



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 9LNX / pdb_00009lnx
Title : Crystal structure of T2R-TTL-YQVB9 Complex
Authors : Wu, C.Y.; Wang, Y.X.; Chen, Q.F.
Deposited on : 2025-01-22
Resolution : 2.59 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:

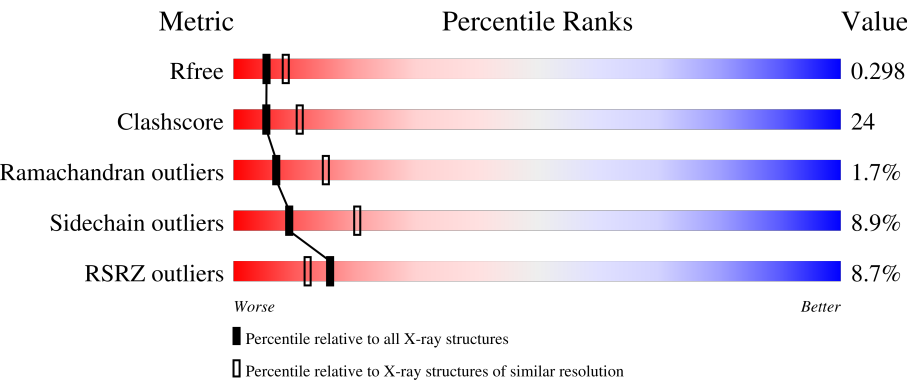
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	450	3% 60% 32% 5%
1	C	450	5% 66% 28% 5%
2	B	445	4% 60% 33%
2	D	445	15% 44% 44% 7% 5%
3	E	143	13% 50% 28% 6% 16%

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Mol	Chain	Length	Quality of chain
4	F	384	15% 47% 32% 7% 14%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17618 atoms, of which 61 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	13	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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	424	Total	C	N	O	S	11	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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

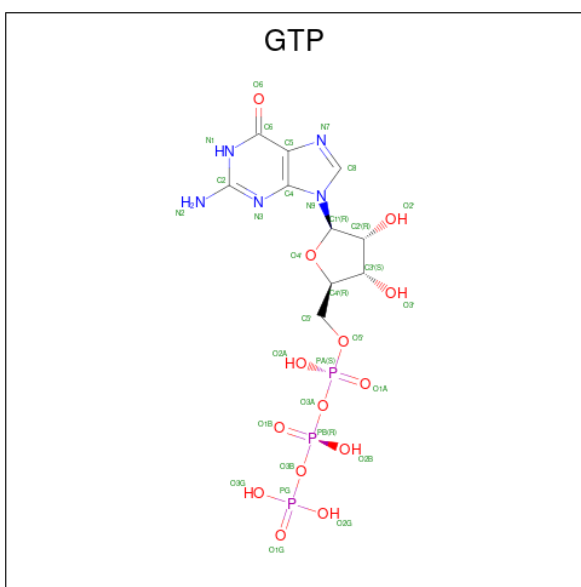
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	9	4	0
			2729	1762	457	496	14			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

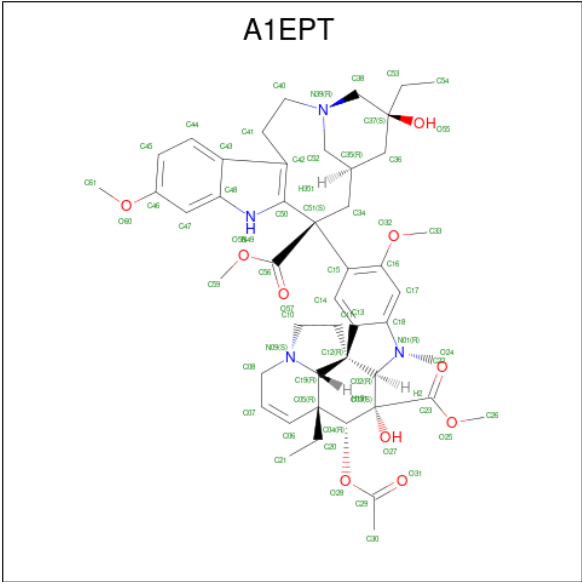
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

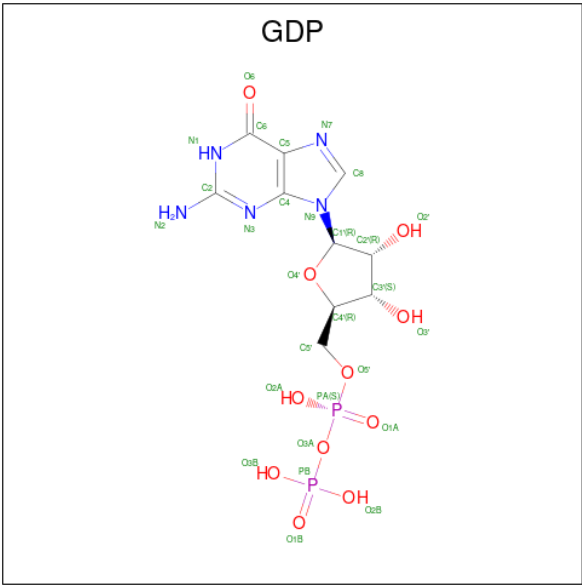
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	1	0
7	C	1	Total Ca 1 1	1	0

- Molecule 8 is 10'-methoxyvinblastine (CCD ID: A1EPT) (formula: $C_{47}H_{60}N_4O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	H	N	O	0	0
			122	47	61	4	10		

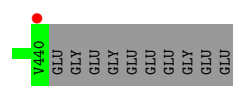
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 10 is water.

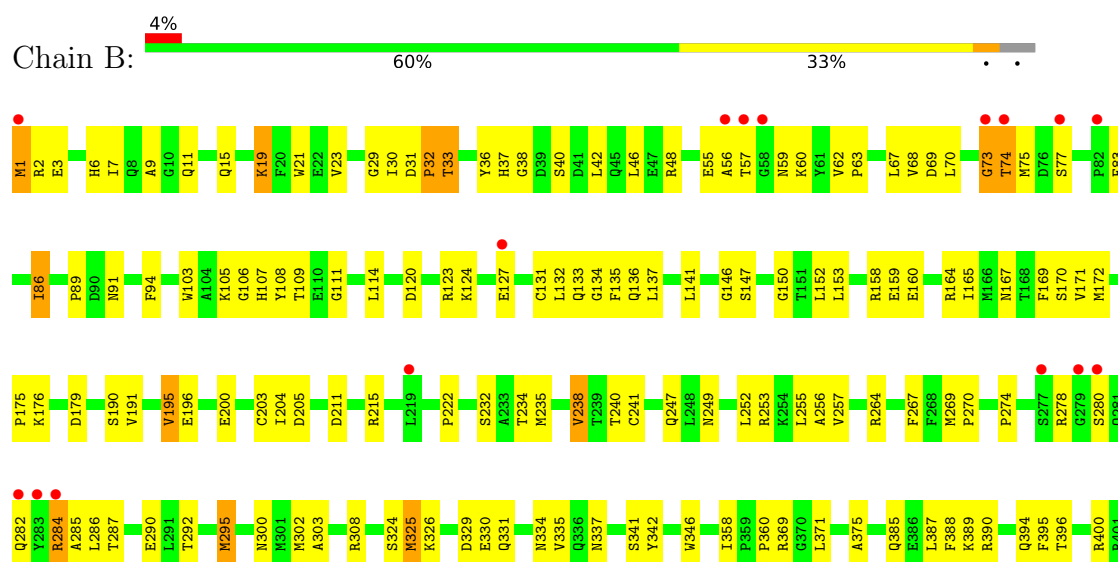
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	5	Total 5	O 5	0	0
10	B	3	Total 3	O 3	0	0

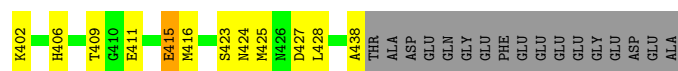


• Molecule 2: Tubulin beta chain

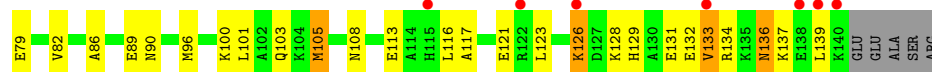
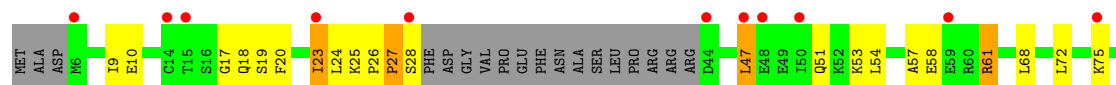


• Molecule 2: Tubulin beta chain

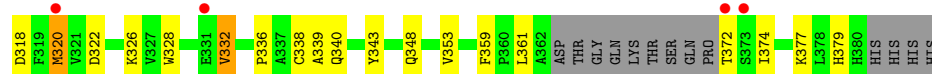
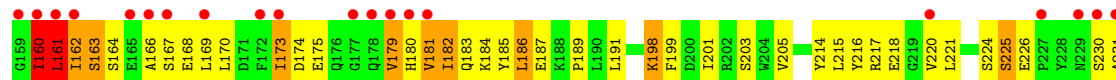
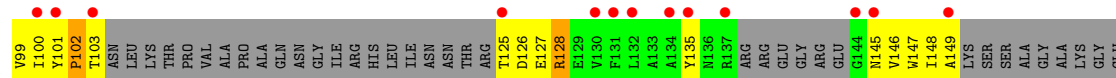
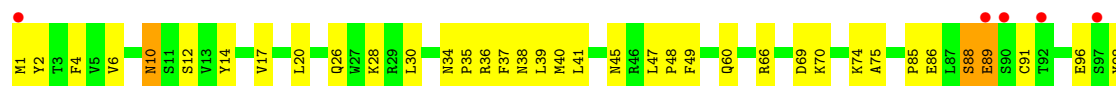




• Molecule 3: Stathmin-4



• 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	105.09Å 156.68Å 183.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.21 – 2.59 91.21 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.0 (91.21-2.59) 99.0 (91.21-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.58Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, R_{free}	0.226 , 0.296 0.230 , 0.298	Depositor DCC
R_{free} test set	4692 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17618	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: MG, A1EPT, GTP, GDP, CA

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	0.38	0/3571	0.57	0/4849
1	C	0.42	0/3565	0.59	0/4842
2	B	0.38	0/3451	0.57	0/4675
2	D	0.32	0/3428	0.50	0/4645
3	E	0.39	0/999	0.52	0/1325
4	F	0.32	0/2802	0.52	0/3789
All	All	0.37	0/17816	0.55	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	C	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	254	GLU	Peptide
2	D	57	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3465	0	3402	165	0
1	C	3466	0	3393	144	0
2	B	3370	0	3250	145	0
2	D	3343	0	3230	219	0
3	E	991	0	1012	48	0
4	F	2729	0	2715	135	0
5	A	32	0	12	0	0
5	C	32	0	12	0	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	61	61	0	16	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	3	0	0	1	0
10	C	5	0	0	5	0
All	All	17557	61	17050	824	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (824) 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)
8:C:504:A1EPT:C12	8:C:504:A1EPT:C02	1.84	1.41
2:D:135:PHE:HB2	2:D:166:MET:HE1	1.32	1.08
1:A:56:THR:HG22	1:A:60:LYS:H	1.13	1.04
1:A:209:ILE:HD11	1:A:302:MET:CE	1.89	1.03
8:C:504:A1EPT:C11	8:C:504:A1EPT:C10	1.80	1.03
2:B:1:MET:HE2	2:B:1:MET:HA	1.41	1.03
2:D:416:MET:HE2	2:D:416:MET:HA	1.40	1.02
3:E:9:ILE:HG22	3:E:10:GLU:HG2	1.39	1.01
2:D:259:MET:HE2	2:D:259:MET:HA	1.40	1.01
2:B:2:ARG:HD3	2:B:133:GLN:HG2	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:149:ALA:HB3	4:F:160:ILE:HB	1.41	0.98
2:D:295:MET:HE3	2:D:377:PHE:HB2	1.45	0.98
1:C:324:VAL:HG22	1:C:327:ASP:HB2	1.46	0.97
1:C:221:ARG:HG2	2:D:325:MET:HE3	1.43	0.96
2:D:20:PHE:HB2	2:D:235:MET:HE3	1.47	0.95
1:A:68[B]:VAL:HG23	1:A:93:ILE:HB	1.47	0.95
1:A:137:VAL:HG21	1:A:154:MET:CE	1.97	0.94
1:A:209:ILE:HD11	1:A:302:MET:HE1	1.49	0.93
2:D:20:PHE:HB2	2:D:235:MET:CE	1.98	0.93
2:B:172:MET:HE2	2:B:387:LEU:HD21	1.51	0.92
2:B:75:MET:HE2	2:B:94:PHE:HB3	1.54	0.88
1:A:72:PRO:HA	1:A:94:THR:HG21	1.53	0.88
2:D:135:PHE:HB2	2:D:166:MET:CE	2.04	0.87
2:D:209:LEU:HD12	2:D:230:LEU:HB2	1.57	0.86
2:D:166:MET:HE3	2:D:166:MET:HA	1.56	0.86
4:F:148:ILE:O	4:F:182:ILE:HD12	1.75	0.85
1:A:56:THR:HG22	1:A:60:LYS:N	1.90	0.85
1:A:225:THR:O	1:A:229:ARG:HG3	1.77	0.85
2:B:132:LEU:HB3	2:B:164:ARG:HH11	1.42	0.85
2:D:108:TYR:CD2	3:E:133:VAL:HG11	2.12	0.84
2:D:142:GLY:O	2:D:186:ASN:ND2	2.08	0.84
2:D:411:GLU:HA	3:E:137:LYS:HD2	1.57	0.84
1:A:209:ILE:HD11	1:A:302:MET:HE3	1.60	0.83
1:A:56:THR:CG2	1:A:60:LYS:HB3	2.08	0.83
1:A:137:VAL:HG21	1:A:154:MET:HE1	1.58	0.83
1:C:252:LEU:HD12	1:C:255:PHE:HB2	1.59	0.83
2:B:264:ARG:NH2	2:B:424:ASN:OD1	2.12	0.82
2:D:286:LEU:H	2:D:286:LEU:HD23	1.45	0.82
1:A:348:PRO:HB2	3:E:23:ILE:HD12	1.62	0.81
1:C:209:ILE:HD11	1:C:302:MET:SD	2.21	0.80
2:B:124:LYS:HA	2:B:127:GLU:HG2	1.63	0.80
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.16	0.80
1:C:313:MET:HE3	1:C:435:VAL:HB	1.64	0.80
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.64	0.80
1:C:324:VAL:HG22	1:C:327:ASP:CB	2.11	0.79
2:D:36:TYR:CE1	2:D:38:GLY:HA3	2.18	0.79
1:C:163:LYS:HG2	3:E:90:ASN:OD1	1.83	0.79
2:D:120:ASP:OD1	2:D:123:ARG:NH1	2.15	0.79
3:E:105:MET:HE2	3:E:105:MET:HA	1.64	0.78
8:C:504:A1EPT:C33	2:B:222:PRO:HD2	2.13	0.78
2:D:141:LEU:HD11	2:D:170:SER:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:320:ARG:HA	2:D:356:CYS:O	1.83	0.78
2:B:278:ARG:HD3	10:B:601:HOH:O	1.83	0.78
2:D:7:ILE:O	2:D:137:LEU:HD12	1.84	0.78
1:A:287:SER:OG	1:A:290:GLU:HG3	1.84	0.78
4:F:237:THR:O	4:F:246:GLN:NE2	2.17	0.78
1:A:56:THR:CG2	1:A:60:LYS:H	1.96	0.77
1:A:155:GLU:HA	1:A:197:HIS:CD2	2.20	0.77
2:D:217:LEU:HD21	2:D:276:THR:HA	1.67	0.77
4:F:147:TRP:CB	4:F:182:ILE:HD11	2.15	0.77
2:B:36:TYR:OH	2:B:40:SER:O	2.02	0.77
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.66	0.77
1:A:317:LEU:HD21	1:A:377:MET:HE2	1.68	0.76
2:B:73:GLY:O	2:B:75:MET:N	2.17	0.76
1:A:132:LEU:HD23	1:A:164:LYS:HE2	1.66	0.76
2:B:42:LEU:HD23	2:B:358:ILE:HD11	1.65	0.76
2:D:209:LEU:HB3	2:D:227:LEU:HD22	1.67	0.76
1:A:336:LYS:HG2	3:E:24:LEU:HD23	1.70	0.74
1:A:210:TYR:OH	1:A:221:ARG:HD2	1.88	0.74
1:A:285:GLN:HG2	1:A:372[B]:GLN:HG3	1.70	0.74
1:A:295:CYS:HB3	1:A:377:MET:HE3	1.70	0.74
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.68	0.74
1:A:336:LYS:HG2	3:E:24:LEU:CD2	2.18	0.74
1:C:275:VAL:HG13	1:C:368:LEU:HD11	1.68	0.73
2:D:180:THR:O	2:D:182:VAL:N	2.22	0.73
4:F:103:THR:HG22	4:F:174:ASP:OD1	1.88	0.73
4:F:225:SER:HB2	4:F:260:ASN:HD21	1.52	0.73
1:A:234:ILE:HD13	1:A:302:MET:CE	2.18	0.73
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.07	0.73
4:F:277[A]:THR:OG1	4:F:278:THR:N	2.18	0.73
2:B:215:ARG:HH11	2:B:215:ARG:HB3	1.53	0.73
1:C:101:ASN:OD1	2:D:254:LYS:HD3	1.89	0.73
3:E:136:ASN:HA	3:E:139:LEU:HD13	1.69	0.73
4:F:102:PRO:HB3	4:F:173:ILE:O	1.88	0.73
4:F:231:ALA:O	4:F:232:ASN:HB3	1.88	0.73
1:C:337:THR:O	1:C:338:LYS:HG2	1.88	0.72
1:C:356:ASN:HB3	10:C:602:HOH:O	1.88	0.72
4:F:244:CYS:SG	4:F:245:ILE:HG13	2.29	0.72
4:F:149:ALA:CB	4:F:160:ILE:HB	2.18	0.72
1:A:56:THR:HG21	1:A:60:LYS:HB3	1.72	0.72
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.70	0.72
2:B:29:GLY:O	2:B:36:TYR:HA	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.20	0.72
2:D:176:LYS:HB3	2:D:210:TYR:CE2	2.25	0.72
1:A:209:ILE:CD1	1:A:302:MET:HE1	2.20	0.71
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.71	0.71
2:D:79:ARG:HH22	2:D:94:PHE:HE2	1.36	0.71
2:D:287:THR:HG23	2:D:290:GLU:OE1	1.90	0.71
1:A:158:SER:OG	1:A:166:LYS:HE3	1.90	0.71
1:A:298:PRO:O	1:A:301:GLN:HG3	1.89	0.71
2:B:36:TYR:OH	2:B:38:GLY:HA3	1.89	0.71
2:B:123:ARG:NH1	2:B:160:GLU:OE2	2.23	0.71
4:F:148:ILE:HG12	4:F:149:ALA:H	1.55	0.71
2:B:191:VAL:CB	2:B:425:MET:HE3	2.21	0.71
4:F:147:TRP:HB3	4:F:182:ILE:HD11	1.72	0.70
2:B:326:LYS:HE2	2:B:330:GLU:OE2	1.90	0.70
2:D:153:LEU:O	2:D:157:ILE:HG13	1.91	0.70
1:A:88:HIS:O	1:A:91:GLN:HG3	1.91	0.70
1:C:328:VAL:HG21	8:C:504:A1EPT:O60	1.90	0.70
1:A:362:VAL:HG21	1:A:368:LEU:O	1.92	0.70
2:B:1:MET:HA	2:B:1:MET:CE	2.20	0.70
1:C:1:MET:O	1:C:2:ARG:NE	2.25	0.69
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.73	0.69
1:A:227:LEU:O	1:A:231:ILE:HG13	1.92	0.69
1:A:295:CYS:CB	1:A:377:MET:HE3	2.21	0.69
2:B:191:VAL:HB	2:B:425:MET:HE3	1.75	0.69
2:D:326:LYS:HE2	2:D:330:GLU:OE2	1.91	0.69
1:A:137:VAL:HG21	1:A:154:MET:HE3	1.75	0.69
1:A:68[B]:VAL:HG21	1:A:118:VAL:CG2	2.23	0.69
2:B:19:LYS:O	2:B:23:VAL:HG23	1.93	0.69
2:D:191:VAL:HG11	2:D:425:MET:HG3	1.74	0.69
4:F:304:THR:HG22	4:F:307:LEU:HD23	1.75	0.68
1:A:311:LYS:NZ	1:A:342:GLN:HG2	2.07	0.68
2:D:223:THR:HG22	2:D:226:ASP:OD2	1.93	0.68
2:D:223:THR:HG23	2:D:226:ASP:H	1.57	0.68
1:A:41:THR:OG1	1:A:44:GLY:O	2.12	0.68
2:D:12:CYS:HB3	2:D:140:SER:OG	1.94	0.68
1:A:311:LYS:HZ2	1:A:342:GLN:HG2	1.59	0.67
2:D:101:ASN:OD1	2:D:180:THR:HG21	1.93	0.67
2:B:132:LEU:HB3	2:B:164:ARG:NH1	2.08	0.67
2:B:36:TYR:C	2:B:37:HIS:HD1	2.03	0.67
4:F:280:GLU:HA	4:F:284[B]:LEU:HD12	1.77	0.67
2:B:29:GLY:C	2:B:30:ILE:HD12	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:262:MET:HE2	4:F:266:GLU:OE1	1.94	0.67
1:A:285:GLN:HG2	1:A:372[B]:GLN:OE1	1.96	0.66
2:D:119:LEU:O	2:D:123:ARG:HG3	1.96	0.66
3:E:126:LYS:HE2	3:E:126:LYS:HA	1.77	0.66
2:D:31:ASP:CG	2:D:33:THR:HG23	2.21	0.66
1:C:22:GLU:HG3	1:C:83:TYR:OH	1.97	0.65
2:D:34:GLY:O	2:D:60:LYS:HA	1.95	0.65
2:B:274:PRO:HB3	2:B:286:LEU:HD21	1.78	0.65
1:C:335:ILE:HG22	1:C:341:ILE:HD11	1.78	0.65
2:D:27:GLU:OE2	2:D:236:SER:OG	2.12	0.65
2:B:55:GLU:OE2	2:B:59:ASN:ND2	2.29	0.65
1:A:56:THR:HG22	1:A:60:LYS:HB3	1.77	0.65
2:D:287:THR:N	2:D:290:GLU:OE1	2.27	0.65
4:F:184:LYS:HE2	4:F:185:TYR:O	1.97	0.65
1:A:180:ALA:O	1:A:183:GLU:HG3	1.96	0.64
1:A:96:LYS:H	1:A:96:LYS:HD2	1.62	0.64
2:D:112:ALA:O	2:D:115:VAL:HG12	1.97	0.64
4:F:135:TYR:OH	4:F:164:SER:O	2.08	0.64
1:A:88:HIS:CE1	1:A:90:GLU:HB2	2.33	0.64
2:B:416:MET:HA	2:B:416:MET:HE2	1.78	0.64
1:A:88:HIS:N	1:A:91:GLN:OE1	2.25	0.64
1:A:68[B]:VAL:HG21	1:A:118:VAL:HG21	1.78	0.64
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.79	0.64
2:D:104:ALA:HB2	2:D:413:MET:HE3	1.80	0.64
4:F:170:LEU:HD23	4:F:173:ILE:HD11	1.80	0.64
2:D:20:PHE:HB2	2:D:235:MET:HE1	1.79	0.64
1:A:3:GLU:HG2	1:A:64:ARG:NH2	2.13	0.64
1:C:1:MET:HG3	1:C:131:GLY:HA3	1.79	0.64
2:D:119:LEU:HA	2:D:122:VAL:HG23	1.80	0.64
4:F:148:ILE:HG12	4:F:149:ALA:N	2.12	0.64
1:A:76:ASP:HA	1:A:79:ARG:HG3	1.80	0.63
2:D:83:PHE:O	2:D:86:ILE:HG22	1.97	0.63
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.33	0.63
1:C:301:GLN:NE2	1:C:307:PRO:HG2	2.13	0.63
2:D:297:ASP:OD2	2:D:299:LYS:HE3	1.98	0.63
2:B:124:LYS:HA	2:B:127:GLU:CG	2.28	0.63
1:A:335:ILE:C	1:A:335:ILE:HD12	2.22	0.63
1:C:298:PRO:HA	1:C:301:GLN:NE2	2.14	0.63
4:F:47:LEU:HD23	4:F:48:PRO:HD2	1.80	0.63
2:B:215:ARG:HB3	2:B:215:ARG:NH1	2.13	0.63
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:ARG:HG2	2:B:342:TYR:CZ	2.34	0.62
2:D:416:MET:HA	2:D:416:MET:CE	2.23	0.62
4:F:146:VAL:HG23	4:F:187:GLU:OE2	1.98	0.62
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.82	0.62
1:A:90:GLU:O	1:A:121:ARG:HD2	1.99	0.62
1:C:313:MET:HG2	1:C:346:TRP:CH2	2.35	0.62
2:D:73:GLY:HA2	2:D:76:ASP:CG	2.24	0.62
2:D:274:PRO:HB3	2:D:286:LEU:HD21	1.81	0.62
2:D:209:LEU:HD12	2:D:230:LEU:CB	2.28	0.62
4:F:163:SER:OG	4:F:164:SER:N	2.32	0.61
4:F:286:GLN:O	4:F:290:ILE:HG13	1.99	0.61
2:D:25:SER:HB3	2:D:30:ILE:HG22	1.82	0.61
2:B:31:ASP:O	2:B:33:THR:N	2.33	0.61
2:D:259:MET:HA	2:D:259:MET:CE	2.23	0.61
3:E:101:LEU:O	3:E:105:MET:HG2	2.00	0.61
2:B:284:ARG:HD2	2:B:285:ALA:O	2.00	0.61
4:F:160:ILE:HG12	4:F:161:LEU:N	2.16	0.61
4:F:186:LEU:HD22	4:F:320:MET:HE3	1.83	0.61
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.81	0.61
3:E:72:LEU:HD13	2:B:159:GLU:HB2	1.81	0.61
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.34	0.61
1:C:301:GLN:HE22	1:C:307:PRO:HG2	1.66	0.61
2:D:205:ASP:O	2:D:209:LEU:HD22	2.00	0.61
4:F:89:GLU:OE1	4:F:89:GLU:HA	1.95	0.61
2:B:48:ARG:NH2	2:B:241:CYS:O	2.33	0.61
1:C:190:THR:O	1:C:194[B]:THR:HG23	2.01	0.61
1:C:324:VAL:HG23	1:C:327:ASP:H	1.66	0.61
1:C:353:VAL:HG13	8:C:504:A1EPT:C61	2.31	0.61
2:B:331:GLN:O	2:B:335:VAL:HG23	2.01	0.61
2:D:181:VAL:O	2:D:398:MET:HE1	2.01	0.60
4:F:272:MET:HE3	4:F:278:THR:HG22	1.83	0.60
4:F:147:TRP:HB2	4:F:182:ILE:HD11	1.81	0.60
1:C:401:LYS:HD2	1:C:401:LYS:N	2.15	0.60
4:F:217:ARG:HG2	4:F:374:ILE:O	2.01	0.60
4:F:225:SER:H	4:F:246:GLN:HE22	1.50	0.60
2:D:210:TYR:CD1	2:D:222:PRO:HG3	2.36	0.60
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.36	0.60
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.36	0.60
4:F:199:PHE:CD2	4:F:221:LEU:HG	2.36	0.60
2:B:83:PHE:O	2:B:86:ILE:HG23	2.02	0.60
1:C:348:PRO:O	1:C:350:GLY:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:HIS:O	1:C:284:GLU:HB3	2.00	0.60
3:E:47:LEU:HD12	3:E:47:LEU:O	2.01	0.60
2:D:176:LYS:HB3	2:D:210:TYR:HE2	1.67	0.59
2:D:179:ASP:O	2:D:181:VAL:N	2.31	0.59
2:D:405:LEU:C	2:D:405:LEU:HD23	2.27	0.59
2:B:2:ARG:HA	2:B:131:CYS:O	2.02	0.59
1:A:48:SER:O	1:A:51[A]:THR:HG23	2.02	0.59
1:C:324:VAL:CG2	1:C:327:ASP:H	2.14	0.59
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.20	0.59
2:D:75:MET:HE2	2:D:94:PHE:CD2	2.37	0.59
1:C:18:ASN:OD1	1:C:78:VAL:HG22	2.03	0.59
4:F:100:ILE:O	4:F:179:VAL:HG23	2.03	0.58
2:D:36:TYR:CZ	2:D:38:GLY:HA3	2.37	0.58
2:D:123:ARG:O	2:D:127:GLU:HG2	2.03	0.58
2:B:31:ASP:C	2:B:33:THR:H	2.10	0.58
2:D:104:ALA:HB2	2:D:413:MET:CE	2.33	0.58
1:C:108:TYR:CD2	3:E:105:MET:HE1	2.38	0.58
2:D:119:LEU:HA	2:D:122:VAL:CG2	2.33	0.58
2:B:2:ARG:NH1	2:B:133:GLN:HA	2.19	0.58
2:B:141:LEU:HD11	2:B:170:SER:HB3	1.86	0.58
2:D:259:MET:CE	2:D:314:THR:HB	2.33	0.58
4:F:20:LEU:HD22	4:F:348:GLN:OE1	2.04	0.58
1:C:238:ILE:HG23	1:C:252:LEU:HD22	1.86	0.58
3:E:126:LYS:HA	3:E:126:LYS:CE	2.34	0.58
1:C:180:ALA:O	1:C:183:GLU:HG3	2.04	0.58
2:D:29:GLY:O	2:D:36:TYR:HA	2.04	0.57
3:E:47:LEU:O	3:E:51:GLN:HG2	2.04	0.57
2:B:120:ASP:OD1	2:B:123:ARG:NH2	2.37	0.57
1:A:10:GLY:O	1:A:14:VAL:HG23	2.04	0.57
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.86	0.57
1:C:313:MET:HG2	1:C:346:TRP:CZ2	2.39	0.57
1:A:96:LYS:HE2	1:A:113:GLU:OE2	2.05	0.57
8:C:504:A1EPT:C02	8:C:504:A1EPT:C19	2.71	0.57
2:D:223:THR:HG22	2:D:226:ASP:CG	2.30	0.57
1:C:401:LYS:NZ	2:D:439:THR:O	2.32	0.57
1:A:311:LYS:HG3	1:A:436:GLY:HA2	1.87	0.57
1:C:400:ALA:C	1:C:401:LYS:HD2	2.29	0.57
2:D:39:ASP:N	2:D:39:ASP:OD1	2.36	0.57
4:F:89:GLU:C	4:F:91:CYS:H	2.13	0.57
4:F:245:ILE:HG22	4:F:245:ILE:O	2.05	0.57
1:C:271:THR:HG23	1:C:300:ASN:C	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:OG1	1:A:41:THR:O	2.23	0.56
1:C:301:GLN:HE22	1:C:307:PRO:CD	2.18	0.56
3:E:9:ILE:HG22	3:E:10:GLU:N	2.20	0.56
3:E:129:HIS:HA	3:E:132:GLU:OE1	2.04	0.56
1:C:317:LEU:C	1:C:318:LEU:HD12	2.31	0.56
2:D:30:ILE:HA	2:D:35:SER:O	2.05	0.56
2:D:32:PRO:HB3	2:D:83:PHE:HA	1.87	0.56
2:D:118:VAL:O	2:D:122:VAL:HG23	2.05	0.56
3:E:75:LYS:O	3:E:79:GLU:HG3	2.05	0.56
3:E:126:LYS:HE2	3:E:126:LYS:CA	2.36	0.56
2:B:38:GLY:C	2:B:40:SER:H	2.13	0.56
2:D:67:LEU:N	2:D:67:LEU:HD12	2.20	0.56
4:F:199:PHE:HD2	4:F:221:LEU:HG	1.70	0.56
2:D:294:GLN:O	2:D:297:ASP:HB3	2.05	0.56
1:A:34:GLY:HA3	1:A:60:LYS:HD3	1.86	0.56
1:C:221:ARG:HG3	1:C:221:ARG:HH11	1.69	0.56
2:B:191:VAL:HG11	2:B:425:MET:HE3	1.87	0.56
1:A:34:GLY:O	1:A:61:HIS:N	2.34	0.56
1:C:335:ILE:CG2	1:C:341:ILE:HD11	2.35	0.56
4:F:74:LYS:HB3	4:F:181:VAL:HG11	1.88	0.56
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.41	0.56
2:D:75:MET:HE3	2:D:92:PHE:HD2	1.70	0.56
2:B:195:VAL:HG11	2:B:424:ASN:HD21	1.72	0.55
1:C:252:LEU:C	1:C:254:GLU:H	2.13	0.55
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.06	0.55
2:D:191:VAL:O	2:D:195:VAL:HG23	2.06	0.55
4:F:377:LYS:HG2	4:F:379:HIS:CD2	2.41	0.55
2:B:123:ARG:O	2:B:127:GLU:HG2	2.07	0.55
2:B:191:VAL:HG21	2:B:425:MET:CE	2.35	0.55
1:A:285:GLN:HG2	1:A:372[B]:GLN:CG	2.36	0.55
2:D:65:ALA:C	2:D:66:ILE:HD12	2.31	0.55
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.40	0.55
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.87	0.55
1:A:340:SER:C	1:A:341:ILE:HD12	2.31	0.55
1:C:63:PRO:HG2	1:C:87:PHE:CE2	2.42	0.55
4:F:269:GLN:HA	4:F:272:MET:HG3	1.87	0.55
2:B:191:VAL:CG1	2:B:425:MET:HE3	2.36	0.55
4:F:163:SER:HB3	4:F:169:LEU:HD21	1.88	0.55
1:A:339:ARG:HB3	1:A:341:ILE:CD1	2.38	0.54
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.41	0.54
4:F:4:PHE:HE1	4:F:6:VAL:HG23	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:162:ILE:HD12	4:F:163:SER:N	2.21	0.54
2:B:195:VAL:HG11	2:B:424:ASN:ND2	2.22	0.54
1:A:187:SER:CB	1:A:391:LEU:HD21	2.36	0.54
2:D:161:TYR:HB3	2:D:164:ARG:HG3	1.90	0.54
1:A:33:ASP:O	1:A:60:LYS:HD3	2.07	0.54
1:C:301:GLN:HE22	1:C:307:PRO:CG	2.20	0.54
2:D:192:HIS:CE1	2:D:424:ASN:HD22	2.24	0.54
1:C:27:GLU:CD	1:C:320:ARG:HH22	2.15	0.54
2:D:105:LYS:HE2	2:D:110:GLU:OE1	2.07	0.54
2:D:217:LEU:HD11	2:D:276:THR:O	2.07	0.54
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.43	0.54
2:B:11:GLN:HG3	2:B:74:THR:CG2	2.38	0.54
1:A:409:VAL:HA	1:A:413:MET:O	2.07	0.54
1:C:108:TYR:O	1:C:112:LYS:HG2	2.07	0.54
2:D:135:PHE:CB	2:D:166:MET:HE1	2.22	0.54
3:E:26:PRO:HB2	3:E:27:PRO:HD2	1.89	0.54
2:D:159:GLU:HG3	3:E:123:LEU:HD13	1.89	0.54
1:A:231:ILE:O	1:A:235:VAL:HG23	2.07	0.54
2:D:223:THR:HG23	2:D:226:ASP:N	2.23	0.54
2:D:387:LEU:HD23	2:D:387:LEU:C	2.32	0.54
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.89	0.54
1:C:335:ILE:HG22	1:C:341:ILE:CD1	2.38	0.54
3:E:96:MET:HE3	3:E:96:MET:HA	1.90	0.54
2:D:295:MET:SD	2:D:375:ALA:HB1	2.48	0.53
4:F:244:CYS:O	4:F:246:GLN:N	2.38	0.53
4:F:244:CYS:C	4:F:246:GLN:H	2.16	0.53
1:A:348:PRO:CB	3:E:23:ILE:HD12	2.36	0.53
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.43	0.53
2:B:402:LYS:HE2	2:B:415:GLU:OE1	2.08	0.53
4:F:86:GLU:CD	4:F:86:GLU:H	2.16	0.53
1:A:76:ASP:OD1	1:A:79:ARG:HD2	2.09	0.53
1:A:296:PHE:CE2	1:A:377:MET:HE1	2.44	0.53
1:A:72:PRO:HA	1:A:94:THR:CG2	2.33	0.53
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.73	0.53
2:D:141:LEU:HD22	2:D:172:MET:SD	2.49	0.53
4:F:160:ILE:HD13	4:F:160:ILE:H	1.73	0.53
1:A:39:ASP:OD1	1:A:41:THR:N	2.42	0.53
1:A:83:TYR:HD2	1:A:86:LEU:HD22	1.74	0.53
1:A:298:PRO:HA	1:A:301:GLN:CD	2.34	0.53
1:C:1:MET:C	1:C:2:ARG:HG3	2.34	0.53
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:192:HIS:ND1	2:D:421:ALA:HA	2.24	0.53
1:A:412:GLY:HA3	3:E:57:ALA:HB1	1.92	0.52
1:C:313:MET:HE1	1:C:435:VAL:HG21	1.92	0.52
2:D:259:MET:HE1	2:D:314:THR:HB	1.92	0.52
2:B:134:GLY:HA2	2:B:164:ARG:HB3	1.91	0.52
2:B:284:ARG:HH11	2:B:284:ARG:CG	2.22	0.52
1:A:285:GLN:CG	1:A:372[B]:GLN:HG3	2.39	0.52
2:B:169:PHE:CE2	2:B:235:MET:HG2	2.45	0.52
1:C:363[A]:VAL:HG13	1:C:364:PRO:HD2	1.91	0.52
2:B:124:LYS:CA	2:B:127:GLU:HG2	2.35	0.52
2:B:234:THR:O	2:B:238:VAL:HG13	2.09	0.52
1:A:221:ARG:NE	2:B:329:ASP:OD2	2.42	0.52
4:F:96:GLU:O	4:F:183:GLN:HA	2.10	0.52
4:F:10:ASN:OD1	4:F:10:ASN:N	2.43	0.52
2:B:416:MET:HA	2:B:416:MET:CE	2.39	0.52
1:C:28:HIS:O	1:C:36:MET:HE3	2.10	0.52
2:D:325:MET:SD	2:D:355:VAL:HG21	2.50	0.52
4:F:36:ARG:HB3	2:B:337:ASN:OD1	2.10	0.52
4:F:244:CYS:SG	4:F:245:ILE:N	2.82	0.52
2:B:292:THR:CG2	2:B:335:VAL:HG21	2.39	0.52
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.44	0.52
8:C:504:A1EPT:C33	2:B:222:PRO:CD	2.85	0.52
2:D:414:ASP:N	2:D:414:ASP:OD1	2.41	0.52
1:C:12:ALA:HB3	1:C:140:SER:HB3	1.92	0.52
3:E:131:GLU:OE1	3:E:131:GLU:HA	2.09	0.52
4:F:100:ILE:HD13	4:F:170:LEU:HD21	1.92	0.52
1:C:1:MET:CG	1:C:2:ARG:H	2.23	0.51
2:D:82:PRO:O	2:D:83:PHE:HB2	2.10	0.51
1:C:358:GLN:HB2	10:C:602:HOH:O	2.11	0.51
2:D:28:HIS:CE1	2:D:243:ARG:HB3	2.45	0.51
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.43	0.51
2:D:7:ILE:O	2:D:137:LEU:HA	2.10	0.51
3:E:68:LEU:HD23	3:E:68:LEU:C	2.35	0.51
2:B:215:ARG:HH11	2:B:215:ARG:CB	2.22	0.51
1:C:337:THR:C	1:C:338:LYS:HG2	2.35	0.51
2:D:23:VAL:HG21	2:D:232:SER:OG	2.10	0.51
2:D:248:LEU:HD13	2:D:352:LYS:HB3	1.93	0.51
2:B:253:ARG:O	2:B:257:VAL:HG23	2.10	0.51
1:C:349:THR:C	10:C:603:HOH:O	2.53	0.51
4:F:224:SER:OG	4:F:238:CYS:HA	2.10	0.51
4:F:225:SER:CB	4:F:260:ASN:HD21	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:191:VAL:HG21	2:D:425:MET:HE2	1.91	0.51
3:E:82:VAL:HG11	2:B:108:TYR:CG	2.45	0.51
4:F:85:PRO:HG2	4:F:86:GLU:OE2	2.11	0.51
2:B:282:GLN:HA	2:B:282:GLN:OE1	2.10	0.51
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.46	0.51
1:C:107:HIS:CD2	1:C:152:LEU:HB2	2.45	0.51
2:D:227:LEU:O	2:D:230:LEU:N	2.41	0.51
2:D:306:ASP:HB3	2:D:309:HIS:ND1	2.25	0.51
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.46	0.51
2:B:287:THR:N	2:B:290:GLU:OE1	2.41	0.51
4:F:75:ALA:HB1	4:F:99:VAL:HG12	1.93	0.51
1:A:426:ALA:O	1:A:430:LYS:HE3	2.11	0.51
2:B:416:MET:HE2	2:B:416:MET:CA	2.40	0.51
1:A:3:GLU:HG2	1:A:64:ARG:NE	2.26	0.50
1:A:415:GLU:O	1:A:418:PHE:HB2	2.11	0.50
2:D:102:ASN:HB3	2:D:105:LYS:HG3	1.93	0.50
2:D:301:MET:HE1	2:D:377:PHE:CD2	2.46	0.50
1:C:282:TYR:O	1:C:283:HIS:O	2.27	0.50
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.27	0.50
1:C:398:MET:HE3	2:D:347:ILE:HG23	1.93	0.50
1:C:271:THR:HG23	1:C:300:ASN:O	2.12	0.50
4:F:160:ILE:O	4:F:161:LEU:HB2	2.12	0.50
4:F:280:GLU:CA	4:F:284[B]:LEU:HD12	2.40	0.50
1:A:107:HIS:HD2	1:A:152:LEU:HB2	1.75	0.50
2:D:324:SER:HB3	2:D:327:GLU:HB2	1.94	0.50
1:C:248:LEU:HD12	1:C:357:TYR:CE2	2.47	0.50
4:F:236:LYS:HD3	4:F:240:LEU:HD12	1.93	0.50
1:A:7:ILE:HG23	1:A:66[A]:VAL:HG13	1.94	0.50
4:F:231:ALA:O	4:F:232:ASN:CB	2.59	0.50
2:B:424:ASN:O	2:B:427:ASP:HB2	2.12	0.50
2:D:136:GLN:HA	2:D:167:ASN:O	2.12	0.50
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.94	0.50
4:F:160:ILE:HD13	4:F:160:ILE:N	2.25	0.50
2:D:147:SER:O	2:D:151:THR:HG23	2.12	0.49
4:F:148:ILE:O	4:F:182:ILE:HA	2.12	0.49
4:F:166:ALA:O	4:F:168:GLU:N	2.45	0.49
8:C:504:A1EPT:C33	2:B:222:PRO:CG	2.89	0.49
2:B:11:GLN:HA	2:B:74:THR:HG21	1.93	0.49
1:A:98:ASP:C	1:A:98:ASP:OD1	2.55	0.49
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.94	0.49
1:C:335:ILE:O	1:C:339:ARG:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.47	0.49
2:D:286:LEU:HD23	2:D:286:LEU:N	2.22	0.49
2:D:2:ARG:HD2	2:D:131:CYS:SG	2.52	0.49
2:B:171:VAL:HA	2:B:204:ILE:O	2.12	0.49
2:D:94:PHE:HD1	2:D:94:PHE:O	1.95	0.49
2:D:274:PRO:HB3	2:D:286:LEU:CD2	2.41	0.49
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.95	0.49
1:A:2:ARG:O	1:A:51[B]:THR:HG23	2.12	0.49
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.47	0.49
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.93	0.49
2:D:274:PRO:HD2	2:D:371:LEU:HD13	1.94	0.49
1:C:165:SER:HA	1:C:199:ASP:OD2	2.12	0.49
1:C:324:VAL:HG22	1:C:327:ASP:CG	2.37	0.49
1:C:325:PRO:HB3	8:C:504:A1EPT:C48	2.43	0.49
2:B:36:TYR:CZ	2:B:38:GLY:CA	2.93	0.49
2:B:308:ARG:HA	2:B:342:TYR:CE1	2.48	0.49
2:B:390:ARG:O	2:B:394:GLN:HG3	2.13	0.49
2:B:396:THR:HG21	2:B:400:ARG:HH21	1.78	0.49
1:A:119:LEU:HD11	1:A:156:ARG:CB	2.43	0.49
2:D:191:VAL:CG1	2:D:425:MET:HG3	2.42	0.49
2:D:310:GLY:HA2	2:D:436:GLN:OE1	2.12	0.49
1:A:56:THR:HG23	1:A:58:ALA:H	1.78	0.48
2:D:18:ALA:O	2:D:22:GLU:HG3	2.13	0.48
2:B:234:THR:HG21	2:B:270:PRO:HB2	1.93	0.48
1:A:285:GLN:HG2	1:A:372[B]:GLN:CD	2.38	0.48
2:D:75:MET:HE1	2:D:93:VAL:H	1.78	0.48
2:B:30:ILE:HD12	2:B:30:ILE:N	2.28	0.48
2:B:200:GLU:OE2	2:B:256:ALA:HB2	2.13	0.48
1:A:1:MET:HE2	1:A:50:ASN:CB	2.42	0.48
2:D:287:THR:O	2:D:290:GLU:N	2.46	0.48
1:A:339:ARG:HB3	1:A:341:ILE:HD11	1.94	0.48
4:F:162:ILE:HD12	4:F:163:SER:H	1.79	0.48
1:A:329:ASN:HD21	3:E:20:PHE:HE2	1.61	0.48
1:C:108:TYR:CD2	3:E:108:ASN:CG	2.92	0.48
3:E:86:ALA:HB2	2:B:411:GLU:C	2.38	0.48
2:D:30:ILE:HG22	2:D:30:ILE:O	2.14	0.48
2:B:195:VAL:HG12	2:B:196:GLU:HG2	1.94	0.48
1:A:341:ILE:HD12	1:A:341:ILE:N	2.28	0.48
2:D:191:VAL:HG21	2:D:425:MET:CE	2.44	0.48
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.94	0.48
1:A:1:MET:HE2	1:A:50:ASN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:ASP:OD1	2:D:76:ASP:N	2.47	0.48
2:D:115:VAL:HG13	2:D:116:ASP:N	2.28	0.48
2:D:416:MET:O	2:D:418:PHE:N	2.46	0.48
3:E:58:GLU:O	3:E:58:GLU:HG2	2.12	0.48
4:F:314:LEU:HD23	4:F:336:PRO:HG2	1.96	0.48
1:A:25:CYS:HB3	1:A:30:ILE:O	2.14	0.48
1:C:336:LYS:NZ	10:C:601:HOH:O	2.17	0.48
2:D:31:ASP:OD2	2:D:33:THR:HG23	2.14	0.48
2:D:109:THR:HG21	2:D:411:GLU:HB3	1.95	0.48
2:B:89:PRO:C	2:B:91:ASN:H	2.22	0.48
2:B:295:MET:SD	2:B:375:ALA:HB1	2.53	0.48
1:A:96:LYS:HD2	1:A:96:LYS:N	2.29	0.47
1:A:221:ARG:HG2	2:B:325:MET:HB2	1.95	0.47
4:F:170:LEU:HD23	4:F:173:ILE:CD1	2.43	0.47
4:F:186:LEU:CD2	4:F:320:MET:HE3	2.44	0.47
2:B:2:ARG:H	2:B:131:CYS:HB3	1.79	0.47
1:A:113:GLU:O	1:A:113:GLU:HG3	2.14	0.47
1:A:234:ILE:O	1:A:238:ILE:HG13	2.14	0.47
2:D:75:MET:HE2	2:D:94:PHE:HD2	1.79	0.47
2:D:416:MET:HE2	2:D:416:MET:CA	2.28	0.47
1:C:255:PHE:CD1	1:C:316:CYS:HB3	2.50	0.47
2:D:103:TRP:CD1	2:D:148:GLY:HA2	2.50	0.47
2:D:297:ASP:CG	2:D:299:LYS:HE3	2.39	0.47
2:D:396:THR:C	2:D:398:MET:H	2.22	0.47
1:C:334:THR:O	1:C:335:ILE:C	2.57	0.47
2:D:70:LEU:H	2:D:145:THR:HG21	1.78	0.47
2:D:72:PRO:HG2	2:D:96:GLN:OE1	2.14	0.47
2:D:259:MET:HE2	2:D:314:THR:HB	1.97	0.47
4:F:135:TYR:CD2	4:F:166:ALA:HB2	2.49	0.47
2:B:146:GLY:O	2:B:150:GLY:HA3	2.14	0.47
1:A:249:ASN:OD1	1:A:258:ASN:ND2	2.45	0.47
1:A:67:PHE:HD1	1:A:67:PHE:N	2.12	0.47
1:A:383:ALA:O	1:A:386:GLU:HG3	2.14	0.47
1:C:114:ILE:O	1:C:114:ILE:HG12	2.14	0.47
1:C:313:MET:HE3	1:C:346:TRP:HZ2	1.80	0.47
1:C:325:PRO:HB3	8:C:504:A1EPT:C43	2.45	0.47
2:D:66:ILE:HD11	2:D:125:GLU:HG3	1.96	0.47
2:D:295:MET:HE3	2:D:377:PHE:CB	2.32	0.47
2:D:382:THR:HA	2:D:432:TYR:HD1	1.80	0.47
4:F:338:CYS:HB3	4:F:343:TYR:CZ	2.50	0.47
4:F:338:CYS:SG	4:F:339:ALA:N	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PHE:N	1:A:67:PHE:CD1	2.82	0.47
1:C:250:VAL:HG21	10:C:604:HOH:O	2.15	0.47
2:D:93:VAL:HG21	2:D:121:VAL:HG21	1.97	0.47
4:F:69:ASP:OD1	4:F:69:ASP:N	2.44	0.47
1:C:1:MET:H1	1:C:1:MET:HE3	1.79	0.47
1:C:334:THR:HG23	1:C:338:LYS:HE2	1.97	0.47
4:F:88:SER:OG	4:F:89:GLU:N	2.46	0.47
2:B:31:ASP:C	2:B:33:THR:N	2.73	0.47
1:A:7:ILE:HG12	1:A:66[A]:VAL:CG1	2.45	0.47
2:D:69:ASP:OD2	2:D:74:THR:OG1	2.33	0.47
2:D:119:LEU:CA	2:D:122:VAL:HG23	2.45	0.47
2:D:234:THR:O	2:D:237:GLY:N	2.48	0.47
4:F:28:LYS:HD3	4:F:30:LEU:CD2	2.45	0.47
1:A:1:MET:HE2	1:A:50:ASN:C	2.40	0.46
1:A:76:ASP:HA	1:A:79:ARG:CG	2.44	0.46
1:C:313:MET:HE3	1:C:435:VAL:CB	2.41	0.46
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.50	0.46
2:D:214:PHE:O	2:D:218:LYS:HA	2.15	0.46
3:E:9:ILE:HG22	3:E:10:GLU:CG	2.28	0.46
4:F:146:VAL:C	4:F:147:TRP:CD1	2.93	0.46
1:C:112:LYS:HG3	1:C:113:GLU:N	2.29	0.46
1:C:252:LEU:O	1:C:254:GLU:N	2.45	0.46
2:D:210:TYR:CE1	2:D:222:PRO:HG3	2.49	0.46
4:F:75:ALA:HB1	4:F:99:VAL:CG1	2.45	0.46
4:F:272:MET:HE2	4:F:272:MET:HB3	1.81	0.46
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.42	0.46
2:D:322:ARG:O	2:D:323:MET:HB3	2.14	0.46
1:C:93:ILE:CG2	1:C:114:ILE:HD11	2.46	0.46
2:D:71:GLU:HB2	2:D:98:GLY:HA2	1.97	0.46
2:D:191:VAL:HB	2:D:425:MET:HE3	1.96	0.46
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.98	0.46
2:B:36:TYR:C	2:B:37:HIS:ND1	2.72	0.46
2:B:325:MET:HB3	2:B:325:MET:HE3	1.45	0.46
1:A:258:ASN:O	1:A:314:ALA:HB1	2.15	0.46
4:F:162:ILE:HG13	4:F:233:PHE:HB2	1.96	0.46
2:B:308:ARG:HG2	2:B:342:TYR:OH	2.16	0.46
1:A:83:TYR:CD2	1:A:86:LEU:HD22	2.50	0.46
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.16	0.46
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.56	0.46
1:A:23:LEU:HD23	1:A:236:SER:HB2	1.97	0.46
1:C:255:PHE:CD1	1:C:352:LYS:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:MET:HE2	1:A:418:PHE:CE2	2.51	0.46
3:E:24:LEU:N	3:E:24:LEU:HD12	2.30	0.46
1:A:110:ILE:O	1:A:110:ILE:HG22	2.14	0.46
8:C:504:A1EPT:C02	8:C:504:A1EPT:C11	2.59	0.46
4:F:160:ILE:HG12	4:F:161:LEU:H	1.78	0.46
4:F:322:ASP:C	4:F:322:ASP:OD1	2.59	0.46
1:A:401:LYS:HE3	2:B:438:ALA:HB1	1.99	0.46
1:C:285:GLN:HG2	1:C:372:GLN:OE1	2.16	0.46
2:D:248:LEU:HD23	2:D:354:ALA:CB	2.41	0.46
4:F:233:PHE:CD1	4:F:233:PHE:N	2.84	0.46
2:B:135:PHE:CD1	2:B:135:PHE:N	2.85	0.45
1:A:56:THR:HG23	1:A:58:ALA:N	2.31	0.45
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.47	0.45
1:C:39:ASP:C	1:C:40:LYS:HD3	2.40	0.45
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.97	0.45
2:D:31:ASP:OD1	2:D:31:ASP:N	2.49	0.45
2:B:9:ALA:HA	2:B:68:VAL:O	2.15	0.45
1:A:56:THR:HG22	1:A:60:LYS:CB	2.46	0.45
1:C:63:PRO:HD3	1:C:86:LEU:HG	1.98	0.45
2:D:174:SER:HB2	2:D:207:GLU:N	2.31	0.45
2:D:275:LEU:HD23	2:D:275:LEU:HA	1.79	0.45
4:F:224:SER:HA	4:F:246:GLN:NE2	2.30	0.45
1:C:1:MET:O	1:C:2:ARG:CZ	2.63	0.45
1:C:108:TYR:CD2	3:E:105:MET:CE	3.00	0.45
1:C:221:ARG:HG3	1:C:221:ARG:NH1	2.31	0.45
2:D:274:PRO:CG	2:D:371:LEU:HD13	2.47	0.45
4:F:146:VAL:HG12	4:F:185:TYR:HB3	1.98	0.45
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.51	0.45
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.31	0.45
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.97	0.45
4:F:38:ASN:O	4:F:60:GLN:HA	2.16	0.45
4:F:235:ASP:OD1	4:F:235:ASP:N	2.47	0.45
2:D:104:ALA:HB1	2:D:411:GLU:HB2	1.98	0.45
2:D:405:LEU:HD23	2:D:406:HIS:N	2.32	0.45
3:E:136:ASN:O	3:E:139:LEU:HB2	2.17	0.45
1:A:146:GLY:O	1:A:150:THR:HB	2.17	0.45
1:A:234:ILE:HD13	1:A:302:MET:SD	2.57	0.45
2:B:105:LYS:HA	2:B:109:THR:OG1	2.15	0.45
2:B:107:HIS:O	2:B:152:LEU:HD22	2.17	0.45
2:D:247:GLN:HA	2:D:247:GLN:NE2	2.31	0.45
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:VAL:HG11	2:B:425:MET:CE	2.46	0.45
1:C:9:VAL:HG22	1:C:68[B]:VAL:CG1	2.47	0.45
8:C:504:A1EPT:C33	2:B:222:PRO:HG2	2.46	0.45
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.99	0.45
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.99	0.45
4:F:100:ILE:HG21	4:F:173:ILE:CD1	2.46	0.45
2:B:136:GLN:HA	2:B:167:ASN:O	2.17	0.45
1:A:270:ALA:HB3	1:A:302:MET:CG	2.47	0.45
1:A:304:LYS:O	1:A:305:CYS:HB3	2.16	0.45
1:A:335:ILE:HD12	1:A:336:LYS:N	2.31	0.45
1:C:48:SER:HB3	1:C:243:ARG:O	2.17	0.45
2:D:171:VAL:HG12	2:D:206:ASN:HD21	1.82	0.45
2:D:401:ARG:O	2:D:403:ALA:N	2.50	0.45
3:E:23:ILE:HD11	3:E:26:PRO:HA	1.99	0.45
1:C:397:LEU:HD23	1:C:397:LEU:HA	1.81	0.44
2:D:402:LYS:O	2:D:405:LEU:HB3	2.18	0.44
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.51	0.44
2:B:141:LEU:HD12	2:B:172:MET:SD	2.57	0.44
1:A:7:ILE:HG12	1:A:66[A]:VAL:HG12	1.98	0.44
1:C:234:ILE:O	1:C:238:ILE:HD12	2.17	0.44
2:D:174:SER:HB3	2:D:206:ASN:HB2	1.99	0.44
4:F:147:TRP:O	4:F:162:ILE:HD12	2.17	0.44
4:F:236:LYS:HD3	4:F:240:LEU:CD1	2.47	0.44
2:B:284:ARG:CD	2:B:285:ALA:O	2.64	0.44
1:A:155:GLU:HG2	1:A:197:HIS:NE2	2.32	0.44
2:D:402:LYS:HB3	2:D:402:LYS:HE2	1.80	0.44
2:B:32:PRO:O	2:B:86:ILE:HG22	2.18	0.44
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.99	0.44
2:D:346:TRP:CD1	2:D:346:TRP:H	2.36	0.44
4:F:201:ILE:HG12	4:F:221:LEU:CD1	2.47	0.44
1:C:192:HIS:CG	1:C:421:ALA:HA	2.53	0.44
2:B:396:THR:CG2	2:B:400:ARG:HH21	2.30	0.44
1:C:318:LEU:HD12	1:C:318:LEU:N	2.33	0.44
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.53	0.44
2:D:174:SER:O	2:D:177:VAL:N	2.50	0.44
2:D:209:LEU:CB	2:D:227:LEU:HD22	2.42	0.44
3:E:9:ILE:CG2	3:E:10:GLU:N	2.81	0.44
2:D:67:LEU:HD12	2:D:67:LEU:H	1.82	0.44
2:D:185:TYR:CD1	2:D:418:PHE:HE2	2.36	0.44
2:D:211:ASP:O	2:D:215:ARG:HD2	2.18	0.44
2:D:382:THR:HA	2:D:432:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:399:PHE:CE1	2:D:418:PHE:HB3	2.52	0.44
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.99	0.44
2:B:388:PHE:HD1	2:B:425:MET:HE2	1.82	0.44
1:A:234:ILE:HD13	1:A:302:MET:HE2	1.97	0.44
2:D:67:LEU:CD2	2:D:78:VAL:HG11	2.48	0.44
4:F:146:VAL:CG1	4:F:162:ILE:HD11	2.47	0.44
1:A:123:ARG:HG3	1:A:123:ARG:HH11	1.83	0.43
1:A:162:GLY:C	1:A:163:LYS:HE3	2.43	0.43
1:C:318:LEU:N	1:C:318:LEU:CD1	2.81	0.43
3:E:134:ARG:C	3:E:136:ASN:H	2.26	0.43
1:A:427:ALA:O	1:A:430:LYS:HB2	2.18	0.43
2:D:27:GLU:O	2:D:45:GLN:NE2	2.46	0.43
2:D:72:PRO:HG3	2:D:95:GLY:O	2.18	0.43
4:F:135:TYR:O	4:F:145:ASN:ND2	2.51	0.43
4:F:326:LYS:HD3	4:F:328:TRP:CZ2	2.53	0.43
1:A:1:MET:SD	1:A:1:MET:C	3.01	0.43
2:D:190:SER:O	2:D:193:GLN:N	2.51	0.43
4:F:269:GLN:NE2	4:F:273:ASP:OD2	2.50	0.43
2:B:195:VAL:CG1	2:B:424:ASN:HD21	2.32	0.43
1:C:208:ALA:HB2	1:C:304:LYS:HG3	2.00	0.43
2:D:70:LEU:HD13	2:D:110:GLU:HB3	2.00	0.43
2:D:171:VAL:HG22	2:D:204:ILE:HG21	2.01	0.43
2:D:188:THR:O	2:D:188:THR:HG22	2.19	0.43
2:B:106:GLY:O	2:B:111:GLY:HA3	2.18	0.43
1:C:40:LYS:HD3	1:C:40:LYS:N	2.34	0.43
2:D:102:ASN:OD1	2:D:104:ALA:HB3	2.18	0.43
2:D:179:ASP:C	2:D:181:VAL:H	2.24	0.43
2:D:326:LYS:O	2:D:330:GLU:HG3	2.18	0.43
4:F:101:TYR:O	4:F:128:ARG:NH1	2.51	0.43
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.53	0.43
1:A:75:ILE:O	1:A:79:ARG:HG2	2.19	0.43
1:A:281:ALA:O	1:A:282:TYR:O	2.36	0.43
1:A:439:SER:OG	4:F:70:LYS:CG	2.67	0.43
2:D:176:LYS:HB3	2:D:210:TYR:CD2	2.53	0.43
2:D:269:MET:HB2	2:D:269:MET:HE3	1.58	0.43
2:D:400:ARG:HD2	2:D:400:ARG:HA	1.52	0.43
4:F:49:PHE:HB3	4:F:66:ARG:HD2	2.01	0.43
2:B:360:PRO:O	2:B:369:ARG:C	2.61	0.43
1:A:157:LEU:C	1:A:159:VAL:H	2.27	0.43
1:A:217:LEU:O	1:A:218:ASP:C	2.61	0.43
1:C:164:LYS:HB2	1:C:164:LYS:HE2	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:415:GLU:H	2:D:415:GLU:HG2	1.44	0.43
2:B:387:LEU:C	2:B:387:LEU:HD23	2.44	0.43
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.49	0.43
1:C:395:PHE:CD1	1:C:422:ARG:HD3	2.54	0.43
1:A:179:THR:HG21	2:B:247:GLN:O	2.18	0.42
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.60	0.42
1:C:242:LEU:N	1:C:242:LEU:HD23	2.34	0.42
1:C:391:LEU:HD23	1:C:391:LEU:HA	1.87	0.42
1:C:248:LEU:CD1	1:C:357:TYR:OH	2.67	0.42
1:C:325:PRO:HA	8:C:504:A1EPT:C47	2.48	0.42
2:D:292:THR:O	2:D:296:PHE:HD1	2.02	0.42
4:F:135:TYR:HE1	4:F:145:ASN:CB	2.32	0.42
4:F:168:GLU:HG3	4:F:169:LEU:N	2.34	0.42
2:B:103:TRP:HD1	2:B:147:SER:OG	2.01	0.42
1:A:202:PHE:CE1	1:A:268:PRO:HG2	2.54	0.42
1:C:83:TYR:HD2	1:C:86:LEU:HD22	1.84	0.42
2:B:153:LEU:HA	2:B:153:LEU:HD23	1.86	0.42
1:C:6:SER:O	1:C:65:ALA:HA	2.20	0.42
1:C:90:GLU:O	1:C:121:ARG:HD2	2.19	0.42
1:C:252:LEU:C	1:C:254:GLU:N	2.76	0.42
2:D:68:VAL:O	2:D:69:ASP:HB2	2.19	0.42
4:F:135:TYR:O	4:F:135:TYR:CD1	2.73	0.42
4:F:148:ILE:C	4:F:182:ILE:HD12	2.43	0.42
2:B:176:LYS:NZ	2:B:211:ASP:OD2	2.52	0.42
2:B:292:THR:CG2	2:B:335:VAL:CG2	2.98	0.42
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.19	0.42
1:C:8:HIS:CE1	1:C:17:GLY:HA2	2.55	0.42
1:C:100:ALA:HA	2:D:254:LYS:HE3	2.02	0.42
1:C:398:MET:HE2	1:C:404:PHE:CD2	2.55	0.42
4:F:75:ALA:CB	4:F:99:VAL:HG12	2.50	0.42
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.02	0.42
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.84	0.42
1:A:88:HIS:NE2	1:A:90:GLU:CB	2.82	0.42
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.55	0.42
1:C:41:THR:O	1:C:41:THR:OG1	2.36	0.42
2:D:233:ALA:HB1	2:D:272:PHE:CE2	2.55	0.42
2:D:244:PHE:HB3	2:D:245:PRO:HD2	2.02	0.42
3:E:113:GLU:O	3:E:117:ALA:N	2.47	0.42
4:F:89:GLU:C	4:F:91:CYS:N	2.77	0.42
2:B:23:VAL:HG21	2:B:232:SER:HB2	2.01	0.42
2:B:69:ASP:O	2:B:94:PHE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:VAL:HG22	1:A:327:ASP:OD2	2.20	0.42
1:C:252:LEU:HD12	1:C:252:LEU:O	2.20	0.42
4:F:201:ILE:HG12	4:F:221:LEU:HD11	2.00	0.42
1:A:20:CYS:N	1:A:232:SER:OG	2.53	0.42
2:D:192:HIS:C	2:D:192:HIS:CD2	2.97	0.42
4:F:98:TYR:HA	4:F:127:GLU:OE2	2.20	0.42
1:A:117:LEU:HD12	1:A:117:LEU:O	2.20	0.42
1:C:221:ARG:HG2	2:D:325:MET:CE	2.30	0.42
1:C:252:LEU:CD1	1:C:255:PHE:HB2	2.38	0.42
1:C:355:ILE:CG1	8:C:504:A1EPT:C61	2.98	0.42
3:E:121:GLU:OE1	3:E:121:GLU:HA	2.20	0.42
2:B:70:LEU:HD23	2:B:114:LEU:HD22	2.02	0.42
1:C:86:LEU:HD12	1:C:86:LEU:HA	1.74	0.42
1:C:349:THR:HG21	2:B:175:PRO:HB3	2.02	0.42
2:D:109:THR:HG21	2:D:411:GLU:OE1	2.20	0.42
4:F:201:ILE:O	4:F:318:ASP:HA	2.20	0.42
4:F:205:VAL:HG21	4:F:291:ILE:HD13	2.01	0.42
2:B:7:ILE:O	2:B:137:LEU:HA	2.19	0.42
2:B:31:ASP:CG	2:B:33:THR:HG23	2.45	0.42
2:B:195:VAL:CG2	2:B:428:LEU:HD13	2.50	0.42
1:A:56:THR:HG22	1:A:60:LYS:CA	2.48	0.41
2:D:286:LEU:N	2:D:286:LEU:CD2	2.81	0.41
4:F:99:VAL:HG23	4:F:127:GLU:HG2	2.02	0.41
2:B:36:TYR:CE1	2:B:46:LEU:HG	2.55	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.55	0.41
1:C:88:HIS:O	1:C:89:PRO:C	2.62	0.41
1:C:187:SER:HB3	1:C:391:LEU:HD13	2.02	0.41
1:C:331:ALA:O	1:C:335:ILE:HG12	2.20	0.41
1:A:88:HIS:O	1:A:89:PRO:C	2.62	0.41
1:A:270:ALA:HB3	1:A:302:MET:HG2	2.01	0.41
1:C:305:CYS:HA	1:C:386:GLU:OE1	2.20	0.41
2:D:3:GLU:O	2:D:132:LEU:HD12	2.20	0.41
2:D:210:TYR:HE1	2:D:222:PRO:CD	2.34	0.41
2:D:287:THR:OG1	2:D:289:PRO:HD2	2.20	0.41
3:E:27:PRO:O	3:E:28:SER:OG	2.31	0.41
3:E:57:ALA:O	3:E:61:ARG:HB3	2.20	0.41
4:F:203:SER:HB3	4:F:215:LEU:HD11	2.03	0.41
2:B:1:MET:HE2	2:B:1:MET:CA	2.30	0.41
1:C:108:TYR:CE2	3:E:105:MET:CE	3.04	0.41
2:D:70:LEU:HD23	2:D:70:LEU:HA	1.66	0.41
2:D:406:HIS:CD2	2:D:407:TRP:HD1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.55	0.41
2:B:38:GLY:C	2:B:40:SER:N	2.78	0.41
2:D:75:MET:HE3	2:D:92:PHE:CD2	2.54	0.41
2:D:178:SER:OG	2:D:183:GLU:OE2	2.34	0.41
2:D:210:TYR:HD1	2:D:222:PRO:HG3	1.81	0.41
4:F:189:PRO:O	4:F:191:LEU:HG	2.20	0.41
1:A:215:ARG:NH2	1:A:299:ALA:O	2.53	0.41
1:A:413:MET:CE	1:A:418:PHE:CE2	3.03	0.41
3:E:100:LYS:O	3:E:103:GLN:HG3	2.21	0.41
4:F:248:GLU:O	4:F:249:TYR:CG	2.73	0.41
2:B:67:LEU:N	2:B:67:LEU:HD12	2.36	0.41
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.01	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.55	0.41
1:A:346:TRP:CD1	1:A:346:TRP:H	2.39	0.41
1:C:245:ASP:HA	1:C:249:ASN:HD22	1.86	0.41
2:D:287:THR:HG23	2:D:290:GLU:CD	2.45	0.41
4:F:244:CYS:C	4:F:246:GLN:N	2.79	0.41
2:B:406:HIS:HA	2:B:409:THR:OG1	2.21	0.41
2:D:72:PRO:HD3	2:D:96:GLN:HA	2.02	0.41
2:D:102:ASN:CG	2:D:105:LYS:HG3	2.46	0.41
2:D:105:LYS:CE	2:D:110:GLU:OE1	2.69	0.41
4:F:14:TYR:HA	4:F:17:VAL:HB	2.03	0.41
1:A:40:LYS:O	1:A:42:ILE:N	2.54	0.41
1:A:234:ILE:HD13	1:A:302:MET:HE1	2.02	0.41
1:C:328:VAL:HG21	8:C:504:A1EPT:C61	2.50	0.41
2:D:28:HIS:NE2	2:D:243:ARG:HD2	2.35	0.41
2:D:103:TRP:O	2:D:104:ALA:C	2.64	0.41
2:D:210:TYR:HE1	2:D:222:PRO:HD3	1.86	0.41
2:D:274:PRO:HG2	2:D:371:LEU:HD13	2.02	0.41
2:D:286:LEU:H	2:D:286:LEU:CD2	2.21	0.41
2:D:320:ARG:O	2:D:373:MET:HA	2.20	0.41
4:F:26:GLN:OE1	4:F:361:LEU:HD23	2.21	0.41
4:F:147:TRP:HB3	4:F:182:ILE:CD1	2.45	0.41
4:F:214:TYR:CD2	4:F:353[B]:VAL:HG11	2.56	0.41
4:F:317:PHE:CD2	4:F:332:VAL:HG13	2.55	0.41
2:B:3:GLU:O	2:B:133:GLN:HG3	2.21	0.41
2:B:141:LEU:HD22	2:B:190:SER:HB3	2.02	0.41
2:B:158:ARG:NH1	2:B:196:GLU:O	2.54	0.41
2:B:249:ASN:HB3	2:B:255:LEU:HD13	2.02	0.41
2:B:282:GLN:HG3	2:B:371:LEU:CD2	2.51	0.41
1:A:68[B]:VAL:HG21	1:A:118:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.93	0.41
1:A:401:LYS:HE2	2:B:346:TRP:CD1	2.56	0.41
1:C:68[A]:VAL:HG11	1:C:118:VAL:HG21	2.03	0.41
1:C:348:PRO:O	1:C:349:THR:C	2.64	0.41
2:D:118:VAL:HB	2:D:153:LEU:HD21	2.03	0.41
2:B:395:PHE:CD1	2:B:395:PHE:C	2.99	0.41
1:A:44:GLY:O	1:A:55:GLU:OE2	2.39	0.40
1:C:324:VAL:CG2	1:C:324:VAL:O	2.68	0.40
1:C:355:ILE:HG12	8:C:504:A1EPT:C61	2.52	0.40
2:D:168:THR:OG1	2:D:201:THR:HG23	2.22	0.40
3:E:27:PRO:HB2	3:E:28:SER:H	1.59	0.40
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.51	0.40
1:C:352:LYS:HG3	2:B:179:ASP:OD1	2.20	0.40
2:D:204:ILE:HG23	2:D:209:LEU:HD21	2.02	0.40
2:D:327:GLU:O	2:D:331:GLN:HG2	2.21	0.40
4:F:169:LEU:HD23	4:F:169:LEU:HA	1.89	0.40
1:A:74:VAL:O	1:A:77:GLU:HB2	2.21	0.40
1:A:355:ILE:O	3:E:17:GLY:HA3	2.21	0.40
2:D:165:ILE:HA	2:D:199:ASP:OD2	2.22	0.40
2:D:188:THR:O	2:D:421:ALA:HB1	2.21	0.40
4:F:218:GLU:OE1	4:F:218:GLU:HA	2.21	0.40
4:F:220:VAL:HG12	4:F:263:PHE:HE1	1.85	0.40
2:B:300:ASN:O	2:B:302:MET:HE2	2.21	0.40
1:A:311:LYS:CE	1:A:342:GLN:HG2	2.51	0.40
1:A:209:ILE:CG2	1:A:227:LEU:HD22	2.47	0.40
1:A:414:GLU:O	1:A:415:GLU:C	2.64	0.40
1:C:82:THR:O	1:C:82:THR:HG22	2.20	0.40
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.46	0.40
4:F:242:ASN:O	4:F:246:GLN:HB2	2.21	0.40
2:B:269:MET:HB3	2:B:269:MET:HE2	1.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/450 (99%)	409 (92%)	32 (7%)	5 (1%)	11	25
1	C	445/450 (99%)	419 (94%)	20 (4%)	6 (1%)	9	21
2	B	428/445 (96%)	399 (93%)	25 (6%)	4 (1%)	14	30
2	D	424/445 (95%)	372 (88%)	43 (10%)	9 (2%)	5	11
3	E	116/143 (81%)	108 (93%)	6 (5%)	2 (2%)	7	15
4	F	323/384 (84%)	287 (89%)	25 (8%)	11 (3%)	3	4
All	All	2182/2317 (94%)	1994 (91%)	151 (7%)	37 (2%)	7	15

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	282	TYR
1	A	438	ASP
1	C	283	HIS
1	C	349	THR
4	F	230	SER
4	F	232	ASN
4	F	248	GLU
2	B	74	THR
2	D	143	GLY
2	D	180	THR
2	D	181	VAL
2	D	402	LYS
2	D	417	GLU
3	E	27	PRO
4	F	88	SER
4	F	167	SER
4	F	245	ILE
2	B	280	SER
1	C	41	THR
4	F	160	ILE
4	F	175	GLU
2	B	32	PRO
2	D	323	MET
2	D	360	PRO
4	F	161	LEU
1	A	305	CYS

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Mol	Chain	Res	Type
1	C	253	THR
1	C	284	GLU
1	C	348	PRO
4	F	247	LYS
2	D	69	ASP
3	E	25	LYS
2	D	98	GLY
1	A	114	ILE
4	F	102	PRO
2	B	73	GLY

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	378/378 (100%)	341 (90%)	37 (10%)	7	17
1	C	378/378 (100%)	352 (93%)	26 (7%)	14	32
2	B	369/383 (96%)	349 (95%)	20 (5%)	20	42
2	D	369/383 (96%)	328 (89%)	41 (11%)	6	12
3	E	108/127 (85%)	94 (87%)	14 (13%)	4	8
4	F	303/342 (89%)	268 (88%)	35 (12%)	5	11
All	All	1905/1991 (96%)	1732 (91%)	173 (9%)	9	19

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	41	THR
1	A	60	LYS
1	A	62	VAL
1	A	67	PHE
1	A	71	GLU
1	A	74	VAL
1	A	79	ARG

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Mol	Chain	Res	Type
1	A	88	HIS
1	A	90	GLU
1	A	91	GLN
1	A	96	LYS
1	A	112	LYS
1	A	113	GLU
1	A	118	VAL
1	A	132	LEU
1	A	136[A]	LEU
1	A	136[B]	LEU
1	A	150	THR
1	A	163	LYS
1	A	176	GLN
1	A	177	VAL
1	A	179	THR
1	A	203	MET
1	A	218	ASP
1	A	220	GLU
1	A	229	ARG
1	A	232	SER
1	A	251	ASP
1	A	257	THR
1	A	259	LEU
1	A	280	LYS
1	A	286	LEU
1	A	301	GLN
1	A	420[A]	GLU
1	A	420[B]	GLU
1	A	430	LYS
1	C	1	MET
1	C	2	ARG
1	C	48	SER
1	C	71	GLU
1	C	97	GLU
1	C	120[A]	ASP
1	C	120[B]	ASP
1	C	158	SER
1	C	188	ILE
1	C	215	ARG
1	C	230	LEU
1	C	234	ILE
1	C	238	ILE

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Mol	Chain	Res	Type
1	C	242	LEU
1	C	248	LEU
1	C	253	THR
1	C	285	GLN
1	C	286	LEU
1	C	290	GLU
1	C	313	MET
1	C	318	LEU
1	C	324	VAL
1	C	353	VAL
1	C	368	LEU
1	C	379	SER
1	C	381	THR
2	D	1	MET
2	D	11	GLN
2	D	24	ILE
2	D	26	ASP
2	D	30	ILE
2	D	33	THR
2	D	35	SER
2	D	46	LEU
2	D	59	ASN
2	D	67	LEU
2	D	75	MET
2	D	76	ASP
2	D	94	PHE
2	D	110	GLU
2	D	117	SER
2	D	121	VAL
2	D	122	VAL
2	D	138	THR
2	D	140	SER
2	D	164	ARG
2	D	177	VAL
2	D	182	VAL
2	D	196	GLU
2	D	207	GLU
2	D	248	LEU
2	D	286	LEU
2	D	287	THR
2	D	325	MET
2	D	335	VAL

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Mol	Chain	Res	Type
2	D	345	GLU
2	D	352	LYS
2	D	393	GLU
2	D	400	ARG
2	D	401	ARG
2	D	405	LEU
2	D	409	THR
2	D	414	ASP
2	D	415	GLU
2	D	425	MET
2	D	429	VAL
2	D	434	GLN
3	E	18	GLN
3	E	19	SER
3	E	23	ILE
3	E	47	LEU
3	E	53	LYS
3	E	54	LEU
3	E	61	ARG
3	E	89	GLU
3	E	105	MET
3	E	116	LEU
3	E	126	LYS
3	E	128	LYS
3	E	133	VAL
3	E	136	ASN
4	F	10	ASN
4	F	12	SER
4	F	45	ASN
4	F	89	GLU
4	F	125	THR
4	F	126	ASP
4	F	128	ARG
4	F	160	ILE
4	F	161	LEU
4	F	162	ILE
4	F	163	SER
4	F	173	ILE
4	F	179	VAL
4	F	180	HIS
4	F	181	VAL
4	F	182	ILE

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Mol	Chain	Res	Type
4	F	186	LEU
4	F	198	LYS
4	F	225	SER
4	F	226	GLU
4	F	233	PHE
4	F	238	CYS
4	F	241	THR
4	F	266	GLU
4	F	272	MET
4	F	277[A]	THR
4	F	277[B]	THR
4	F	284[A]	LEU
4	F	284[B]	LEU
4	F	285	LEU
4	F	286	GLN
4	F	320	MET
4	F	332	VAL
4	F	340	GLN
4	F	372	THR
2	B	1	MET
2	B	15	GLN
2	B	19	LYS
2	B	33	THR
2	B	57	THR
2	B	62	VAL
2	B	77	SER
2	B	86	ILE
2	B	195	VAL
2	B	238	VAL
2	B	240	THR
2	B	284	ARG
2	B	295	MET
2	B	324	SER
2	B	325	MET
2	B	334	ASN
2	B	341	SER
2	B	415	GLU
2	B	423[A]	SER
2	B	423[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	107	HIS
1	A	309	HIS
1	C	11	GLN
1	C	301	GLN
1	C	356	ASN
1	C	393	HIS
2	D	6	HIS
2	D	136	GLN
2	D	206	ASN
2	D	336	GLN
2	D	424	ASN
3	E	103	GLN
4	F	243	HIS
4	F	260	ASN
4	F	333	ASN
2	B	15	GLN
2	B	193	GLN
2	B	331	GLN
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	$\# Z > 2$
9	GDP	B	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
5	GTP	C	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
9	GDP	D	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.75	7 (15%)
8	A1EPT	C	504	-	68,69,69	7.78	34 (50%)	85,111,111	2.56	22 (25%)
5	GTP	A	501	6	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)

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	B	501	-	-	0/16/32/32	0/3/3/3
5	GTP	C	501	-	-	7/22/38/38	0/3/3/3
9	GDP	D	501	-	-	0/16/32/32	0/3/3/3
8	A1EPT	C	504	-	-	13/42/133/133	0/7/9/9
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	504	A1EPT	C11-C12	-25.54	1.00	1.55
8	C	504	A1EPT	C10-N09	-20.83	0.96	1.47
8	C	504	A1EPT	C08-N09	-18.33	1.05	1.47
8	C	504	A1EPT	C18-C13	18.04	1.60	1.39
8	C	504	A1EPT	C11-C10	15.67	1.80	1.52
8	C	504	A1EPT	C18-N01	13.90	1.63	1.39
8	C	504	A1EPT	C05-C06	-13.27	1.27	1.51
8	C	504	A1EPT	C14-C15	12.73	1.57	1.39
8	C	504	A1EPT	C14-C13	12.57	1.57	1.39
8	C	504	A1EPT	C16-C15	11.84	1.61	1.39
8	C	504	A1EPT	C44-C43	11.79	1.57	1.39
8	C	504	A1EPT	C47-C48	11.60	1.57	1.39
8	C	504	A1EPT	C17-C16	11.33	1.58	1.38
8	C	504	A1EPT	C03-C23	8.79	1.73	1.52
8	C	504	A1EPT	C03-C04	-8.66	1.29	1.54
8	C	504	A1EPT	C17-C18	8.53	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	504	A1EPT	C12-C02	8.36	1.84	1.55
8	C	504	A1EPT	C45-C44	8.15	1.52	1.38
8	C	504	A1EPT	O28-C04	8.12	1.61	1.44
8	C	504	A1EPT	C47-C46	7.78	1.51	1.39
8	C	504	A1EPT	C19-N09	7.44	1.59	1.47
8	C	504	A1EPT	C06-C07	-6.97	1.20	1.32
8	C	504	A1EPT	C08-C07	6.60	1.65	1.49
8	C	504	A1EPT	C45-C46	6.44	1.50	1.38
8	C	504	A1EPT	O58-C56	5.72	1.44	1.33
8	C	504	A1EPT	O25-C23	5.08	1.42	1.33
8	C	504	A1EPT	C02-N01	-4.93	1.36	1.47
8	C	504	A1EPT	C41-C42	4.28	1.57	1.51
8	C	504	A1EPT	C12-C13	-3.69	1.45	1.51
8	C	504	A1EPT	C12-C19	-3.67	1.42	1.55
8	C	504	A1EPT	C50-C42	3.65	1.42	1.37
9	D	501	GDP	C5-C4	3.19	1.47	1.38
9	B	501	GDP	C5-C4	3.16	1.47	1.38
8	C	504	A1EPT	O28-C29	3.02	1.41	1.35
8	C	504	A1EPT	C51-C56	2.94	1.57	1.53
9	D	501	GDP	C6-N1	-2.41	1.34	1.38
9	B	501	GDP	C6-N1	-2.36	1.34	1.38
5	C	501	GTP	C2-N3	2.23	1.38	1.33
8	C	504	A1EPT	O60-C46	2.21	1.41	1.37
5	A	501	GTP	C2-N3	2.20	1.38	1.33
9	D	501	GDP	C5-N7	-2.04	1.35	1.39
9	B	501	GDP	C5-N7	-2.03	1.35	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	504	A1EPT	C11-C12-C13	-8.83	96.29	112.36
8	C	504	A1EPT	O32-C16-C15	8.55	125.06	116.59
8	C	504	A1EPT	C11-C12-C02	8.50	128.64	112.17
9	B	501	GDP	C5-C4-N3	-6.15	118.61	128.39
8	C	504	A1EPT	C19-C05-C06	6.14	114.40	108.27
9	D	501	GDP	C5-C4-N3	-5.96	118.91	128.39
8	C	504	A1EPT	O32-C16-C17	-5.52	114.58	124.08
8	C	504	A1EPT	O25-C23-C03	5.43	121.14	112.21
5	C	501	GTP	C5-C4-N3	-5.14	120.21	128.39
5	A	501	GTP	C5-C4-N3	-5.10	120.28	128.39
9	B	501	GDP	C2-N3-C4	5.03	120.96	112.30
9	D	501	GDP	C2-N3-C4	4.92	120.77	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C2-N3-C4	4.66	120.32	112.30
5	A	501	GTP	C2-N3-C4	4.66	120.32	112.30
9	B	501	GDP	N9-C4-N3	4.57	135.10	125.95
9	D	501	GDP	N9-C4-N3	4.44	134.84	125.95
8	C	504	A1EPT	O28-C29-C30	4.32	118.79	111.09
8	C	504	A1EPT	C14-C13-C12	3.92	135.71	129.01
8	C	504	A1EPT	C03-C02-N01	-3.81	107.57	112.81
8	C	504	A1EPT	C14-C13-C18	-3.80	117.12	120.29
8	C	504	A1EPT	O58-C56-C51	3.59	117.01	111.21
8	C	504	A1EPT	C04-O28-C29	-3.41	112.48	117.65
8	C	504	A1EPT	C35-C52-N39	3.39	116.88	111.20
8	C	504	A1EPT	C20-C05-C06	-3.36	103.99	107.99
8	C	504	A1EPT	C02-C03-C23	-3.36	100.79	110.02
5	C	501	GTP	N9-C4-N3	3.35	132.66	125.95
5	A	501	GTP	N9-C4-N3	3.30	132.56	125.95
9	D	501	GDP	C6-C5-N7	3.27	136.24	130.29
8	C	504	A1EPT	C08-C07-C06	-3.26	118.06	123.13
9	B	501	GDP	C6-C5-N7	3.13	136.00	130.29
5	C	501	GTP	C2-N1-C6	-2.94	119.79	125.11
5	A	501	GTP	C2-N1-C6	-2.90	119.86	125.11
8	C	504	A1EPT	O25-C23-O24	-2.79	119.15	123.95
8	C	504	A1EPT	O24-C23-C03	-2.78	119.65	123.92
5	A	501	GTP	N9-C8-N7	-2.60	108.59	113.40
8	C	504	A1EPT	O28-C04-C03	2.54	110.26	106.29
9	D	501	GDP	C4-C5-N7	-2.51	106.69	110.67
9	B	501	GDP	C4-C5-N7	-2.51	106.69	110.67
5	C	501	GTP	C5-C6-N1	2.50	119.62	113.25
5	A	501	GTP	C8-N7-C5	2.49	108.70	104.26
5	C	501	GTP	N9-C8-N7	-2.49	108.78	113.40
5	A	501	GTP	C5-C6-N1	2.48	119.58	113.25
5	C	501	GTP	C8-N7-C5	2.44	108.60	104.26
9	D	501	GDP	C3'-C2'-C1'	2.42	106.04	101.46
5	C	501	GTP	O6-C6-C5	-2.42	120.14	126.53
5	A	501	GTP	O6-C6-C5	-2.42	120.16	126.53
9	B	501	GDP	C3'-C2'-C1'	2.37	105.95	101.46
8	C	504	A1EPT	C12-C02-N01	2.27	109.69	105.38
5	A	501	GTP	C3'-C2'-C1'	2.16	105.54	101.46
5	C	501	GTP	C3'-C2'-C1'	2.14	105.50	101.46
8	C	504	A1EPT	C47-C48-C43	-2.11	120.84	122.52
8	C	504	A1EPT	C05-C19-N09	2.09	116.13	111.72
9	D	501	GDP	O6-C6-C5	-2.09	121.02	126.53
9	B	501	GDP	O6-C6-C5	-2.07	121.08	126.53

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O2A
8	C	504	A1EPT	C03-C23-O25-C26
8	C	504	A1EPT	C30-C29-O28-C04
8	C	504	A1EPT	C15-C16-O32-C33
8	C	504	A1EPT	C45-C46-O60-C61
8	C	504	A1EPT	C47-C46-O60-C61
8	C	504	A1EPT	C17-C16-O32-C33
8	C	504	A1EPT	O31-C29-O28-C04
5	C	501	GTP	C3'-C4'-C5'-O5'
8	C	504	A1EPT	O24-C23-O25-C26
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O5'
5	C	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	C4'-C5'-O5'-PA
8	C	504	A1EPT	N39-C40-C41-C42
8	C	504	A1EPT	O55-C37-C53-C54
5	C	501	GTP	PA-O3A-PB-O1B
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
8	C	504	A1EPT	C41-C40-N39-C38
8	C	504	A1EPT	C04-C03-C23-O24
8	C	504	A1EPT	C04-C03-C23-O25

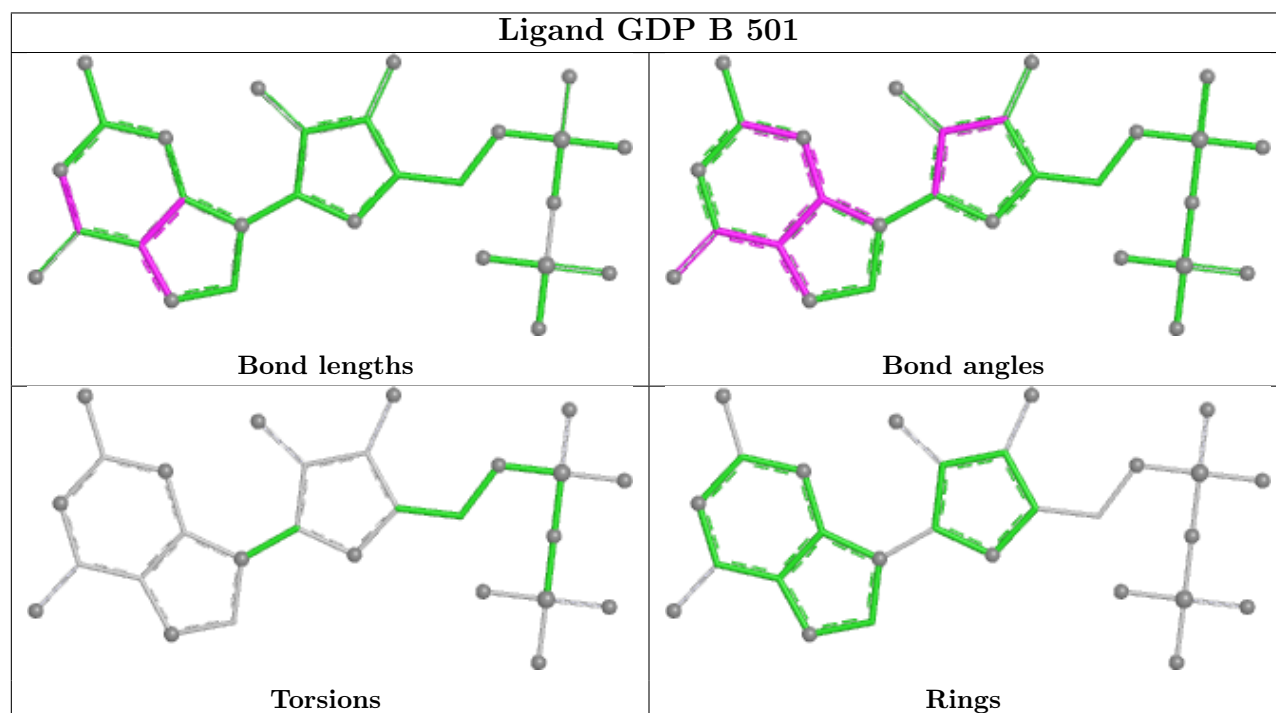
There are no ring outliers.

1 monomer is involved in 16 short contacts:

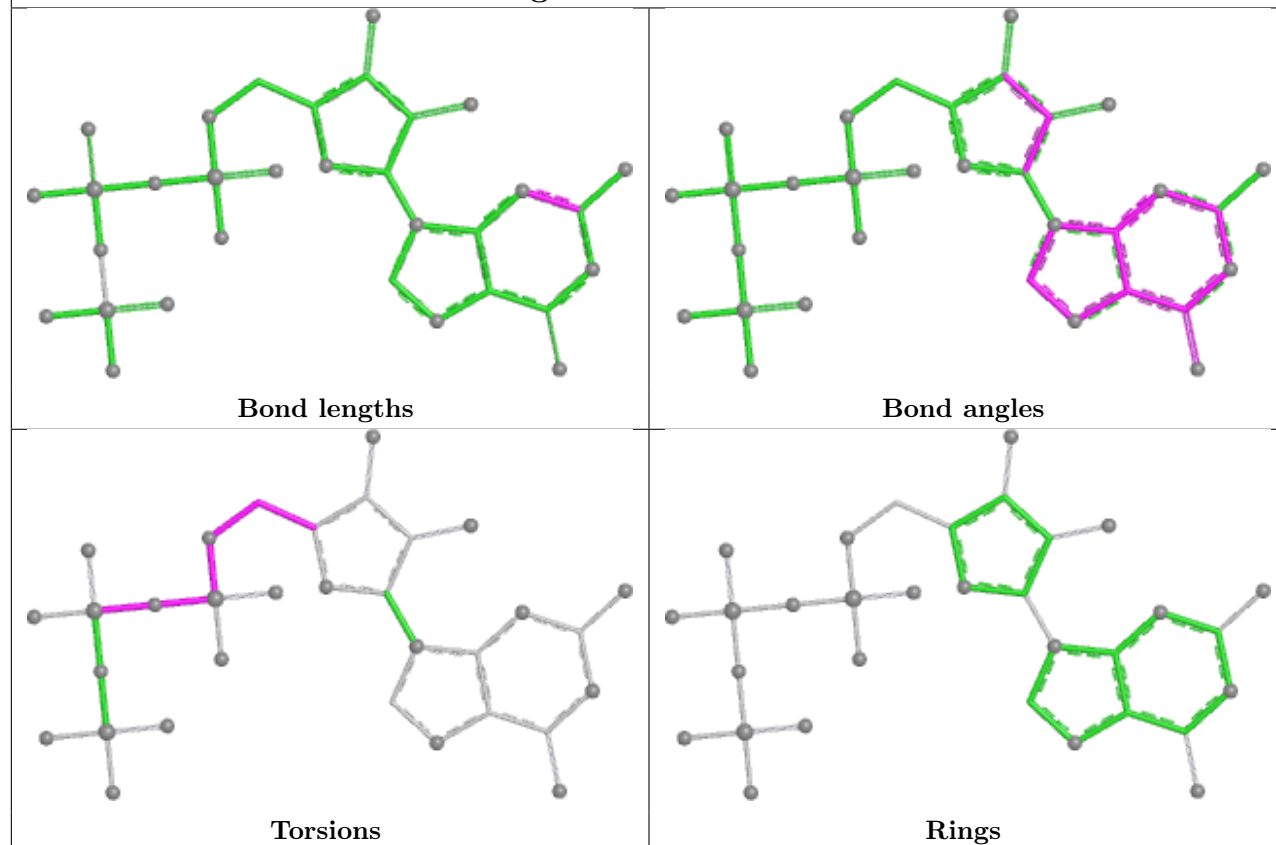
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	504	A1EPT	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

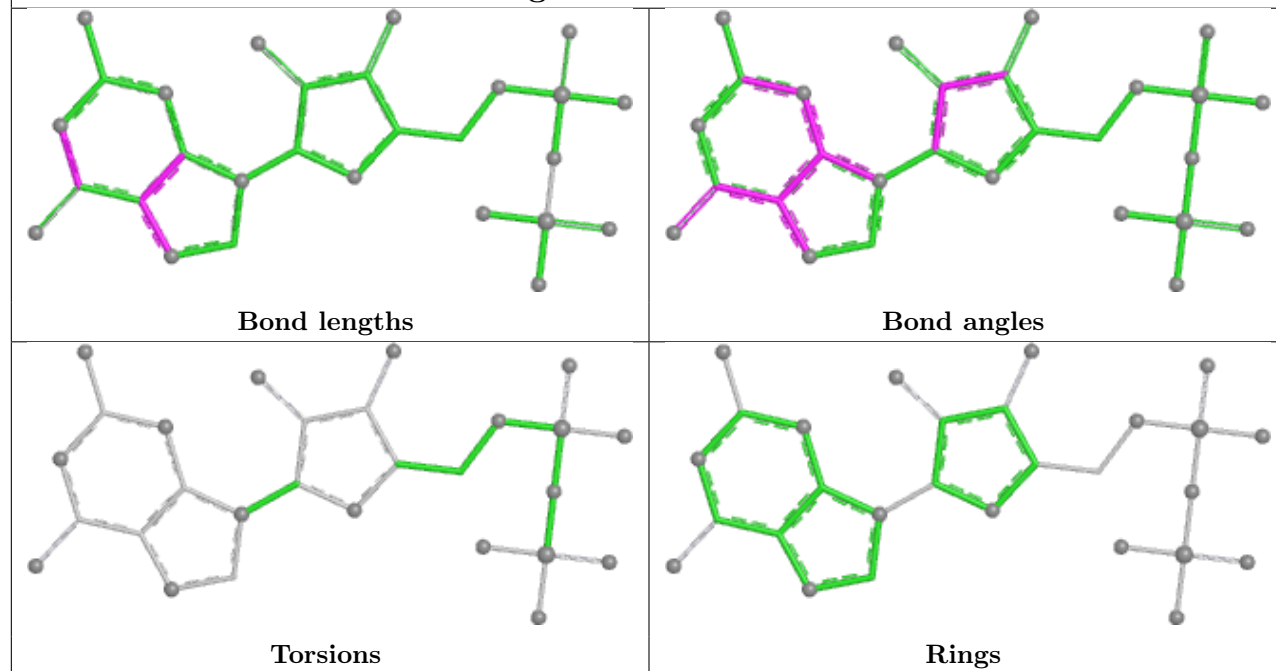
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



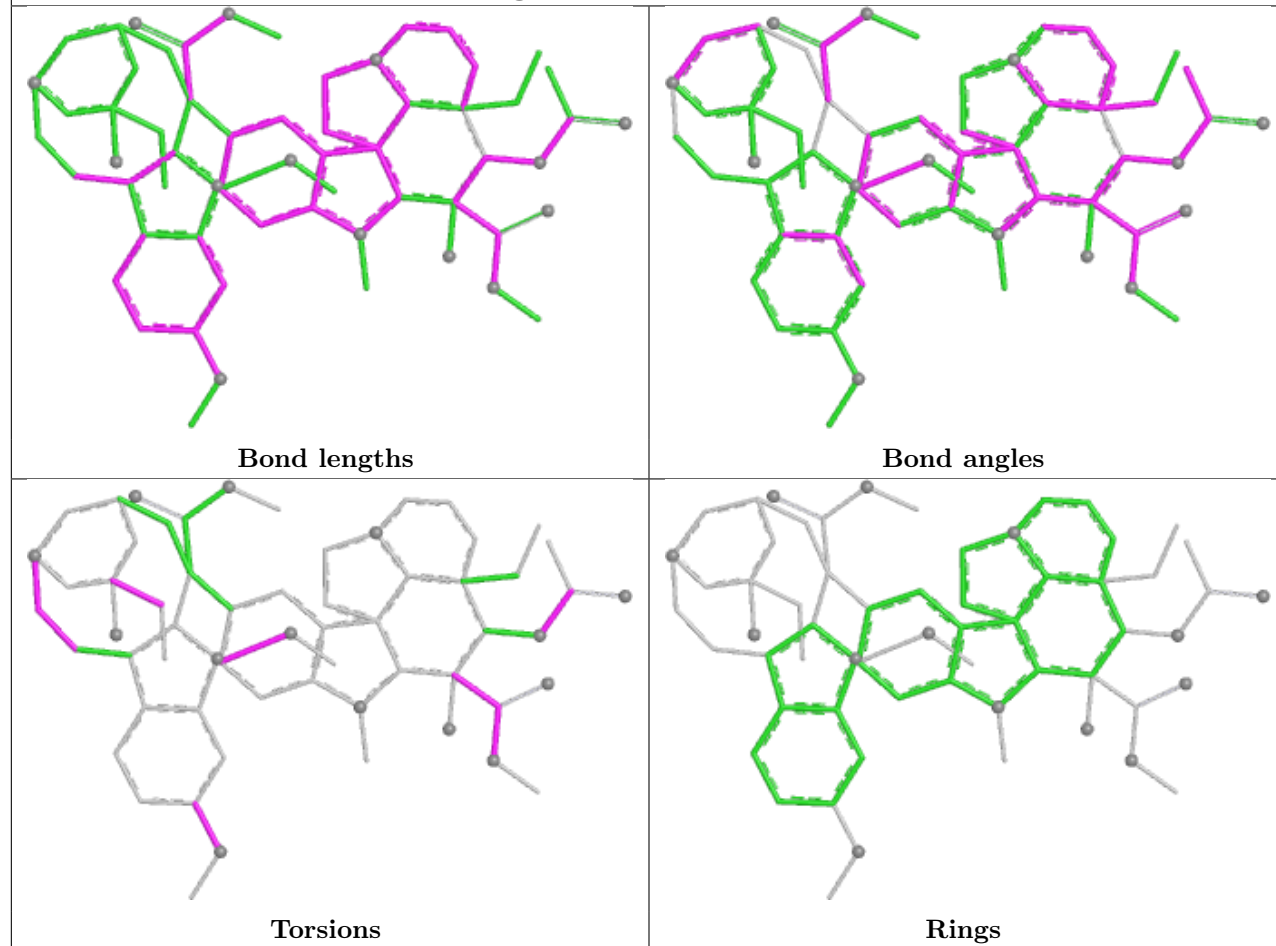
Ligand GTP C 501

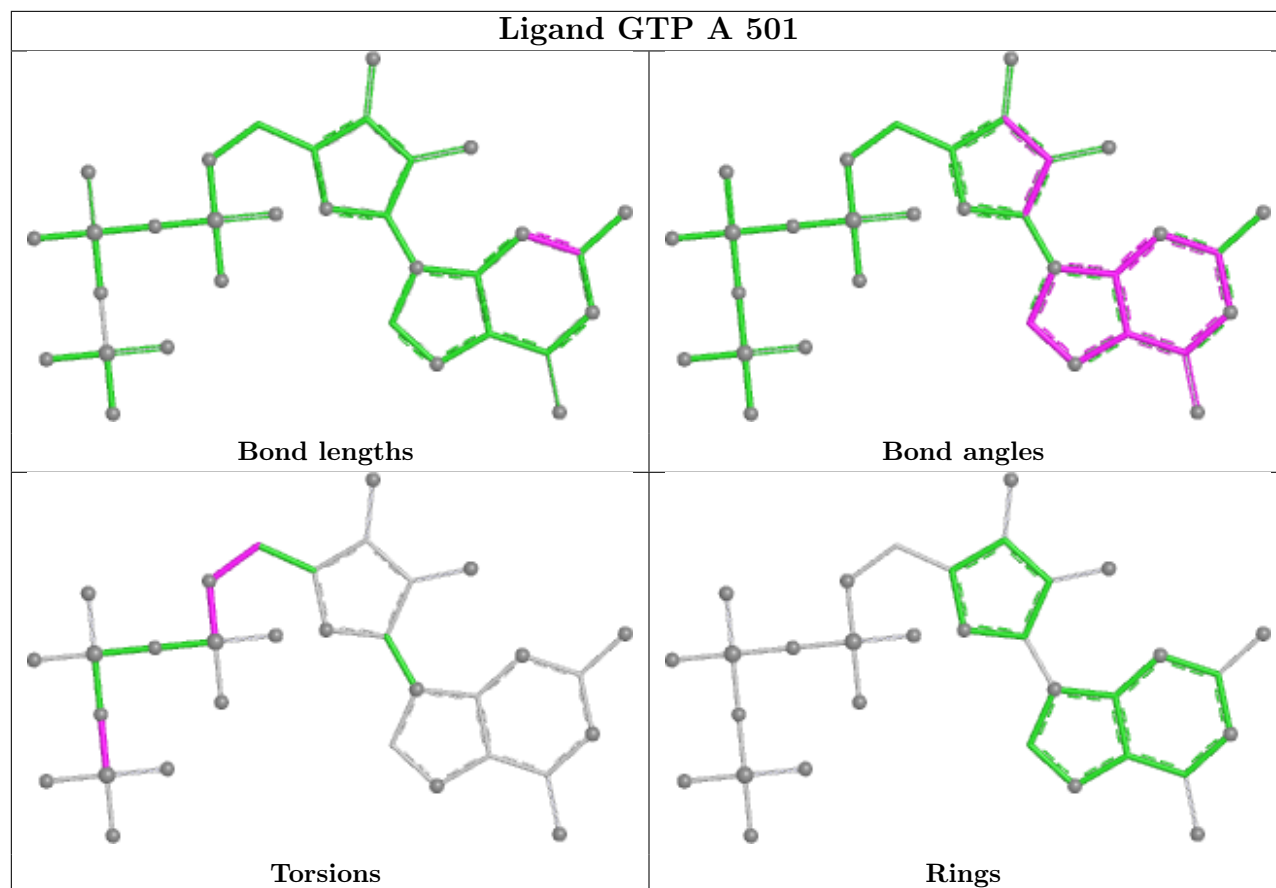


Ligand GDP D 501



Ligand A1EPT C 504





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	439/450 (97%)	0.29	12 (2%)	56	50	26, 45, 69, 104	9 (2%)
1	C	440/450 (97%)	0.10	21 (4%)	35	30	20, 39, 63, 77	7 (1%)
2	B	428/445 (96%)	0.18	16 (3%)	45	39	21, 43, 77, 120	4 (0%)
2	D	424/445 (95%)	1.11	66 (15%)	5	4	34, 64, 93, 113	7 (1%)
3	E	120/143 (83%)	1.02	18 (15%)	5	4	35, 59, 83, 101	0
4	F	331/384 (86%)	0.98	56 (16%)	4	3	34, 64, 115, 125	4 (1%)
All	All	2182/2317 (94%)	0.53	189 (8%)	16	12	20, 50, 91, 125	31 (1%)

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	6.3
2	B	283	TYR	5.8
2	D	285	ALA	5.5
4	F	231	ALA	5.5
1	A	282	TYR	5.3
3	E	140	LYS	5.2
4	F	245	ILE	5.1
4	F	250	SER	5.0
4	F	180	HIS	4.9
4	F	125	THR	4.8
4	F	144	GLY	4.7
4	F	159	GLY	4.7
4	F	161	LEU	4.5
1	A	439	SER	4.3
2	B	280	SER	4.3
4	F	160	ILE	4.2
4	F	179	VAL	4.2
2	D	220	THR	4.1
4	F	244	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	98	GLY	4.1
4	F	149	ALA	4.1
3	E	6	MET	4.1
3	E	59	GLU	4.0
4	F	173	ILE	4.0
4	F	232	ASN	4.0
2	B	1	MET	3.9
2	D	11	GLN	3.9
4	F	162	ILE	3.8
2	D	276	THR	3.8
2	D	1	MET	3.8
2	B	57	THR	3.7
2	D	37	HIS	3.7
1	C	247	ALA	3.6
1	A	281	ALA	3.6
2	D	56	ALA	3.6
4	F	169	LEU	3.5
2	D	82	PRO	3.5
4	F	103	THR	3.4
2	B	58	GLY	3.4
2	D	88	ARG	3.4
4	F	372	THR	3.3
2	D	370	GLY	3.3
3	E	14	CYS	3.3
2	D	284	ARG	3.3
2	D	57	THR	3.3
2	D	219	LEU	3.2
1	C	440	VAL	3.2
4	F	101	TYR	3.2
1	A	283	HIS	3.2
2	D	369	ARG	3.1
4	F	90	SER	3.1
1	A	262	TYR	3.1
2	D	87	PHE	3.1
4	F	259	GLY	3.1
4	F	166	ALA	3.0
2	D	404	PHE	3.0
2	D	216	THR	3.0
2	D	32	PRO	3.0
4	F	236	LYS	3.0
4	F	1	MET	3.0
2	D	405	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	174	SER	2.9
2	D	142	GLY	2.9
2	D	42	LEU	2.9
1	C	251	ASP	2.9
2	D	94	PHE	2.9
2	D	305	CYS	2.8
4	F	132	LEU	2.8
2	D	144	GLY	2.8
2	B	82	PRO	2.8
3	E	139	LEU	2.8
4	F	238	CYS	2.8
2	B	279	GLY	2.8
4	F	240	LEU	2.8
2	D	357	ASP	2.8
4	F	135	TYR	2.8
4	F	130	VAL	2.8
2	D	127	GLU	2.8
2	D	99	ALA	2.7
4	F	234	GLN	2.7
3	E	28	SER	2.7
1	C	253	THR	2.7
2	D	406	HIS	2.7
1	C	280	LYS	2.6
1	C	341	ILE	2.6
2	D	86	ILE	2.6
4	F	320	MET	2.6
1	A	358	GLN	2.6
1	A	88	HIS	2.6
4	F	137	ARG	2.6
2	D	295	MET	2.6
1	C	285	GLN	2.6
2	D	97	SER	2.6
2	B	74	THR	2.6
2	D	372	LYS	2.6
2	D	291	LEU	2.6
3	E	115	HIS	2.6
1	C	350	GLY	2.5
4	F	235	ASP	2.5
2	D	214	PHE	2.5
2	D	96	GLN	2.5
2	B	277	SER	2.5
3	E	44	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	284	GLU	2.5
4	F	134	ALA	2.5
1	A	41	THR	2.5
1	C	248	LEU	2.5
2	D	83	PHE	2.5
2	D	275	LEU	2.5
2	D	441	ASP	2.5
4	F	172	PHE	2.5
2	D	229	HIS	2.4
2	B	56	ALA	2.4
2	D	85	GLN	2.4
2	D	286	LEU	2.4
4	F	89	GLU	2.4
2	D	213	CYS	2.4
4	F	167	SER	2.4
1	C	95	GLY	2.4
2	D	66	ILE	2.4
2	D	130	ASP	2.4
3	E	47	LEU	2.4
4	F	131	PHE	2.4
2	D	65	ALA	2.4
4	F	92	THR	2.3
2	D	321	GLY	2.3
1	A	437	VAL	2.3
4	F	181	VAL	2.3
4	F	229	ASN	2.3
4	F	242	ASN	2.3
4	F	165	GLU	2.3
1	C	232	SER	2.3
2	B	284	ARG	2.3
2	D	15	GLN	2.3
2	B	127	GLU	2.3
2	B	219	LEU	2.3
2	D	402	LYS	2.3
4	F	220	VAL	2.3
3	E	122	ARG	2.3
3	E	15	THR	2.2
1	C	283	HIS	2.2
4	F	178	GLN	2.2
2	D	387	LEU	2.2
3	E	23	ILE	2.2
4	F	100	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	438	ASP	2.2
2	D	414	ASP	2.2
1	C	356	ASN	2.2
4	F	239	HIS	2.2
1	C	218	ASP	2.2
2	D	407	TRP	2.2
3	E	126	LYS	2.2
3	E	75	LYS	2.2
3	E	138	GLU	2.2
2	D	89	PRO	2.2
4	F	227	PRO	2.2
1	C	349	THR	2.1
2	D	409	THR	2.1
2	D	16	ILE	2.1
4	F	373	SER	2.1
1	C	348	PRO	2.1
2	D	13	GLY	2.1
2	D	81	GLY	2.1
3	E	50	ILE	2.1
1	C	290	GLU	2.1
4	F	331	GLU	2.1
4	F	97	SER	2.1
2	D	218	LYS	2.1
2	D	182	VAL	2.1
2	B	282	GLN	2.1
2	D	206	ASN	2.1
4	F	145	ASN	2.1
1	C	308	ARG	2.1
4	F	258	GLU	2.1
2	D	128	SER	2.1
4	F	230	SER	2.1
1	A	435	VAL	2.1
4	F	177	GLY	2.1
2	B	77	SER	2.1
1	A	256	GLN	2.0
2	D	248	LEU	2.0
2	B	73	GLY	2.0
2	D	61	TYR	2.0
2	D	294	GLN	2.0
1	C	255	PHE	2.0
3	E	133	VAL	2.0
3	E	48	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	41	THR	2.0
2	D	77	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](#)

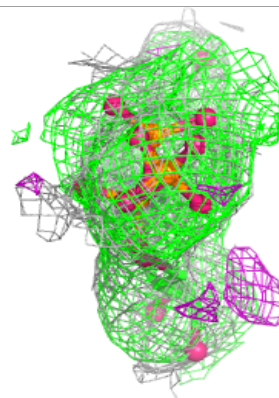
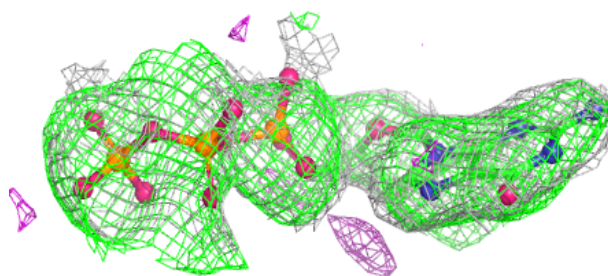
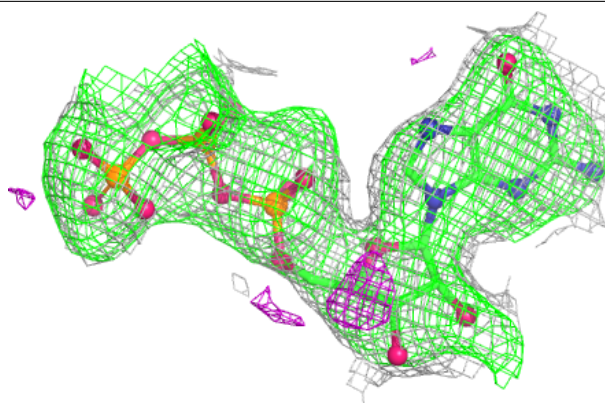
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	A	501	32/32	-	-	32,34,36,39	32
5	GTP	C	501	32/32	-	-	30,31,34,39	32
6	MG	A	502	1/1	-	-	37,37,37,37	1
6	MG	C	502	1/1	-	-	33,33,33,33	1
7	CA	A	503	1/1	-	-	64,64,64,64	1
7	CA	C	503	1/1	-	-	50,50,50,50	1
8	A1EPT	C	504	61/61	0.89	0.10	41,61,73,80	0
9	GDP	D	501	28/28	-	-	65,70,72,73	28
9	GDP	B	501	28/28	-	-	30,38,40,41	28

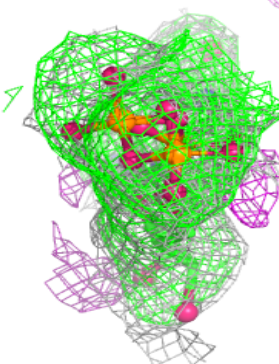
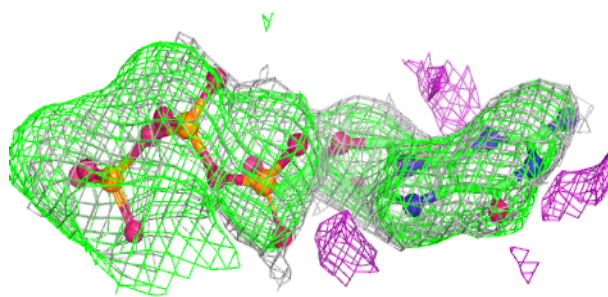
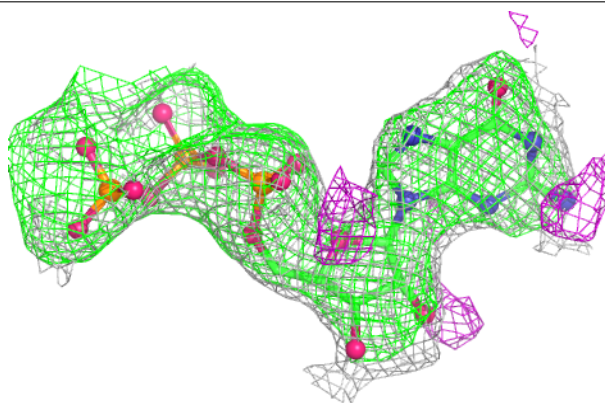
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP A 501:

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

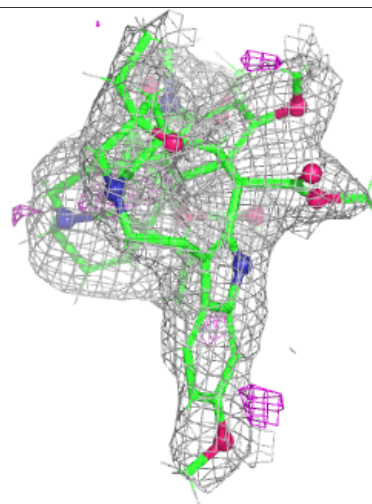
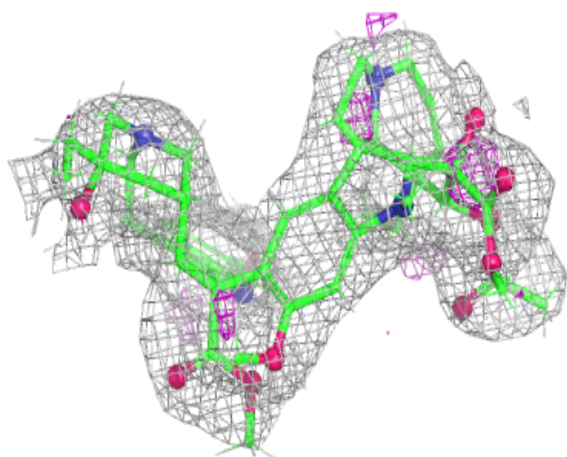
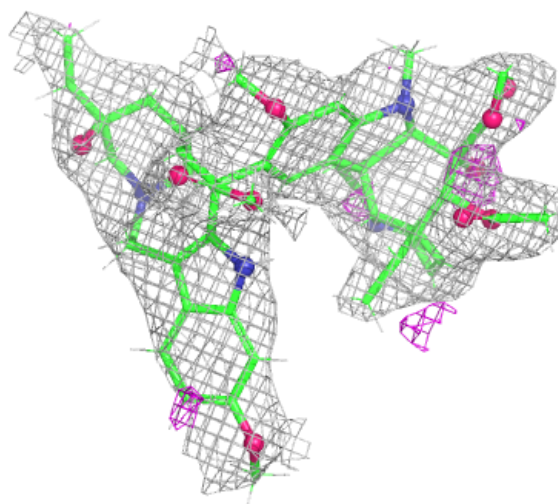
**Electron density around GTP C 501:**

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



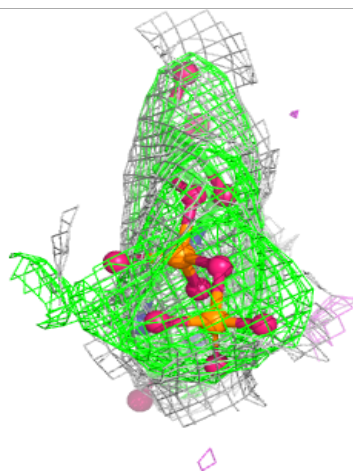
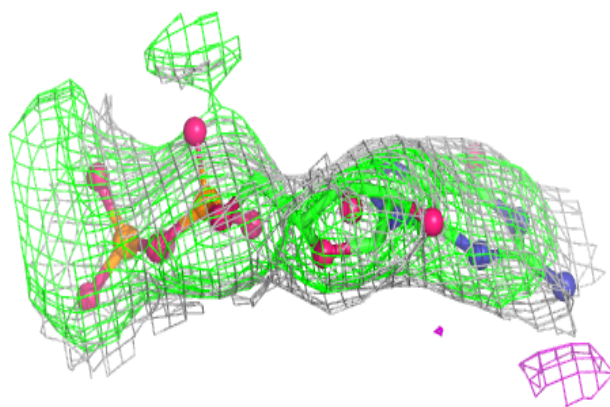
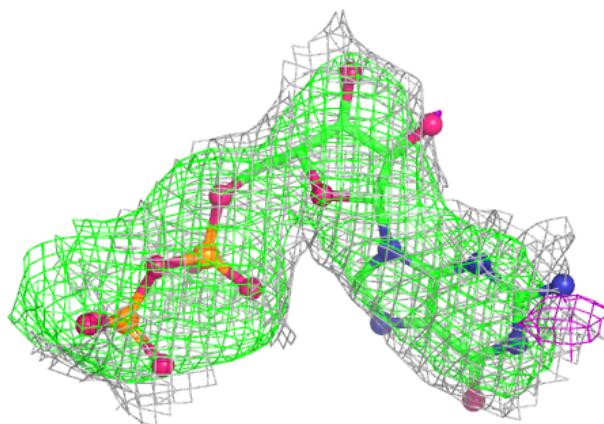
Electron density around A1EPT C 504:

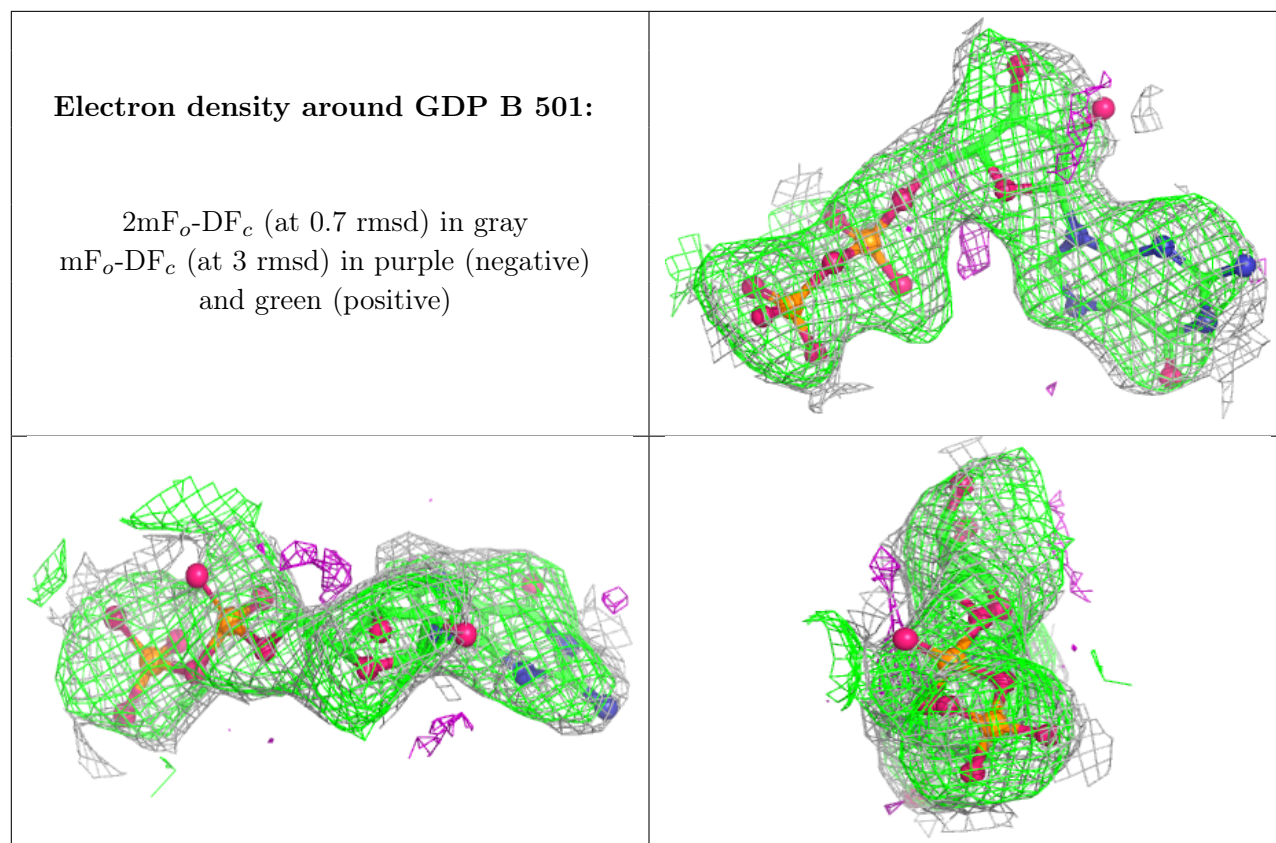
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.