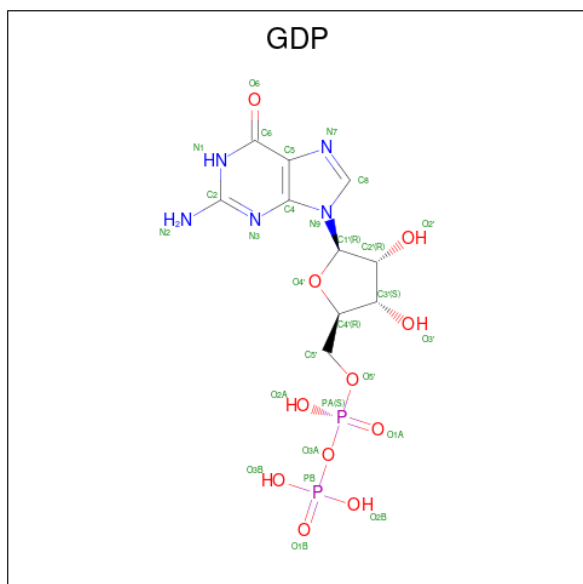
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



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

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

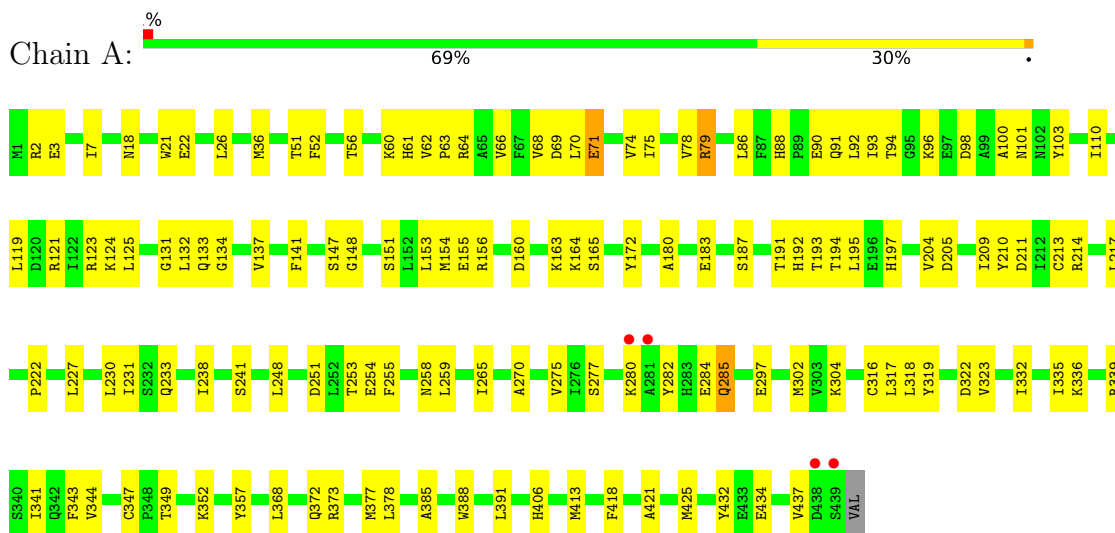
- Molecule 10 is water.

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

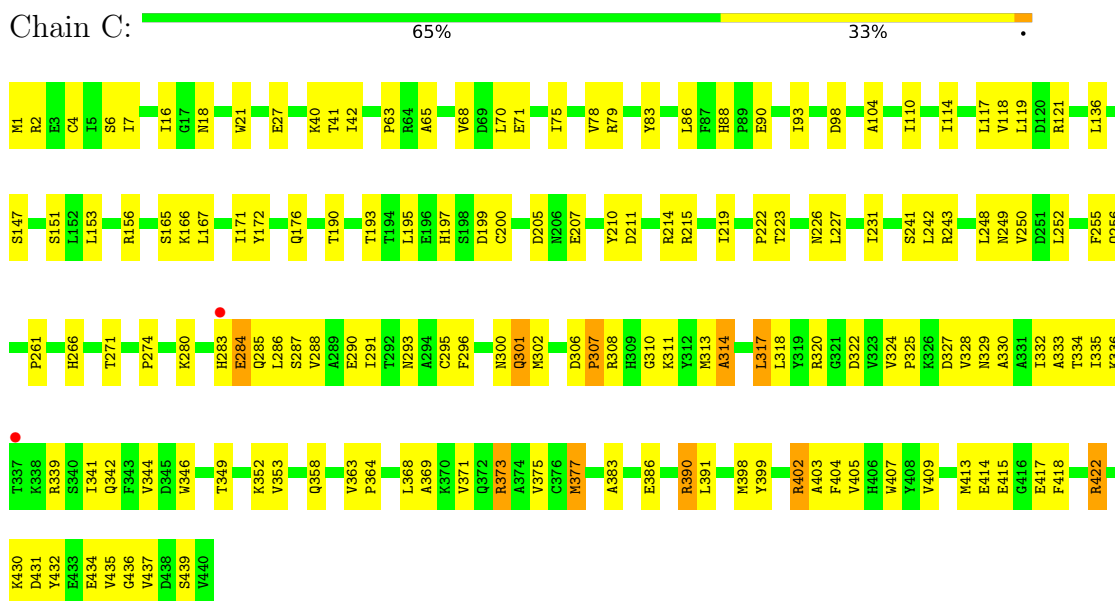
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

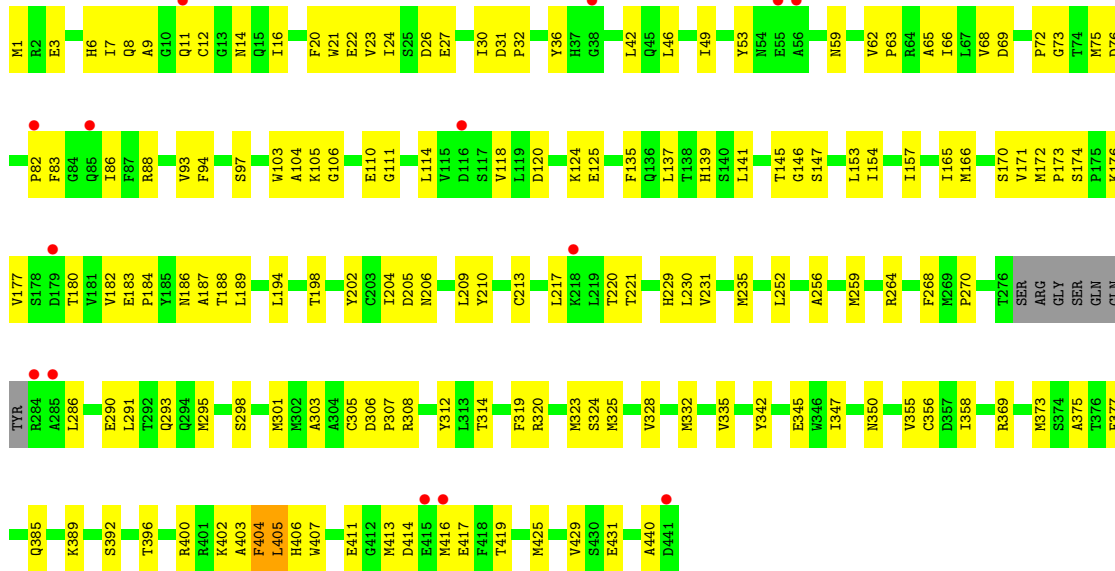
- Molecule 1: Tubulin alpha-1B chain



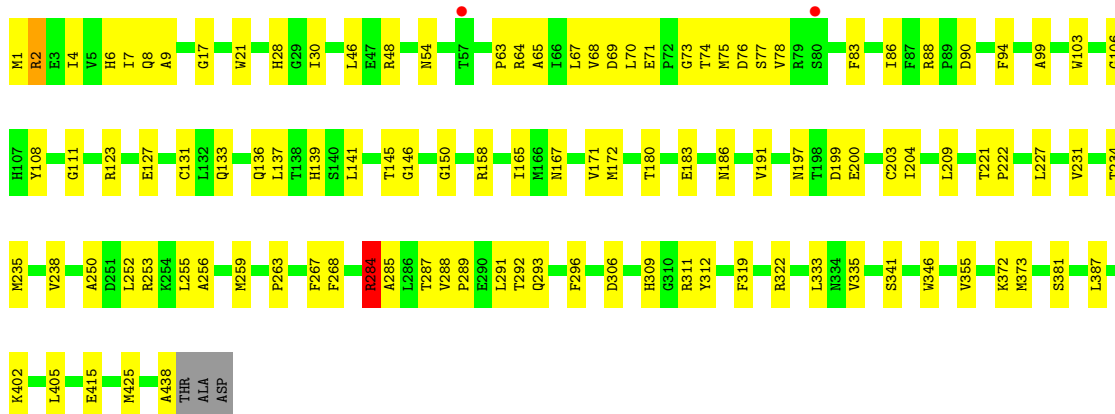
- Molecule 1: Tubulin alpha-1B chain



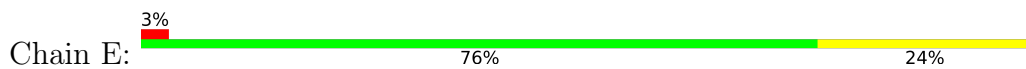
- Molecule 2: Tubulin beta-2B chain



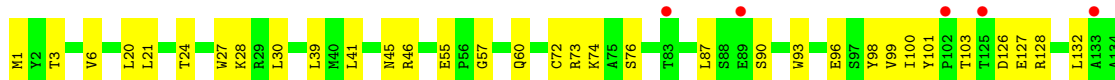
• Molecule 2: Tubulin beta-2B chain

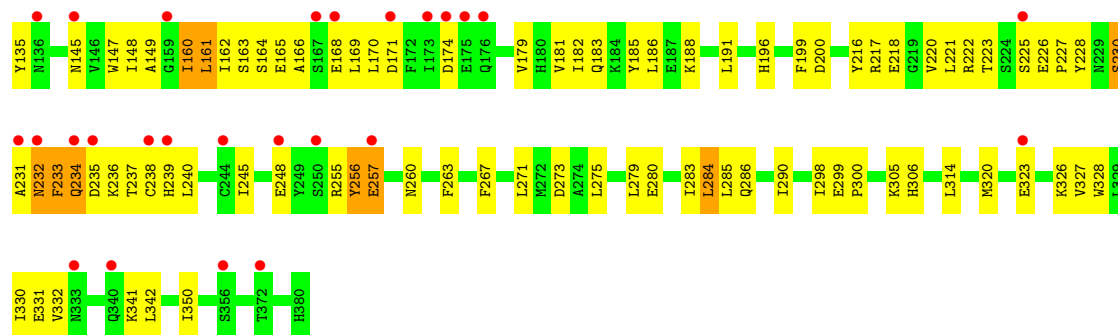


• Molecule 3: Stathmin-4



• 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 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.13-3.20) 76.0 (15.13-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.20_4487	Depositor
R, R_{free}	0.200 , 0.248 0.207 , 0.252	Depositor DCC
R_{free} test set	1999 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 75.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17637	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage'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

5.1 Standard geometry

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

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	0.32	0/3571	0.59	0/4849
1	C	0.47	0/3565	0.66	0/4842
2	B	0.34	0/3451	0.63	0/4675
2	D	0.32	0/3428	0.59	0/4645
3	E	0.34	0/999	0.65	0/1325
4	F	0.38	0/2802	0.62	0/3789
All	All	0.37	0/17816	0.62	0/24125

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

There are no bond length outliers.

There are no bond angle outliers.

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

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Mol	Chain	Res	Type	Group
1	C	390	ARG	Sidechain
1	C	402	ARG	Sidechain
1	C	422	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	121	0
1	C	3466	0	3393	120	1
2	B	3370	0	3250	85	0
2	D	3343	0	3231	139	0
3	E	991	0	1012	27	1
4	F	2729	0	2715	92	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
8	C	59	58	58	15	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	2	0
All	All	17579	58	17109	577	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 17.

All (577) 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
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
1:A:317:LEU:HD21	1:A:377:MET:HE2	1.53	0.91
2:D:402:LYS:CG	2:D:405:LEU:HD13	2.03	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:402:LYS:CE	2:D:405:LEU:HD11	2.06	0.86
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
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: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:209:ILE:HD11	1:A:302:MET:HE3	1.67	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:137:VAL:HG21	1:A:154:MET:HE1	1.72	0.71
1:A:154:MET:HE2	1:A:154:MET:HA	1.72	0.71
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.71	0.71
2:D:166:MET:HE3	2:D:166:MET:HA	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
2:D:259:MET:HE2	2:D:259:MET:HA	1.73	0.70
2:D:319:PHE:HB3	2:D:323:MET:HE1	1.72	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
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.73	0.69
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
2:D:20:PHE:HB2	2:D:235:MET:HE3	1.76	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
2:D:259:MET:HE2	2:D:314:THR:HB	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.80	0.63
4:F:98:TYR:HA	4:F:127:GLU:OE2	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:C:88:HIS:CD2	1:C:90:GLU:HG3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:145:THR:N	9:D:501:GDP:O2B	2.37	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
1:C:75:ILE:HG22	1:C:79:ARG:NH1	2.19	0.56
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
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
2:D:188:THR:HG23	2:D:425:MET:HE3	1.88	0.55
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:30:ILE:HD12	2:B:30:ILE:N	2.23	0.54
1:C:151[A]:SER:HB2	1:C:193:THR:HG21	1.90	0.54
1:C:261:PRO:HG3	1:C:313:MET:HE2	1.90	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
4:F:162:ILE:C	4:F:162:ILE:HD12	2.28	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
2:D:20:PHE:HB2	2:D:235:MET:HE1	1.90	0.53
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
3:E:105:MET:HE2	3:E:105:MET:HA	1.91	0.53
1:A:372[B]:GLN:OE1	1:A:373:ARG:NH1	2.42	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:C:214:ARG:HG2	1:C:219:ILE:O	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:285:GLN:HG3	1:A:372[B]:GLN:CD	2.30	0.52
2:D:166:MET:HA	2:D:166:MET:CE	2.40	0.52
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
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
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.93	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
1:A:317:LEU:CD2	1:A:377:MET:HE2	2.34	0.50
1:A:251:ASP:OD1	1:A:253:THR:HB	2.11	0.50
2:B:322:ARG:O	2:B:373:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:259:MET:HA	2:D:259:MET:CE	2.40	0.49
2:D:301:MET:HA	2:D:301:MET:HE2	1.92	0.49
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
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
1:A:123:ARG:HH22	1:A:160:ASP:HB3	1.76	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:D:416:MET:O	2:D:417:GLU:C	2.49	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
4:F:162:ILE:HD11	4:F:233:PHE:C	2.33	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
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
1:C:241:SER:HB2	1:C:250:VAL:O	2.13	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
1:C:377:MET:HE3	1:C:377:MET:HB3	1.83	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:284:ARG:O	2:B:284:ARG:HG3	2.14	0.48
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
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: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
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
2:B:191:VAL:HG11	2:B:425:MET:HE2	1.93	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: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
2:D:319:PHE:HB3	2:D:323:MET:HE3	1.95	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
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: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
1:A:204:VAL:HG13	1:A:302:MET:HE3	1.97	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
1:C:27:GLU:CD	1:C:320:ARG:HH22	2.19	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
1:C:313:MET:HE2	1:C:346:TRP:HH2	1.81	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
4:F:320:MET:HE1	10:F:404:HOH:O	2.15	0.46
2:B:172:MET:HE2	2:B:387:LEU:HD21	1.98	0.46
1:C:287:SER:H	1:C:290:GLU:CG	2.29	0.46
2:D:20:PHE:CE2	2:D:24:ILE:HD13	2.51	0.46
1:C:335:ILE:O	1:C:336:LYS:C	2.53	0.46
2:D:406:HIS:NE2	2:D:407:TRP:CD1	2.83	0.46
2:B:75:MET:O	2:B:76:ASP:C	2.54	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.98	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
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.41	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
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
1:C:287:SER:H	1:C:290:GLU:CD	2.21	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
4:F:320:MET:CE	10:F:404:HOH:O	2.65	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:385:GLN:HB2	2:D:429:VAL:HG13	1.98	0.44
2:B:1:MET:HE2	2:B:1:MET:HA	1.99	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
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
4:F:320:MET:HE2	4:F:330:ILE:HG13	1.99	0.44
1:A:322:ASP:HB3	1:A:373:ARG:HH21	1.83	0.44
2:D:402:LYS:HG2	2:D:402:LYS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:135:PHE:HB2	2:D:166:MET:HE3	2.00	0.43
2:D:404:PHE:C	2:D:406:HIS:H	2.22	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: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
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.01	0.43
1:C:335:ILE:HG22	1:C:341:ILE:HD11	2.00	0.43
2:D:104:ALA:HB2	2:D:413:MET:HE1	2.01	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
4:F:45:ASN:C	4:F:46:ARG:HG2	2.39	0.43
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.53	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
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:B:203:CYS:SG	2:B:267:PHE:HB3	2.59	0.43
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
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:TRP:CE3	1:A:425:MET:HE1	2.54	0.42
1:C:398:MET:HE3	2:D:347:ILE:HG23	2.00	0.42
1:C:399:TYR:O	1:C:402:ARG:HD3	2.19	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:285:GLN:CG	1:A:372[B]:GLN:CD	2.88	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
1:C:333:ALA:O	1:C:334:THR:C	2.57	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
4:F:271:LEU:C	4:F:273:ASP:H	2.22	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
2:B:387:LEU:C	2:B:387:LEU:HD23	2.40	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
4:F:298:ILE:C	4:F:300:PRO:HD2	2.40	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ALA:HB2	1:C:413:MET:HG3	2.02	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
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
1:C:430:LYS:O	1:C:434:GLU:HG3	2.19	0.41
2:D:404:PHE:C	2:D:406:HIS:N	2.74	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: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
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:308:ARG:C	1:C:310:GLY:H	2.25	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
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.56	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
2:B:287:THR:O	2:B:288:VAL:C	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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%)	34	69
1	C	445/440 (101%)	415 (93%)	27 (6%)	3 (1%)	22	61
2	B	428/431 (99%)	415 (97%)	13 (3%)	0	100	100
2	D	424/431 (98%)	402 (95%)	20 (5%)	2 (0%)	29	67
3	E	116/120 (97%)	113 (97%)	3 (3%)	0	100	100
4	F	323/331 (98%)	295 (91%)	26 (8%)	2 (1%)	25	64
All	All	2182/2193 (100%)	2066 (95%)	107 (5%)	9 (0%)	34	69

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	41	THR
1	C	284	GLU
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/371 (102%)	375 (99%)	3 (1%)	81	93
1	C	378/371 (102%)	364 (96%)	14 (4%)	34	68
2	B	369/372 (99%)	364 (99%)	5 (1%)	67	86
2	D	369/372 (99%)	366 (99%)	3 (1%)	81	93
3	E	108/108 (100%)	106 (98%)	2 (2%)	57	81
4	F	303/299 (101%)	292 (96%)	11 (4%)	35	69
All	All	1905/1893 (101%)	1867 (98%)	38 (2%)	57	80

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

Mol	Chain	Res	Type
1	A	71	GLU
1	A	124	LYS
1	A	285	GLN
1	C	71	GLU
1	C	242	LEU
1	C	280	LYS
1	C	301	GLN
1	C	302	MET
1	C	307	PRO
1	C	317	LEU
1	C	325	PRO
1	C	349	THR
1	C	363[A]	VAL
1	C	363[B]	VAL
1	C	377	MET
1	C	391	LEU
1	C	439	SER
2	D	75	MET
2	D	229	HIS
2	D	405	LEU
3	E	61	ARG
3	E	106	GLU

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Mol	Chain	Res	Type
4	F	160	ILE
4	F	161	LEU
4	F	222	ARG
4	F	230	SER
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	2	ARG
2	B	71	GLU
2	B	77	SER
2	B	139	HIS
2	B	284	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	88	HIS
1	C	256	GLN
1	C	329	ASN
1	C	342	GLN
2	D	349	ASN
4	F	229	ASN
4	F	232	ASN
4	F	234	GLN
4	F	260	ASN
2	B	8	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
9	GDP	D	501	-	24,30,30	0.90	1 (4%)	30,47,47	1.16	4 (13%)
5	GTP	A	501	6	26,34,34	0.99	3 (11%)	32,54,54	0.71	0
9	GDP	B	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.03	2 (6%)
8	VLB	C	501	-	63,67,67	4.03	24 (38%)	79,108,108	2.76	36 (45%)
5	GTP	C	502	6	26,34,34	1.01	3 (11%)	32,54,54	0.73	1 (3%)

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
9	GDP	D	501	-	-	3/12/32/32	0/3/3/3
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
9	GDP	B	501	-	-	2/12/32/32	0/3/3/3
8	VLB	C	501	-	-	12/38/131/131	0/7/9/9
5	GTP	C	502	6	-	7/18/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	501	VLB	C68-C73	25.35	1.74	1.53
8	C	501	VLB	C58-C59	-8.42	1.37	1.52
8	C	501	VLB	C57-N56	6.44	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	501	VLB	O75-C76	-5.51	1.32	1.45
8	C	501	VLB	O32-C33	-5.13	1.27	1.42
8	C	501	VLB	C68-C15	-3.94	1.40	1.54
8	C	501	VLB	O25-C26	-3.77	1.36	1.45
8	C	501	VLB	C5-C6	-3.73	1.44	1.51
8	C	501	VLB	C68-C67	-3.66	1.50	1.53
8	C	501	VLB	C69-N56	3.17	1.52	1.46
8	C	501	VLB	C20-C5	-3.17	1.50	1.55
8	C	501	VLB	C70-C54	3.05	1.58	1.53
8	C	501	VLB	O28-C4	-2.94	1.38	1.44
8	C	501	VLB	C69-C52	2.93	1.56	1.52
8	C	501	VLB	C57-C58	-2.90	1.44	1.52
8	C	501	VLB	C21-C20	2.75	1.63	1.51
5	C	502	GTP	C5-C6	-2.69	1.41	1.47
5	A	501	GTP	C5-C6	-2.67	1.42	1.47
9	B	501	GDP	C6-N1	-2.65	1.33	1.37
8	C	501	VLB	O74-C73	2.63	1.26	1.20
8	C	501	VLB	C19-N9	2.58	1.51	1.47
8	C	501	VLB	O75-C73	2.43	1.37	1.33
8	C	501	VLB	C14-C13	-2.32	1.36	1.39
8	C	501	VLB	O27-C3	-2.31	1.38	1.42
9	D	501	GDP	C6-N1	-2.27	1.34	1.37
8	C	501	VLB	C59-C67	-2.17	1.36	1.39
5	A	501	GTP	C8-N7	-2.13	1.31	1.35
5	C	502	GTP	C8-N7	-2.13	1.31	1.35
8	C	501	VLB	C60-C65	-2.06	1.37	1.42
5	C	502	GTP	C5-C4	-2.04	1.37	1.43
8	C	501	VLB	C51-C68	2.01	1.58	1.56
5	A	501	GTP	C5-C4	-2.00	1.38	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	501	VLB	O32-C16-C15	7.16	123.91	116.58
8	C	501	VLB	O25-C23-C3	7.07	124.10	112.22
8	C	501	VLB	O72-C54-C70	-5.59	99.11	108.75
8	C	501	VLB	C3-C2-N1	-5.58	105.13	112.81
8	C	501	VLB	O75-C73-C68	5.47	119.54	111.32
8	C	501	VLB	C33-O32-C16	-5.25	109.60	117.53
8	C	501	VLB	C22-N1-C2	-4.86	107.35	119.21
8	C	501	VLB	C22-N1-C18	-4.86	105.32	120.84
8	C	501	VLB	O32-C16-C17	-4.76	115.93	124.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	501	VLB	C58-C57-N56	4.56	123.62	113.44
8	C	501	VLB	C57-C58-C59	4.42	122.65	114.30
8	C	501	VLB	O75-C73-O74	-4.34	116.33	123.93
8	C	501	VLB	O24-C23-C3	-3.88	117.91	123.94
8	C	501	VLB	C19-C5-C6	3.84	112.21	108.28
8	C	501	VLB	C13-C18-N1	3.83	115.33	110.98
8	C	501	VLB	O28-C29-C30	3.53	117.58	111.09
8	C	501	VLB	C17-C18-N1	-3.53	122.69	127.61
8	C	501	VLB	O25-C23-O24	-3.39	117.99	123.93
8	C	501	VLB	C18-N1-C2	-3.33	104.57	109.03
8	C	501	VLB	C63-C64-C65	-3.30	115.34	120.08
8	C	501	VLB	C52-C69-N56	3.28	116.42	111.28
8	C	501	VLB	C62-C61-C60	-3.15	116.52	120.89
8	C	501	VLB	C14-C15-C16	2.89	120.91	116.78
8	C	501	VLB	C8-N9-C19	-2.87	104.99	112.50
8	C	501	VLB	C4-C3-C2	-2.62	103.84	109.23
8	C	501	VLB	C76-O75-C73	-2.54	111.65	115.94
8	C	501	VLB	C53-C54-C55	2.48	112.33	109.29
8	C	501	VLB	C69-N56-C55	-2.47	108.06	111.01
9	B	501	GDP	C8-N7-C5	2.44	107.64	102.99
9	D	501	GDP	C3'-C2'-C1'	2.38	104.57	100.98
8	C	501	VLB	C4-O28-C29	-2.38	113.98	117.65
8	C	501	VLB	C7-C8-N9	-2.33	105.47	111.03
8	C	501	VLB	C17-C16-C15	-2.25	120.13	122.20
9	D	501	GDP	C5-C6-N1	2.25	117.92	113.95
9	D	501	GDP	O3B-PB-O3A	2.21	112.05	104.64
9	D	501	GDP	C8-N7-C5	2.19	107.16	102.99
8	C	501	VLB	C61-C60-C65	2.17	121.05	118.17
8	C	501	VLB	C54-C53-C52	2.16	116.37	110.02
8	C	501	VLB	O28-C29-O31	-2.10	118.80	122.96
8	C	501	VLB	C53-C52-C69	2.08	111.15	108.72
9	B	501	GDP	PA-O3A-PB	-2.05	125.80	132.83
5	C	502	GTP	O6-C6-C5	2.03	128.34	124.37
8	C	501	VLB	C4-C3-C23	2.01	115.98	110.85

There are no chirality outliers.

All (29) 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-O1A
5	C	502	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
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-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
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
9	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	502	GTP	C5'-O5'-PA-O2A
5	C	502	GTP	C4'-C5'-O5'-PA
8	C	501	VLB	C58-C57-N56-C55
8	C	501	VLB	C15-C68-C73-O75
8	C	501	VLB	C15-C68-C73-O74
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C3'-C4'-C5'-O5'
5	C	502	GTP	PB-O3A-PA-O2A
8	C	501	VLB	C21-C20-C5-C4

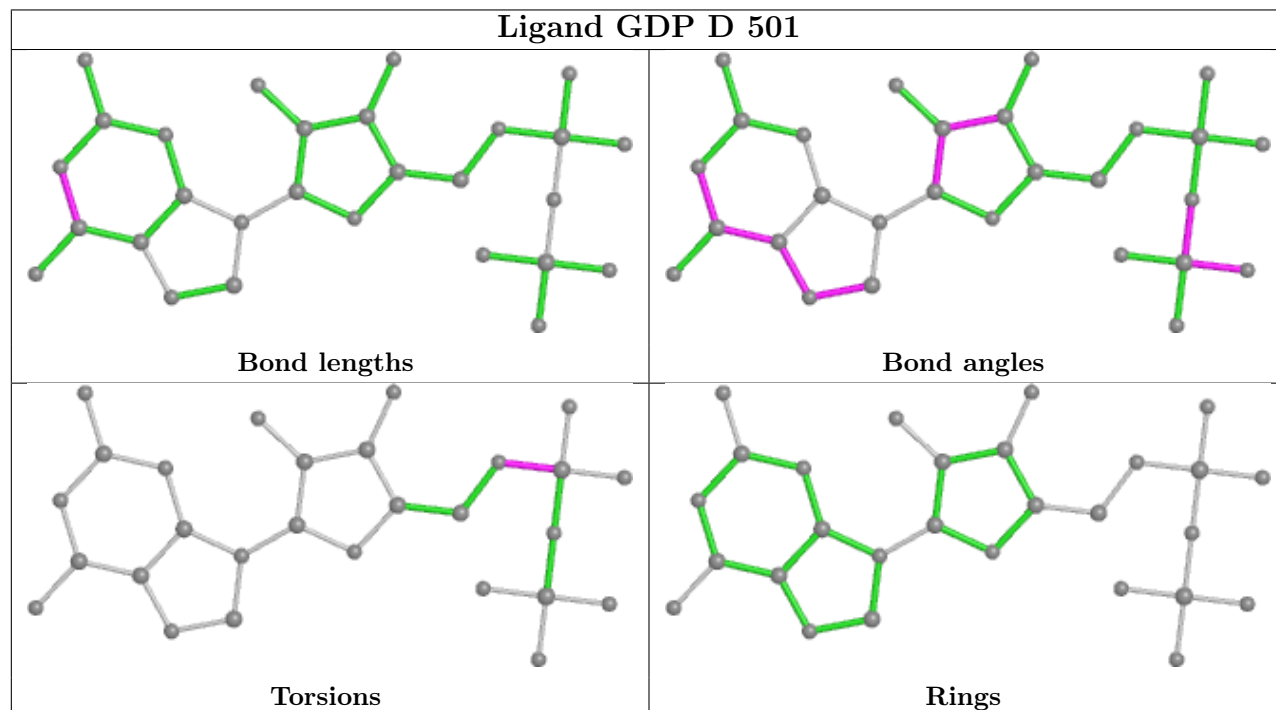
There are no ring outliers.

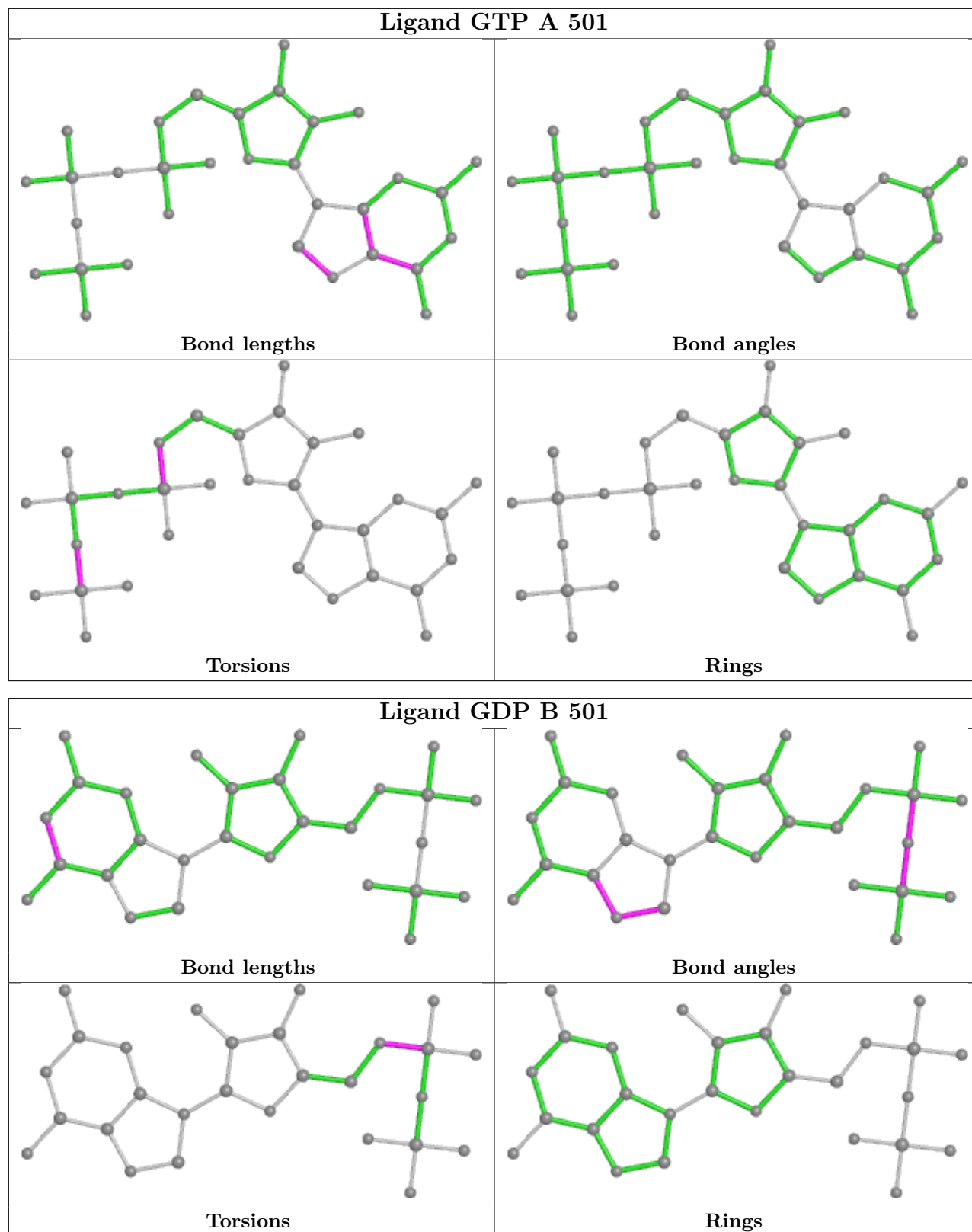
4 monomers are involved in 20 short contacts:

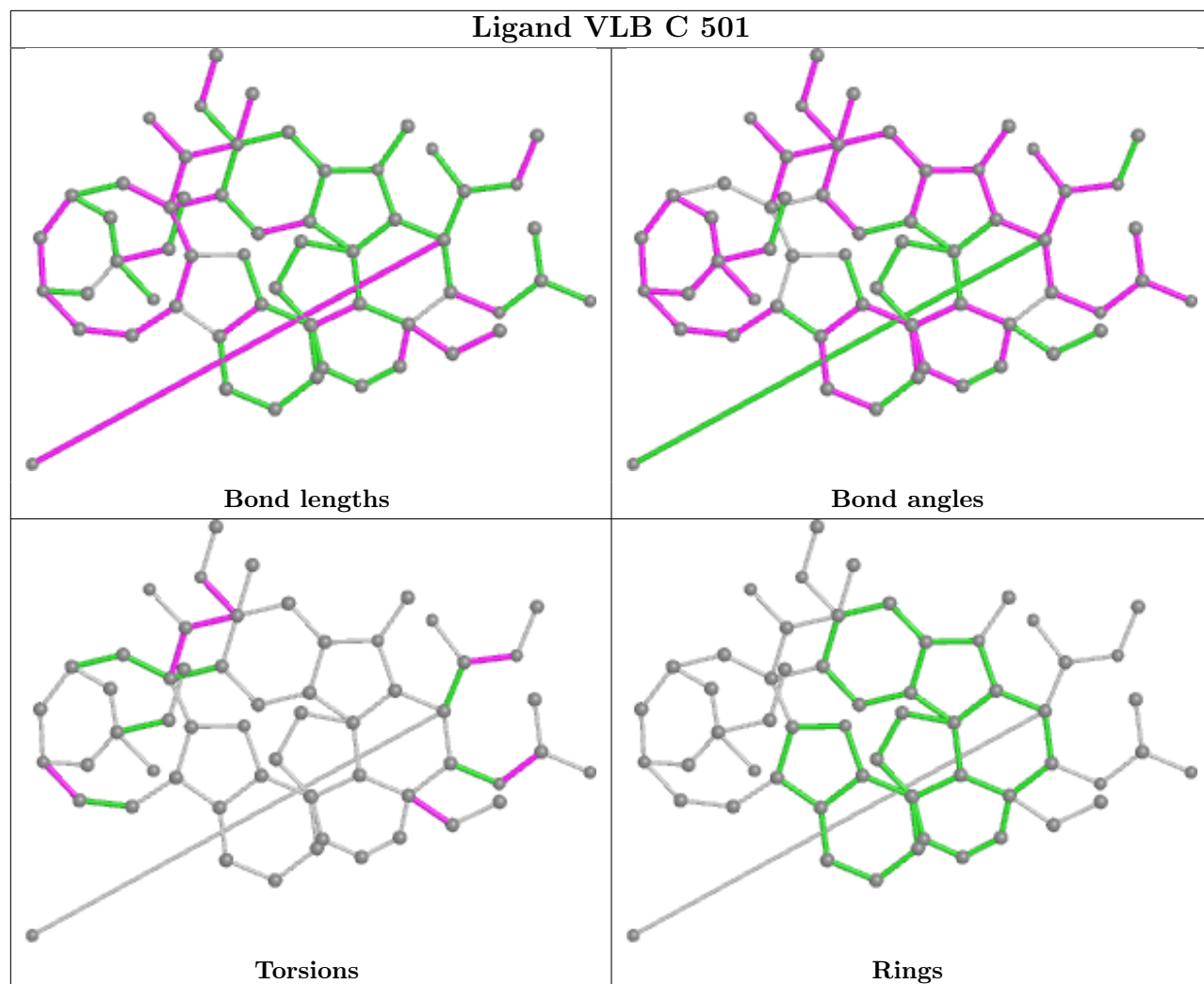
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	3	0
9	B	501	GDP	1	0
8	C	501	VLB	15	0
5	C	502	GTP	1	0

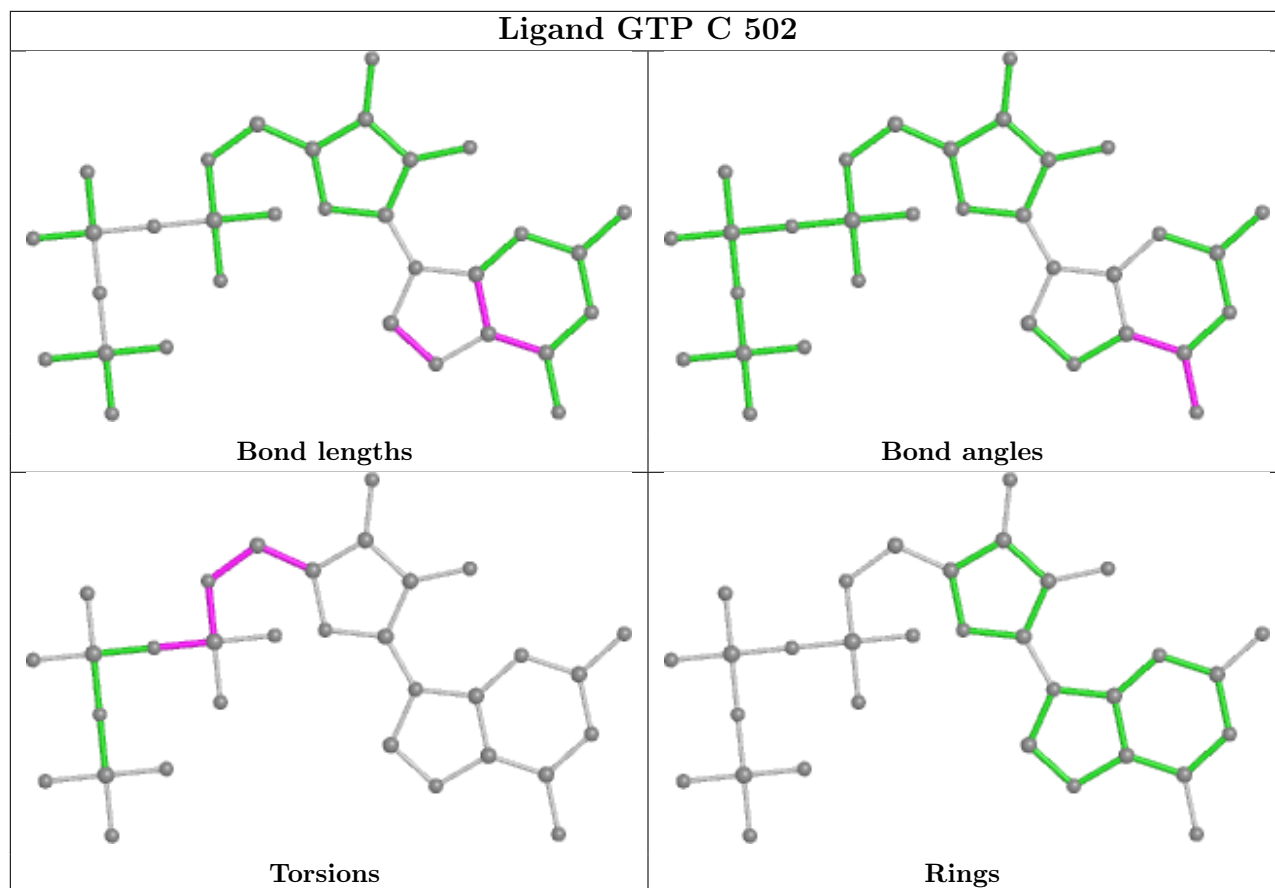
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	137:ARG	C	144:GLY	N	7.47

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.38	4 (0%) 84 75	36, 65, 112, 259	0
1	C	440/440 (100%)	-0.49	2 (0%) 91 86	24, 50, 88, 226	0
2	B	428/431 (99%)	-0.46	2 (0%) 91 86	24, 54, 97, 150	4 (0%)
2	D	424/431 (98%)	-0.14	14 (3%) 46 30	41, 82, 130, 180	1 (0%)
3	E	120/120 (100%)	0.02	4 (3%) 46 30	47, 82, 130, 153	0
4	F	331/331 (100%)	0.26	31 (9%) 8 4	51, 97, 172, 212	0
All	All	2182/2193 (99%)	-0.25	57 (2%) 56 40	24, 68, 134, 259	5 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	175	GLU	8.8
1	A	439	SER	7.3
4	F	238	CYS	6.5
4	F	257	GLU	5.6
4	F	232	ASN	5.3
4	F	372	THR	5.0
4	F	102	PRO	4.6
4	F	231	ALA	4.4
2	D	56	ALA	4.0
4	F	167	SER	4.0
4	F	248	GLU	4.0
3	E	138	GLU	3.9
4	F	176	GLN	3.9
2	D	415	GLU	3.7
2	D	179	ASP	3.6
3	E	103	GLN	3.4
4	F	174	ASP	3.3
4	F	168	GLU	3.2
4	F	125	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	441	ASP	3.1
2	D	285	ALA	3.0
4	F	171	ASP	3.0
4	F	133	ALA	3.0
4	F	234	GLN	2.9
2	D	55	GLU	2.9
4	F	83	THR	2.9
2	B	80	SER	2.9
2	D	11	GLN	2.8
4	F	323	GLU	2.8
4	F	136	ASN	2.8
2	D	218	LYS	2.8
4	F	89	GLU	2.7
4	F	145	ASN	2.7
4	F	340	GLN	2.7
4	F	173	ILE	2.7
4	F	250	SER	2.7
1	A	438	ASP	2.6
2	D	82	PRO	2.6
2	B	57	THR	2.5
2	D	284	ARG	2.5
2	D	416	MET	2.4
4	F	235	ASP	2.3
4	F	244	CYS	2.3
4	F	356	SER	2.2
1	C	337	THR	2.2
4	F	159	GLY	2.2
1	C	283	HIS	2.2
1	A	280	LYS	2.2
4	F	333	ASN	2.2
3	E	140	LYS	2.2
4	F	225	SER	2.2
4	F	239	HIS	2.1
2	D	116	ASP	2.1
2	D	38	GLY	2.1
1	A	281	ALA	2.1
2	D	85	GLN	2.0
3	E	128	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

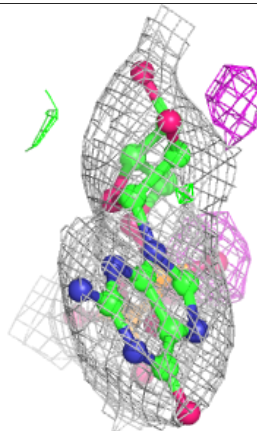
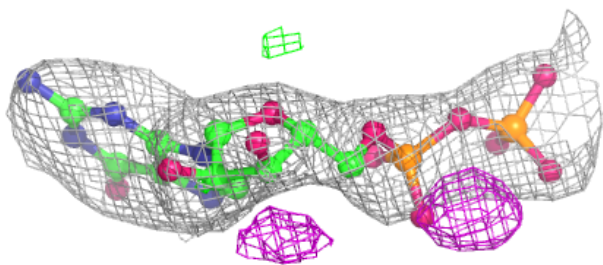
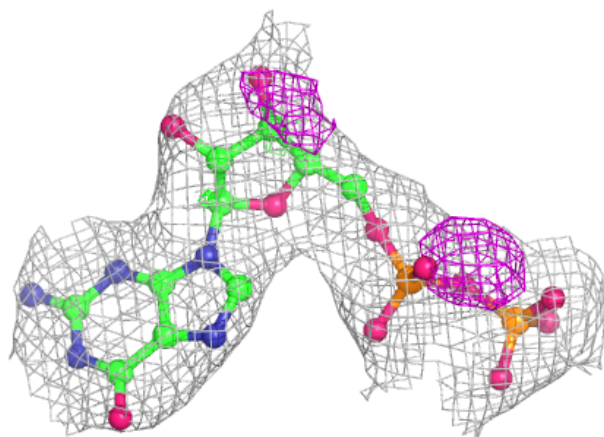
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.89	0.16	74,78,89,101	0
8	VLB	C	501	59/59	0.91	0.15	38,47,55,59	0
6	MG	C	503	1/1	0.91	0.40	41,41,41,41	0
6	MG	A	502	1/1	0.92	0.29	45,45,45,45	0
5	GTP	A	501	32/32	0.94	0.17	49,51,55,55	0
7	CA	C	504	1/1	0.95	0.17	30,30,30,30	0
5	GTP	C	502	32/32	0.95	0.14	41,45,48,48	0
7	CA	A	503	1/1	0.95	0.08	91,91,91,91	0
9	GDP	B	501	28/28	0.95	0.13	36,41,43,44	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.

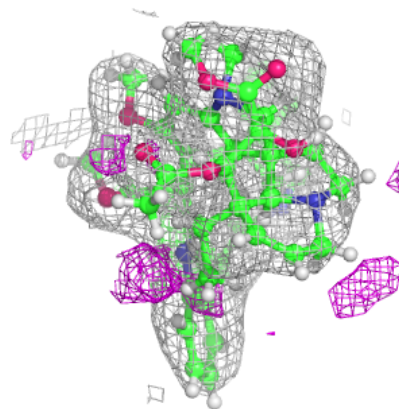
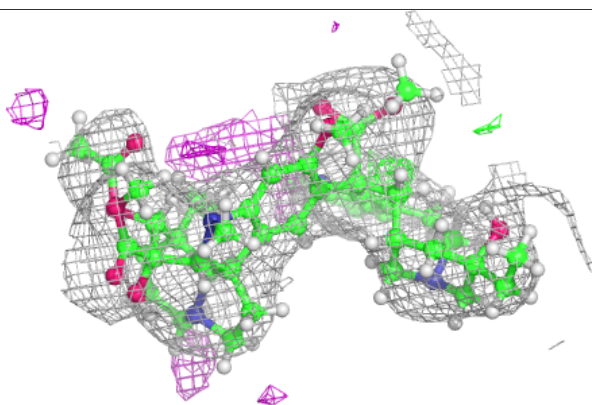
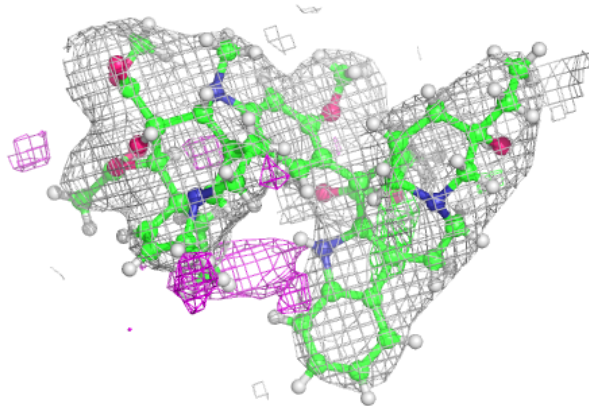
Electron density around GDP D 501:

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



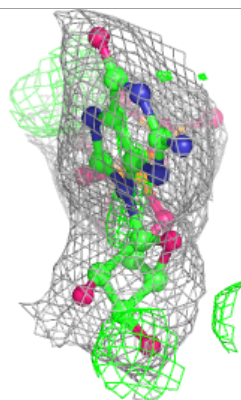
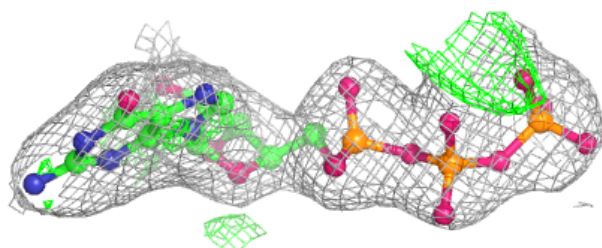
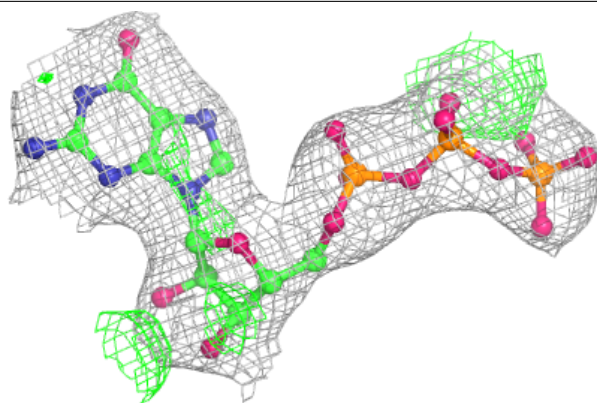
Electron density around VLB C 501:

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

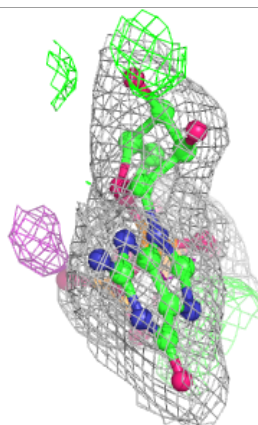
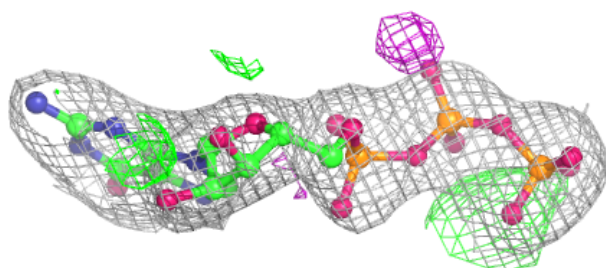
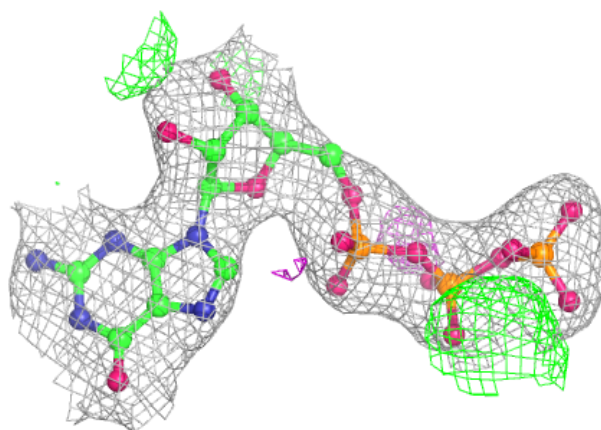


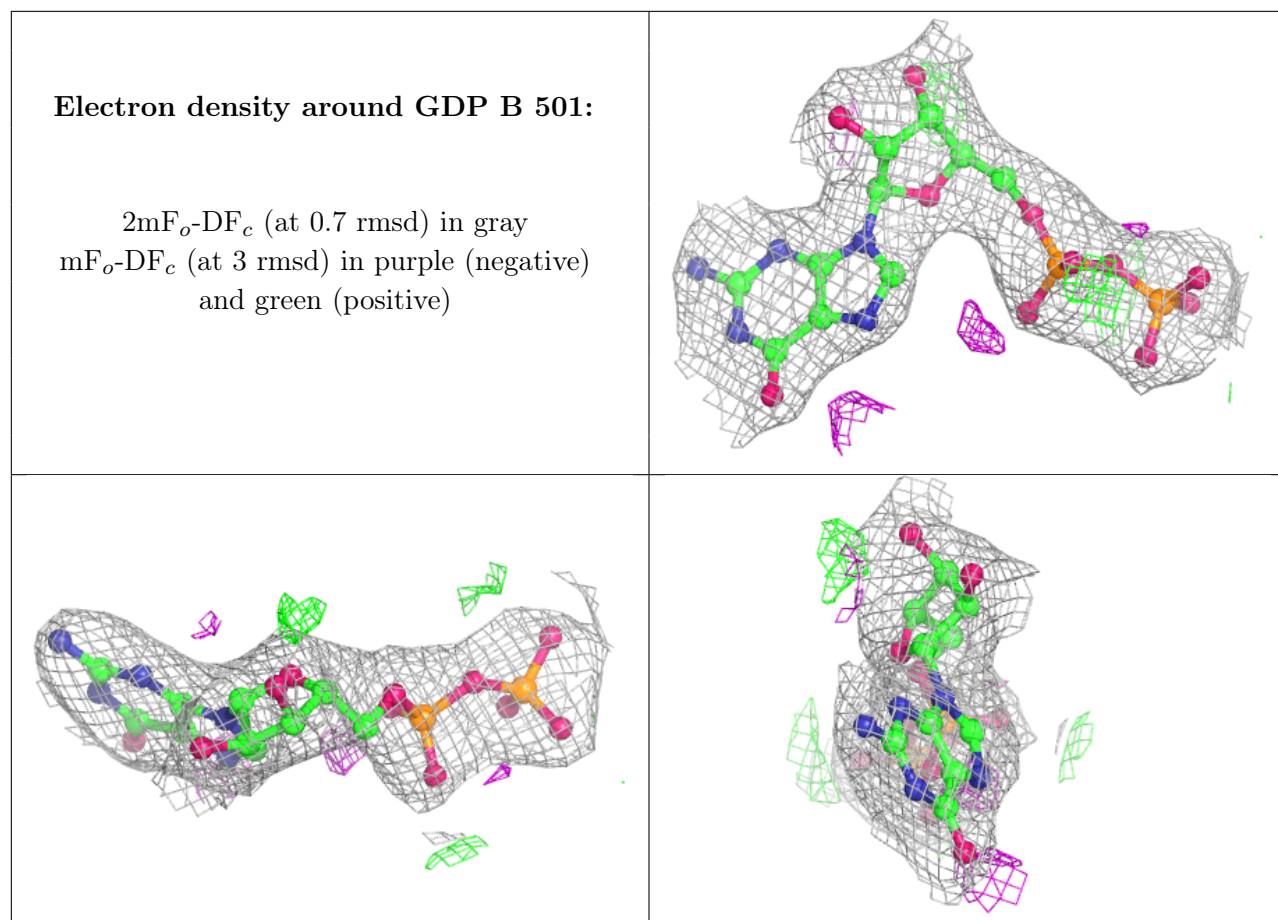
Electron density around GTP A 501:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.