



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 20, 2026 – 08:56 PM JST

PDB ID : 9VYK / pdb_00009vyk
Title : Crystal structure of T2R-TTL-312 complex
Authors : Lun, T.; Chengyong, W.
Deposited on : 2025-07-21
Resolution : 2.65 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:

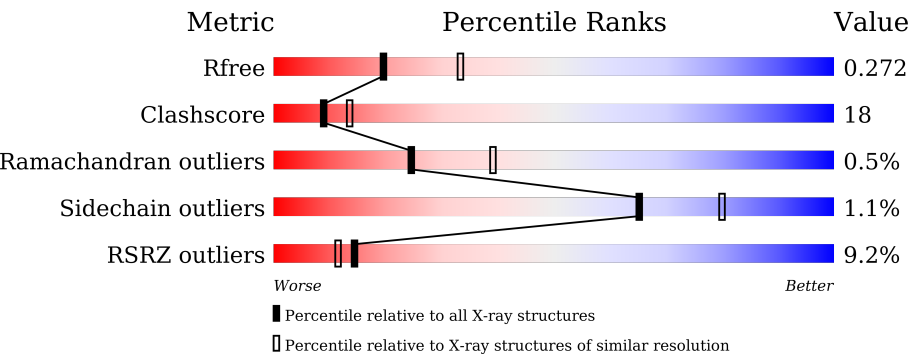
MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	2% 69% 30% ..
1	C	440	2% 71% 29% .
2	B	431	5% 65% 33% ..
2	D	431	21% 58% 39% ..
3	E	136	7% 62% 27% 11%
4	F	380	17% 53% 34% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	A1EUX	B	505	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17419 atoms, of which 25 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	437	Total	C	N	O	S	0	0	0
			3405	2154	580	649	22			
1	C	440	Total	C	N	O	S	0	0	0
			3433	2172	583	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3351	2104	572	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3300	2076	559	638	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

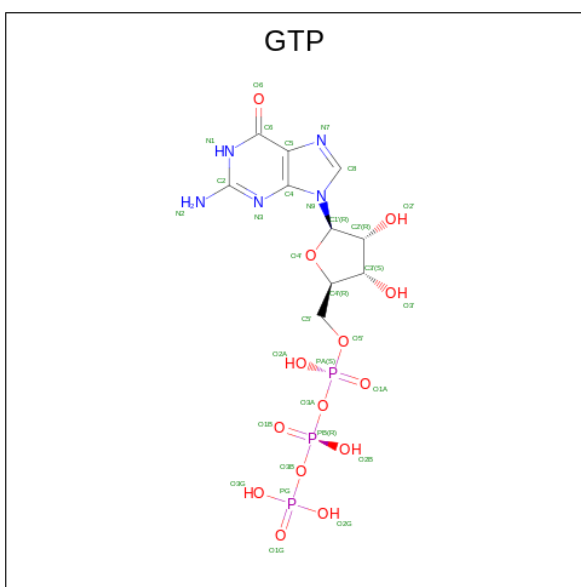
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	0	0
			2713	1740	466	493	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP A0A8C9FGJ1
F	380	HIS	-	expression tag	UNP A0A8C9FGJ1

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



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

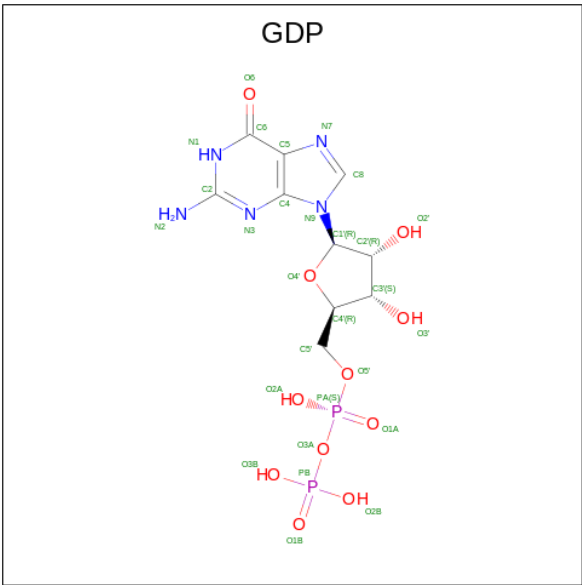
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

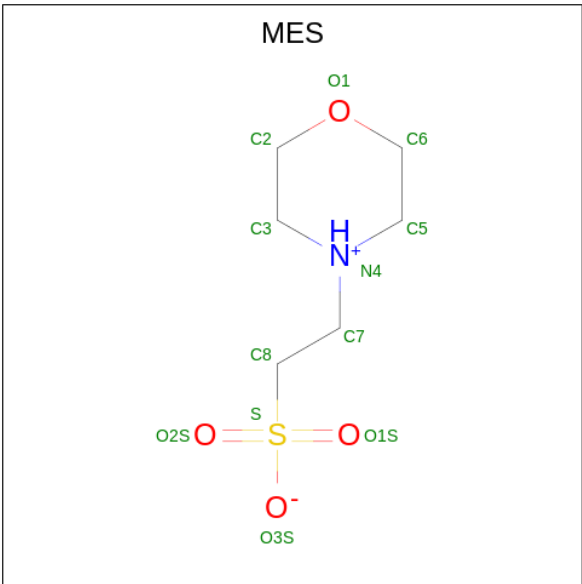
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	1	0
			1	1		
7	B	1	Total	Mg	1	0
			1	1		
7	C	1	Total	Mg	1	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



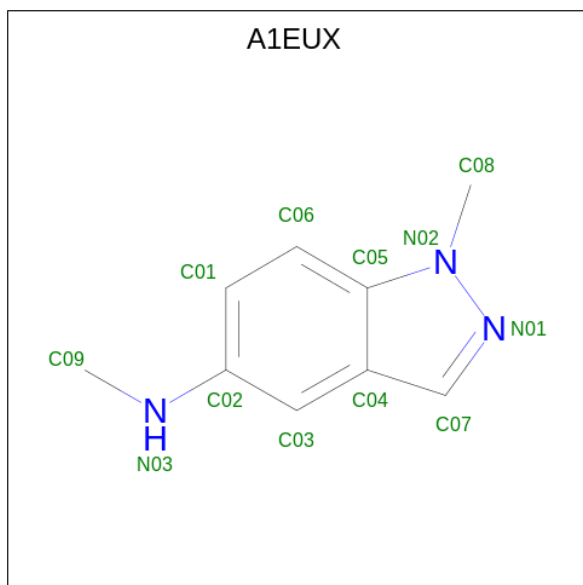
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

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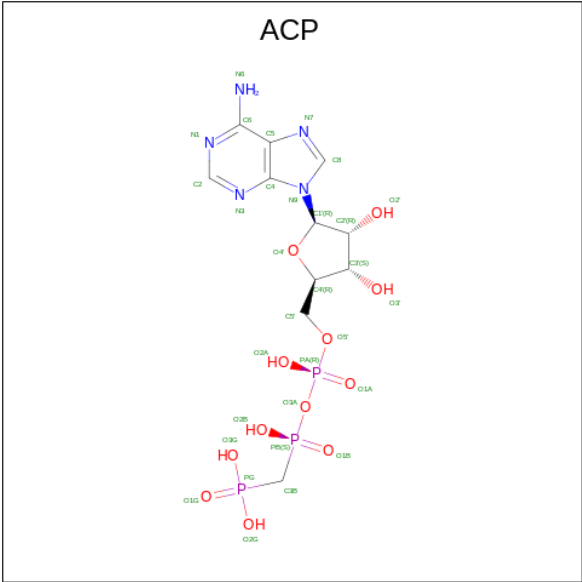
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

- Molecule 10 is {N},1-dimethylindazol-5-amine (CCD ID: A1EUX) (formula: C₉H₁₁N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	N	0	0
			23	9	11	3		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).

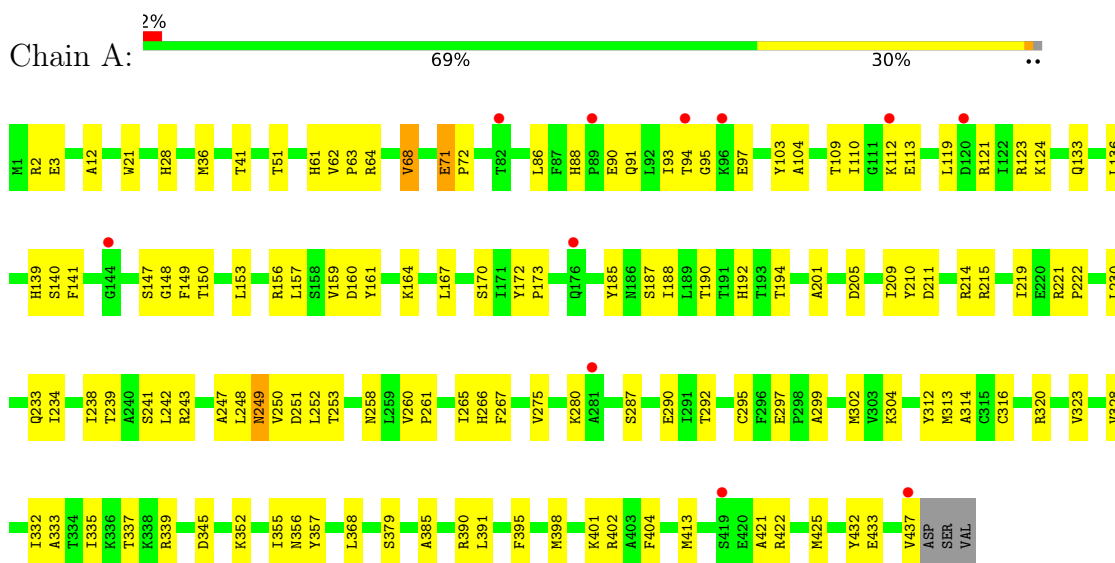


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	
			45	11	14	5	12	3	

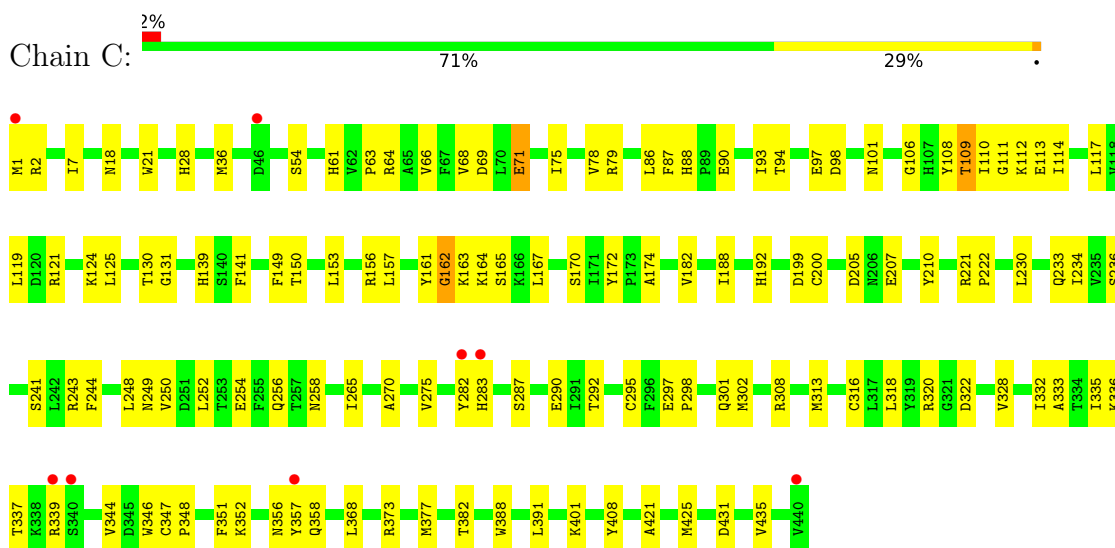
3 Residue-property plots [i](#)

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: Detyrosinated tubulin alpha-1B chain

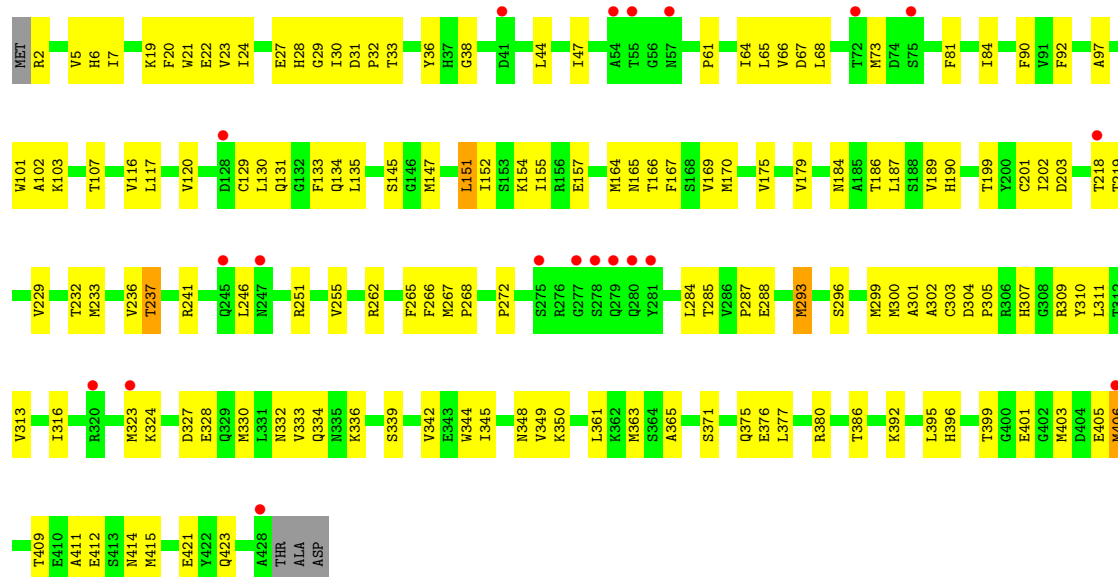


• Molecule 1: Detyrosinated tubulin alpha-1B chain

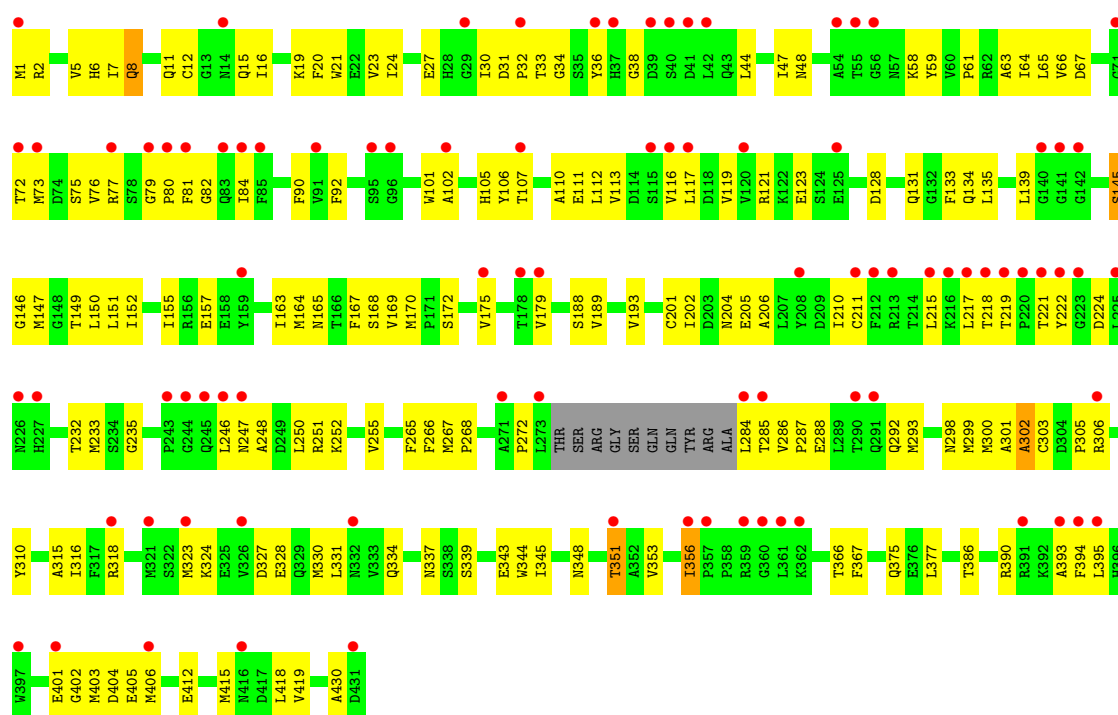


• Molecule 2: Tubulin beta chain

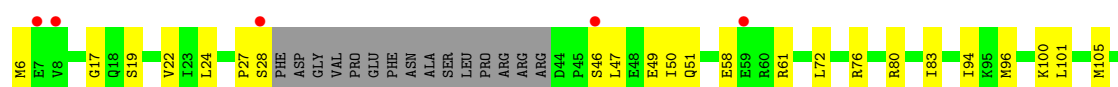




• Molecule 2: Tubulin beta chain

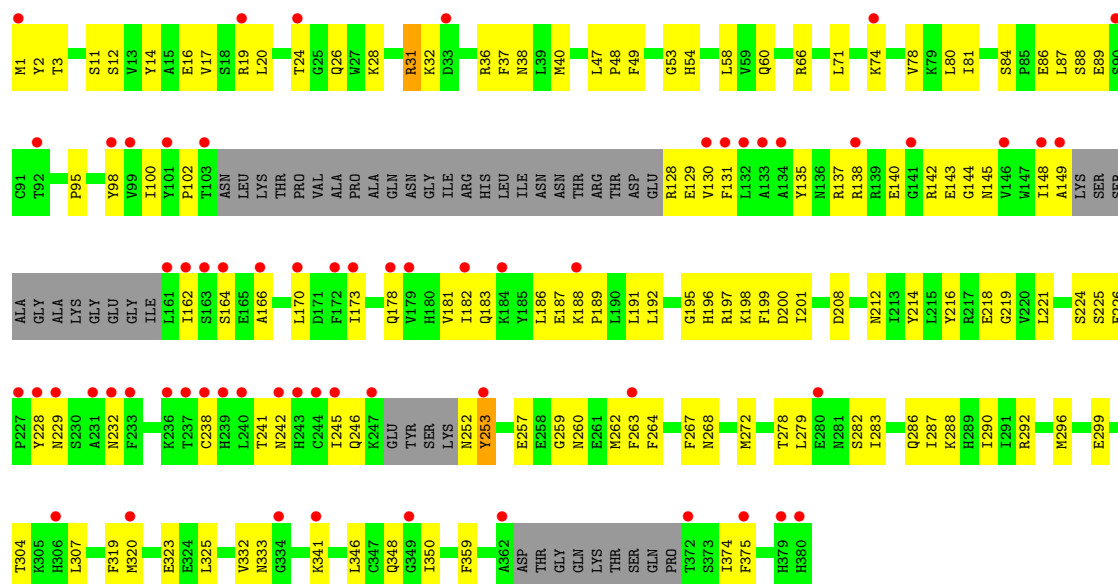


• Molecule 3: Stathmin-4





● 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	104.58Å 156.93Å 180.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.23 – 2.65 59.23 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.6 (59.23-2.65) 98.6 (59.23-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.65Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, R_{free}	0.237 , 0.271 0.239 , 0.272	Depositor DCC
R_{free} test set	4387 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17419	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, A1EUX, ACP, MES, CA, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/3482	0.45	0/4728
1	C	0.35	0/3511	0.47	0/4768
2	B	0.31	0/3426	0.44	0/4643
2	D	0.24	0/3373	0.38	0/4570
3	E	0.28	0/1008	0.37	0/1337
4	F	0.23	0/2775	0.35	0/3752
All	All	0.29	0/17575	0.42	0/23798

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3405	0	3312	113	0
1	C	3433	0	3337	102	1
2	B	3351	0	3216	127	1
2	D	3300	0	3176	152	0
3	E	1000	0	1018	43	0
4	F	2713	0	2659	122	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	B	24	0	26	0	0
10	B	12	11	0	1	0
11	F	31	14	14	0	0
All	All	17394	25	16806	627	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (627) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.44	0.99
2:D:395:LEU:HD21	2:D:405:GLU:HG2	1.46	0.96
4:F:19:ARG:HD3	4:F:20:LEU:HD12	1.48	0.95
2:D:330:MET:HG3	2:D:351:THR:HG21	1.50	0.94
1:A:90:GLU:OE1	1:A:124:LYS:NZ	2.02	0.92
3:E:6:MET:HE2	3:E:24:LEU:HD22	1.53	0.90
2:B:66:VAL:HG12	2:B:147:MET:HE1	1.53	0.88
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.08	0.87
2:D:1:MET:HE3	2:D:128:ASP:HB2	1.55	0.87
2:D:134:GLN:HA	2:D:165:ASN:O	1.77	0.85
2:B:309:ARG:HH21	2:B:342:VAL:HA	1.43	0.84
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.58	0.84
4:F:242:ASN:HB2	4:F:245:ILE:HB	1.60	0.84
2:D:272:PRO:HB3	2:D:284:LEU:HD21	1.61	0.83
1:A:133:GLN:OE1	1:A:252:LEU:N	2.11	0.82
2:B:262:ARG:NH1	2:B:421:GLU:OE1	2.13	0.82
2:D:66:VAL:HG12	2:D:147:MET:HE1	1.61	0.82
1:A:72:PRO:HB3	1:A:94:THR:HG21	1.60	0.81
2:D:315:ALA:HB3	2:D:351:THR:HG22	1.61	0.81
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.65	0.79
2:B:392:LYS:HE3	2:B:405:GLU:OE2	1.81	0.79
4:F:138:ARG:NH1	4:F:144:GLY:O	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:MET:HE2	2:B:377:LEU:HD21	1.64	0.79
4:F:188:LYS:HD3	4:F:323:GLU:OE1	1.84	0.78
2:D:285:THR:HG23	2:D:288:GLU:H	1.48	0.78
4:F:192:LEU:HD21	4:F:262:MET:HE1	1.64	0.78
2:D:73:MET:SD	2:D:92:PHE:HB3	2.24	0.78
1:A:112:LYS:NZ	1:A:113:GLU:OE2	2.15	0.77
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.65	0.77
4:F:100:ILE:HD12	4:F:128:ARG:N	2.00	0.77
2:B:81:PHE:O	2:B:84:ILE:HG22	1.86	0.76
4:F:135:TYR:OH	4:F:164:SER:O	2.03	0.76
2:D:1:MET:HG3	2:D:128:ASP:HB3	1.67	0.76
4:F:278:THR:O	4:F:282:SER:OG	2.02	0.76
4:F:3:THR:HG22	4:F:28:LYS:HG3	1.68	0.76
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.69	0.75
2:D:246:LEU:CD1	2:D:248:ALA:HB2	2.16	0.74
3:E:46:SER:HB3	3:E:49:GLU:HG3	1.69	0.74
4:F:135:TYR:CD2	4:F:166:ALA:HB2	2.22	0.74
2:B:134:GLN:HA	2:B:165:ASN:O	1.88	0.74
2:B:386:THR:HG22	2:B:412:GLU:OE2	1.88	0.73
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.69	0.73
2:D:272:PRO:HB3	2:D:284:LEU:CD2	2.18	0.73
1:C:71:GLU:OE2	2:D:247:ASN:ND2	2.22	0.72
2:D:44:LEU:HA	2:D:47:ILE:HB	1.69	0.72
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.19	0.71
4:F:186:LEU:HD12	4:F:320:MET:CG	2.20	0.70
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.27	0.70
2:D:73:MET:HE3	2:D:90:PHE:HB3	1.72	0.70
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.73	0.70
2:D:63:ALA:O	2:D:64:ILE:HD13	1.91	0.70
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.73	0.70
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.72	0.70
2:B:66:VAL:CG1	2:B:147:MET:HE1	2.22	0.70
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.27	0.69
1:A:88:HIS:N	1:A:91:GLN:OE1	2.22	0.69
4:F:292:ARG:O	4:F:296:MET:HG2	1.91	0.69
1:C:221:ARG:HD2	2:D:327:ASP:OD2	1.92	0.69
2:B:233:MET:O	2:B:237:THR:OG1	2.11	0.69
4:F:221:LEU:HD22	4:F:262:MET:CE	2.24	0.68
4:F:225:SER:HB3	4:F:252:ASN:HB3	1.76	0.68
2:B:237:THR:HB	2:B:241:ARG:HE	1.58	0.68
4:F:137:ARG:O	4:F:137:ARG:NH1	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:CB	1:A:391:LEU:HD21	2.22	0.68
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.29	0.68
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.28	0.68
2:D:73:MET:CE	2:D:90:PHE:HB3	2.24	0.68
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.74	0.67
1:A:402:ARG:HH11	1:A:402:ARG:HG3	1.59	0.67
4:F:144:GLY:HA3	4:F:187:GLU:OE1	1.94	0.67
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.28	0.66
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.31	0.66
3:E:46:SER:O	3:E:50:ILE:HG12	1.95	0.65
1:A:230:LEU:O	1:A:234:ILE:HD12	1.95	0.65
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.78	0.65
2:D:5:VAL:HB	2:D:133:PHE:CD2	2.31	0.65
2:D:80:PRO:O	2:D:81:PHE:HB2	1.96	0.65
1:A:221:ARG:HD2	2:B:327:ASP:OD2	1.96	0.65
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.15	0.64
1:C:101:ASN:ND2	2:D:252:LYS:HE2	2.12	0.64
2:D:395:LEU:HD21	2:D:405:GLU:CG	2.25	0.64
2:B:350:LYS:HG2	10:B:505:A1EUX:C06	2.28	0.64
2:D:5:VAL:HB	2:D:133:PHE:HD2	1.62	0.64
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.30	0.64
2:D:285:THR:HG22	2:D:288:GLU:CG	2.27	0.64
2:D:272:PRO:HG3	2:D:284:LEU:HD13	1.77	0.64
2:B:406:MET:HE3	2:B:406:MET:HA	1.79	0.64
3:E:130:ALA:HA	3:E:133:VAL:HG12	1.77	0.64
2:B:189:VAL:HB	2:B:415:MET:CE	2.27	0.64
4:F:31:ARG:NH2	4:F:32:LYS:HG3	2.13	0.64
2:D:306:ARG:NH2	2:D:337:ASN:OD1	2.31	0.64
2:B:189:VAL:HG11	2:B:415:MET:HE2	1.80	0.64
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.33	0.64
2:B:101:TRP:CE3	2:B:187:LEU:HD13	2.34	0.63
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.33	0.63
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.35	0.62
2:D:66:VAL:CG1	2:D:147:MET:HE1	2.29	0.62
2:D:267:MET:HG2	2:D:301:ALA:HB3	1.82	0.62
1:A:247:ALA:HB3	3:E:19:SER:OG	1.99	0.62
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.00	0.62
2:D:266:PHE:O	2:D:268:PRO:HD3	2.00	0.62
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.30	0.61
2:B:232:THR:OG1	2:B:300:MET:HE3	2.00	0.61
2:B:324:LYS:HE3	2:B:328:GLU:OE2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:HG2	1:A:72:PRO:N	2.14	0.61
2:D:330:MET:O	2:D:334:GLN:HG3	2.00	0.61
2:D:65:LEU:HD22	2:D:90:PHE:CE2	2.36	0.61
2:D:110:ALA:O	2:D:113:VAL:HG12	2.01	0.61
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.83	0.61
1:A:398:MET:HE3	1:A:404:PHE:CD2	2.36	0.61
2:D:30:ILE:HD13	2:D:59:TYR:HB2	1.82	0.60
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.16	0.60
2:B:293:MET:CE	2:B:365:ALA:HB1	2.31	0.60
2:D:189:VAL:HG11	2:D:415:MET:HE2	1.84	0.60
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.37	0.60
1:A:97:GLU:O	1:A:110:ILE:HD13	2.01	0.60
2:B:301:ALA:O	2:B:303:CYS:N	2.35	0.60
2:D:179:VAL:HG21	2:D:394:PHE:CZ	2.37	0.60
2:B:330:MET:O	2:B:334:GLN:HG3	2.01	0.60
1:A:136:LEU:HD23	1:A:167:LEU:HB2	1.84	0.60
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.83	0.60
2:D:19:LYS:O	2:D:23:VAL:HG23	2.02	0.60
2:D:402:GLY:C	3:E:133:VAL:HG23	2.27	0.60
1:C:320:ARG:HA	1:C:356:ASN:O	2.02	0.60
2:B:345:ILE:HG22	2:B:348:ASN:HB3	1.83	0.59
3:E:96:MET:HE3	3:E:100:LYS:HE2	1.83	0.59
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.83	0.59
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.84	0.59
4:F:224:SER:OG	4:F:238:CYS:HA	2.02	0.59
2:B:251:ARG:O	2:B:255:VAL:HG23	2.02	0.59
1:A:97:GLU:HG3	2:B:2:ARG:NH1	2.18	0.59
2:B:309:ARG:NH2	2:B:342:VAL:HA	2.16	0.59
2:D:81:PHE:O	2:D:84:ILE:HG22	2.02	0.59
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.38	0.59
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.38	0.59
4:F:192:LEU:HD21	4:F:262:MET:CE	2.33	0.59
3:E:96:MET:O	3:E:100:LYS:HD3	2.02	0.59
2:D:1:MET:HE3	2:D:128:ASP:CB	2.32	0.58
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.37	0.58
1:A:398:MET:HE3	1:A:404:PHE:HD2	1.68	0.58
1:C:230:LEU:O	1:C:234:ILE:HD12	2.02	0.58
1:C:332:ILE:HG22	1:C:336:LYS:HE2	1.85	0.58
2:B:61:PRO:HD3	2:B:84:ILE:HG12	1.83	0.58
2:D:375:GLN:HB2	2:D:419:VAL:HG13	1.85	0.58
2:D:7:ILE:O	2:D:135:LEU:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:HIS:O	1:C:36:MET:HE3	2.04	0.58
4:F:197:ARG:HH22	4:F:257:GLU:CD	2.10	0.58
2:D:106:TYR:CD1	3:E:133:VAL:HG11	2.39	0.58
4:F:74:LYS:HB3	4:F:181:VAL:HG11	1.85	0.58
1:A:62:VAL:HG13	1:A:86:LEU:O	2.04	0.58
2:D:327:ASP:O	2:D:331:LEU:HD13	2.03	0.58
1:A:63:PRO:CD	1:A:86:LEU:HG	2.34	0.58
1:A:192:HIS:CG	1:A:421:ALA:HA	2.39	0.58
2:D:401:GLU:HA	3:E:137:LYS:HD2	1.84	0.58
1:A:323:VAL:HG12	1:A:355:ILE:HD13	1.85	0.57
2:B:101:TRP:HD1	2:B:145:SER:OG	1.87	0.57
3:E:6:MET:HE2	3:E:24:LEU:CD2	2.31	0.57
4:F:286:GLN:O	4:F:290:ILE:HG13	2.05	0.57
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.86	0.57
2:D:221:THR:HG23	2:D:224:ASP:H	1.70	0.57
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.87	0.57
2:B:65:LEU:HD22	2:B:90:PHE:CE2	2.40	0.57
4:F:3:THR:HG22	4:F:28:LYS:CG	2.35	0.57
2:B:406:MET:CE	2:B:409:THR:HB	2.35	0.57
4:F:20:LEU:O	4:F:24:THR:HG23	2.05	0.57
4:F:87:LEU:O	4:F:88:SER:OG	2.21	0.57
2:D:301:ALA:O	2:D:303:CYS:N	2.35	0.57
4:F:135:TYR:CE1	4:F:145:ASN:HB3	2.40	0.57
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.40	0.56
2:D:172:SER:OG	2:D:205:GLU:HB2	2.05	0.56
1:A:88:HIS:HE1	1:A:90:GLU:HG3	1.69	0.56
2:B:5:VAL:HB	2:B:133:PHE:CD2	2.40	0.56
2:B:316:ILE:N	2:B:316:ILE:HD12	2.21	0.56
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.70	0.56
2:D:102:ALA:HB2	2:D:403:MET:SD	2.46	0.56
4:F:128:ARG:N	4:F:128:ARG:HD2	2.21	0.56
2:B:189:VAL:CB	2:B:415:MET:HE2	2.35	0.56
4:F:262:MET:HE3	4:F:267:PHE:HB2	1.87	0.56
1:A:333:ALA:O	1:A:337:THR:HG23	2.06	0.56
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.41	0.56
4:F:135:TYR:HD2	4:F:166:ALA:HB2	1.69	0.56
4:F:226:GLU:OE2	4:F:252:ASN:HB2	2.06	0.56
1:A:104:ALA:HB2	1:A:413:MET:SD	2.46	0.56
2:B:29:GLY:C	2:B:30:ILE:HD12	2.31	0.56
3:E:121:GLU:O	3:E:124:GLN:HG3	2.06	0.56
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:138:ARG:HB3	4:F:145:ASN:OD1	2.06	0.56
2:B:2:ARG:HB3	2:B:131:GLN:CG	2.36	0.56
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.88	0.56
2:B:203:ASP:CG	2:B:380:ARG:HH22	2.13	0.56
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.41	0.55
2:B:166:THR:OG1	2:B:199:THR:HG22	2.06	0.55
1:A:242:LEU:HD23	1:A:250:VAL:O	2.07	0.55
2:D:386:THR:HG22	2:D:412:GLU:OE2	2.06	0.55
1:A:28:HIS:O	1:A:36:MET:HE3	2.06	0.55
2:D:323:MET:SD	2:D:353:VAL:HG11	2.46	0.55
3:E:130:ALA:O	3:E:133:VAL:HG12	2.06	0.55
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.41	0.55
4:F:287:ILE:HG23	4:F:319:PHE:CE1	2.41	0.55
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.88	0.55
1:C:241:SER:HA	1:C:249:ASN:OD1	2.06	0.55
2:D:206:ALA:O	2:D:210:ILE:HG13	2.06	0.55
2:D:345:ILE:CG2	2:D:348:ASN:HB3	2.35	0.55
1:A:265:ILE:HD12	1:A:265:ILE:N	2.21	0.55
1:C:109:THR:HG22	1:C:110:ILE:HD13	1.89	0.55
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.89	0.55
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.42	0.55
2:D:101:TRP:NE1	2:D:146:GLY:HA2	2.20	0.55
4:F:16:GLU:OE2	4:F:19:ARG:HD2	2.06	0.55
2:B:73:MET:HE3	2:B:90:PHE:HD2	1.70	0.55
2:B:101:TRP:HB2	2:B:184:ASN:OD1	2.06	0.55
4:F:178:GLN:N	4:F:178:GLN:OE1	2.40	0.55
2:B:5:VAL:HB	2:B:133:PHE:HD2	1.72	0.54
1:A:261:PRO:HG3	1:A:313:MET:HB3	1.89	0.54
1:C:97:GLU:HG3	2:D:2:ARG:NH1	2.23	0.54
2:D:63:ALA:C	2:D:64:ILE:HD13	2.32	0.54
3:E:131:GLU:OE1	3:E:134:ARG:NH2	2.31	0.54
1:A:320:ARG:HA	1:A:356:ASN:O	2.07	0.54
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.89	0.54
2:B:189:VAL:CG1	2:B:415:MET:HE2	2.37	0.54
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.38	0.54
2:D:324:LYS:HE2	2:D:328:GLU:OE2	2.07	0.54
4:F:148:ILE:HD13	4:F:162:ILE:HG12	1.88	0.54
4:F:346:LEU:O	4:F:350:ILE:HG13	2.08	0.54
3:E:47:LEU:HD12	3:E:47:LEU:O	2.08	0.54
1:A:402:ARG:HG3	1:A:402:ARG:NH1	2.22	0.54
1:A:210:TYR:OH	1:A:221:ARG:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:LEU:C	2:B:377:LEU:HD23	2.32	0.54
2:D:36:TYR:CE1	2:D:38:GLY:HA3	2.43	0.54
2:B:293:MET:HE3	2:B:365:ALA:HB1	1.90	0.53
4:F:195:GLY:HA3	4:F:197:ARG:HD2	1.91	0.53
4:F:229:ASN:ND2	4:F:232:ASN:OD1	2.41	0.53
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.24	0.53
1:A:248:LEU:HD12	1:A:249:ASN:H	1.72	0.53
1:C:254:GLU:HG2	1:C:352:LYS:CE	2.35	0.53
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.44	0.53
2:D:101:TRP:HD1	2:D:145:SER:OG	1.90	0.53
1:C:153:LEU:O	1:C:157:LEU:HG	2.09	0.53
2:D:23:VAL:O	2:D:27:GLU:HG3	2.08	0.53
1:A:28:HIS:NE2	1:A:243:ARG:HD2	2.23	0.53
2:B:19:LYS:O	2:B:23:VAL:HG23	2.09	0.53
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.44	0.53
2:B:67:ASP:O	2:B:92:PHE:HA	2.09	0.53
2:D:105:HIS:O	2:D:150:LEU:HD22	2.08	0.53
3:E:131:GLU:OE1	3:E:131:GLU:HA	2.08	0.52
2:D:286:VAL:HB	2:D:287:PRO:HD3	1.91	0.52
3:E:101:LEU:O	3:E:105:MET:HG2	2.09	0.52
4:F:191:LEU:HA	4:F:197:ARG:O	2.09	0.52
1:A:328:VAL:O	1:A:332:ILE:HG13	2.09	0.52
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.92	0.52
1:C:192:HIS:CG	1:C:421:ALA:HA	2.44	0.52
4:F:135:TYR:HE1	4:F:145:ASN:HB3	1.73	0.52
1:A:94:THR:HG22	1:A:95:GLY:O	2.09	0.52
2:D:251:ARG:O	2:D:255:VAL:HG23	2.09	0.52
1:A:260:VAL:HG11	1:A:266:HIS:HB3	1.92	0.52
4:F:225:SER:CB	4:F:252:ASN:HB3	2.39	0.52
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.45	0.52
2:B:44:LEU:HA	2:B:47:ILE:HB	1.91	0.52
2:B:310:TYR:CD1	2:B:371:SER:HB2	2.45	0.52
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.24	0.52
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.39	0.52
2:D:64:ILE:HD12	2:D:119:VAL:HG12	1.92	0.52
4:F:31:ARG:HG3	4:F:32:LYS:N	2.25	0.52
1:A:292:THR:O	1:A:295:CYS:HB2	2.10	0.52
2:D:293:MET:CG	2:D:367:PHE:HB2	2.40	0.52
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.91	0.51
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.40	0.51
2:D:221:THR:HG22	2:D:224:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:PHE:O	2:B:268:PRO:HD3	2.10	0.51
2:D:64:ILE:HD12	2:D:119:VAL:CG1	2.40	0.51
1:C:79:ARG:NH2	1:C:94:THR:HG23	2.26	0.51
2:D:404:ASP:OD1	2:D:405:GLU:N	2.43	0.51
2:B:64:ILE:HD12	2:B:120:VAL:HG22	1.92	0.51
2:D:65:LEU:HD23	2:D:76:VAL:HG11	1.93	0.51
2:D:272:PRO:HG3	2:D:284:LEU:CD1	2.41	0.51
4:F:195:GLY:C	4:F:197:ARG:HG3	2.36	0.51
1:A:147:SER:HB2	1:A:190:THR:HB	1.92	0.51
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.46	0.51
4:F:142:ARG:O	4:F:142:ARG:HG2	2.11	0.51
1:C:265:ILE:HG22	1:C:265:ILE:O	2.10	0.51
1:C:333:ALA:O	1:C:337:THR:HG23	2.11	0.51
2:D:193:VAL:HG22	2:D:265:PHE:CE2	2.46	0.51
1:C:287:SER:OG	1:C:290:GLU:HG3	2.09	0.51
1:A:401:LYS:HG3	2:B:344:TRP:CE3	2.46	0.51
1:C:298:PRO:O	1:C:301:GLN:HG3	2.11	0.51
2:B:73:MET:CE	2:B:90:PHE:HB3	2.41	0.51
2:D:65:LEU:N	2:D:65:LEU:HD12	2.26	0.51
2:B:2:ARG:HA	2:B:129:CYS:O	2.11	0.50
2:B:36:TYR:CE1	2:B:38:GLY:HA3	2.44	0.50
1:C:66:VAL:HG23	1:C:125:LEU:HD12	1.93	0.50
1:A:187:SER:HB2	1:A:391:LEU:HD21	1.93	0.50
2:B:116:VAL:HG11	2:B:151:LEU:HD21	1.92	0.50
2:B:272:PRO:HD2	2:B:361:LEU:HD13	1.93	0.50
2:B:313:VAL:HB	2:B:349:VAL:HG22	1.94	0.50
2:D:145:SER:OG	2:D:188:SER:OG	2.27	0.50
2:D:377:LEU:C	2:D:377:LEU:HD23	2.36	0.50
4:F:138:ARG:HB3	4:F:145:ASN:CG	2.35	0.50
4:F:138:ARG:HB3	4:F:145:ASN:ND2	2.26	0.50
2:D:72:THR:O	2:D:76:VAL:HG23	2.12	0.50
2:B:186:THR:HA	2:B:415:MET:HE1	1.93	0.50
3:E:119:MET:O	3:E:122:ARG:HG2	2.10	0.50
2:D:107:THR:O	2:D:111:GLU:HG3	2.11	0.50
2:D:157:GLU:CA	3:E:123:LEU:HD13	2.42	0.50
1:A:401:LYS:HG3	2:B:344:TRP:CD2	2.47	0.50
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.93	0.50
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.47	0.49
2:B:330:MET:O	2:B:333:VAL:HG12	2.11	0.49
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.42	0.49
2:B:169:VAL:HA	2:B:202:ILE:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:157:GLU:HA	3:E:123:LEU:HD13	1.94	0.49
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.77	0.49
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.94	0.49
2:B:332:ASN:ND2	2:B:336:LYS:HE2	2.27	0.49
1:C:244:PHE:CZ	1:C:358:GLN:OE1	2.66	0.49
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.94	0.49
2:D:292:GLN:HB3	2:D:298:ASN:ND2	2.27	0.49
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.42	0.49
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.44	0.49
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.94	0.49
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.46	0.49
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.95	0.49
1:C:270:ALA:HB3	1:C:302:MET:CG	2.43	0.49
4:F:137:ARG:NH2	4:F:143:GLU:OE2	2.46	0.49
2:B:116:VAL:CG1	2:B:151:LEU:HD21	2.42	0.49
1:A:433:GLU:O	1:A:437:VAL:HG23	2.12	0.48
2:B:73:MET:HE3	2:B:90:PHE:CD2	2.48	0.48
1:C:165:SER:HA	1:C:199:ASP:OD2	2.13	0.48
2:D:64:ILE:HD11	2:D:123:GLU:HG3	1.94	0.48
4:F:131:PHE:CG	4:F:182:ILE:HD11	2.47	0.48
4:F:95:PRO:HB2	4:F:183:GLN:HG2	1.96	0.48
4:F:208:ASP:OD2	4:F:212:ASN:HB2	2.13	0.48
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.94	0.48
2:B:65:LEU:N	2:B:65:LEU:HD12	2.28	0.48
1:C:162:GLY:CA	3:E:94:ILE:HD11	2.39	0.48
1:A:390:ARG:HD3	4:F:54:HIS:CD2	2.49	0.48
2:B:395:LEU:HD21	2:B:405:GLU:HG2	1.94	0.48
2:D:285:THR:CG2	2:D:288:GLU:HG3	2.44	0.48
4:F:49:PHE:CB	4:F:66:ARG:HD2	2.43	0.48
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.48	0.48
1:A:345:ASP:O	3:E:28:SER:N	2.46	0.48
1:C:302:MET:N	1:C:302:MET:HE2	2.28	0.48
2:D:44:LEU:O	2:D:47:ILE:HG22	2.13	0.48
2:D:145:SER:HG	2:D:188:SER:HG	1.58	0.48
3:E:72:LEU:O	3:E:76:ARG:HG2	2.14	0.48
2:D:1:MET:HB3	2:D:48:ASN:ND2	2.29	0.48
4:F:1:MET:HG2	4:F:26:GLN:HA	1.96	0.48
2:B:304:ASP:HB3	2:B:307:HIS:CG	2.49	0.48
4:F:192:LEU:CD2	4:F:262:MET:HE1	2.38	0.48
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.49	0.48
1:A:221:ARG:NH2	2:B:323:MET:SD	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:LEU:O	2:D:155:ILE:HG13	2.13	0.48
1:A:241:SER:HB2	1:A:249:ASN:O	2.14	0.47
2:D:152:ILE:HG23	2:D:164:MET:HG2	1.96	0.47
2:D:1:MET:HG3	2:D:128:ASP:CB	2.42	0.47
2:D:285:THR:OG1	2:D:287:PRO:HD2	2.15	0.47
2:D:330:MET:HE2	2:D:351:THR:CG2	2.44	0.47
2:B:296:SER:HA	2:B:299:MET:HG2	1.96	0.47
4:F:135:TYR:HE2	4:F:166:ALA:H	1.62	0.47
4:F:198:LYS:HG2	4:F:199:PHE:N	2.29	0.47
2:B:117:LEU:HD11	2:B:154:LYS:HD3	1.96	0.47
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.97	0.47
2:D:285:THR:HG22	2:D:288:GLU:HG3	1.95	0.47
2:D:404:ASP:CG	2:D:406:MET:HG2	2.40	0.47
4:F:135:TYR:HE2	4:F:166:ALA:N	2.13	0.47
1:A:215:ARG:CZ	1:A:299:ALA:HB1	2.44	0.47
2:B:61:PRO:CD	2:B:84:ILE:HG12	2.44	0.47
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.96	0.47
1:A:28:HIS:CE1	1:A:243:ARG:HB3	2.50	0.47
2:B:103:LYS:HA	2:B:107:THR:OG1	2.15	0.47
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.96	0.47
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.97	0.47
4:F:170:LEU:O	4:F:173:ILE:HG12	2.15	0.47
4:F:268:ASN:O	4:F:272:MET:HG3	2.15	0.47
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.97	0.47
1:A:201:ALA:HB3	1:A:267:PHE:CD2	2.50	0.47
1:C:282:TYR:O	1:C:283:HIS:HB2	2.15	0.47
2:D:285:THR:HG22	2:D:288:GLU:CD	2.39	0.47
2:D:11:GLN:HG2	2:D:15:GLN:OE1	2.15	0.47
2:D:12:CYS:O	2:D:16:ILE:HG23	2.15	0.47
3:E:80:ARG:HA	3:E:83:ILE:HG22	1.95	0.47
2:B:189:VAL:HB	2:B:415:MET:HE2	1.94	0.47
1:C:108:TYR:O	1:C:112:LYS:HG2	2.15	0.47
2:D:75:SER:O	2:D:79:GLY:N	2.46	0.47
2:D:246:LEU:HD12	2:D:248:ALA:HB2	1.93	0.47
2:B:332:ASN:HD21	2:B:336:LYS:HE2	1.80	0.46
2:D:20:PHE:CE1	2:D:24:ILE:HG21	2.50	0.46
2:D:235:GLY:HA3	2:D:366:THR:OG1	2.15	0.46
4:F:148:ILE:O	4:F:182:ILE:HA	2.15	0.46
2:B:190:HIS:CD2	2:B:411:ALA:HA	2.51	0.46
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.33	0.46
1:A:287:SER:OG	1:A:290:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.98	0.46
1:C:163:LYS:HD3	1:C:163:LYS:HA	1.78	0.46
2:D:20:PHE:CD1	2:D:233:MET:HE2	2.51	0.46
1:A:395:PHE:CD1	1:A:422:ARG:HD3	2.50	0.46
2:B:152:ILE:HG23	2:B:164:MET:HG2	1.97	0.46
1:C:101:ASN:HD21	2:D:252:LYS:HE2	1.80	0.46
4:F:197:ARG:HB3	4:F:224:SER:O	2.15	0.46
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.98	0.46
1:C:401:LYS:HG3	2:D:344:TRP:CD2	2.51	0.46
3:E:139:LEU:O	3:E:139:LEU:HG	2.16	0.46
2:B:30:ILE:HD12	2:B:30:ILE:N	2.30	0.46
1:C:161:TYR:O	1:C:162:GLY:C	2.59	0.46
1:C:265:ILE:N	1:C:265:ILE:HD12	2.30	0.46
2:B:396:HIS:HA	2:B:399:THR:OG1	2.15	0.46
2:D:206:ALA:HB2	2:D:302:ALA:N	2.30	0.46
4:F:86:GLU:C	4:F:87:LEU:HD23	2.41	0.46
4:F:100:ILE:HG23	4:F:128:ARG:N	2.30	0.46
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.51	0.45
4:F:191:LEU:HD23	4:F:196:HIS:C	2.40	0.45
2:D:7:ILE:HG21	2:D:151:LEU:CD2	2.46	0.45
1:C:164:LYS:HE2	1:C:164:LYS:HB2	1.66	0.45
2:D:139:LEU:HD21	2:D:168:SER:HB3	1.98	0.45
2:D:170:MET:O	2:D:204:ASN:HB2	2.16	0.45
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.97	0.45
2:B:311:LEU:HD23	2:B:342:VAL:HG11	1.98	0.45
1:C:21:TRP:CH2	1:C:63:PRO:HB3	2.52	0.45
3:E:96:MET:CE	3:E:100:LYS:HE2	2.47	0.45
2:D:316:ILE:N	2:D:316:ILE:HD12	2.32	0.45
1:A:133:GLN:OE1	1:A:251:ASP:HA	2.17	0.45
4:F:296:MET:HE1	4:F:299:GLU:OE1	2.17	0.45
1:C:63:PRO:HD3	1:C:86:LEU:HG	1.99	0.45
1:C:313:MET:HE2	1:C:382:THR:HG23	1.98	0.45
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.47	0.45
2:D:31:ASP:OD1	2:D:33:THR:HG22	2.17	0.45
1:A:124:LYS:HE2	1:A:124:LYS:HB3	1.76	0.45
2:B:199:THR:OG1	2:B:265:PHE:CD1	2.70	0.45
1:C:2:ARG:HA	1:C:131:GLY:O	2.17	0.45
4:F:19:ARG:CD	4:F:20:LEU:HD12	2.34	0.45
2:B:157:GLU:HB2	3:E:72:LEU:HD13	1.98	0.45
2:D:232:THR:OG1	2:D:300:MET:HE3	2.17	0.45
4:F:47:LEU:C	4:F:47:LEU:HD23	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:HE2	1:A:280:LYS:HB3	1.79	0.44
2:B:31:ASP:CG	2:B:33:THR:HG22	2.42	0.44
2:D:201:CYS:SG	2:D:265:PHE:HB3	2.58	0.44
4:F:148:ILE:HG13	4:F:149:ALA:N	2.32	0.44
1:A:209:ILE:HD11	1:A:302:MET:SD	2.57	0.44
2:B:28:HIS:HB3	2:B:47:ILE:HD13	1.97	0.44
2:B:36:TYR:CD2	2:B:44:LEU:HD11	2.52	0.44
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.52	0.44
2:D:218:THR:HG23	2:D:219:THR:N	2.31	0.44
2:D:315:ALA:HB3	2:D:351:THR:CG2	2.40	0.44
2:D:344:TRP:CE3	2:D:345:ILE:HG13	2.53	0.44
4:F:20:LEU:HD23	4:F:348:GLN:OE1	2.17	0.44
4:F:148:ILE:HD13	4:F:162:ILE:CG1	2.48	0.44
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.51	0.44
2:B:64:ILE:CD1	2:B:120:VAL:HG22	2.47	0.44
2:B:179:VAL:HG22	1:C:258:ASN:OD1	2.18	0.44
1:C:236:SER:OG	1:C:243:ARG:NH2	2.50	0.44
1:C:335:ILE:HG23	1:C:339:ARG:CG	2.43	0.44
2:D:32:PRO:O	2:D:84:ILE:HB	2.17	0.44
4:F:253:TYR:CZ	4:F:259:GLY:HA2	2.52	0.44
1:C:292:THR:O	1:C:295:CYS:HB2	2.17	0.44
2:D:113:VAL:O	2:D:117:LEU:HG	2.18	0.44
2:D:117:LEU:O	2:D:121:ARG:HG3	2.18	0.44
4:F:95:PRO:HD2	4:F:183:GLN:NE2	2.33	0.44
4:F:192:LEU:HD12	4:F:192:LEU:N	2.31	0.44
1:A:123:ARG:HH22	1:A:160:ASP:HB3	1.81	0.44
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.52	0.44
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.33	0.44
2:B:309:ARG:NH1	2:B:339:SER:O	2.50	0.44
1:C:332:ILE:HG23	1:C:351:PHE:CD2	2.53	0.44
2:D:167:PHE:CE2	2:D:233:MET:HG2	2.52	0.44
2:B:324:LYS:O	2:B:328:GLU:HG3	2.18	0.44
1:C:244:PHE:CE1	1:C:358:GLN:OE1	2.71	0.44
1:A:12:ALA:CB	1:A:140:SER:HB3	2.48	0.44
1:A:123:ARG:NH2	1:A:160:ASP:HB3	2.33	0.44
1:A:312:TYR:CE2	1:A:379:SER:HB2	2.53	0.44
2:B:284:LEU:O	2:B:363:MET:CE	2.66	0.44
4:F:374:ILE:O	4:F:374:ILE:HG13	2.17	0.44
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.00	0.44
1:C:316:CYS:O	1:C:377:MET:HG3	2.17	0.44
4:F:189:PRO:O	4:F:191:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:MET:HE3	2:B:409:THR:HB	2.00	0.44
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.98	0.44
2:D:267:MET:CE	2:D:299:MET:HG3	2.48	0.44
4:F:71:LEU:O	4:F:332:VAL:HB	2.18	0.44
4:F:282:SER:CB	4:F:325:LEU:HD13	2.48	0.44
1:A:221:ARG:NE	2:B:323:MET:HB3	2.33	0.43
1:A:90:GLU:O	1:A:121:ARG:HD2	2.18	0.43
1:A:97:GLU:HG3	2:B:2:ARG:HH12	1.82	0.43
1:A:159:VAL:HG12	1:A:160:ASP:OD1	2.18	0.43
1:A:234:ILE:O	1:A:238:ILE:HG13	2.17	0.43
4:F:47:LEU:HD23	4:F:48:PRO:N	2.33	0.43
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.53	0.43
2:B:102:ALA:HB2	2:B:403:MET:SD	2.58	0.43
2:B:218:THR:HG23	2:B:219:THR:N	2.33	0.43
1:C:97:GLU:O	1:C:110:ILE:HG21	2.19	0.43
2:D:330:MET:HE2	2:D:351:THR:HG23	2.00	0.43
4:F:137:ARG:NH1	4:F:140:GLU:HB3	2.34	0.43
2:B:307:HIS:ND1	2:B:376:GLU:OE2	2.44	0.43
1:C:1:MET:HG3	1:C:2:ARG:H	1.83	0.43
2:D:112:LEU:O	2:D:116:VAL:HG23	2.18	0.43
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.52	0.43
2:B:285:THR:HB	2:B:287:PRO:HD2	2.00	0.43
2:B:310:TYR:CE1	2:B:371:SER:HB2	2.54	0.43
1:C:18:ASN:HD21	1:C:78:VAL:CG2	2.31	0.43
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.99	0.43
1:A:258:ASN:O	1:A:314:ALA:HB1	2.18	0.43
2:B:68:LEU:HD12	2:B:97:ALA:HB2	2.00	0.43
2:B:202:ILE:HG21	2:B:229:VAL:HG22	2.01	0.43
1:C:322:ASP:HB3	1:C:373:ARG:HH21	1.84	0.43
4:F:11:SER:OG	4:F:14:TYR:HB2	2.17	0.43
1:A:316:CYS:HA	1:A:352:LYS:O	2.19	0.43
2:B:21:TRP:CE3	2:B:61:PRO:HB3	2.54	0.43
1:C:139:HIS:CG	1:C:150:THR:HG21	2.53	0.43
1:A:112:LYS:HE2	3:E:61:ARG:NH2	2.34	0.43
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.58	0.43
4:F:14:TYR:HA	4:F:17:VAL:HB	2.00	0.43
4:F:31:ARG:HG3	4:F:32:LYS:H	1.83	0.43
1:A:323:VAL:HG12	1:A:355:ILE:CD1	2.48	0.43
2:B:167:PHE:HE2	2:B:236:VAL:HG21	1.84	0.43
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.96	0.42
1:C:54:SER:HB3	1:C:64:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LYS:HE2	1:C:124:LYS:HB3	1.77	0.42
1:C:328:VAL:O	1:C:332:ILE:HG13	2.17	0.42
1:A:153:LEU:O	1:A:157:LEU:HG	2.20	0.42
1:C:79:ARG:HH22	1:C:94:THR:HG23	1.85	0.42
1:C:119:LEU:HD12	1:C:156:ARG:NH2	2.33	0.42
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.00	0.42
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.54	0.42
1:C:401:LYS:HG3	2:D:344:TRP:CE3	2.54	0.42
2:D:7:ILE:HD13	2:D:151:LEU:HD21	2.00	0.42
2:D:193:VAL:CG2	2:D:418:LEU:HD22	2.49	0.42
4:F:3:THR:O	4:F:38:ASN:HB2	2.18	0.42
4:F:80:LEU:HD12	4:F:84:SER:OG	2.18	0.42
4:F:130:VAL:HG12	4:F:130:VAL:O	2.19	0.42
1:C:388:TRP:CE3	1:C:425:MET:HE1	2.54	0.42
2:D:6:HIS:HE2	2:D:8:GLN:HG2	1.83	0.42
4:F:135:TYR:HE1	4:F:145:ASN:CB	2.31	0.42
1:A:2:ARG:O	1:A:51:THR:HG22	2.20	0.42
1:A:302:MET:N	1:A:302:MET:HE2	2.35	0.42
1:A:345:ASP:HB2	3:E:28:SER:HB2	2.01	0.42
1:C:69:ASP:O	1:C:94:THR:HA	2.20	0.42
1:A:68:VAL:HG21	1:A:149:PHE:CE2	2.55	0.42
1:A:93:ILE:CD1	1:A:121:ARG:HG3	2.50	0.42
1:A:172:TYR:CG	1:A:173:PRO:HD2	2.54	0.42
2:B:190:HIS:CE1	2:B:414:ASN:HD22	2.37	0.42
1:C:1:MET:HB3	1:C:130:THR:OG1	2.20	0.42
2:D:267:MET:HE1	2:D:305:PRO:HG3	2.00	0.42
4:F:78:VAL:HG21	4:F:181:VAL:HG21	2.01	0.42
4:F:138:ARG:HD2	4:F:143:GLU:HB2	2.01	0.42
4:F:191:LEU:HD22	4:F:196:HIS:CD2	2.54	0.42
2:B:284:LEU:O	2:B:363:MET:HE1	2.20	0.42
2:D:175:VAL:CG1	2:D:222:TYR:HE1	2.32	0.42
3:E:22:VAL:HG13	3:E:22:VAL:O	2.19	0.42
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.43	0.42
2:D:21:TRP:CH2	2:D:61:PRO:HB3	2.55	0.42
4:F:31:ARG:HH21	4:F:32:LYS:HG3	1.84	0.42
4:F:36:ARG:HA	4:F:58:LEU:CD1	2.50	0.42
4:F:53:GLY:N	4:F:60:GLN:OE1	2.43	0.42
4:F:98:TYR:O	4:F:181:VAL:HG23	2.20	0.42
4:F:102:PRO:HG3	4:F:178:GLN:O	2.20	0.42
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.50	0.42
1:A:72:PRO:CB	1:A:94:THR:HG21	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:HB3	1:C:98:ASP:HB3	2.01	0.42
1:C:106:GLY:O	1:C:111:GLY:HA3	2.20	0.42
2:D:211:CYS:O	2:D:215:LEU:HB2	2.20	0.42
2:D:386:THR:O	2:D:390:ARG:HG2	2.20	0.42
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.54	0.42
2:B:5:VAL:HG23	2:B:130:LEU:CD1	2.50	0.42
3:E:138:GLU:C	3:E:140:LYS:H	2.27	0.42
2:B:44:LEU:O	2:B:47:ILE:HG22	2.20	0.41
2:B:66:VAL:CG1	2:B:147:MET:CE	2.94	0.41
1:C:248:LEU:CD1	1:C:357:TYR:OH	2.68	0.41
1:C:318:LEU:HD12	1:C:318:LEU:N	2.35	0.41
2:D:272:PRO:HB3	2:D:284:LEU:HD22	2.01	0.41
3:E:101:LEU:HD12	3:E:101:LEU:HA	1.82	0.41
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.92	0.41
1:A:265:ILE:O	1:A:265:ILE:HG22	2.20	0.41
1:A:357:TYR:CD2	3:E:17:GLY:HA2	2.55	0.41
2:B:267:MET:HE1	2:B:305:PRO:HG3	2.00	0.41
3:E:130:ALA:HA	3:E:133:VAL:CG1	2.47	0.41
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.02	0.41
2:B:2:ARG:O	2:B:131:GLN:NE2	2.35	0.41
2:B:7:ILE:O	2:B:135:LEU:HA	2.20	0.41
2:B:332:ASN:O	2:B:336:LYS:HG3	2.20	0.41
2:B:375:GLN:OE1	2:B:423:GLN:HG2	2.19	0.41
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.38	0.41
4:F:2:TYR:CE2	4:F:359:PHE:HB3	2.55	0.41
4:F:16:GLU:O	4:F:20:LEU:HD13	2.20	0.41
1:A:72:PRO:HB3	1:A:94:THR:CG2	2.42	0.41
1:C:68:VAL:HG11	1:C:149:PHE:CE2	2.55	0.41
3:E:127:ASP:O	3:E:131:GLU:HG2	2.21	0.41
1:A:185:TYR:CZ	1:A:398:MET:HE2	2.55	0.41
1:A:194:THR:O	1:A:194:THR:HG22	2.21	0.41
2:B:28:HIS:NE2	2:B:241:ARG:HB3	2.35	0.41
1:C:391:LEU:HD23	1:C:391:LEU:HA	1.84	0.41
2:D:267:MET:HE2	2:D:267:MET:HB3	1.85	0.41
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.50	0.41
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.02	0.41
2:D:77:ARG:O	2:D:82:GLY:HA3	2.20	0.41
2:D:318:ARG:HH21	2:D:356:ILE:HG12	1.85	0.41
2:B:23:VAL:O	2:B:27:GLU:HG3	2.21	0.41
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.34	0.41
2:D:67:ASP:O	2:D:92:PHE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:343:GLU:HG3	2:D:430:ALA:HB2	2.03	0.41
4:F:232:ASN:OD1	4:F:232:ASN:N	2.51	0.41
4:F:288:LYS:HB2	4:F:288:LYS:HE3	1.88	0.41
1:A:214:ARG:HG2	1:A:219:ILE:O	2.21	0.41
2:B:103:LYS:HE2	2:B:401:GLU:OE2	2.20	0.41
2:B:237:THR:O	2:B:241:ARG:HG3	2.21	0.41
2:B:285:THR:O	2:B:288:GLU:N	2.54	0.41
1:C:252:LEU:O	1:C:256:GLN:HG3	2.21	0.41
1:C:270:ALA:HB3	1:C:302:MET:HG2	2.02	0.41
2:D:34:GLY:C	2:D:58:LYS:HD3	2.46	0.41
2:D:169:VAL:HA	2:D:202:ILE:O	2.21	0.41
3:E:51:GLN:OE1	3:E:51:GLN:HA	2.20	0.41
2:D:2:ARG:HB3	2:D:131:GLN:CG	2.51	0.41
2:D:293:MET:HG3	2:D:367:PHE:HB2	2.02	0.41
4:F:87:LEU:HD23	4:F:87:LEU:N	2.34	0.41
4:F:138:ARG:HD3	4:F:138:ARG:HA	1.81	0.41
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.56	0.40
2:B:151:LEU:O	2:B:155:ILE:HG13	2.20	0.40
1:C:431:ASP:O	1:C:435:VAL:HG13	2.21	0.40
2:D:31:ASP:CG	2:D:33:THR:HG22	2.46	0.40
2:D:145:SER:O	2:D:149:THR:HG23	2.21	0.40
2:D:393:ALA:HB1	2:D:394:PHE:CD1	2.56	0.40
3:E:130:ALA:C	3:E:133:VAL:HG12	2.46	0.40
4:F:191:LEU:HD23	4:F:196:HIS:O	2.21	0.40
4:F:148:ILE:HG22	4:F:183:GLN:O	2.21	0.40
4:F:191:LEU:HD21	4:F:228:TYR:HB3	2.03	0.40
1:C:182:VAL:HB	1:C:408:TYR:OH	2.20	0.40
1:C:250:VAL:HG11	1:C:352:LYS:CE	2.49	0.40
2:D:7:ILE:O	2:D:135:LEU:HA	2.21	0.40
3:E:130:ALA:CA	3:E:133:VAL:HG12	2.46	0.40
2:D:211:CYS:HB3	2:D:217:LEU:HD12	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:GLU:OE1	1:C:282:TYR:OH[4_545]	2.18	0.02

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	435/440 (99%)	425 (98%)	8 (2%)	2 (0%)	24	39
1	C	438/440 (100%)	426 (97%)	10 (2%)	2 (0%)	24	39
2	B	425/431 (99%)	411 (97%)	12 (3%)	2 (0%)	24	39
2	D	417/431 (97%)	401 (96%)	14 (3%)	2 (0%)	24	39
3	E	117/136 (86%)	113 (97%)	3 (3%)	1 (1%)	14	24
4	F	322/380 (85%)	301 (94%)	19 (6%)	2 (1%)	21	34
All	All	2154/2258 (95%)	2077 (96%)	66 (3%)	11 (0%)	24	39

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	302	ALA
4	F	129	GLU
2	B	302	ALA
2	B	175	VAL
1	C	109	THR
3	E	27	PRO
1	A	109	THR
1	A	249	ASN
4	F	253	TYR
2	D	145	SER
1	C	162	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/371 (99%)	361 (99%)	5 (1%)	59	76
1	C	370/371 (100%)	367 (99%)	3 (1%)	73	85
2	B	367/372 (99%)	362 (99%)	5 (1%)	59	76
2	D	362/372 (97%)	358 (99%)	4 (1%)	65	80
3	E	109/122 (89%)	109 (100%)	0	100	100
4	F	295/338 (87%)	291 (99%)	4 (1%)	59	76
All	All	1869/1946 (96%)	1848 (99%)	21 (1%)	65	80

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	68	VAL
1	A	71	GLU
1	A	253	THR
1	A	297	GLU
2	B	151	LEU
2	B	237	THR
2	B	246	LEU
2	B	293	MET
2	B	406	MET
1	C	71	GLU
1	C	297	GLU
1	C	347	CYS
2	D	8	GLN
2	D	339	SER
2	D	351	THR
2	D	356	ILE
4	F	12	SER
4	F	31	ARG
4	F	89	GLU
4	F	333	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	C	133	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\# Z > 2$
8	GDP	B	501	7	28,30,30	1.14	3 (10%)	44,47,47	1.84	8 (18%)
10	A1EUX	B	505	-	13,13,13	4.34	7 (53%)	17,18,18	8.32	8 (47%)
9	MES	B	503	-	12,12,12	1.12	1 (8%)	14,16,16	0.86	1 (7%)
5	GTP	C	501	7	30,34,34	0.83	1 (3%)	46,54,54	1.77	10 (21%)
11	ACP	F	401	-	30,33,33	2.04	2 (6%)	45,52,52	0.94	3 (6%)
5	GTP	A	501	7	30,34,34	0.82	1 (3%)	46,54,54	1.76	10 (21%)
8	GDP	D	501	-	28,30,30	1.14	3 (10%)	44,47,47	1.86	8 (18%)
9	MES	B	502	-	12,12,12	1.14	1 (8%)	14,16,16	0.86	1 (7%)

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
8	GDP	B	501	7	-	3/16/32/32	0/3/3/3
10	A1EUX	B	505	-	-	2/2/2/2	0/2/2/2
9	MES	B	503	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	7	-	4/22/38/38	0/3/3/3
11	ACP	F	401	-	-	1/19/38/38	0/3/3/3
5	GTP	A	501	7	-	7/22/38/38	0/3/3/3
8	GDP	D	501	-	-	4/16/32/32	0/3/3/3
9	MES	B	502	-	-	0/6/14/14	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	A1EUX	N02-N01	-12.24	1.30	1.37
11	F	401	ACP	PB-O3A	10.28	1.69	1.58
10	B	505	A1EUX	C02-N03	5.04	1.46	1.37
10	B	505	A1EUX	C04-C07	4.91	1.48	1.42
10	B	505	A1EUX	C04-C05	3.95	1.47	1.41
10	B	505	A1EUX	C05-N02	3.41	1.44	1.36
8	B	501	GDP	C5-C4	3.14	1.47	1.38
8	D	501	GDP	C5-C4	3.10	1.47	1.38
9	B	502	MES	C8-S	3.04	1.81	1.77
9	B	503	MES	C8-S	2.99	1.81	1.77
8	B	501	GDP	C6-N1	-2.43	1.34	1.38
10	B	505	A1EUX	C06-C01	2.43	1.43	1.38
8	D	501	GDP	C6-N1	-2.41	1.34	1.38
5	C	501	GTP	C2-N3	2.26	1.38	1.33
11	F	401	ACP	PB-O2B	-2.21	1.51	1.56
5	A	501	GTP	C2-N3	2.21	1.38	1.33
8	B	501	GDP	C5-N7	-2.13	1.35	1.39
8	D	501	GDP	C5-N7	-2.12	1.35	1.39
10	B	505	A1EUX	C07-N01	-2.04	1.29	1.32

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	A1EUX	C05-N02-N01	19.12	122.11	111.62
10	B	505	A1EUX	C04-C05-N02	-16.14	100.84	106.68
10	B	505	A1EUX	C04-C07-N01	13.77	122.50	112.06
10	B	505	A1EUX	C07-N01-N02	-11.99	96.71	106.42
10	B	505	A1EUX	C05-C04-C07	-11.03	97.84	104.48
10	B	505	A1EUX	C08-N02-C05	-6.73	119.75	128.39
8	B	501	GDP	C5-C4-N3	-6.11	118.55	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C4-N3	-5.97	118.77	128.46
5	C	501	GTP	C5-C4-N3	-4.97	120.39	128.46
5	A	501	GTP	C5-C4-N3	-4.95	120.44	128.46
8	B	501	GDP	C2-N3-C4	4.86	120.95	112.30
8	D	501	GDP	C2-N3-C4	4.83	120.91	112.30
10	B	505	A1EUX	C03-C04-C07	4.80	143.32	135.50
10	B	505	A1EUX	C06-C05-N02	4.59	138.28	132.07
8	B	501	GDP	N9-C4-N3	4.59	135.15	125.94
8	D	501	GDP	N9-C4-N3	4.52	135.01	125.94
5	C	501	GTP	C2-N3-C4	4.46	120.24	112.30
5	A	501	GTP	C2-N3-C4	4.43	120.20	112.30
8	D	501	GDP	PA-O3A-PB	-3.82	119.70	132.83
5	A	501	GTP	PA-O3A-PB	-3.67	120.22	132.83
5	C	501	GTP	PA-O3A-PB	-3.66	120.26	132.83
5	A	501	GTP	PB-O3B-PG	-3.59	120.50	132.83
5	C	501	GTP	PB-O3B-PG	-3.58	120.54	132.83
8	B	501	GDP	PA-O3A-PB	-3.33	121.38	132.83
5	C	501	GTP	N9-C4-N3	3.22	132.41	125.94
5	A	501	GTP	N9-C4-N3	3.20	132.36	125.94
8	D	501	GDP	C6-C5-N7	3.20	136.19	130.25
8	B	501	GDP	C6-C5-N7	3.10	136.01	130.25
11	F	401	ACP	O2B-PB-O1B	3.05	120.24	110.07
5	C	501	GTP	C2-N1-C6	-2.88	119.85	125.10
5	A	501	GTP	C2-N1-C6	-2.88	119.85	125.10
11	F	401	ACP	O1G-PG-C3B	-2.63	105.58	111.24
11	F	401	ACP	PB-O3A-PA	-2.59	124.33	132.56
8	B	501	GDP	C4-C5-N7	-2.56	106.67	110.72
8	D	501	GDP	C4-C5-N7	-2.55	106.68	110.72
5	C	501	GTP	C5-C6-N1	2.53	119.60	113.19
5	A	501	GTP	C5-C6-N1	2.52	119.58	113.19
5	C	501	GTP	N9-C8-N7	-2.51	108.66	113.39
5	A	501	GTP	N9-C8-N7	-2.50	108.69	113.39
5	A	501	GTP	C8-N7-C5	2.48	108.72	104.24
5	C	501	GTP	C8-N7-C5	2.47	108.72	104.24
8	B	501	GDP	C3'-C2'-C1'	2.43	106.05	101.43
5	A	501	GTP	O6-C6-C5	-2.40	120.24	126.60
5	C	501	GTP	O6-C6-C5	-2.38	120.30	126.60
8	D	501	GDP	C3'-C2'-C1'	2.16	105.53	101.43
8	D	501	GDP	O6-C6-C5	-2.14	120.93	126.60
8	B	501	GDP	O6-C6-C5	-2.11	121.00	126.60
9	B	502	MES	O2S-S-C8	-2.08	104.41	106.92
9	B	503	MES	O2S-S-C8	-2.05	104.44	106.92

There are no chirality outliers.

All (21) torsion outliers are listed below:

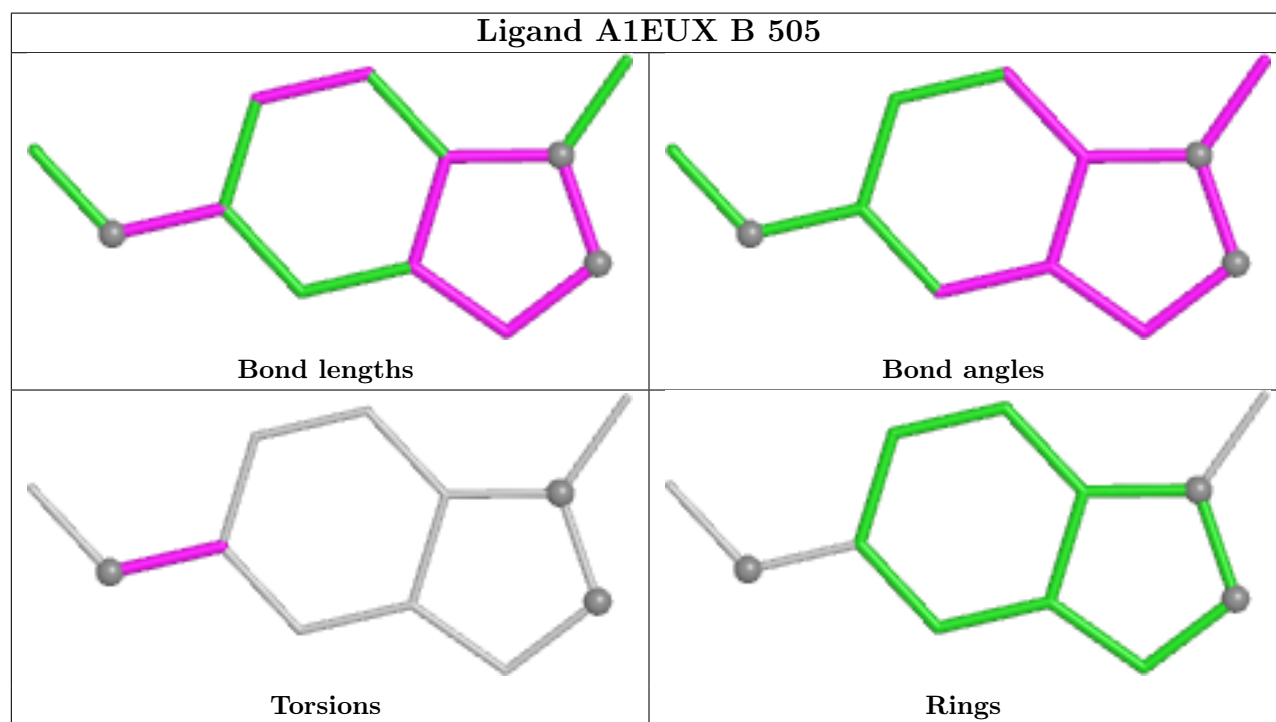
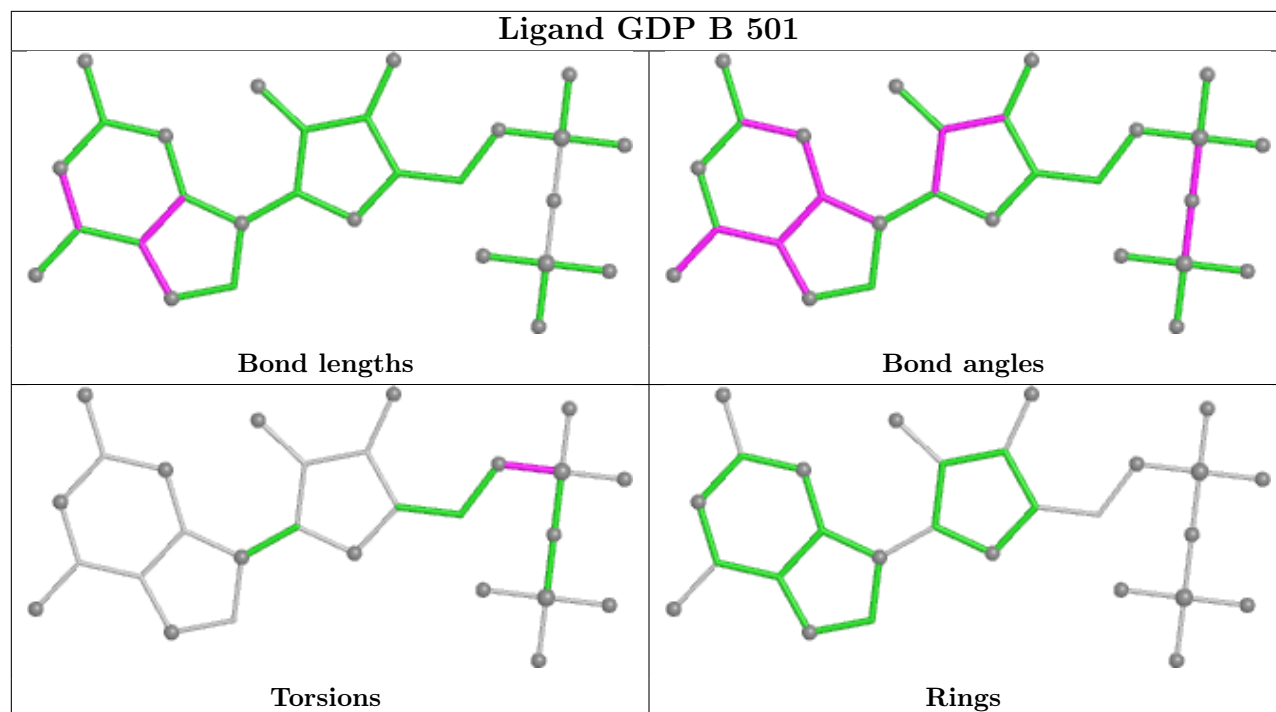
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	PA-O3A-PB-O3B
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
10	B	505	A1EUX	C01-C02-N03-C09
10	B	505	A1EUX	C03-C02-N03-C09
8	D	501	GDP	PA-O3A-PB-O1B
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
8	B	501	GDP	C5'-O5'-PA-O3A
11	F	401	ACP	O4'-C4'-C5'-O5'

There are no ring outliers.

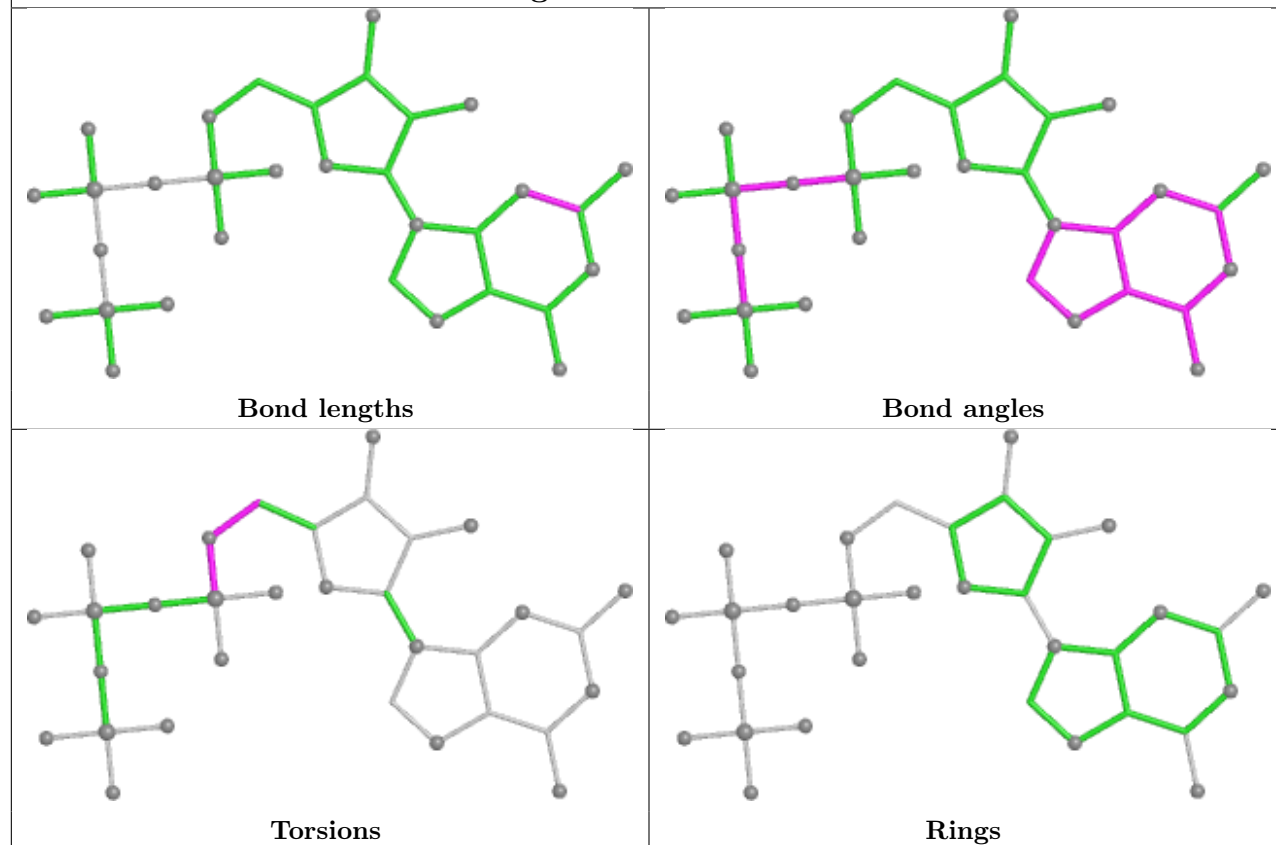
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	A1EUX	1	0

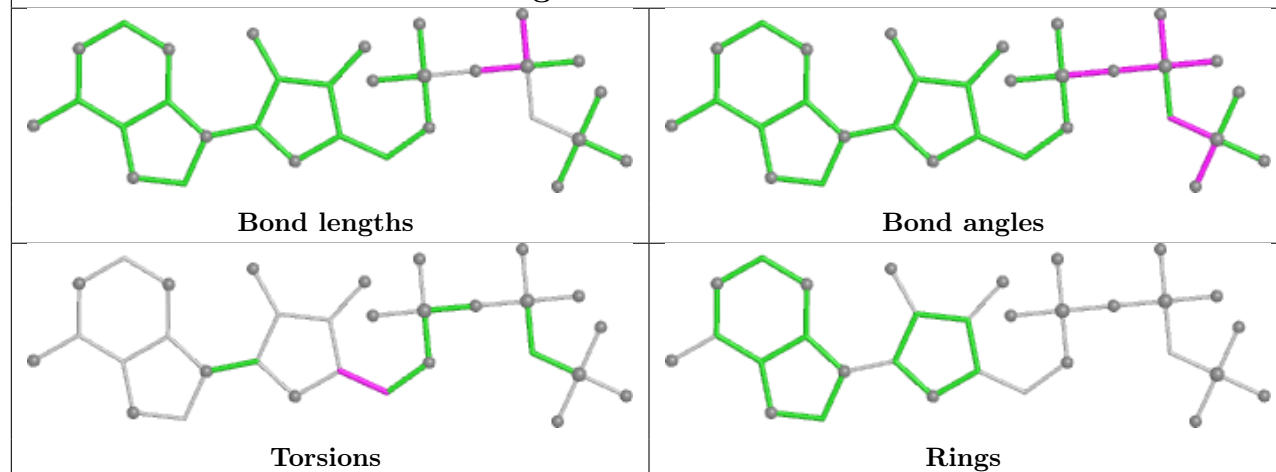
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

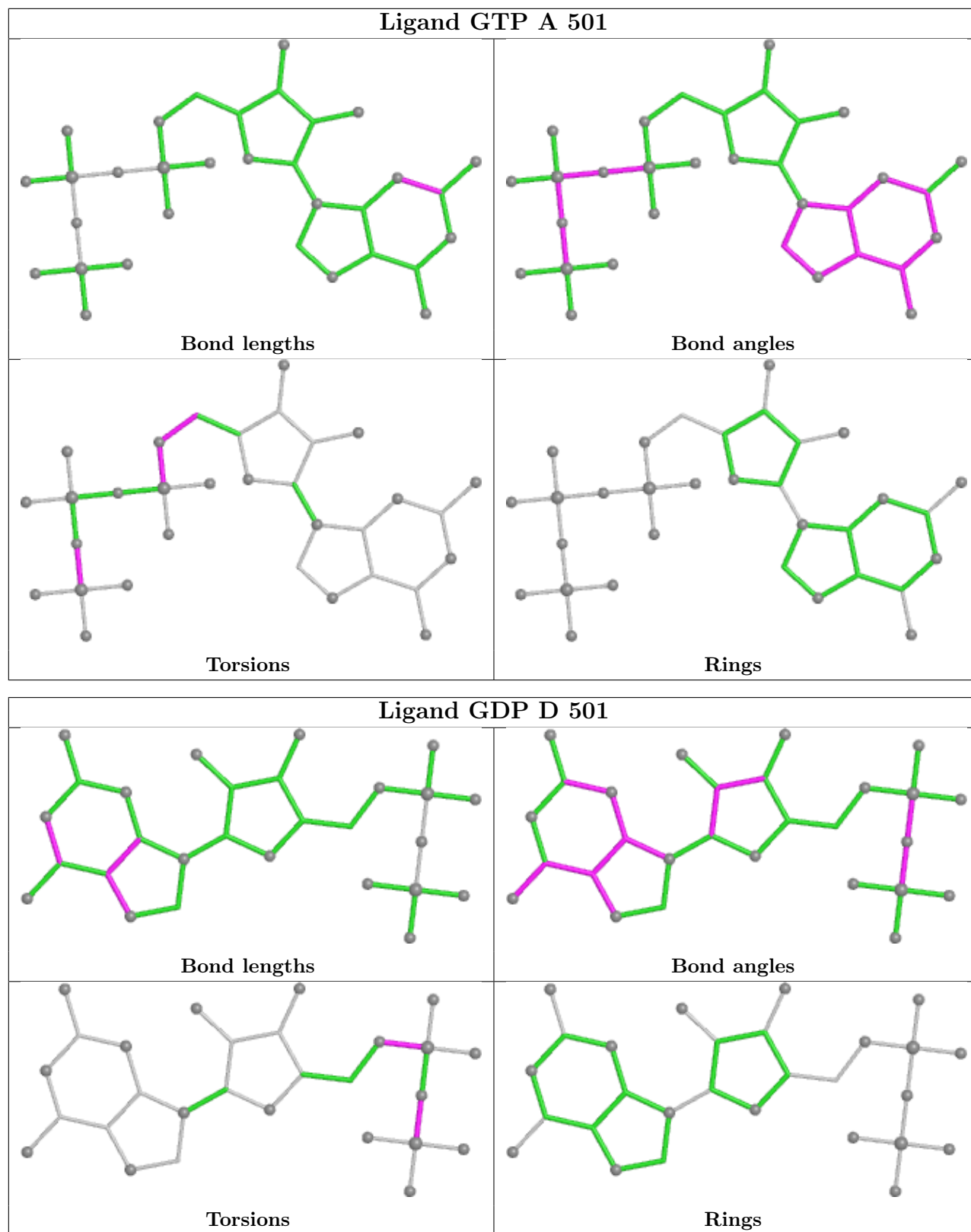


Ligand GTP C 501



Ligand ACP F 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/440 (99%)	0.34	11 (2%) 58 52	33, 49, 68, 83	0
1	C	440/440 (100%)	0.02	8 (1%) 67 63	25, 41, 60, 78	0
2	B	427/431 (99%)	0.37	20 (4%) 36 28	30, 49, 77, 108	0
2	D	421/431 (97%)	1.29	89 (21%) 2 1	39, 73, 104, 123	0
3	E	121/136 (88%)	0.86	10 (8%) 17 12	42, 60, 92, 103	0
4	F	332/380 (87%)	1.04	63 (18%) 3 2	43, 69, 129, 142	0
All	All	2178/2258 (96%)	0.60	201 (9%) 14 11	25, 54, 99, 142	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	247	ASN	5.8
2	D	141	GLY	5.2
4	F	362	ALA	4.5
2	D	212	PHE	4.4
4	F	161	LEU	4.4
2	B	218	THR	4.4
2	D	323	MET	4.3
2	D	431	ASP	4.2
2	D	80	PRO	4.2
2	D	179	VAL	4.1
2	D	397	TRP	4.0
2	B	72	THR	4.0
2	D	219	THR	3.9
2	D	208	TYR	3.8
4	F	173	ILE	3.8
2	D	362	LYS	3.8
2	D	216	LYS	3.8
2	D	32	PRO	3.7
2	D	220	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
4	F	149	ALA	3.6
4	F	253	TYR	3.6
2	B	55	THR	3.5
4	F	233	PHE	3.5
2	D	55	THR	3.4
2	B	278	SER	3.4
4	F	103	THR	3.4
4	F	162	ILE	3.3
2	D	218	THR	3.3
2	D	72	THR	3.3
3	E	115	HIS	3.3
1	A	437	VAL	3.3
2	D	360	GLY	3.2
2	D	54	ALA	3.2
2	D	85	PHE	3.2
2	D	394	PHE	3.2
4	F	99	VAL	3.2
1	A	96	LYS	3.2
4	F	74	LYS	3.2
2	B	279	GLN	3.2
2	D	356	ILE	3.2
4	F	245	ILE	3.2
2	D	91	VAL	3.2
2	B	280	GLN	3.1
4	F	146	VAL	3.1
2	D	221	THR	3.1
2	D	273	LEU	3.1
2	D	71	GLY	3.1
2	B	428	ALA	3.1
4	F	182	ILE	3.1
1	A	82	THR	3.1
1	C	339	ARG	3.1
2	B	275	SER	3.1
2	D	215	LEU	3.0
4	F	372	THR	3.0
2	D	217	LEU	3.0
2	D	395	LEU	3.0
3	E	28	SER	2.9
2	B	128	ASP	2.9
2	D	96	GLY	2.9
2	B	54	ALA	2.9
2	D	227	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	73	MET	2.9
4	F	242	ASN	2.9
4	F	170	LEU	2.9
2	D	245	GLN	2.8
4	F	101	TYR	2.8
2	D	361	LEU	2.8
4	F	237	THR	2.8
4	F	239	HIS	2.8
4	F	263	PHE	2.8
2	D	1	MET	2.8
4	F	247	LYS	2.8
2	D	284	LEU	2.8
4	F	172	PHE	2.8
4	F	243	HIS	2.8
4	F	33	ASP	2.8
4	F	244	CYS	2.8
2	B	281	TYR	2.8
2	D	223	GLY	2.7
1	A	94	THR	2.7
3	E	59	GLU	2.7
4	F	231	ALA	2.7
2	B	277	GLY	2.7
4	F	379	HIS	2.7
2	D	359	ARG	2.7
4	F	134	ALA	2.7
2	D	211	CYS	2.7
3	E	139	LEU	2.7
2	D	244	GLY	2.7
1	C	440	VAL	2.7
3	E	8	VAL	2.7
4	F	131	PHE	2.7
4	F	179	VAL	2.7
4	F	148	ILE	2.7
4	F	380	HIS	2.7
4	F	334	GLY	2.6
1	C	340	SER	2.6
4	F	130	VAL	2.6
2	D	81	PHE	2.6
4	F	164	SER	2.6
2	D	178	THR	2.6
2	D	41	ASP	2.6
2	B	406	MET	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	166	ALA	2.6
2	B	75	SER	2.6
2	D	83	GLN	2.6
2	D	393	ALA	2.6
1	A	281	ALA	2.5
2	D	222	TYR	2.5
2	B	323	MET	2.5
2	D	290	THR	2.5
2	D	42	LEU	2.5
4	F	280	GLU	2.5
2	D	77	ARG	2.5
2	D	115	SER	2.5
1	C	1	MET	2.5
4	F	1	MET	2.5
4	F	133	ALA	2.5
2	D	306	ARG	2.4
4	F	227	PRO	2.4
4	F	188	LYS	2.4
2	D	159	TYR	2.4
2	D	175	VAL	2.4
4	F	306	HIS	2.4
4	F	141	GLY	2.4
2	D	120	VAL	2.4
4	F	240	LEU	2.4
2	D	291	GLN	2.4
4	F	178	GLN	2.4
2	B	247	ASN	2.3
2	D	40	SER	2.3
3	E	135	LYS	2.3
4	F	236	LYS	2.3
2	D	84	ILE	2.3
1	C	282	TYR	2.3
4	F	92	THR	2.3
4	F	232	ASN	2.3
4	F	163	SER	2.3
2	D	351	THR	2.3
3	E	128	LYS	2.3
2	D	391	ARG	2.3
1	C	283	HIS	2.3
2	D	107	THR	2.3
2	D	321	MET	2.3
4	F	341	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	419	SER	2.3
2	D	243	PRO	2.3
2	D	140	GLY	2.3
2	D	37	HIS	2.2
2	D	116	VAL	2.2
2	D	246	LEU	2.2
4	F	132	LEU	2.2
3	E	141	GLU	2.2
4	F	229	ASN	2.2
2	D	357	PRO	2.2
2	D	285	THR	2.2
4	F	19	ARG	2.2
2	D	332	ASN	2.2
4	F	98	TYR	2.2
4	F	228	TYR	2.2
2	D	29	GLY	2.2
2	D	225	LEU	2.2
2	B	320	ARG	2.2
2	D	213	ARG	2.2
2	D	39	ASP	2.2
3	E	46	SER	2.2
4	F	375	PHE	2.2
4	F	238	CYS	2.1
2	B	57	ASN	2.1
2	D	226	ASN	2.1
1	C	357	TYR	2.1
2	D	79	GLY	2.1
2	B	41	ASP	2.1
2	D	95	SER	2.1
2	D	326	VAL	2.1
2	D	271	ALA	2.1
2	D	125	GLU	2.1
1	A	176	GLN	2.1
2	B	245	GLN	2.1
2	D	416	ASN	2.1
2	D	142	GLY	2.1
4	F	138	ARG	2.1
4	F	24	THR	2.1
1	A	89	PRO	2.1
4	F	320	MET	2.1
2	D	14	ASN	2.1
2	D	56	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	46	ASP	2.1
4	F	90	SER	2.1
2	D	401	GLU	2.1
1	A	112	LYS	2.1
4	F	184	LYS	2.1
2	D	117	LEU	2.1
2	D	318	ARG	2.0
3	E	7	GLU	2.0
2	D	36	TYR	2.0
1	A	120	ASP	2.0
2	D	102	ALA	2.0
2	D	406	MET	2.0
1	A	144	GLY	2.0
4	F	349	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

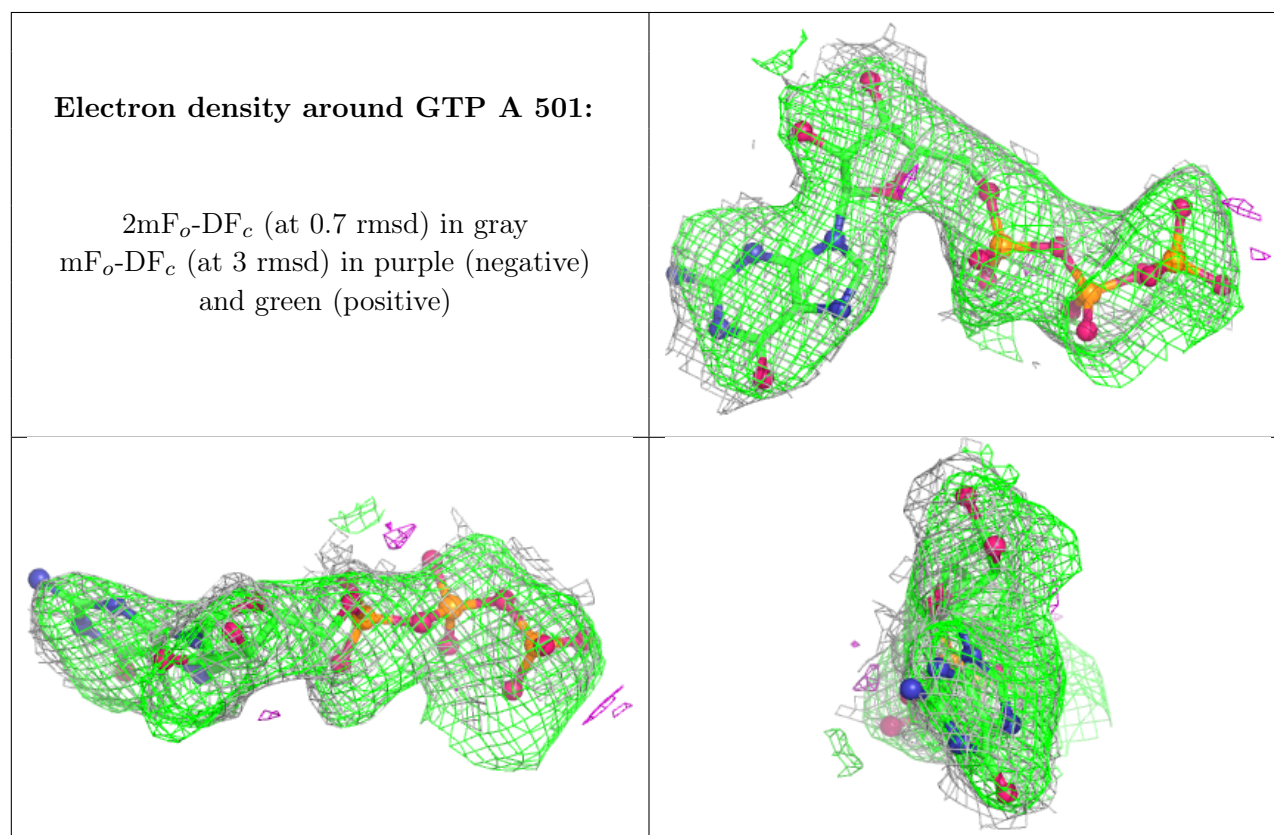
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GTP	A	501	32/32	-	-	40,41,43,43	32
5	GTP	C	501	32/32	-	-	33,36,39,40	32
6	CA	A	502	1/1	-	-	69,69,69,69	1
6	CA	C	502	1/1	-	-	53,53,53,53	1
7	MG	A	503	1/1	-	-	45,45,45,45	1
7	MG	B	504	1/1	-	-	47,47,47,47	1
7	MG	C	503	1/1	-	-	42,42,42,42	1
8	GDP	B	501	28/28	-	-	36,41,43,44	28
8	GDP	D	501	28/28	-	-	71,76,79,80	28

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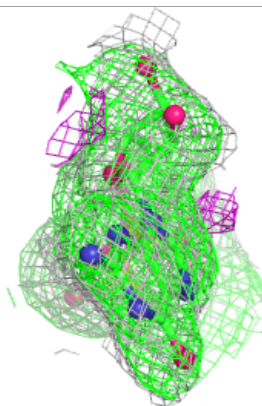
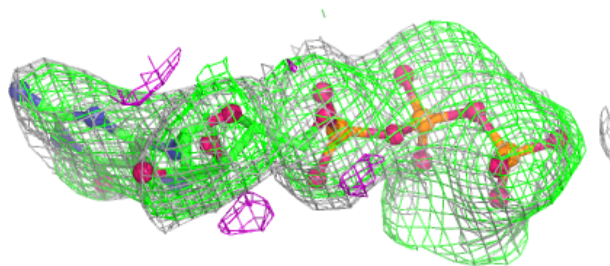
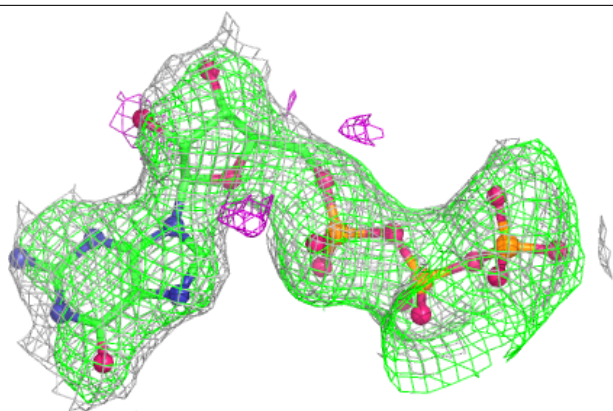
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MES	B	502	12/12	-	-	42,43,45,45	12
9	MES	B	503	12/12	-	-	53,53,54,54	12
10	A1EUX	B	505	12/12	0.71	0.21	44,53,63,71	0
11	ACP	F	401	31/31	-	-	74,87,104,105	45

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



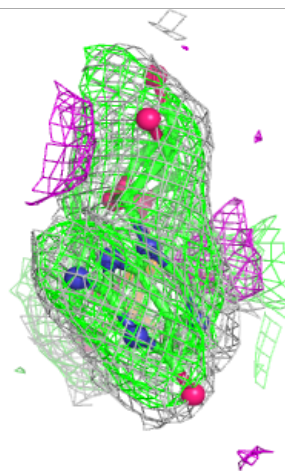
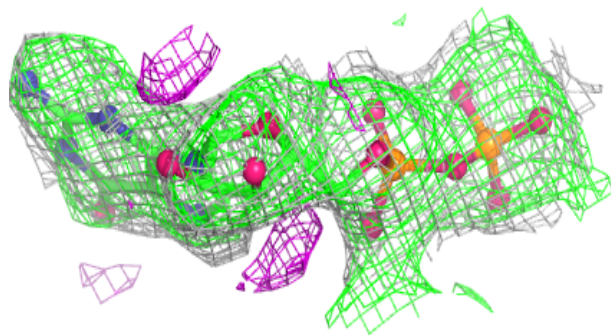
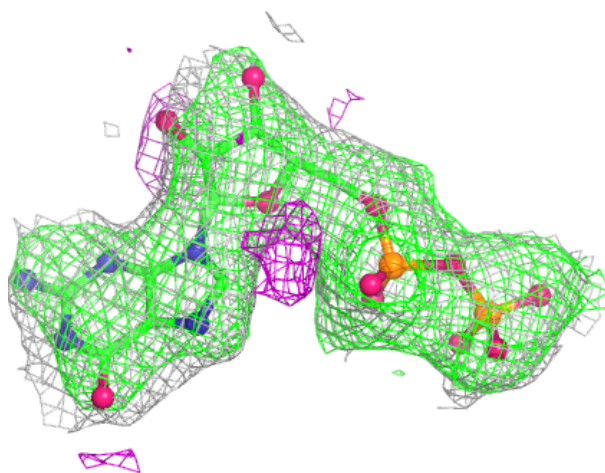
Electron density around GTP C 501:

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



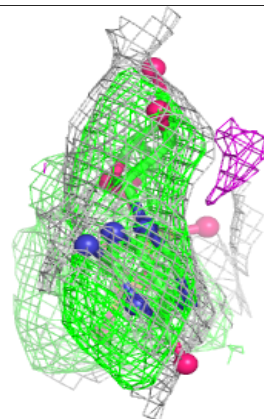
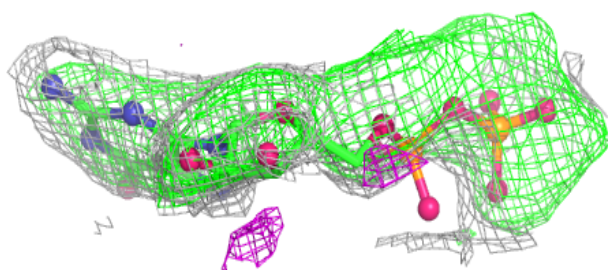
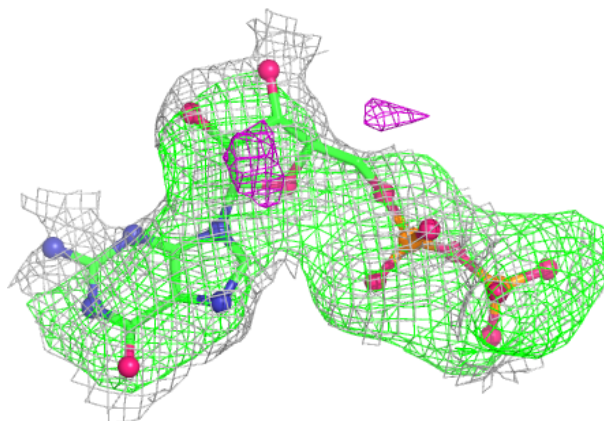
Electron density around GDP B 501:

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

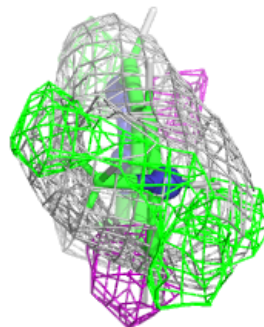
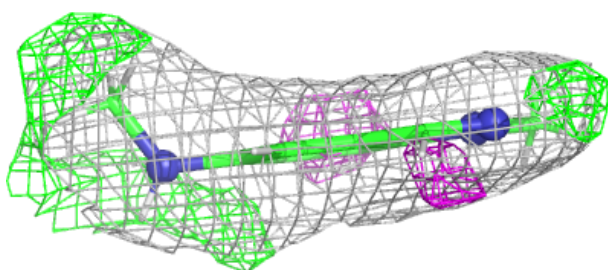
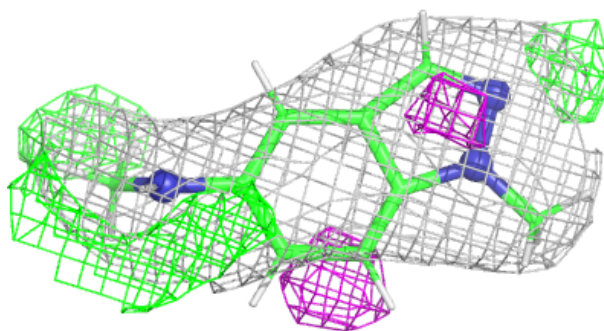


Electron density around GDP D 501:

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

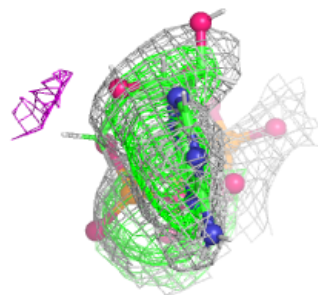
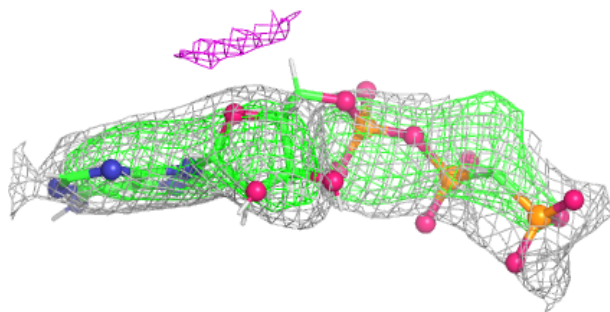
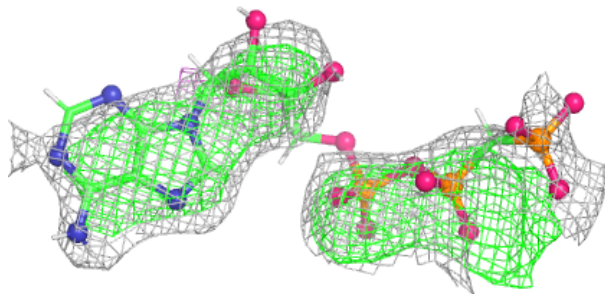
**Electron density around A1EUX B 505:**

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



Electron density around ACP F 401:

$2mF_o - DF_c$ (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.