



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:43 AM UTC

PDB ID : 8YEM / pdb_00008yem
Title : Tubulin-RB3_SLD-TTL in complex with compound 9
Authors : Wu, C.Y.; Wang, Y.X.
Deposited on : 2024-02-22
Resolution : 2.74 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

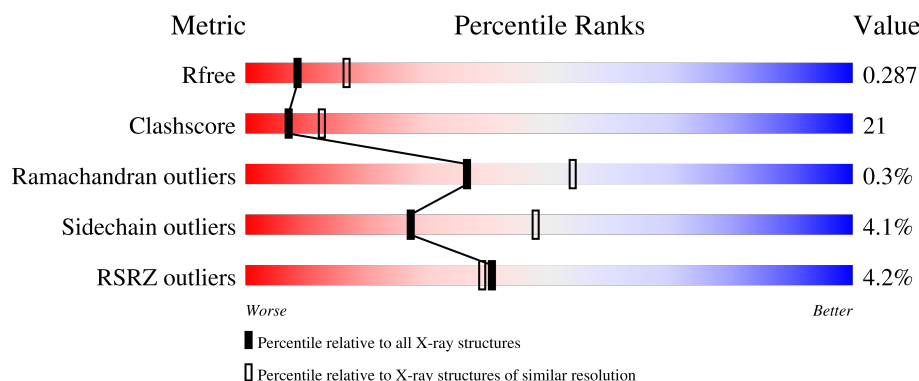
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	7% 67% 31% ..
1	C	440	7% 71% 28% .
2	B	431	7% 68% 30% ..
2	D	431	7% 56% 41% ..
3	E	136	2% 57% 29% . 11%

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Mol	Chain	Length	Quality of chain
4	F	380	12% 41% 43% • 14%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17437 atoms, of which 38 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			

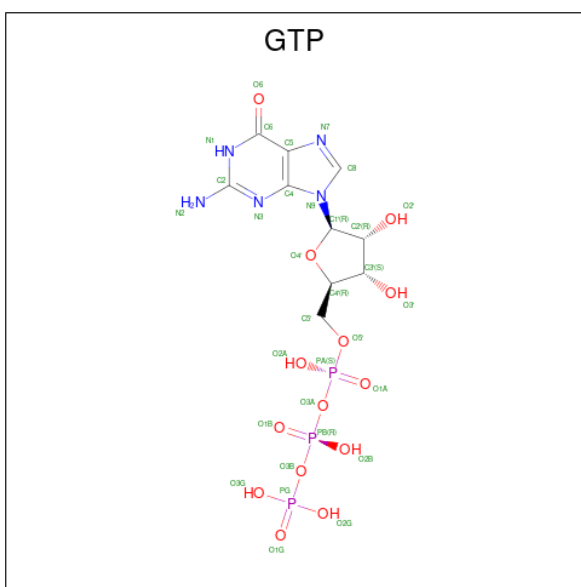
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	328	Total	C	N	O	S	0	0	0
			2680	1722	458	486	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		

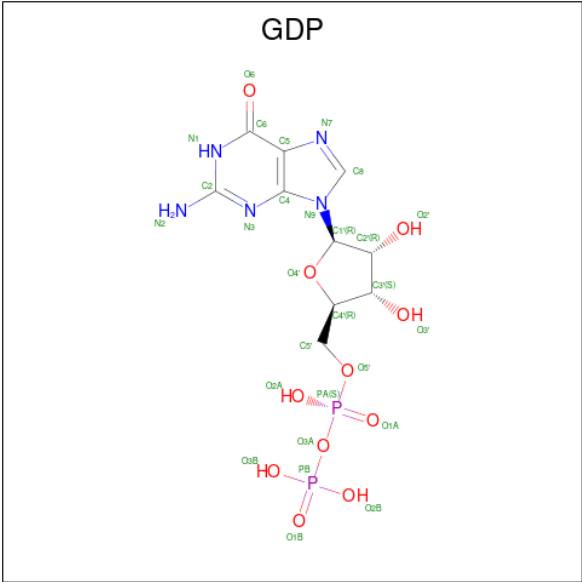
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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).

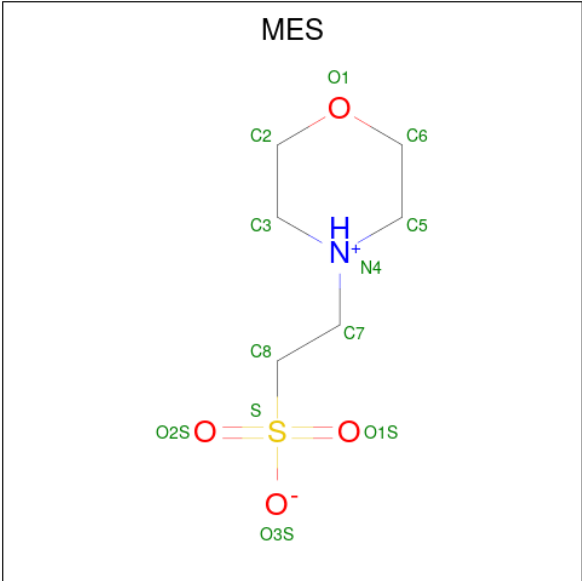
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	1	0
			1	1		
7	B	1	Total	Mg	1	0
			1	1		
7	C	1	Total	Mg	1	0
			1	1		

- 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).



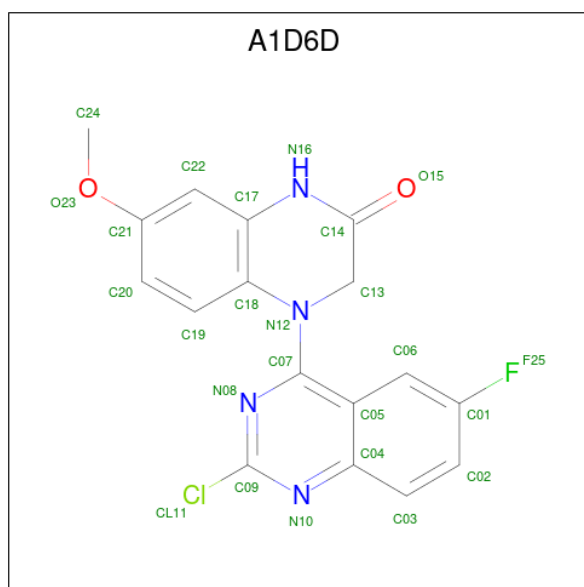
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

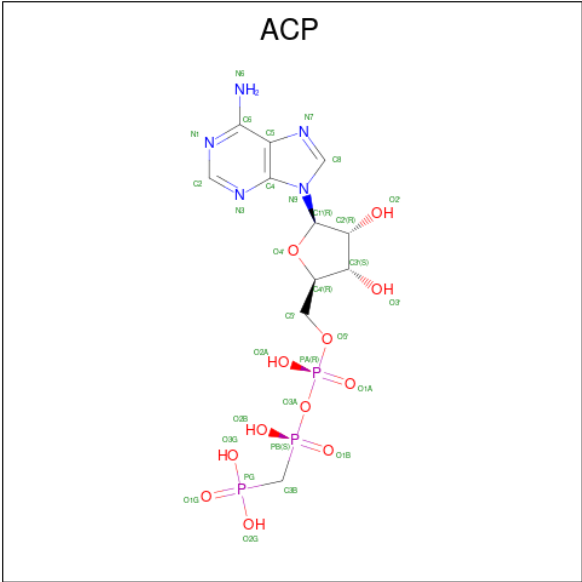
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

- Molecule 10 is 4-(2-chloranyl-6-fluoranyl-quinazolin-4-yl)-7-methoxy-1,3-dihydroquinoxalin-2-one (CCD ID: A1D6D) (formula: $C_{17}H_{12}ClFN_4O_2$) (labeled as "Ligand of Interest" by depositor).



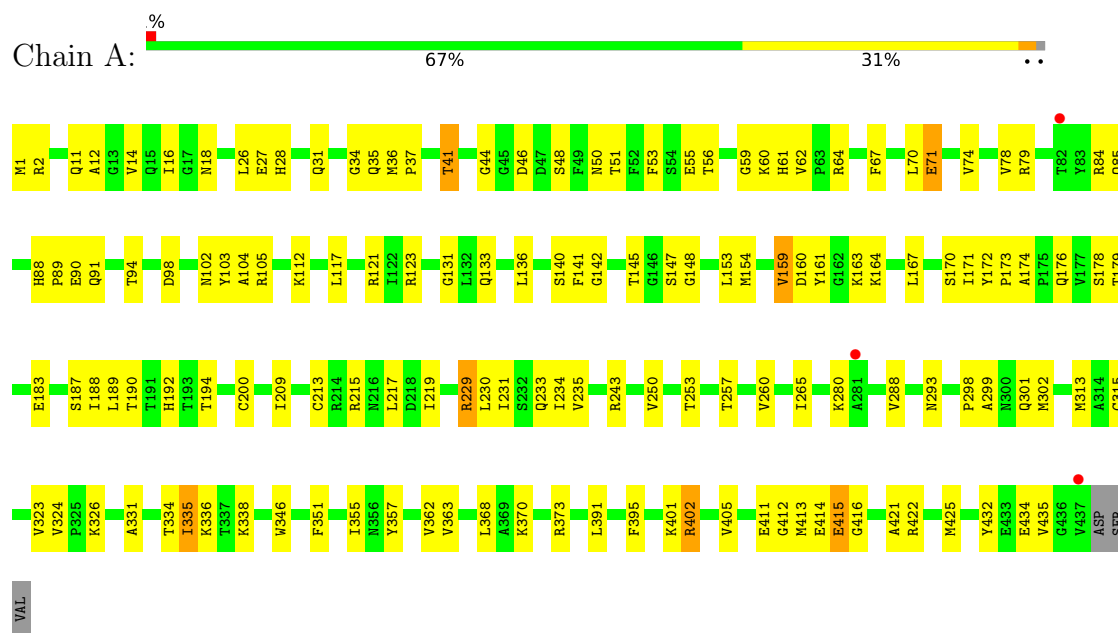


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	
			45	11	14	5	12	3	

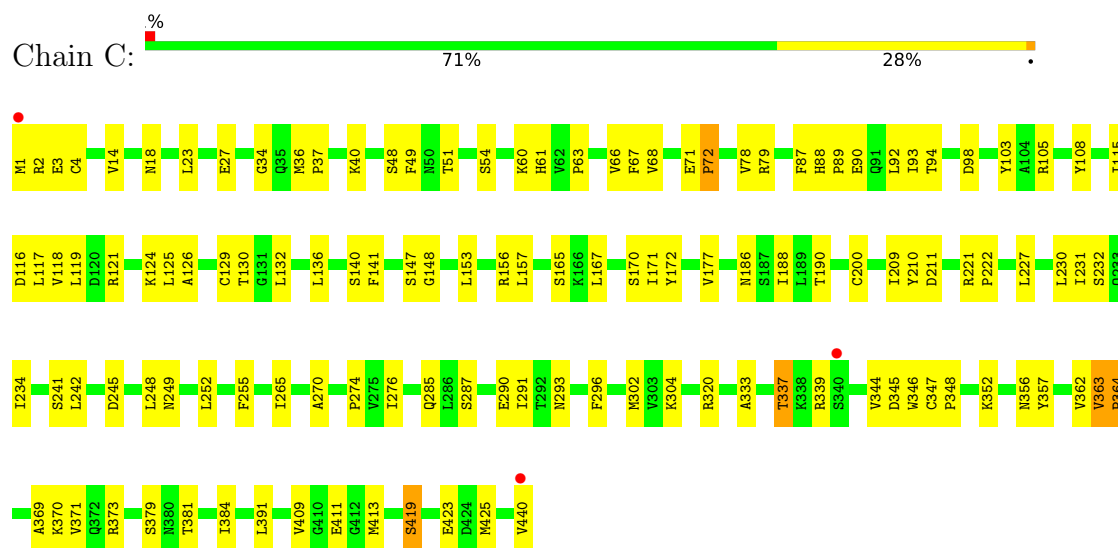
3 Residue-property plots [i](#)

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.

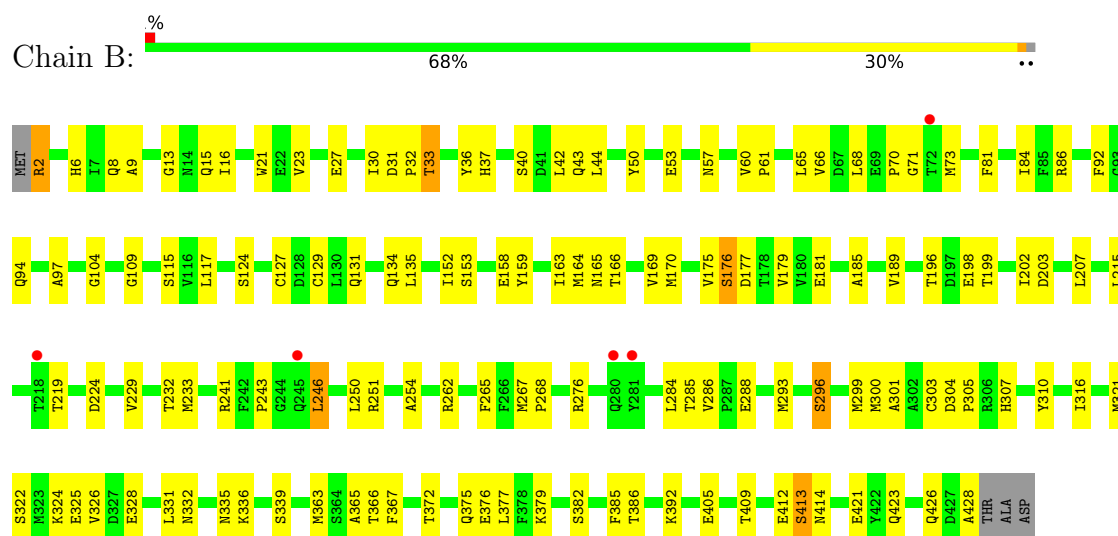
• Molecule 1: Detyrosinated tubulin alpha-1B chain



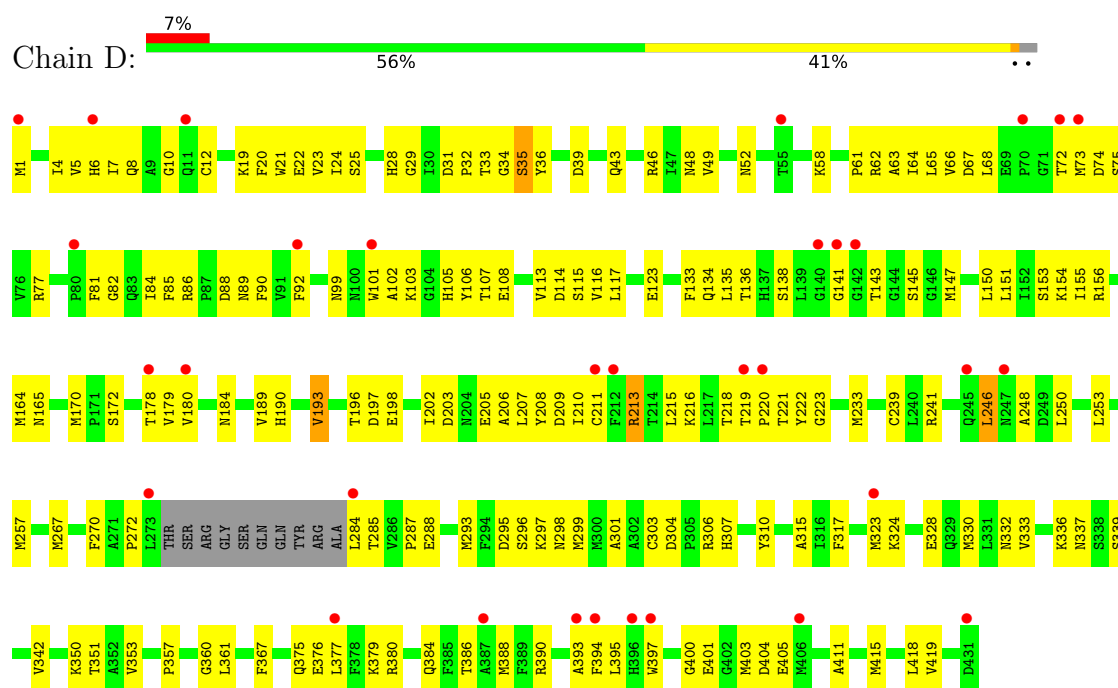
• Molecule 1: Detyrosinated tubulin alpha-1B chain



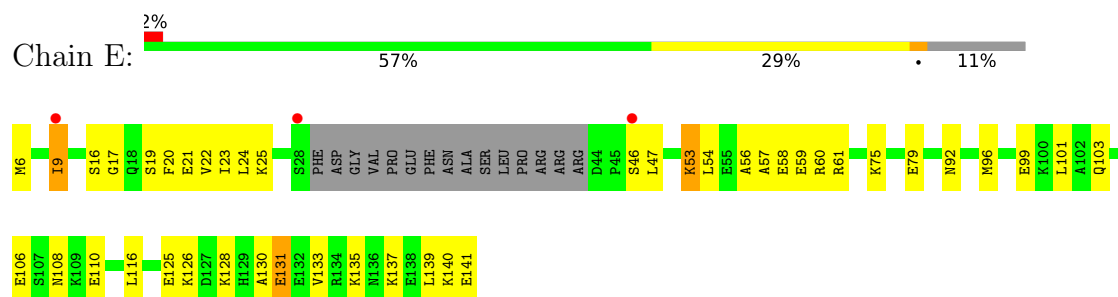
• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain

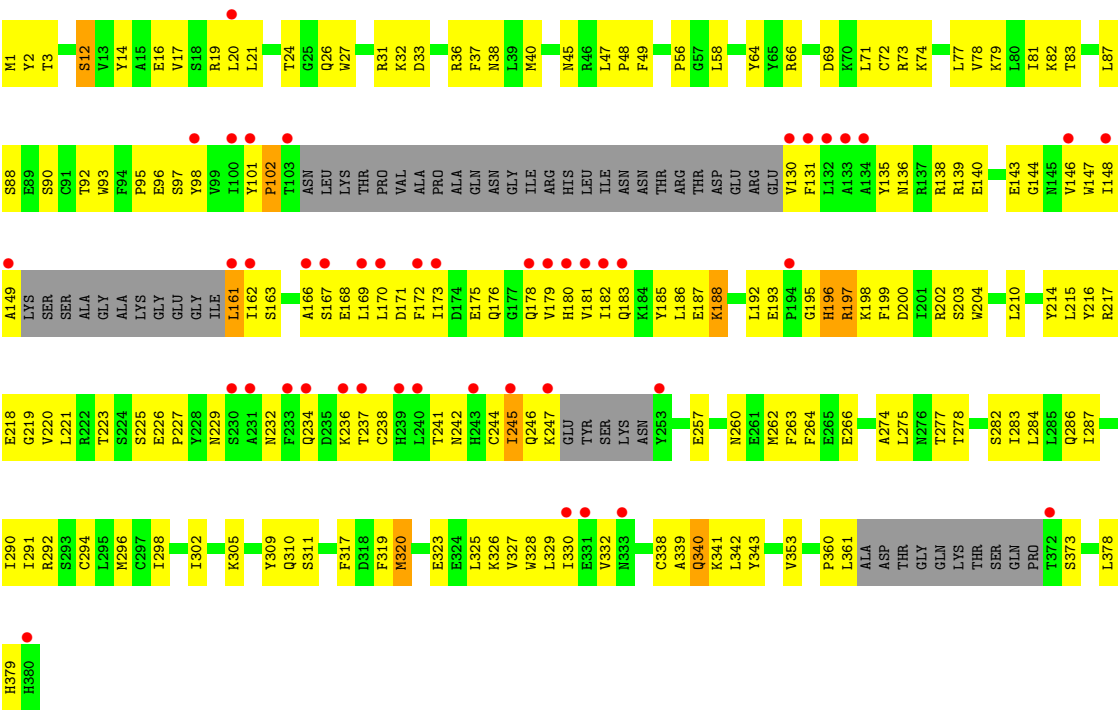


• Molecule 3: Stathmin-4



• 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	104.94Å 156.81Å 182.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.72 – 2.74 43.72 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.72-2.74) 99.9 (43.72-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.217 , 0.284 (Not available) , 0.287	Depositor DCC
R_{free} test set	2000 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17437	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: GDP, A1D6D, GTP, MG, MES, ACP, 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	0.39	0/3482	0.59	0/4728
1	C	0.45	0/3511	0.63	0/4768
2	B	0.41	0/3426	0.61	0/4643
2	D	0.33	0/3373	0.54	0/4570
3	E	0.39	0/1008	0.60	0/1337
4	F	0.30	0/2742	0.50	0/3708
All	All	0.39	0/17542	0.58	0/23754

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	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
2	B	2	ARG	Sidechain
2	B	251	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3405	0	3312	140	0
1	C	3433	0	3337	93	0
2	B	3351	0	3216	114	0
2	D	3300	0	3175	175	0
3	E	1000	0	1018	39	0
4	F	2680	0	2629	167	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	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	24	0	0
10	B	25	12	0	0	0
10	D	25	12	0	1	0
11	F	31	14	14	0	0
All	All	17399	38	16773	709	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 21.

All (709) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ALA:HB2	1:A:413:MET:HE3	1.33	1.10
4:F:192:LEU:CD2	4:F:262:MET:HE1	1.88	1.03
1:A:79:ARG:HH22	1:A:94:THR:HG22	1.25	0.99
1:A:79:ARG:HH12	1:A:94:THR:HG21	1.29	0.96
2:B:336:LYS:HA	2:B:336:LYS:HE3	1.47	0.95
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.46	0.95
4:F:192:LEU:HD21	4:F:262:MET:HE1	1.45	0.94
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:LEU:O	2:D:155:ILE:HG13	1.66	0.94
1:A:88:HIS:NE2	1:A:90:GLU:HG3	1.83	0.94
2:D:134:GLN:HA	2:D:165:ASN:O	1.66	0.94
2:D:350:LYS:HB2	10:D:502:A1D6D:C24	1.98	0.93
2:D:102:ALA:HB2	2:D:403:MET:CE	1.99	0.92
2:D:315:ALA:HB3	2:D:351:THR:HG22	1.49	0.92
2:D:73:MET:HE3	2:D:77:ARG:HH22	1.34	0.91
1:A:313:MET:HE2	1:A:435:VAL:HG11	1.55	0.89
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.38	0.88
4:F:263:PHE:CE1	4:F:341:LYS:HD3	2.08	0.88
2:D:375:GLN:HB2	2:D:419:VAL:HG13	1.54	0.88
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.57	0.86
1:A:323:VAL:HG12	1:A:355:ILE:HD13	1.58	0.84
2:B:293:MET:HE3	2:B:365:ALA:HB1	1.58	0.84
2:B:332:ASN:O	2:B:336:LYS:HG2	1.76	0.83
2:D:21:TRP:O	2:D:25:SER:OG	1.95	0.83
2:B:392:LYS:HE3	2:B:405:GLU:OE2	1.79	0.83
2:D:170:MET:HE2	2:D:377:LEU:HD11	1.60	0.83
2:D:141:GLY:HA2	2:D:184:ASN:HD22	1.43	0.82
1:A:104:ALA:HB2	1:A:413:MET:CE	2.09	0.82
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.45	0.82
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.61	0.81
2:B:375:GLN:OE1	2:B:379:LYS:HE3	1.80	0.81
2:B:293:MET:CE	2:B:365:ALA:HB1	2.11	0.80
4:F:24:THR:HG21	4:F:361:LEU:HD13	1.64	0.79
2:B:286:VAL:HG22	2:B:321:MET:HE2	1.63	0.79
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.16	0.78
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.16	0.78
2:D:81:PHE:O	2:D:84:ILE:HG22	1.82	0.78
4:F:149:ALA:HB3	4:F:161:LEU:CD1	2.14	0.78
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.66	0.77
1:C:362:VAL:HG22	1:C:370:LYS:HG3	1.64	0.77
2:D:73:MET:HE3	2:D:77:ARG:NH2	1.99	0.77
4:F:226:GLU:HG3	4:F:237:THR:HG22	1.66	0.77
2:D:73:MET:CE	2:D:77:ARG:HH22	1.97	0.76
1:A:56:THR:O	1:A:59:GLY:N	2.17	0.76
3:E:135:LYS:O	3:E:139:LEU:HD23	1.86	0.76
2:B:31:ASP:OD1	2:B:33:THR:HG23	1.86	0.75
3:E:92:ASN:OD1	3:E:96:MET:HE3	1.85	0.75
1:A:88:HIS:O	1:A:91:GLN:HG3	1.87	0.75
2:D:12:CYS:HB3	2:D:138:SER:HB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:LEU:HD22	2:B:243:PRO:HG2	1.69	0.74
2:D:22:GLU:HG2	2:D:81:PHE:CD1	2.23	0.74
4:F:234:GLN:O	4:F:234:GLN:NE2	2.21	0.74
1:A:1:MET:HE2	1:A:50:ASN:CB	2.18	0.74
1:A:90:GLU:HA	1:A:121:ARG:HH21	1.52	0.74
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.23	0.74
2:B:166:THR:OG1	2:B:199:THR:HG22	1.87	0.74
1:C:293:ASN:OD1	1:C:339:ARG:NH1	2.20	0.74
2:B:170:MET:HB2	2:B:203:ASP:HA	1.70	0.73
2:D:63:ALA:C	2:D:64:ILE:HD13	2.14	0.73
4:F:195:GLY:HA3	4:F:197:ARG:HD2	1.71	0.73
1:A:79:ARG:HH12	1:A:94:THR:CG2	2.01	0.73
2:D:22:GLU:HG2	2:D:81:PHE:HD1	1.54	0.73
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.19	0.72
3:E:130:ALA:HA	3:E:133:VAL:HG12	1.70	0.72
4:F:193:GLU:OE2	4:F:196:HIS:ND1	2.19	0.72
1:C:419:SER:O	1:C:423:GLU:HG3	1.89	0.72
4:F:138:ARG:NH1	4:F:144:GLY:O	2.22	0.72
4:F:262:MET:SD	4:F:266:GLU:HG2	2.30	0.72
2:D:330:MET:HG3	2:D:351:THR:HG21	1.73	0.71
4:F:262:MET:HG3	4:F:266:GLU:HG2	1.72	0.71
4:F:326:LYS:HE2	4:F:328:TRP:CZ2	2.26	0.70
3:E:47:LEU:HD12	3:E:47:LEU:O	1.91	0.70
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.27	0.70
2:D:73:MET:SD	2:D:92:PHE:HD1	2.14	0.70
1:A:209:ILE:HD11	1:A:302:MET:SD	2.30	0.70
1:C:287:SER:OG	1:C:290:GLU:HG3	1.91	0.70
4:F:33:ASP:OD1	4:F:33:ASP:O	2.09	0.70
1:A:234:ILE:HG12	1:A:302:MET:HE3	1.73	0.69
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.26	0.69
4:F:163:SER:OG	4:F:168:GLU:HG3	1.92	0.69
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.74	0.69
4:F:147:TRP:O	4:F:162:ILE:HG23	1.93	0.69
4:F:149:ALA:HB2	4:F:161:LEU:HB2	1.75	0.69
3:E:24:LEU:O	3:E:25:LYS:HG3	1.93	0.69
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.10	0.68
1:C:4:CYS:HB3	1:C:136:LEU:CD1	2.24	0.68
1:A:70:LEU:HG	1:A:145:THR:HG23	1.74	0.68
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.28	0.68
2:B:36:TYR:C	2:B:37:HIS:HD1	2.01	0.68
4:F:149:ALA:CB	4:F:161:LEU:HB2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.29	0.68
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.29	0.68
2:D:210:ILE:HG22	2:D:215:LEU:HD23	1.76	0.68
1:A:154:MET:HG3	1:A:194:THR:HG23	1.76	0.68
2:B:134:GLN:HA	2:B:165:ASN:O	1.94	0.68
2:D:33:THR:O	2:D:58:LYS:HD2	1.93	0.68
2:D:67:ASP:OD2	2:D:72:THR:OG1	2.05	0.68
4:F:81:ILE:HD13	4:F:87:LEU:CD1	2.24	0.67
2:B:316:ILE:HG23	2:B:366:THR:HB	1.76	0.67
4:F:138:ARG:HD2	4:F:143:GLU:HB2	1.75	0.67
1:A:28:HIS:O	1:A:36:MET:HE3	1.95	0.67
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.30	0.67
4:F:148:ILE:HD12	4:F:149:ALA:H	1.57	0.67
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.28	0.67
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.59	0.67
2:D:19:LYS:O	2:D:23:VAL:HG23	1.94	0.67
1:C:71:GLU:CG	1:C:98:ASP:HB3	2.23	0.67
2:D:46:ARG:HG3	2:D:46:ARG:HH11	1.59	0.67
2:B:170:MET:HG3	2:B:377:LEU:HD21	1.77	0.66
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.30	0.66
4:F:149:ALA:HB3	4:F:161:LEU:HD13	1.76	0.66
2:D:106:TYR:CD2	3:E:133:VAL:HG11	2.30	0.66
4:F:135:TYR:HD1	4:F:135:TYR:O	1.79	0.66
4:F:186:LEU:HD12	4:F:320:MET:HG3	1.78	0.66
2:D:332:ASN:OD1	2:D:336:LYS:HD2	1.95	0.66
4:F:296:MET:HE3	4:F:296:MET:HA	1.77	0.66
4:F:186:LEU:HD12	4:F:320:MET:CG	2.26	0.66
2:D:107:THR:OG1	2:D:108:GLU:N	2.29	0.65
2:D:141:GLY:HA2	2:D:184:ASN:ND2	2.10	0.65
4:F:210:LEU:O	4:F:305:LYS:NZ	2.30	0.65
1:A:323:VAL:HG12	1:A:355:ILE:CD1	2.25	0.65
2:B:176:SER:HB2	2:B:181:GLU:OE1	1.97	0.65
4:F:192:LEU:HD11	4:F:199:PHE:CD1	2.32	0.65
1:A:90:GLU:HB3	1:A:121:ARG:HE	1.61	0.65
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.31	0.65
2:D:206:ALA:O	2:D:210:ILE:HG13	1.96	0.65
3:E:75:LYS:HD3	3:E:79:GLU:OE2	1.97	0.65
2:B:372:THR:OG1	2:B:426:GLN:HG3	1.97	0.65
2:D:285:THR:OG1	2:D:288:GLU:HG3	1.97	0.65
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.79	0.64
1:A:1:MET:HE2	1:A:50:ASN:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:247:LYS:H	4:F:247:LYS:HD3	1.62	0.64
2:B:316:ILE:CG2	2:B:366:THR:HB	2.28	0.64
1:C:79:ARG:HH22	1:C:94:THR:HG23	1.63	0.64
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.33	0.64
3:E:130:ALA:HA	3:E:133:VAL:CG1	2.27	0.64
2:B:2:ARG:HA	2:B:129:CYS:O	1.98	0.64
2:D:102:ALA:HB2	2:D:403:MET:HE2	1.76	0.64
2:D:65:LEU:HD12	2:D:90:PHE:CE2	2.33	0.64
4:F:16:GLU:O	4:F:20:LEU:HG	1.98	0.63
4:F:262:MET:CG	4:F:266:GLU:HG2	2.28	0.63
4:F:95:PRO:HB2	4:F:183:GLN:HG2	1.79	0.63
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.33	0.63
1:A:362:VAL:HG21	1:A:370:LYS:HG3	1.81	0.63
2:B:293:MET:HE3	2:B:365:ALA:CB	2.29	0.63
4:F:16:GLU:HG2	4:F:19:ARG:HH21	1.64	0.63
2:D:52:ASN:OD1	2:D:62:ARG:NH1	2.31	0.63
2:D:32:PRO:HB3	2:D:81:PHE:HA	1.79	0.63
2:D:393:ALA:HB1	2:D:394:PHE:CD1	2.33	0.63
4:F:171:ASP:O	4:F:175:GLU:HG2	1.99	0.63
4:F:217:ARG:NH1	4:F:373:SER:O	2.31	0.63
1:A:178:SER:OG	1:A:183:GLU:OE2	2.14	0.62
4:F:292:ARG:HD3	4:F:379:HIS:O	1.98	0.62
1:A:117:LEU:HD11	1:A:121:ARG:NH1	2.14	0.62
2:D:12:CYS:CB	2:D:138:SER:HB3	2.29	0.62
1:A:104:ALA:CB	1:A:413:MET:HE3	2.21	0.62
1:A:229:ARG:HH11	1:A:363:VAL:HG21	1.65	0.62
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.81	0.62
1:A:79:ARG:NH2	1:A:94:THR:HG22	2.07	0.62
2:B:324:LYS:O	2:B:328:GLU:HG3	1.99	0.62
1:C:248:LEU:CD1	1:C:357:TYR:OH	2.48	0.62
2:D:64:ILE:HD11	2:D:123:GLU:HG3	1.81	0.62
2:D:293:MET:CG	2:D:367:PHE:HB2	2.30	0.62
4:F:170:LEU:H	4:F:170:LEU:HD12	1.64	0.62
2:D:99:ASN:ND2	2:D:178:THR:HG21	2.14	0.62
1:A:79:ARG:NH1	1:A:94:THR:HG21	2.08	0.61
2:D:179:VAL:O	2:D:388:MET:HE1	2.00	0.61
2:D:360:GLY:O	2:D:361:LEU:HD12	2.00	0.61
3:E:53:LYS:HG3	3:E:54:LEU:N	2.15	0.61
4:F:97:SER:OG	4:F:183:GLN:HG3	1.99	0.61
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.32	0.61
2:B:322:SER:O	2:B:326:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:131:GLU:OE1	3:E:131:GLU:HA	1.99	0.61
2:D:210:ILE:HG22	2:D:215:LEU:CD2	2.31	0.61
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.66	0.61
1:A:217:LEU:HB2	1:A:219:ILE:HD12	1.81	0.61
2:D:272:PRO:HB3	2:D:284:LEU:HD22	1.82	0.61
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.36	0.61
1:A:293:ASN:CA	1:A:335:ILE:HD11	2.31	0.61
1:C:37:PRO:O	1:C:40:LYS:HE2	2.01	0.61
1:C:79:ARG:NH2	1:C:94:THR:HG23	2.16	0.61
4:F:236:LYS:O	4:F:237:THR:HB	2.01	0.61
1:C:209:ILE:HD11	1:C:302:MET:SD	2.40	0.61
2:D:4:ILE:HG12	2:D:250:LEU:HD11	1.83	0.61
2:D:7:ILE:O	2:D:135:LEU:HD12	2.01	0.61
4:F:199:PHE:CG	4:F:221:LEU:HD23	2.35	0.61
4:F:196:HIS:O	4:F:227:PRO:HA	2.01	0.60
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.18	0.60
1:C:119:LEU:HD12	1:C:156:ARG:NH2	2.16	0.60
2:D:375:GLN:O	2:D:379:LYS:HG3	2.00	0.60
4:F:223:THR:O	4:F:260:ASN:HB3	2.02	0.60
1:A:288:VAL:HG22	1:A:323:VAL:HG22	1.84	0.60
4:F:87:LEU:O	4:F:88:SER:HB3	2.02	0.60
1:C:68:VAL:HG11	1:C:118:VAL:HG21	1.82	0.60
2:D:323:MET:HG2	2:D:353:VAL:HG21	1.82	0.60
4:F:135:TYR:HE2	4:F:166:ALA:HB2	1.66	0.60
4:F:218:GLU:HG3	4:F:342:LEU:HD22	1.82	0.60
4:F:226:GLU:CG	4:F:237:THR:HG22	2.31	0.60
4:F:82:LYS:NZ	4:F:97:SER:O	2.34	0.59
1:A:117:LEU:HD11	1:A:121:ARG:HH11	1.67	0.59
2:D:4:ILE:HG12	2:D:250:LEU:CD1	2.32	0.59
1:C:221:ARG:NH1	2:D:323:MET:HB3	2.17	0.59
2:B:81:PHE:O	2:B:84:ILE:HG22	2.03	0.59
2:D:267:MET:HE2	2:D:303:CYS:HB2	1.85	0.59
4:F:81:ILE:HD13	4:F:87:LEU:HD13	1.84	0.59
2:B:229:VAL:HG12	2:B:233:MET:HE2	1.85	0.59
1:C:320:ARG:HA	1:C:356:ASN:O	2.03	0.59
4:F:98:TYR:O	4:F:181:VAL:HG23	2.03	0.59
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.85	0.59
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.38	0.58
2:D:107:THR:HG21	2:D:401:GLU:OE1	2.03	0.58
1:A:331:ALA:HA	1:A:334:THR:HG22	1.84	0.58
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:THR:OG1	2:B:300:MET:HE3	2.02	0.58
2:B:322:SER:OG	2:B:325:GLU:HB2	2.03	0.58
2:D:48:ASN:O	2:D:62:ARG:NH2	2.37	0.58
2:D:285:THR:HB	2:D:287:PRO:HD2	1.85	0.58
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.86	0.58
1:A:187:SER:CB	1:A:391:LEU:HD21	2.33	0.58
1:A:331:ALA:O	1:A:334:THR:HG22	2.03	0.58
4:F:101:TYR:CD1	4:F:179:VAL:HG22	2.39	0.58
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.40	0.57
2:B:307:HIS:ND1	2:B:376:GLU:OE2	2.33	0.57
1:C:227:LEU:O	1:C:231:ILE:HG13	2.04	0.57
4:F:320:MET:HB2	4:F:330:ILE:HD11	1.87	0.57
2:D:77:ARG:HA	2:D:82:GLY:HA3	1.87	0.57
4:F:185:TYR:OH	4:F:198:LYS:HE3	2.04	0.57
2:D:24:ILE:HG22	2:D:241:ARG:CZ	2.34	0.57
2:D:394:PHE:HB3	2:D:397:TRP:HD1	1.70	0.57
4:F:282:SER:HB2	4:F:325:LEU:HD22	1.86	0.57
4:F:166:ALA:O	4:F:169:LEU:N	2.37	0.57
1:A:41:THR:HB	1:A:44:GLY:O	2.05	0.56
4:F:148:ILE:HD11	4:F:161:LEU:HD12	1.87	0.56
4:F:172:PHE:HE1	4:F:176:GLN:HE21	1.53	0.56
2:B:285:THR:O	2:B:288:GLU:N	2.36	0.56
1:A:298:PRO:HA	1:A:301:GLN:CD	2.31	0.56
2:B:301:ALA:O	2:B:303:CYS:N	2.38	0.56
1:A:174:ALA:O	1:A:178:SER:HB2	2.04	0.56
1:A:293:ASN:HA	1:A:335:ILE:HD11	1.87	0.56
2:B:224:ASP:OD1	2:B:276:ARG:NH1	2.38	0.56
1:A:18:ASN:HD21	1:A:78:VAL:CG2	2.15	0.56
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.35	0.56
2:D:215:LEU:N	2:D:215:LEU:HD22	2.20	0.56
2:D:270:PHE:O	2:D:298:ASN:HB3	2.06	0.56
2:D:333:VAL:O	2:D:337:ASN:HB2	2.04	0.56
2:D:34:GLY:O	2:D:58:LYS:HA	2.06	0.56
1:A:90:GLU:HB3	1:A:121:ARG:NE	2.20	0.56
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.36	0.56
2:B:60:VAL:HG11	2:B:86:ARG:HB2	1.88	0.55
1:A:176:GLN:CD	4:F:56:PRO:HB3	2.30	0.55
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.88	0.55
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.42	0.55
2:D:323:MET:HE2	2:D:353:VAL:HG21	1.87	0.55
1:C:90:GLU:O	1:C:121:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293:MET:O	2:D:299:MET:HE1	2.06	0.55
2:D:92:PHE:HD2	2:D:92:PHE:O	1.89	0.55
4:F:136:ASN:O	4:F:140:GLU:HG3	2.07	0.55
2:D:28:HIS:HA	2:D:43:GLN:HB3	1.88	0.55
4:F:148:ILE:HD13	4:F:162:ILE:HG12	1.89	0.55
2:B:42:LEU:HD22	2:B:243:PRO:CG	2.36	0.55
2:B:262:ARG:NH2	2:B:414:ASN:OD1	2.40	0.55
2:D:74:ASP:HA	2:D:77:ARG:NH1	2.22	0.55
1:A:2:ARG:HB2	1:A:133:GLN:NE2	2.18	0.54
2:B:409:THR:O	2:B:413:SER:HB2	2.06	0.54
2:D:193:VAL:CG2	2:D:418:LEU:HD22	2.37	0.54
4:F:81:ILE:HD13	4:F:87:LEU:HD12	1.88	0.54
4:F:188:LYS:HG2	4:F:323:GLU:OE1	2.07	0.54
1:A:373:ARG:HG2	1:A:373:ARG:HH11	1.71	0.54
2:D:6:HIS:HD1	2:D:21:TRP:NE1	2.05	0.54
2:D:202:ILE:HG22	2:D:207:LEU:HD11	1.89	0.54
2:D:304:ASP:HB3	2:D:307:HIS:ND1	2.23	0.54
4:F:277:THR:HG23	4:F:278:THR:N	2.21	0.54
1:A:163:LYS:H	1:A:164:LYS:HZ2	1.54	0.54
1:A:84:ARG:HG2	1:A:85:GLN:N	2.23	0.53
2:D:65:LEU:N	2:D:65:LEU:HD23	2.23	0.53
4:F:274:ALA:O	4:F:275:LEU:HD23	2.08	0.53
1:A:1:MET:HE2	1:A:50:ASN:HB2	1.90	0.53
4:F:3:THR:OG1	4:F:37:PHE:HA	2.09	0.53
1:A:217:LEU:CB	1:A:219:ILE:HD12	2.39	0.53
2:D:189:VAL:HB	2:D:415:MET:HE3	1.91	0.53
4:F:229:ASN:OD1	4:F:232:ASN:HB3	2.08	0.53
1:A:1:MET:CE	1:A:50:ASN:HB3	2.38	0.53
2:D:63:ALA:O	2:D:64:ILE:HD13	2.08	0.53
4:F:148:ILE:CD1	4:F:149:ALA:H	2.21	0.53
4:F:149:ALA:HB3	4:F:161:LEU:HD12	1.90	0.53
4:F:263:PHE:HE1	4:F:341:LYS:HD3	1.69	0.53
1:C:339:ARG:HG3	1:C:339:ARG:HH11	1.73	0.53
2:D:46:ARG:HG3	2:D:46:ARG:NH1	2.22	0.53
3:E:99:GLU:O	3:E:103:GLN:HG3	2.09	0.53
4:F:77:LEU:O	4:F:81:ILE:HG12	2.09	0.53
2:B:336:LYS:HA	2:B:336:LYS:CE	2.28	0.52
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.91	0.52
2:D:73:MET:SD	2:D:92:PHE:CD1	2.98	0.52
2:D:190:HIS:ND1	2:D:411:ALA:HA	2.23	0.52
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.40	0.52
1:C:153:LEU:O	1:C:157:LEU:HG	2.09	0.52
4:F:192:LEU:HD21	4:F:262:MET:CE	2.29	0.52
1:A:373:ARG:HG2	1:A:373:ARG:NH1	2.24	0.52
3:E:23:ILE:HD13	3:E:23:ILE:N	2.24	0.52
4:F:247:LYS:HD3	4:F:247:LYS:N	2.24	0.52
2:B:40:SER:H	2:B:43:GLN:HE21	1.58	0.52
2:D:86:ARG:NH1	2:D:88:ASP:HB2	2.25	0.52
4:F:195:GLY:HA3	4:F:197:ARG:CD	2.38	0.52
1:A:60:LYS:HG2	1:A:62:VAL:HG23	1.92	0.52
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.92	0.52
2:B:170:MET:HE3	2:B:377:LEU:HD22	1.92	0.52
2:D:6:HIS:HD2	2:D:7:ILE:H	1.57	0.52
2:D:310:TYR:O	2:D:342:VAL:HG22	2.09	0.52
2:B:61:PRO:HD3	2:B:84:ILE:HG12	1.91	0.52
1:C:117:LEU:O	1:C:121:ARG:HG2	2.09	0.52
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.90	0.52
4:F:202:ARG:HD3	4:F:204:TRP:NE1	2.25	0.52
2:B:386:THR:HG22	2:B:412:GLU:OE2	2.10	0.52
2:B:36:TYR:CG	2:B:44:LEU:HD11	2.44	0.52
2:D:6:HIS:CD2	2:D:7:ILE:N	2.78	0.52
1:A:1:MET:HB3	1:A:46:ASP:HB2	1.92	0.51
2:B:179:VAL:CG1	1:C:348:PRO:HG2	2.31	0.51
4:F:88:SER:HG	4:F:90:SER:HG	1.46	0.51
4:F:166:ALA:HB1	4:F:170:LEU:CD1	2.40	0.51
1:A:79:ARG:HH22	1:A:94:THR:CG2	2.12	0.51
2:D:303:CYS:SG	2:D:377:LEU:HB2	2.51	0.51
4:F:78:VAL:HG13	4:F:82:LYS:HZ3	1.75	0.51
4:F:78:VAL:HG13	4:F:82:LYS:NZ	2.25	0.51
3:E:53:LYS:HG3	3:E:54:LEU:H	1.75	0.51
2:D:64:ILE:HD13	2:D:64:ILE:N	2.24	0.51
2:B:2:ARG:HB3	2:B:131:GLN:CG	2.41	0.51
2:D:323:MET:HE2	2:D:353:VAL:CG2	2.39	0.51
4:F:47:LEU:C	4:F:47:LEU:HD23	2.36	0.51
2:D:189:VAL:HG11	2:D:415:MET:CE	2.41	0.51
2:D:239:CYS:O	2:D:248:ALA:HB3	2.11	0.51
1:A:402:ARG:HG2	1:A:405:VAL:HG21	1.93	0.51
2:D:5:VAL:HG22	2:D:62:ARG:HD2	1.93	0.51
1:A:159:VAL:HG12	1:A:160:ASP:OD1	2.11	0.51
1:A:414:GLU:O	1:A:416:GLY:N	2.44	0.51
2:B:73:MET:CE	2:B:92:PHE:CD1	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:GLN:HB2	2:B:165:ASN:HD22	1.76	0.51
4:F:166:ALA:HB1	4:F:170:LEU:HD11	1.93	0.51
3:E:21:GLU:HG2	3:E:23:ILE:HD11	1.92	0.50
1:A:60:LYS:HD3	1:A:62:VAL:CG2	2.41	0.50
1:C:36:MET:HE1	1:C:49:PHE:CD2	2.45	0.50
3:E:61:ARG:HG3	3:E:61:ARG:HH11	1.77	0.50
1:A:229:ARG:NH1	1:A:363:VAL:HG21	2.25	0.50
1:A:234:ILE:HD12	1:A:234:ILE:N	2.27	0.50
1:A:362:VAL:CG2	1:A:370:LYS:HG3	2.41	0.50
4:F:12:SER:HB2	4:F:343:TYR:OH	2.11	0.50
4:F:131:PHE:C	4:F:131:PHE:CD2	2.88	0.50
2:B:335:ASN:OD1	4:F:36:ARG:NE	2.39	0.50
2:D:7:ILE:HG22	2:D:135:LEU:CD1	2.41	0.50
2:D:103:LYS:HE3	2:D:401:GLU:OE2	2.11	0.50
2:D:323:MET:CG	2:D:353:VAL:HG21	2.41	0.50
3:E:21:GLU:HG2	3:E:23:ILE:CD1	2.42	0.50
4:F:287:ILE:HG22	4:F:291:ILE:HD12	1.92	0.50
2:B:53:GLU:OE2	2:B:57:ASN:ND2	2.45	0.50
2:D:6:HIS:HD2	2:D:7:ILE:N	2.10	0.50
2:D:293:MET:HG3	2:D:367:PHE:HB2	1.94	0.50
3:E:130:ALA:CA	3:E:133:VAL:HG12	2.39	0.50
2:D:267:MET:CE	2:D:303:CYS:HB2	2.41	0.50
3:E:128:LYS:HD2	3:E:128:LYS:O	2.12	0.50
2:B:2:ARG:NE	2:B:131:GLN:HG2	2.26	0.50
2:D:189:VAL:HG11	2:D:415:MET:HE2	1.94	0.49
2:D:215:LEU:HD22	2:D:215:LEU:H	1.77	0.49
2:D:317:PHE:O	2:D:353:VAL:HA	2.12	0.49
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.47	0.49
1:A:414:GLU:C	1:A:416:GLY:N	2.70	0.49
2:D:20:PHE:O	2:D:24:ILE:HG12	2.12	0.49
3:E:19:SER:O	3:E:20:PHE:HB3	2.13	0.49
3:E:59:GLU:OE1	3:E:59:GLU:HA	2.11	0.49
4:F:14:TYR:HA	4:F:17:VAL:HB	1.94	0.49
2:B:36:TYR:CD2	2:B:44:LEU:HD11	2.47	0.49
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.31	0.49
2:D:386:THR:O	2:D:390:ARG:HB2	2.12	0.49
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.95	0.49
2:B:336:LYS:NZ	4:F:1:MET:O	2.39	0.49
2:D:6:HIS:ND1	2:D:21:TRP:NE1	2.60	0.49
2:D:377:LEU:HD13	2:D:377:LEU:C	2.36	0.49
2:D:404:ASP:OD1	2:D:405:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:209:ASP:O	2:D:213:ARG:HD2	2.12	0.49
1:A:34:GLY:O	1:A:61:HIS:N	2.40	0.49
2:B:262:ARG:HD3	2:B:421:GLU:OE1	2.13	0.49
2:B:284:LEU:N	2:B:284:LEU:HD12	2.28	0.49
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.94	0.49
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.93	0.49
4:F:72:CYS:O	4:F:73:ARG:HD2	2.12	0.49
1:C:23:LEU:O	1:C:27:GLU:HG3	2.13	0.49
3:E:56:ALA:HB1	3:E:60:ARG:HH12	1.76	0.49
2:B:135:LEU:HD22	2:B:152:ILE:HD11	1.93	0.48
1:C:270:ALA:HB3	1:C:302:MET:HG2	1.95	0.48
2:D:68:LEU:HG	2:D:143:THR:HG23	1.94	0.48
4:F:136:ASN:HA	4:F:139:ARG:HB3	1.95	0.48
4:F:247:LYS:H	4:F:247:LYS:CD	2.26	0.48
2:D:317:PHE:HB2	2:D:353:VAL:HG12	1.95	0.48
1:A:117:LEU:HD12	1:A:117:LEU:O	2.12	0.48
1:A:192:HIS:CG	1:A:421:ALA:HA	2.49	0.48
1:A:414:GLU:O	1:A:415:GLU:C	2.55	0.48
4:F:286:GLN:O	4:F:290:ILE:HG13	2.13	0.48
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.95	0.48
1:A:213:CYS:O	1:A:217:LEU:HB2	2.13	0.48
2:D:113:VAL:CG1	2:D:114:ASP:N	2.76	0.48
2:D:301:ALA:O	2:D:303:CYS:N	2.43	0.48
1:C:296:PHE:CB	1:C:339:ARG:HD2	2.44	0.48
2:D:395:LEU:HD23	2:D:395:LEU:HA	1.69	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.48	0.48
1:C:88:HIS:O	1:C:89:PRO:C	2.57	0.48
1:C:209:ILE:HG22	1:C:227:LEU:CD2	2.38	0.48
4:F:26:GLN:HB2	4:F:361:LEU:HD22	1.94	0.48
4:F:292:ARG:O	4:F:296:MET:HG2	2.14	0.48
2:B:30:ILE:N	2:B:30:ILE:HD13	2.29	0.48
2:D:203:ASP:CG	2:D:380:ARG:HH22	2.21	0.48
2:D:400:GLY:O	3:E:137:LYS:HG3	2.14	0.48
1:A:2:ARG:O	1:A:51:THR:HG22	2.14	0.48
1:A:402:ARG:HH11	1:A:402:ARG:HG3	1.79	0.48
2:B:8:GLN:HB2	2:B:13:GLY:O	2.12	0.48
4:F:47:LEU:HD23	4:F:48:PRO:N	2.29	0.48
1:A:153:LEU:HD12	1:A:153:LEU:O	2.14	0.47
2:B:158:GLU:HB3	2:B:159:TYR:CD1	2.49	0.47
2:D:156:ARG:HG3	2:D:156:ARG:HH11	1.79	0.47
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.47
2:B:198:GLU:OE2	2:B:254:ALA:HB2	2.14	0.47
1:C:66:VAL:HG23	1:C:125:LEU:HD12	1.95	0.47
2:D:86:ARG:HD3	2:D:89:ASN:OD1	2.14	0.47
2:D:116:VAL:HG21	2:D:147:MET:CE	2.44	0.47
4:F:96:GLU:O	4:F:183:GLN:HA	2.14	0.47
2:B:296:SER:HB2	2:B:305:PRO:HD3	1.96	0.47
1:C:291:ILE:HD13	1:C:373:ARG:HG3	1.96	0.47
4:F:72:CYS:HA	4:F:332:VAL:O	2.14	0.47
1:C:409:VAL:HA	1:C:413:MET:O	2.14	0.47
2:D:32:PRO:HA	2:D:81:PHE:CD2	2.50	0.47
4:F:338:CYS:SG	4:F:339:ALA:N	2.88	0.47
2:B:68:LEU:HD12	2:B:97:ALA:HB2	1.95	0.47
2:B:73:MET:HE2	2:B:92:PHE:HB3	1.96	0.47
4:F:93:TRP:HZ3	4:F:329:LEU:HD23	1.78	0.47
1:A:55:GLU:HA	1:A:60:LYS:O	2.15	0.47
1:A:103:TYR:HD2	1:A:189:LEU:HD13	1.77	0.47
1:A:260:VAL:HG12	1:A:260:VAL:O	2.14	0.47
2:B:104:GLY:O	2:B:109:GLY:HA3	2.15	0.47
2:B:203:ASP:O	2:B:207:LEU:HG	2.15	0.47
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.78	0.47
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.80	0.47
2:D:1:MET:HA	2:D:48:ASN:ND2	2.29	0.47
4:F:292:ARG:NH1	4:F:378:LEU:HB3	2.30	0.47
1:A:402:ARG:HG3	1:A:402:ARG:NH1	2.28	0.47
1:A:70:LEU:HG	1:A:145:THR:CG2	2.42	0.47
4:F:195:GLY:HA3	4:F:197:ARG:CG	2.45	0.47
1:A:331:ALA:C	1:A:334:THR:HG22	2.40	0.47
1:C:108:TYR:CD2	3:E:108:ASN:CG	2.94	0.47
2:D:324:LYS:O	2:D:328:GLU:HG3	2.15	0.47
4:F:21:LEU:HD22	4:F:27:TRP:CD1	2.50	0.47
1:C:140:SER:HA	1:C:171:ILE:HB	1.97	0.46
4:F:192:LEU:HD12	4:F:192:LEU:H	1.79	0.46
4:F:79:LYS:O	4:F:83:THR:OG1	2.28	0.46
1:A:105:ARG:NH1	1:A:411:GLU:OE2	2.46	0.46
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.16	0.46
2:D:92:PHE:O	2:D:92:PHE:CD2	2.68	0.46
2:D:393:ALA:HB1	2:D:394:PHE:CE1	2.51	0.46
4:F:192:LEU:HD12	4:F:192:LEU:N	2.30	0.46
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.51	0.46
2:B:23:VAL:O	2:B:27:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:MET:HE3	2:B:377:LEU:CD2	2.45	0.46
1:C:3:GLU:O	1:C:132:LEU:HD12	2.15	0.46
2:D:193:VAL:HG21	2:D:418:LEU:HD22	1.97	0.46
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.98	0.46
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.97	0.46
1:C:230:LEU:O	1:C:234:ILE:HD12	2.16	0.46
2:D:197:ASP:C	2:D:198:GLU:HG3	2.40	0.46
4:F:149:ALA:HB3	4:F:161:LEU:HB2	1.97	0.46
2:D:4:ILE:HD12	2:D:49:VAL:CG1	2.46	0.46
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.51	0.46
1:C:276:ILE:HG23	1:C:369:ALA:HB3	1.97	0.46
4:F:148:ILE:CD1	4:F:161:LEU:HD12	2.46	0.46
1:A:2:ARG:O	1:A:133:GLN:NE2	2.49	0.46
2:B:2:ARG:HB3	2:B:131:GLN:HG2	1.98	0.46
2:B:73:MET:CE	2:B:92:PHE:HB3	2.46	0.46
2:B:199:THR:OG1	2:B:265:PHE:CD1	2.68	0.46
1:C:66:VAL:HG23	1:C:125:LEU:HD11	1.98	0.46
1:C:147:SER:HB2	1:C:190:THR:HB	1.98	0.46
1:C:296:PHE:HB3	1:C:339:ARG:HD2	1.97	0.46
4:F:148:ILE:O	4:F:182:ILE:HA	2.15	0.46
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.51	0.45
2:B:215:LEU:N	2:B:215:LEU:HD23	2.31	0.45
2:B:219:THR:O	2:B:219:THR:HG22	2.16	0.45
1:C:105:ARG:NH1	1:C:411:GLU:OE2	2.44	0.45
2:D:221:THR:C	2:D:223:GLY:N	2.73	0.45
4:F:135:TYR:O	4:F:135:TYR:CD1	2.65	0.45
4:F:242:ASN:HB2	4:F:245:ILE:HB	1.97	0.45
4:F:203:SER:HB3	4:F:215:LEU:HD11	1.97	0.45
2:B:2:ARG:HD2	2:B:129:CYS:SG	2.57	0.45
2:B:9:ALA:HA	2:B:66:VAL:O	2.17	0.45
2:D:117:LEU:HD11	2:D:154:LYS:HB3	1.98	0.45
4:F:81:ILE:CD1	4:F:87:LEU:HD13	2.45	0.45
4:F:102:PRO:HG3	4:F:178:GLN:O	2.17	0.45
1:A:172:TYR:CG	1:A:173:PRO:HD2	2.52	0.45
2:B:185:ALA:O	2:B:189:VAL:HG23	2.17	0.45
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.99	0.45
2:D:99:ASN:HD21	2:D:178:THR:HG21	1.81	0.45
4:F:173:ILE:HG22	4:F:180:HIS:HB2	1.99	0.45
1:A:123:ARG:O	1:A:123:ARG:HG3	2.16	0.45
2:B:267:MET:HE1	2:B:299:MET:HG3	1.99	0.45
1:C:1:MET:HE3	1:C:1:MET:HB2	1.91	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:87:LEU:N	4:F:87:LEU:HD23	2.31	0.45
4:F:88:SER:C	4:F:90:SER:H	2.25	0.45
4:F:237:THR:HG23	4:F:246:GLN:HE22	1.82	0.45
1:C:93:ILE:HD11	1:C:121:ARG:CG	2.41	0.45
2:B:31:ASP:CG	2:B:33:THR:HG23	2.42	0.45
2:D:73:MET:HE1	2:D:92:PHE:CD1	2.52	0.45
2:D:102:ALA:HB2	2:D:403:MET:HE1	1.91	0.45
2:D:113:VAL:HG13	2:D:114:ASP:N	2.31	0.45
4:F:64:TYR:O	4:F:311:SER:HB3	2.17	0.45
4:F:199:PHE:CD2	4:F:199:PHE:C	2.95	0.45
2:B:2:ARG:HE	2:B:131:GLN:HG2	1.82	0.45
2:B:73:MET:HE1	2:B:92:PHE:CD1	2.52	0.45
2:B:73:MET:HE1	2:B:92:PHE:HD1	1.82	0.45
2:D:5:VAL:O	2:D:133:PHE:HA	2.16	0.45
2:D:208:TYR:CD1	2:D:220:PRO:HG2	2.52	0.45
1:A:231:ILE:O	1:A:235:VAL:HG23	2.17	0.44
2:B:135:LEU:CD2	2:B:152:ILE:HD11	2.46	0.44
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.47	0.44
2:D:272:PRO:HB3	2:D:284:LEU:CD2	2.46	0.44
3:E:22:VAL:HG13	3:E:22:VAL:O	2.17	0.44
4:F:309:TYR:C	4:F:310:GLN:HG2	2.43	0.44
2:B:203:ASP:HB2	2:B:301:ALA:HA	1.99	0.44
2:B:336:LYS:HE3	2:B:336:LYS:CA	2.25	0.44
2:B:385:PHE:CE1	2:B:412:GLU:HB2	2.52	0.44
2:D:29:GLY:O	2:D:36:TYR:HA	2.17	0.44
1:C:71:GLU:HB2	1:C:72:PRO:CD	2.48	0.44
1:C:255:PHE:CD1	1:C:352:LYS:HD3	2.52	0.44
2:D:8:GLN:CD	2:D:65:LEU:HD22	2.42	0.44
2:D:65:LEU:HD11	2:D:85:PHE:CD1	2.53	0.44
4:F:226:GLU:HG3	4:F:237:THR:CG2	2.41	0.44
1:C:285:GLN:OE1	1:C:285:GLN:HA	2.17	0.44
2:D:101:TRP:HD1	2:D:145:SER:OG	2.00	0.44
4:F:40:MET:HE3	4:F:40:MET:HB2	1.86	0.44
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.53	0.44
1:A:331:ALA:CA	1:A:334:THR:HG22	2.47	0.44
2:B:177:ASP:O	1:C:352:LYS:HE2	2.17	0.44
2:B:232:THR:HG21	2:B:268:PRO:HB2	1.99	0.44
2:D:330:MET:HE3	2:D:330:MET:HA	2.00	0.44
4:F:92:THR:O	4:F:326:LYS:NZ	2.43	0.44
1:C:221:ARG:HH12	2:D:323:MET:HB3	1.81	0.44
4:F:58:LEU:HA	4:F:58:LEU:HD23	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LYS:HE3	2:B:428:ALA:HB1	1.99	0.44
2:B:124:SER:O	2:B:127:CYS:HB2	2.18	0.44
1:C:1:MET:O	1:C:51:THR:HG22	2.17	0.44
1:C:71:GLU:HB2	1:C:72:PRO:HD2	1.99	0.44
2:D:73:MET:CG	2:D:77:ARG:HH22	2.31	0.44
1:A:36:MET:O	1:A:37:PRO:C	2.61	0.44
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.00	0.44
2:B:363:MET:HB3	2:B:363:MET:HE3	1.68	0.44
2:D:73:MET:SD	2:D:77:ARG:NH2	2.89	0.44
4:F:38:ASN:ND2	4:F:58:LEU:HD22	2.33	0.44
1:C:274:PRO:HG2	1:C:371:VAL:HG11	2.00	0.43
1:A:84:ARG:HG2	1:A:85:GLN:HG3	1.99	0.43
1:A:215:ARG:CZ	1:A:299:ALA:HB1	2.48	0.43
1:A:326:LYS:HE2	1:A:326:LYS:HB3	1.76	0.43
1:A:331:ALA:HA	1:A:334:THR:CG2	2.47	0.43
2:D:77:ARG:HG3	2:D:77:ARG:HH11	1.84	0.43
2:D:221:THR:C	2:D:223:GLY:H	2.26	0.43
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.48	0.43
2:B:169:VAL:HA	2:B:202:ILE:O	2.18	0.43
2:B:246:LEU:HD23	2:B:246:LEU:HA	1.73	0.43
1:C:4:CYS:HB3	1:C:136:LEU:HD11	2.00	0.43
2:D:5:VAL:CG2	2:D:62:ARG:HD2	2.47	0.43
2:D:20:PHE:CZ	2:D:24:ILE:CD1	3.00	0.43
4:F:130:VAL:HG12	4:F:130:VAL:O	2.18	0.43
1:A:147:SER:HB2	1:A:190:THR:HB	1.99	0.43
2:B:36:TYR:O	2:B:37:HIS:ND1	2.46	0.43
1:C:234:ILE:HD13	1:C:302:MET:SD	2.58	0.43
2:D:31:ASP:OD1	2:D:33:THR:CG2	2.66	0.43
4:F:73:ARG:O	4:F:74:LYS:C	2.61	0.43
4:F:283:ILE:HG23	4:F:327:VAL:CG2	2.48	0.43
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.54	0.43
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.93	0.43
1:A:357:TYR:CD2	3:E:17:GLY:HA2	2.53	0.43
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.53	0.43
1:C:221:ARG:NH2	2:D:323:MET:CB	2.81	0.43
2:D:20:PHE:CE1	2:D:24:ILE:HD13	2.52	0.43
2:D:31:ASP:OD1	2:D:33:THR:HG23	2.18	0.43
2:D:295:ASP:OD2	2:D:297:LYS:HE3	2.17	0.43
3:E:116:LEU:HD23	3:E:116:LEU:HA	1.81	0.43
3:E:131:GLU:OE1	3:E:131:GLU:CA	2.66	0.43
1:A:56:THR:HG23	1:A:60:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASP:C	1:A:98:ASP:OD1	2.62	0.43
2:B:70:PRO:HG3	2:B:94:GLN:CD	2.43	0.43
2:D:164:MET:HG3	2:D:196:THR:HG22	2.00	0.43
4:F:192:LEU:CD1	4:F:199:PHE:HD1	2.31	0.43
4:F:202:ARG:HA	4:F:317:PHE:O	2.18	0.43
1:A:41:THR:O	1:A:44:GLY:O	2.37	0.43
1:A:136:LEU:HD12	1:A:136:LEU:N	2.34	0.43
1:C:1:MET:HG2	1:C:130:THR:OG1	2.19	0.43
1:C:413:MET:HE2	1:C:413:MET:HB3	1.87	0.43
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.36	0.43
4:F:146:VAL:HG23	4:F:187:GLU:OE2	2.19	0.43
2:B:164:MET:HG3	2:B:196:THR:HG22	2.01	0.43
3:E:6:MET:HE2	3:E:24:LEU:HG	2.01	0.43
3:E:75:LYS:O	3:E:79:GLU:HG3	2.19	0.43
4:F:172:PHE:HE1	4:F:176:GLN:NE2	2.16	0.43
4:F:234:GLN:O	4:F:234:GLN:CG	2.67	0.43
4:F:2:TYR:OH	4:F:360:PRO:O	2.37	0.43
1:A:102:ASN:HB3	1:A:105:ARG:HB3	2.00	0.42
2:B:61:PRO:CD	2:B:84:ILE:HG12	2.49	0.42
4:F:218:GLU:OE1	4:F:218:GLU:HA	2.19	0.42
4:F:326:LYS:HG2	4:F:328:TRP:NE1	2.33	0.42
1:C:124:LYS:HA	1:C:124:LYS:HD3	1.83	0.42
1:A:173:PRO:HB3	1:A:183:GLU:OE1	2.19	0.42
3:E:47:LEU:HD12	3:E:47:LEU:C	2.44	0.42
1:A:31:GLN:HG3	1:A:35:GLN:O	2.18	0.42
1:C:126:ALA:O	1:C:129:CYS:HB2	2.20	0.42
1:C:345:ASP:OD1	1:C:345:ASP:C	2.63	0.42
2:D:246:LEU:HD12	2:D:248:ALA:HB2	2.01	0.42
4:F:220:VAL:HG23	4:F:263:PHE:CD2	2.54	0.42
1:A:142:GLY:HA3	1:A:183:GLU:OE1	2.18	0.42
2:B:375:GLN:HE22	2:B:423:GLN:HG2	1.83	0.42
2:D:66:VAL:HG21	2:D:116:VAL:CG1	2.50	0.42
2:D:105:HIS:O	2:D:150:LEU:HD22	2.19	0.42
1:A:2:ARG:HB3	1:A:131:GLY:O	2.19	0.42
1:A:112:LYS:NZ	3:E:54:LEU:HB3	2.35	0.42
1:A:141:PHE:O	1:A:147:SER:HB3	2.20	0.42
2:B:31:ASP:OD1	2:B:33:THR:CG2	2.63	0.42
2:B:267:MET:HB3	2:B:267:MET:HE3	1.58	0.42
1:C:363:VAL:O	1:C:364:PRO:C	2.62	0.42
2:D:67:ASP:OD1	2:D:68:LEU:N	2.51	0.42
4:F:71:LEU:HD11	4:F:294:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:78:VAL:HG21	4:F:181:VAL:HG21	2.02	0.42
4:F:131:PHE:CD1	4:F:182:ILE:CD1	3.03	0.42
2:B:8:GLN:NE2	2:B:65:LEU:HD23	2.35	0.42
2:B:196:THR:OG1	2:B:199:THR:HG23	2.18	0.42
2:D:33:THR:HG23	2:D:35:SER:OG	2.19	0.42
2:D:34:GLY:HA3	2:D:58:LYS:HG3	2.02	0.42
4:F:148:ILE:HD13	4:F:162:ILE:CG1	2.49	0.42
4:F:195:GLY:C	4:F:197:ARG:HG2	2.44	0.42
4:F:237:THR:HG23	4:F:246:GLN:NE2	2.35	0.42
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.55	0.42
1:A:153:LEU:HD12	1:A:153:LEU:C	2.45	0.42
1:C:252:LEU:HD12	1:C:252:LEU:O	2.20	0.42
2:B:165:ASN:HA	2:B:198:GLU:O	2.20	0.42
2:D:246:LEU:CD1	2:D:248:ALA:HB2	2.50	0.42
1:A:88:HIS:O	1:A:89:PRO:C	2.62	0.41
1:A:88:HIS:CD2	1:A:90:GLU:HG3	2.52	0.41
2:B:310:TYR:CE1	2:B:367:PHE:HZ	2.38	0.41
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.55	0.41
4:F:192:LEU:CD1	4:F:199:PHE:CD1	3.03	0.41
1:C:48:SER:OG	1:C:245:ASP:OD1	2.39	0.41
4:F:78:VAL:O	4:F:82:LYS:HG3	2.21	0.41
2:B:73:MET:HE3	2:B:73:MET:HB3	1.78	0.41
1:C:4:CYS:SG	1:C:242:LEU:HD13	2.60	0.41
2:D:253:LEU:O	2:D:257:MET:HB2	2.19	0.41
4:F:101:TYR:CD1	4:F:179:VAL:HG13	2.55	0.41
1:A:421:ALA:O	1:A:425:MET:HG2	2.20	0.41
1:C:1:MET:HB2	1:C:2:ARG:H	1.55	0.41
1:C:79:ARG:HG3	1:C:92:LEU:HD12	2.02	0.41
2:D:10:GLY:HA2	2:D:143:THR:HB	2.02	0.41
2:D:62:ARG:HG3	2:D:123:GLU:OE1	2.20	0.41
4:F:148:ILE:HD11	4:F:161:LEU:CD1	2.49	0.41
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.01	0.41
1:A:395:PHE:CD1	1:A:395:PHE:C	2.97	0.41
2:B:50:TYR:CD2	2:B:241:ARG:HG2	2.56	0.41
2:B:117:LEU:HA	2:B:117:LEU:HD23	1.79	0.41
2:D:7:ILE:HG22	2:D:135:LEU:HD12	2.01	0.41
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.55	0.41
1:C:147:SER:OG	1:C:186:ASN:HB3	2.20	0.41
1:A:90:GLU:CA	1:A:121:ARG:HH21	2.30	0.41
2:B:321:MET:HE3	2:B:363:MET:SD	2.60	0.41
4:F:192:LEU:HD11	4:F:199:PHE:HD1	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLN:HG3	1:A:74:VAL:HG21	2.03	0.41
1:A:346:TRP:CH2	1:A:435:VAL:HG13	2.56	0.41
1:C:71:GLU:HG2	1:C:98:ASP:CB	2.33	0.41
1:C:115:ILE:HG23	1:C:116:ASP:N	2.36	0.41
2:D:20:PHE:CD1	2:D:233:MET:HE2	2.56	0.41
3:E:106:GLU:O	3:E:110:GLU:HG3	2.20	0.41
2:B:296:SER:HA	2:B:299:MET:HG2	2.02	0.41
2:B:331:LEU:HD11	4:F:56:PRO:HB2	2.02	0.41
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.52	0.41
2:D:172:SER:HB2	2:D:205:GLU:N	2.35	0.41
2:D:202:ILE:CG2	2:D:207:LEU:HD11	2.49	0.41
2:D:233:MET:HE3	2:D:233:MET:HB3	1.94	0.41
2:D:357:PRO:HB2	2:D:361:LEU:O	2.21	0.41
3:E:58:GLU:O	3:E:58:GLU:HG3	2.21	0.41
4:F:49:PHE:CB	4:F:66:ARG:HD2	2.51	0.41
1:A:395:PHE:CD1	1:A:422:ARG:HD3	2.56	0.41
1:C:103:TYR:CE2	1:C:148:GLY:HA2	2.56	0.41
2:D:5:VAL:HB	2:D:133:PHE:CD1	2.56	0.41
2:D:154:LYS:HA	2:D:154:LYS:HD2	1.80	0.41
3:E:101:LEU:HD23	3:E:101:LEU:HA	1.84	0.41
1:A:280:LYS:HB3	1:A:280:LYS:HE2	1.93	0.40
1:A:293:ASN:CB	1:A:335:ILE:HD11	2.51	0.40
2:D:332:ASN:OD1	2:D:336:LYS:NZ	2.30	0.40
3:E:125:GLU:OE1	3:E:125:GLU:HA	2.21	0.40
3:E:140:LYS:HB3	3:E:141:GLU:OE2	2.21	0.40
4:F:31:ARG:NE	4:F:32:LYS:H	2.19	0.40
4:F:166:ALA:O	4:F:167:SER:C	2.64	0.40
1:A:53:PHE:O	1:A:64:ARG:NH2	2.52	0.40
1:A:70:LEU:HD23	1:A:70:LEU:HA	1.81	0.40
1:C:333:ALA:O	1:C:337:THR:HG23	2.21	0.40
2:D:395:LEU:CD1	2:D:405:GLU:HG3	2.51	0.40
4:F:149:ALA:CB	4:F:161:LEU:CB	2.97	0.40
4:F:214:TYR:CE2	4:F:353:VAL:CG1	3.05	0.40
1:A:351:PHE:N	1:A:351:PHE:CD1	2.88	0.40
1:C:54:SER:O	1:C:61:HIS:HA	2.21	0.40
2:D:380:ARG:O	2:D:384:GLN:HG3	2.22	0.40
4:F:21:LEU:HD22	4:F:27:TRP:CG	2.56	0.40
4:F:21:LEU:HD23	4:F:21:LEU:HA	1.90	0.40
1:A:401:LYS:CE	2:B:428:ALA:HB1	2.52	0.40
1:A:412:GLY:HA3	3:E:57:ALA:HB1	2.03	0.40
2:B:304:ASP:OD2	2:B:307:HIS:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:HIS:O	2:B:426:GLN:NE2	2.55	0.40
2:D:61:PRO:HD3	2:D:84:ILE:HG12	2.02	0.40
2:D:189:VAL:CB	2:D:415:MET:HE3	2.51	0.40
2:D:303:CYS:HA	2:D:376:GLU:OE1	2.22	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	435/440 (99%)	406 (93%)	28 (6%)	1 (0%)	43	62
1	C	438/440 (100%)	415 (95%)	21 (5%)	2 (0%)	24	40
2	B	425/431 (99%)	405 (95%)	19 (4%)	1 (0%)	43	62
2	D	417/431 (97%)	388 (93%)	28 (7%)	1 (0%)	43	62
3	E	117/136 (86%)	107 (92%)	10 (8%)	0	100	100
4	F	318/380 (84%)	294 (92%)	23 (7%)	1 (0%)	36	54
All	All	2150/2258 (95%)	2015 (94%)	129 (6%)	6 (0%)	36	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	GLU
2	B	71	GLY
2	D	222	TYR
4	F	102	PRO
1	C	364	PRO
1	C	72	PRO

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%)	351 (96%)	15 (4%)	27	48
1	C	370/371 (100%)	357 (96%)	13 (4%)	32	54
2	B	367/372 (99%)	355 (97%)	12 (3%)	33	55
2	D	362/372 (97%)	346 (96%)	16 (4%)	25	45
3	E	109/122 (89%)	103 (94%)	6 (6%)	19	35
4	F	292/338 (86%)	278 (95%)	14 (5%)	23	42
All	All	1866/1946 (96%)	1790 (96%)	76 (4%)	27	48

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	48	SER
1	A	71	GLU
1	A	159	VAL
1	A	179	THR
1	A	229	ARG
1	A	250	VAL
1	A	253	THR
1	A	257	THR
1	A	315	CYS
1	A	324	VAL
1	A	335	ILE
1	A	338	LYS
1	A	402	ARG
1	A	434	GLU
2	B	15	GLN
2	B	16	ILE
2	B	33	THR
2	B	115	SER
2	B	153	SER
2	B	175	VAL
2	B	176	SER

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Mol	Chain	Res	Type
2	B	246	LEU
2	B	296	SER
2	B	339	SER
2	B	382	SER
2	B	413	SER
1	C	165	SER
1	C	177	VAL
1	C	232	SER
1	C	241	SER
1	C	265	ILE
1	C	337	THR
1	C	347	CYS
1	C	363	VAL
1	C	379	SER
1	C	381	THR
1	C	384	ILE
1	C	419	SER
1	C	440	VAL
2	D	35	SER
2	D	39	ASP
2	D	75	SER
2	D	115	SER
2	D	136	THR
2	D	153	SER
2	D	180	VAL
2	D	193	VAL
2	D	213	ARG
2	D	216	LYS
2	D	218	THR
2	D	219	THR
2	D	246	LEU
2	D	296	SER
2	D	306	ARG
2	D	339	SER
3	E	9	ILE
3	E	16	SER
3	E	46	SER
3	E	53	LYS
3	E	126	LYS
3	E	131	GLU
4	F	12	SER
4	F	45	ASN

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Mol	Chain	Res	Type
4	F	69	ASP
4	F	161	LEU
4	F	188	LYS
4	F	196	HIS
4	F	197	ARG
4	F	225	SER
4	F	238	CYS
4	F	244	CYS
4	F	245	ILE
4	F	284	LEU
4	F	320	MET
4	F	340	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	102	ASN
1	A	309	HIS
2	B	8	GLN
2	B	43	GLN
2	B	291	GLN
2	B	337	ASN
1	C	256	GLN
1	C	380	ASN
1	C	393	HIS
2	D	99	ASN
2	D	426	GLN
3	E	84	GLN
3	E	103	GLN
3	E	108	ASN
4	F	26	GLN
4	F	145	ASN
4	F	310	GLN

5.3.3 RNA ⓘ

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 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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
10	A1D6D	D	502	-	28,28,28	2.69	9 (32%)	36,41,41	2.37	10 (27%)
5	GTP	A	501	7	33,34,34	0.96	1 (3%)	50,54,54	1.58	9 (18%)
10	A1D6D	B	505	-	28,28,28	2.65	12 (42%)	36,41,41	2.81	11 (30%)
11	ACP	F	401	-	31,33,33	0.52	1 (3%)	47,52,52	1.17	1 (2%)
9	MES	B	502	-	12,12,12	2.33	1 (8%)	15,16,16	1.83	3 (20%)
8	GDP	B	501	7	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
5	GTP	C	501	7	33,34,34	0.98	2 (6%)	50,54,54	1.58	8 (16%)
8	GDP	D	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
9	MES	B	503	-	12,12,12	2.34	1 (8%)	15,16,16	1.87	2 (13%)

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
10	A1D6D	D	502	-	-	5/6/18/18	0/4/4/4
5	GTP	A	501	7	-	8/22/38/38	0/3/3/3
10	A1D6D	B	505	-	-	2/6/18/18	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ACP	F	401	-	-	4/19/38/38	0/3/3/3
9	MES	B	502	-	-	0/6/14/14	0/1/1/1
8	GDP	B	501	7	-	3/16/32/32	0/3/3/3
5	GTP	C	501	7	-	10/22/38/38	0/3/3/3
8	GDP	D	501	-	-	2/16/32/32	0/3/3/3
9	MES	B	503	-	-	4/6/14/14	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	A1D6D	C14-N16	8.85	1.45	1.35
10	B	505	A1D6D	C14-N16	8.02	1.44	1.35
9	B	503	MES	C8-S	-7.82	1.66	1.77
9	B	502	MES	C8-S	-7.79	1.66	1.77
10	B	505	A1D6D	C17-N16	5.69	1.49	1.39
10	D	502	A1D6D	C17-N16	5.22	1.48	1.39
10	B	505	A1D6D	C05-C04	-4.13	1.36	1.42
10	D	502	A1D6D	C18-N12	4.03	1.47	1.40
10	D	502	A1D6D	C07-N12	3.63	1.47	1.39
10	D	502	A1D6D	C05-C04	-3.41	1.37	1.42
10	D	502	A1D6D	C13-C14	3.39	1.55	1.51
10	B	505	A1D6D	C13-C14	3.38	1.55	1.51
8	B	501	GDP	C5-C4	3.18	1.47	1.38
10	B	505	A1D6D	C07-N12	3.17	1.46	1.39
8	D	501	GDP	C5-C4	3.14	1.47	1.38
10	B	505	A1D6D	C17-C18	-3.12	1.37	1.40
10	B	505	A1D6D	C18-N12	2.90	1.45	1.40
10	D	502	A1D6D	C09-N10	2.86	1.32	1.30
10	B	505	A1D6D	C09-N10	2.76	1.32	1.30
11	F	401	ACP	PB-O3A	2.69	1.61	1.58
10	D	502	A1D6D	C17-C18	-2.52	1.37	1.40
10	B	505	A1D6D	C06-C01	2.50	1.40	1.36
8	B	501	GDP	C6-N1	-2.43	1.34	1.38
8	D	501	GDP	C6-N1	-2.38	1.34	1.38
10	B	505	A1D6D	O15-C14	-2.26	1.18	1.23
5	A	501	GTP	C2-N3	2.22	1.38	1.33
5	C	501	GTP	C2-N3	2.20	1.38	1.33
10	B	505	A1D6D	C07-N08	2.18	1.34	1.32
10	B	505	A1D6D	C13-N12	-2.14	1.42	1.46
10	D	502	A1D6D	C13-N12	-2.08	1.42	1.46
5	C	501	GTP	PA-O3A	2.07	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	GDP	C5-N7	-2.03	1.35	1.39
8	B	501	GDP	C5-N7	-2.02	1.35	1.39

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	A1D6D	N10-C09-N08	-11.94	118.74	130.58
10	D	502	A1D6D	N10-C09-N08	-9.08	121.58	130.58
11	F	401	ACP	PB-O3A-PA	-6.68	110.57	132.37
8	B	501	GDP	C5-C4-N3	-6.11	118.67	128.39
8	D	501	GDP	C5-C4-N3	-6.08	118.71	128.39
5	C	501	GTP	C5-C4-N3	-5.02	120.39	128.39
5	A	501	GTP	C5-C4-N3	-5.02	120.41	128.39
8	B	501	GDP	C2-N3-C4	5.01	120.93	112.30
8	D	501	GDP	C2-N3-C4	5.00	120.91	112.30
10	D	502	A1D6D	C07-C05-C04	4.94	118.75	115.47
10	B	505	A1D6D	CL11-C09-N10	4.77	119.66	115.72
5	A	501	GTP	C2-N3-C4	4.63	120.27	112.30
5	C	501	GTP	C2-N3-C4	4.62	120.26	112.30
10	B	505	A1D6D	CL11-C09-N08	4.56	121.59	115.17
8	D	501	GDP	N9-C4-N3	4.53	135.01	125.95
9	B	503	MES	C5-N4-C3	4.52	118.58	108.84
8	B	501	GDP	N9-C4-N3	4.51	134.97	125.95
9	B	502	MES	C5-N4-C3	4.30	118.11	108.84
10	B	505	A1D6D	C09-N08-C07	4.14	123.25	111.13
10	B	505	A1D6D	C17-N16-C14	-3.69	120.03	124.45
10	D	502	A1D6D	C09-N08-C07	3.63	121.77	111.13
10	D	502	A1D6D	CL11-C09-N08	3.43	120.00	115.17
10	B	505	A1D6D	C02-C01-C06	-3.41	119.35	123.32
10	D	502	A1D6D	CL11-C09-N10	3.26	118.42	115.72
8	B	501	GDP	C6-C5-N7	3.24	136.19	130.29
5	C	501	GTP	N9-C4-N3	3.21	132.38	125.95
8	D	501	GDP	C6-C5-N7	3.19	136.10	130.29
5	A	501	GTP	N9-C4-N3	3.18	132.32	125.95
10	B	505	A1D6D	C13-C14-N16	-2.94	112.47	116.13
10	D	502	A1D6D	C05-C04-N10	-2.94	119.69	122.80
10	B	505	A1D6D	C01-C06-C05	2.91	121.05	118.75
10	B	505	A1D6D	C18-N12-C07	2.91	124.57	119.21
5	C	501	GTP	C2-N1-C6	-2.90	119.85	125.11
5	A	501	GTP	C2-N1-C6	-2.86	119.93	125.11
10	D	502	A1D6D	C02-C01-C06	-2.80	120.06	123.32
10	D	502	A1D6D	C01-C06-C05	2.68	120.86	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N9-C8-N7	-2.66	108.47	113.40
5	A	501	GTP	N9-C8-N7	-2.66	108.47	113.40
10	D	502	A1D6D	C17-N16-C14	-2.64	121.29	124.45
9	B	502	MES	C6-C5-N4	-2.61	106.15	110.12
10	B	505	A1D6D	O15-C14-N16	2.59	124.14	121.39
8	B	501	GDP	C4-C5-N7	-2.57	106.60	110.67
5	C	501	GTP	C8-N7-C5	2.55	108.81	104.26
5	A	501	GTP	C8-N7-C5	2.54	108.78	104.26
5	C	501	GTP	C5-C6-N1	2.52	119.67	113.25
8	D	501	GDP	C4-C5-N7	-2.52	106.67	110.67
5	A	501	GTP	C5-C6-N1	2.48	119.57	113.25
9	B	503	MES	C6-C5-N4	-2.48	106.36	110.12
10	D	502	A1D6D	C05-C07-N08	-2.44	117.71	122.44
5	C	501	GTP	O6-C6-C5	-2.41	120.17	126.53
5	A	501	GTP	O6-C6-C5	-2.39	120.23	126.53
9	B	502	MES	O2S-S-C8	2.28	110.17	106.73
8	D	501	GDP	C3'-C2'-C1'	2.11	105.46	101.46
8	B	501	GDP	O6-C6-C5	-2.10	120.98	126.53
8	D	501	GDP	O6-C6-C5	-2.08	121.04	126.53
8	B	501	GDP	C3'-C2'-C1'	2.07	105.38	101.46
5	A	501	GTP	C3'-C2'-C1'	2.04	105.32	101.46
10	B	505	A1D6D	C24-O23-C21	-2.01	113.18	117.50

There are no chirality outliers.

All (38) 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-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
9	B	503	MES	C7-C8-S-O3S
10	D	502	A1D6D	C05-C07-N12-C18

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Mol	Chain	Res	Type	Atoms
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
10	D	502	A1D6D	C20-C21-O23-C24
10	D	502	A1D6D	C22-C21-O23-C24
5	A	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	C3'-C4'-C5'-O5'
10	D	502	A1D6D	N08-C07-N12-C13
9	B	503	MES	C8-C7-N4-C3
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O1A
10	B	505	A1D6D	N08-C07-N12-C18
10	D	502	A1D6D	N08-C07-N12-C18
11	F	401	ACP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O3G
10	B	505	A1D6D	N08-C07-N12-C13
5	C	501	GTP	O4'-C4'-C5'-O5'
5	C	501	GTP	PB-O3A-PA-O1A
11	F	401	ACP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3A-PA-O2A

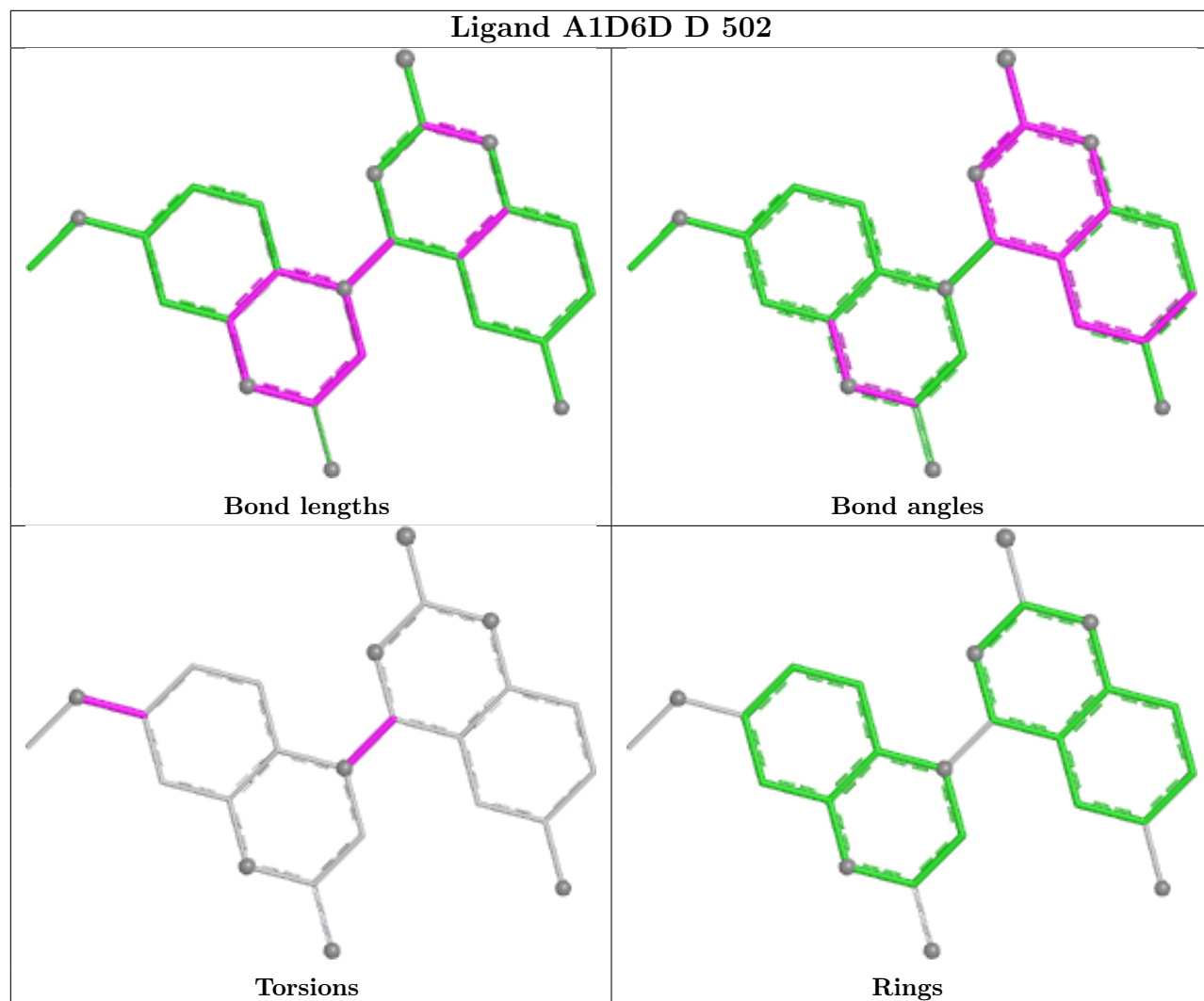
There are no ring outliers.

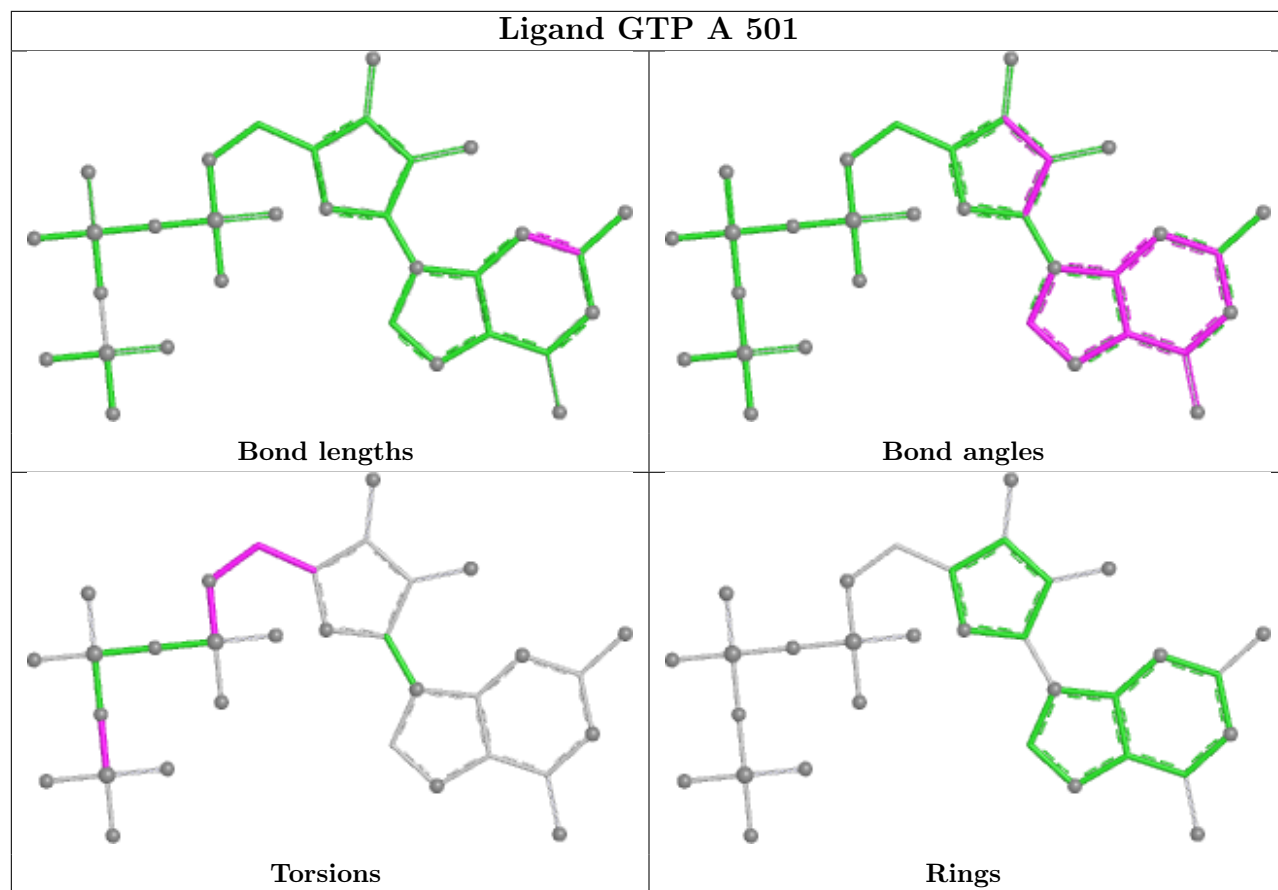
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	502	A1D6D	1	0

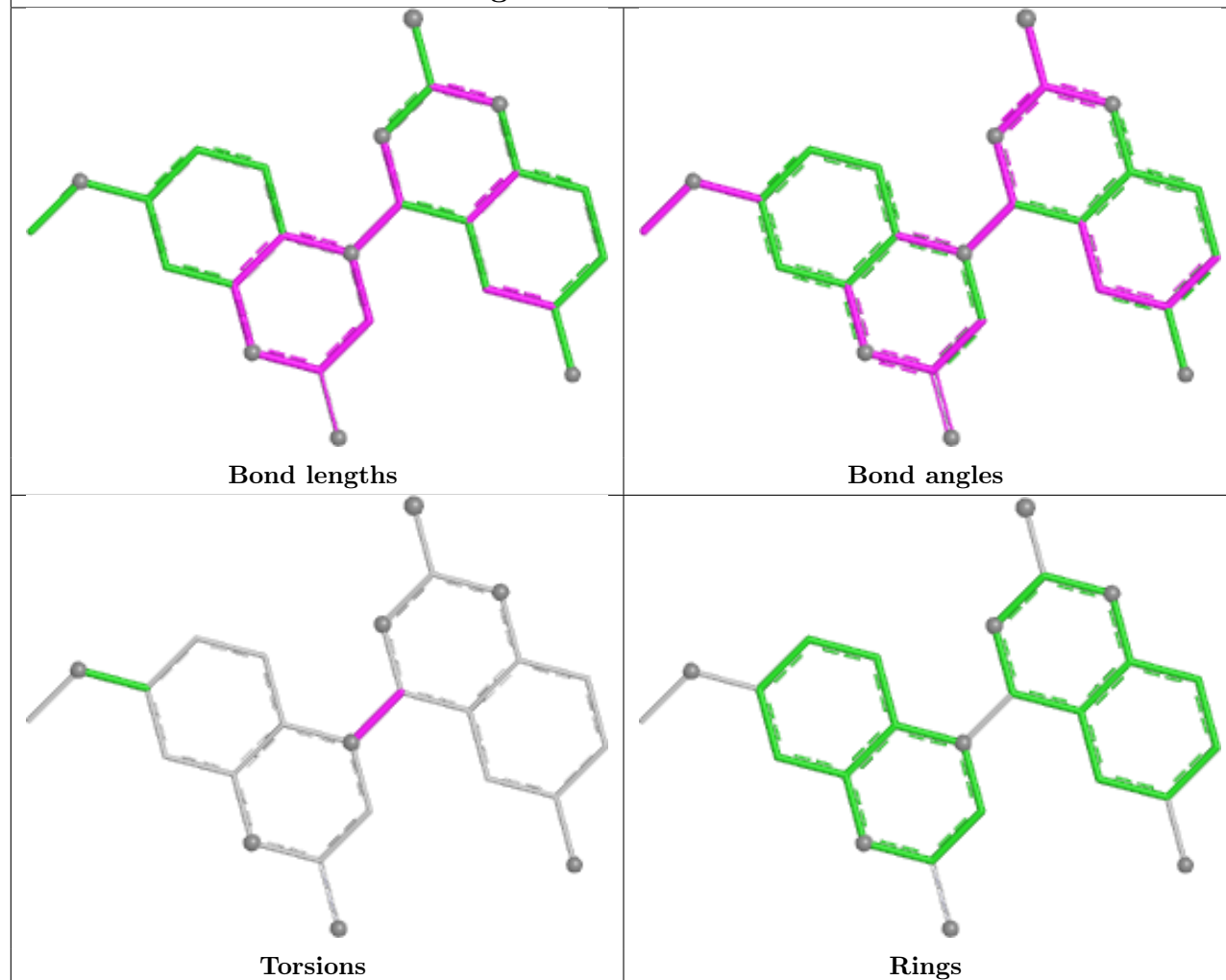
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A1D6D D 502

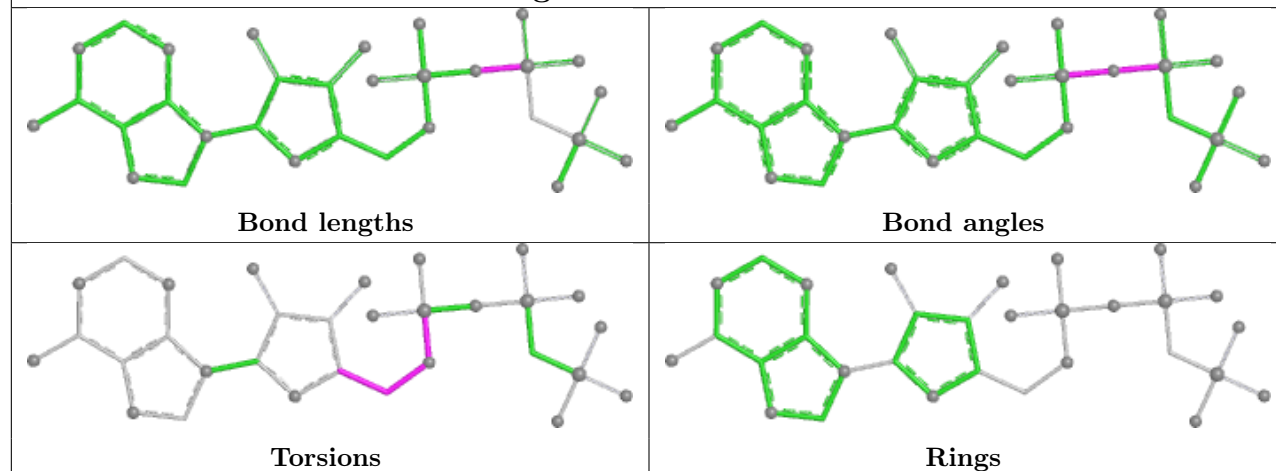


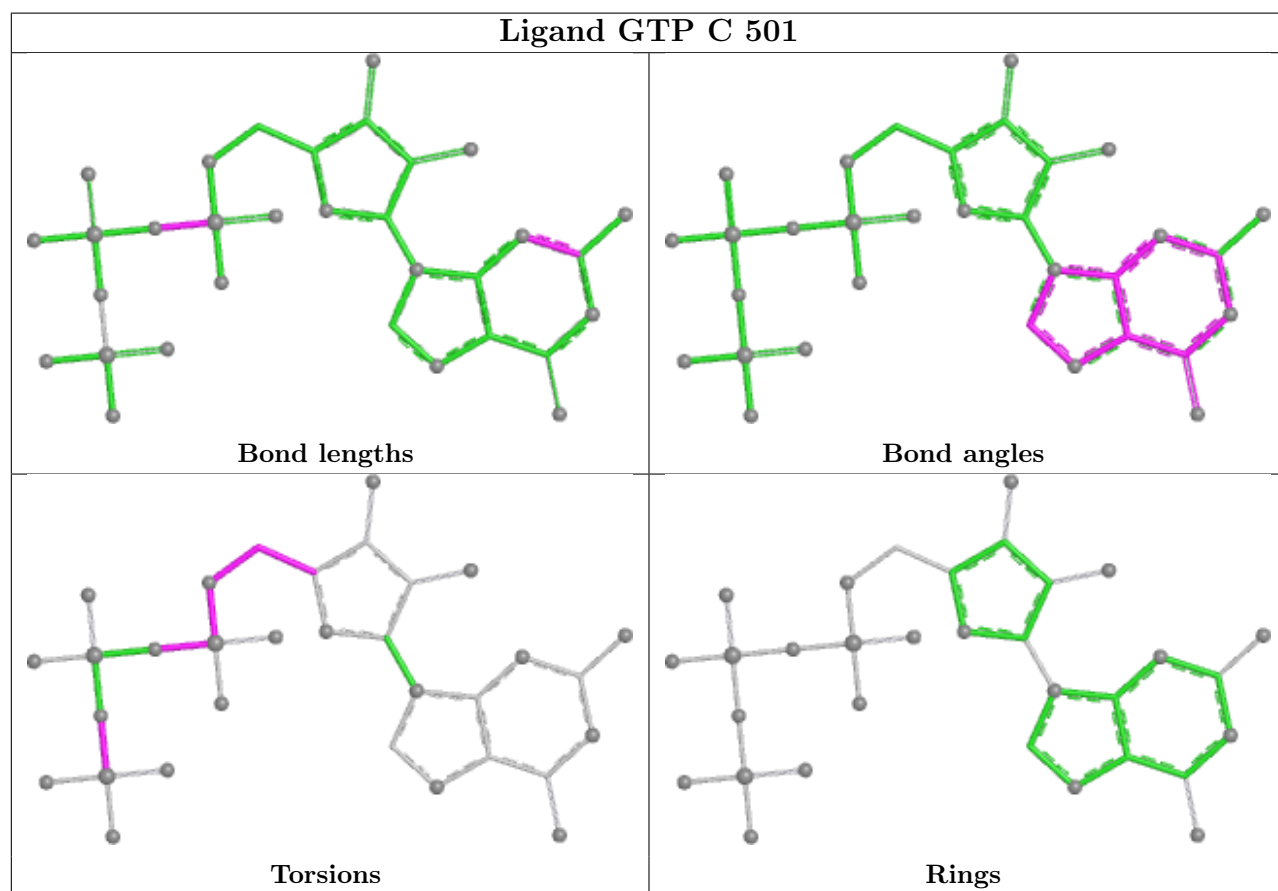
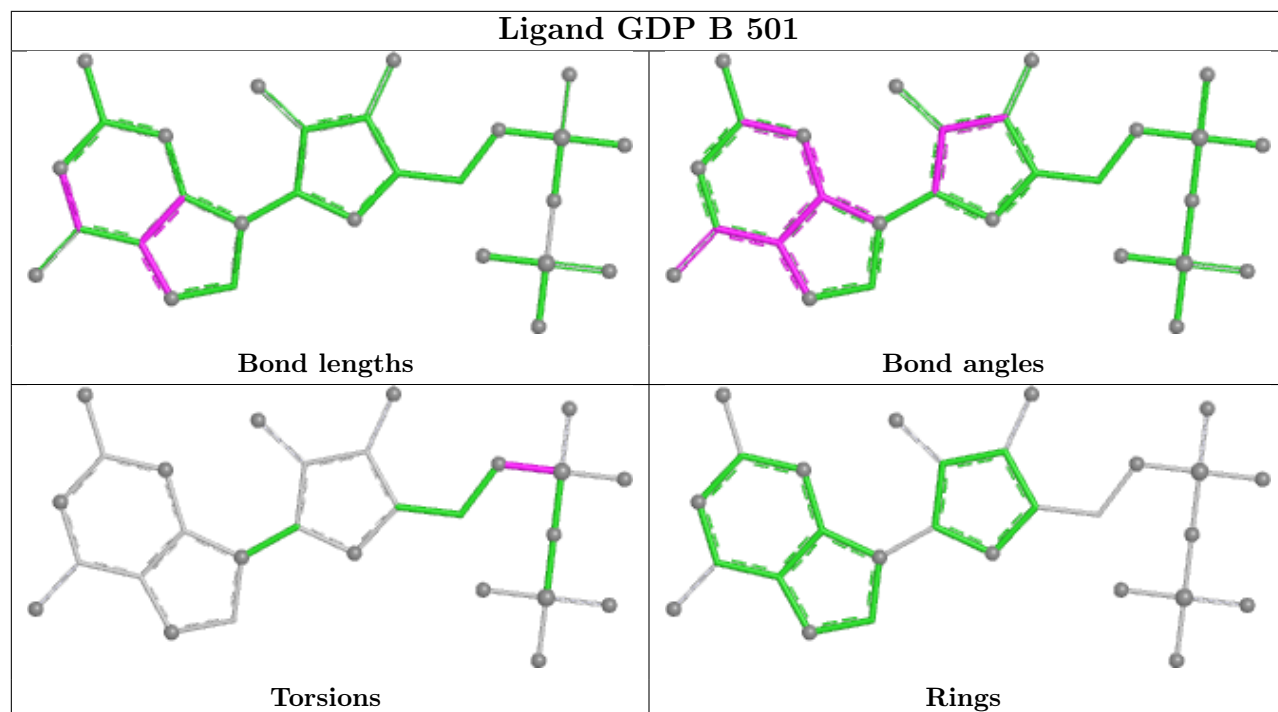


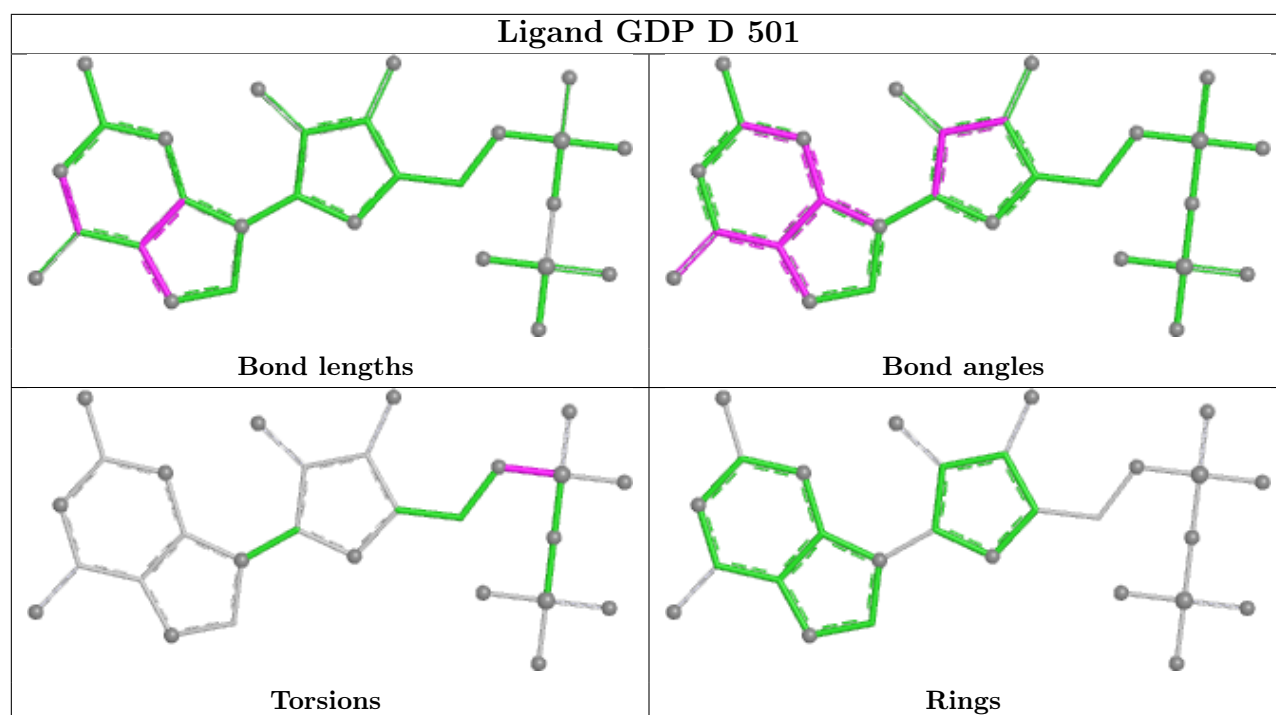
Ligand A1D6D B 505



Ligand ACP F 401







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	437/440 (99%)	0.09	3 (0%)	84 84	33, 53, 72, 100	0
1	C	440/440 (100%)	-0.30	3 (0%)	84 84	27, 42, 61, 74	0
2	B	427/431 (99%)	-0.03	5 (1%)	76 75	30, 48, 74, 118	0
2	D	421/431 (97%)	0.63	32 (7%)	20 19	34, 70, 98, 114	0
3	E	121/136 (88%)	0.47	3 (2%)	58 55	40, 63, 91, 112	0
4	F	328/380 (86%)	0.87	45 (13%)	6 6	45, 76, 137, 147	0
All	All	2174/2258 (96%)	0.23	91 (4%)	40 39	27, 56, 100, 147	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	5.3
2	D	141	GLY	4.9
4	F	149	ALA	4.7
4	F	161	LEU	4.5
4	F	100	ILE	4.2
4	F	132	LEU	3.8
4	F	173	ILE	3.7
4	F	130	VAL	3.7
4	F	133	ALA	3.6
2	D	73	MET	3.6
2	D	397	TRP	3.5
4	F	170	LEU	3.5
3	E	9	ILE	3.4
4	F	182	ILE	3.4
2	D	1	MET	3.4
2	D	323	MET	3.3
2	D	178	THR	3.3
4	F	103	THR	3.3
1	A	437	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	247	LYS	3.1
4	F	240	LEU	3.0
4	F	253	TYR	3.0
2	D	180	VAL	3.0
4	F	181	VAL	2.9
2	D	431	ASP	2.9
2	D	55	THR	2.9
2	D	393	ALA	2.9
4	F	167	SER	2.8
4	F	237	THR	2.8
4	F	180	HIS	2.8
2	D	80	PRO	2.8
4	F	98	TYR	2.7
4	F	179	VAL	2.7
4	F	380	HIS	2.7
1	C	440	VAL	2.7
2	D	92	PHE	2.7
4	F	169	LEU	2.6
2	D	394	PHE	2.6
4	F	245	ILE	2.6
1	A	281	ALA	2.6
2	D	72	THR	2.5
4	F	178	GLN	2.6
2	D	6	HIS	2.5
4	F	166	ALA	2.5
3	E	28	SER	2.5
4	F	330	ILE	2.5
2	D	377	LEU	2.5
4	F	230	SER	2.5
4	F	331	GLU	2.5
4	F	101	TYR	2.5
2	B	72	THR	2.5
2	D	211	CYS	2.5
2	D	284	LEU	2.5
2	B	280	GLN	2.4
4	F	234	GLN	2.4
2	D	140	GLY	2.4
4	F	134	ALA	2.4
4	F	20	LEU	2.3
4	F	236	LYS	2.3
2	D	11	GLN	2.3
2	D	142	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	231	ALA	2.3
2	B	218	THR	2.3
2	D	247	ASN	2.3
4	F	183	GLN	2.3
2	D	212	PHE	2.3
4	F	239	HIS	2.3
2	B	281	TYR	2.3
4	F	243	HIS	2.2
1	C	340	SER	2.2
4	F	131	PHE	2.2
2	D	219	THR	2.2
4	F	333	ASN	2.2
4	F	194	PRO	2.2
2	D	396	HIS	2.2
2	D	406	MET	2.2
4	F	146	VAL	2.2
2	D	70	PRO	2.1
2	D	220	PRO	2.1
3	E	46	SER	2.1
4	F	372	THR	2.1
2	D	245	GLN	2.1
4	F	148	ILE	2.1
4	F	162	ILE	2.1
4	F	172	PHE	2.1
2	D	387	ALA	2.0
1	A	82	THR	2.0
2	B	245	GLN	2.0
1	C	1	MET	2.0
2	D	101	TRP	2.0
2	D	273	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

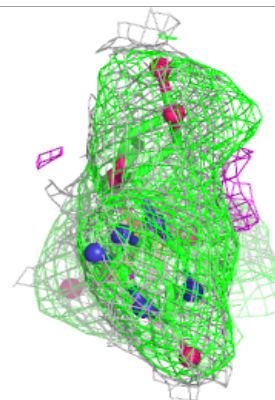
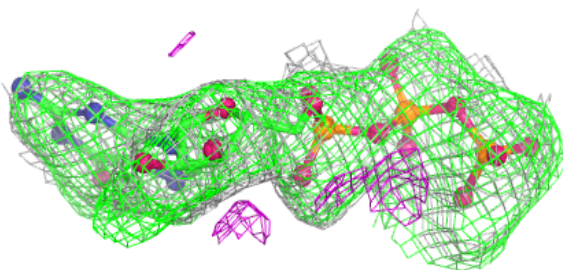
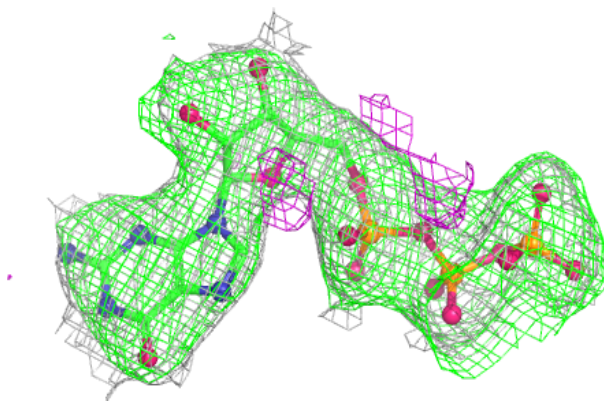
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GTP	A	501	32/32	-	-	41,42,45,47	32
5	GTP	C	501	32/32	-	-	31,33,37,38	32
6	CA	A	502	1/1	-	-	71,71,71,71	1
6	CA	C	502	1/1	-	-	59,59,59,59	1
7	MG	A	503	1/1	-	-	50,50,50,50	1
7	MG	B	504	1/1	-	-	45,45,45,45	1
7	MG	C	503	1/1	-	-	39,39,39,39	1
8	GDP	B	501	28/28	-	-	34,38,40,41	28
8	GDP	D	501	28/28	-	-	71,78,81,82	28
9	MES	B	502	12/12	-	-	39,40,43,43	12
9	MES	B	503	12/12	-	-	54,55,57,57	12
10	A1D6D	B	505	25/25	0.93	0.12	36,45,57,132	0
10	A1D6D	D	502	25/25	0.93	0.12	44,57,69,132	0
11	ACP	F	401	31/31	-	-	91,103,125,125	45

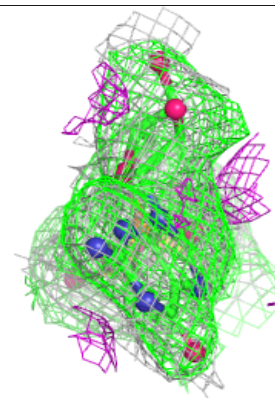
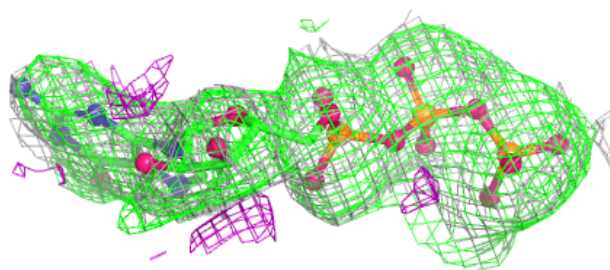
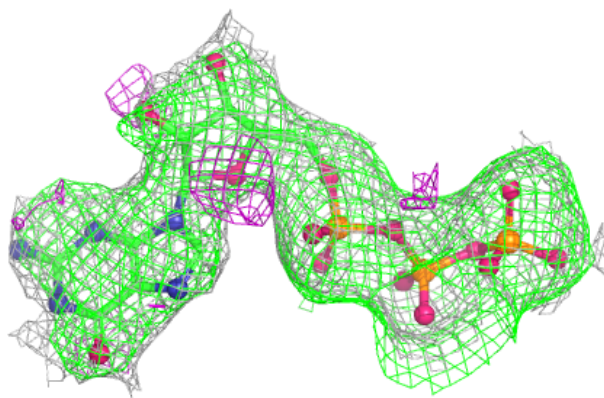
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP 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)

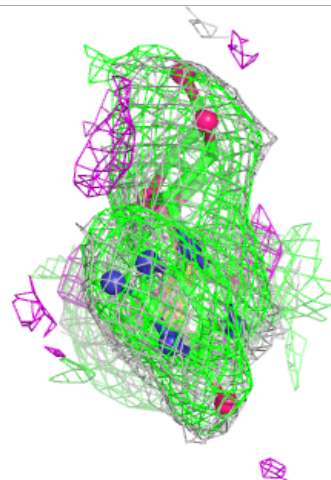
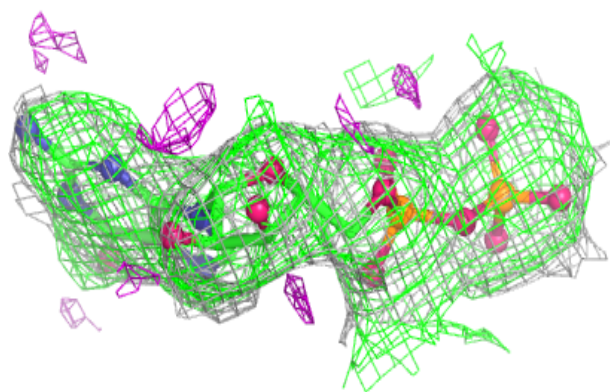
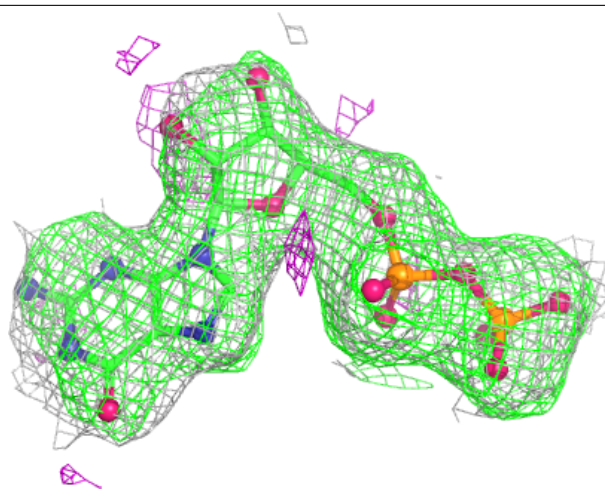
**Electron density around GTP C 501:**

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



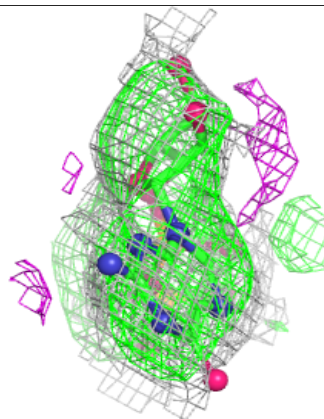
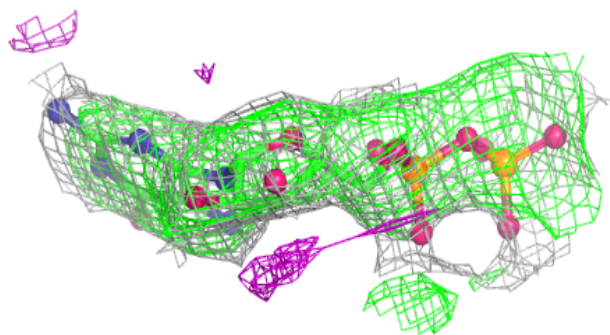
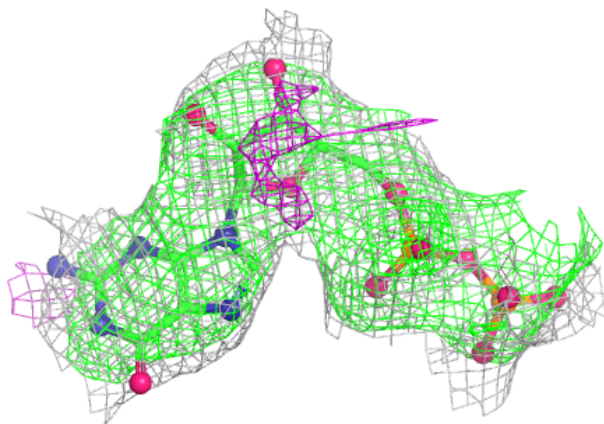
Electron density around GDP B 501:

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



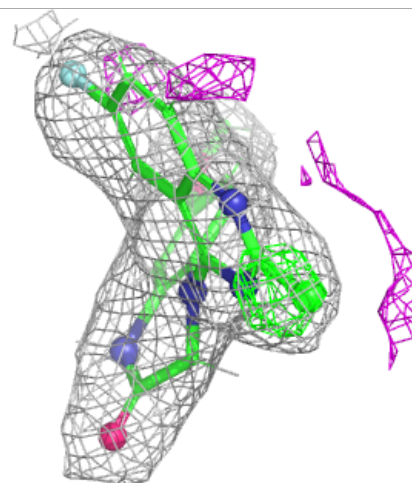
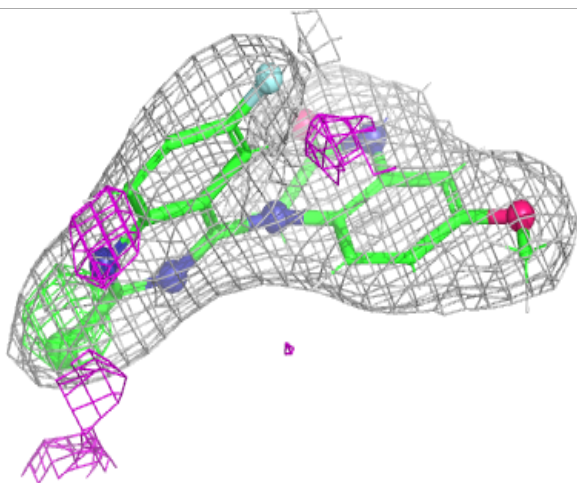
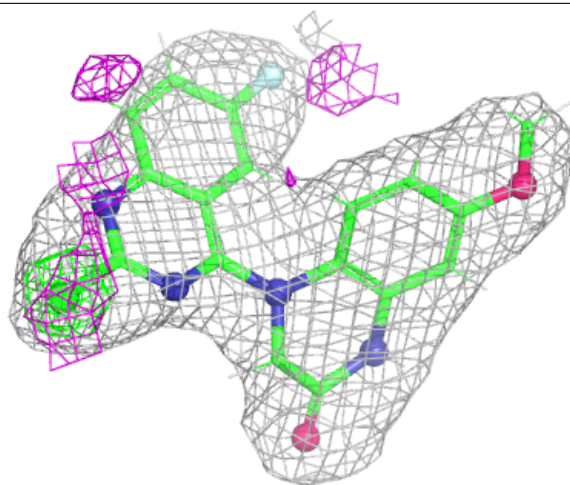
Electron density around GDP D 501:

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



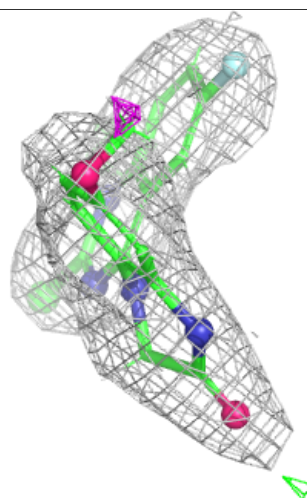
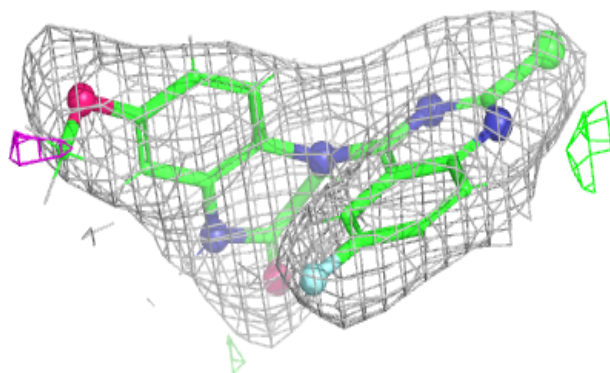
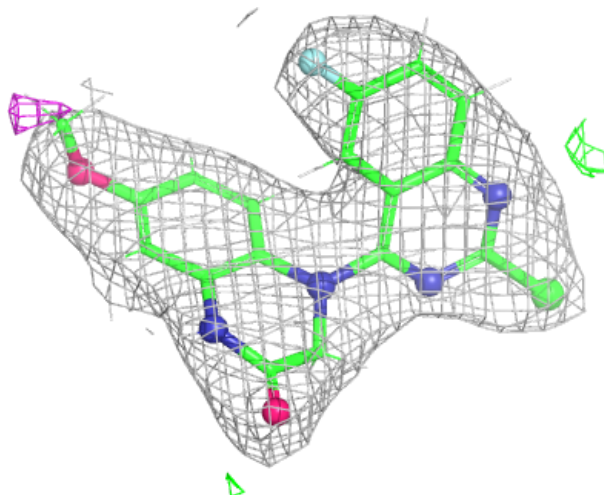
Electron density around A1D6D B 505:

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



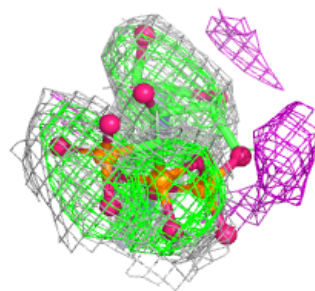
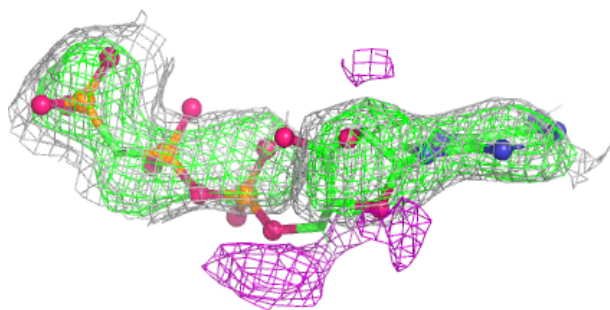
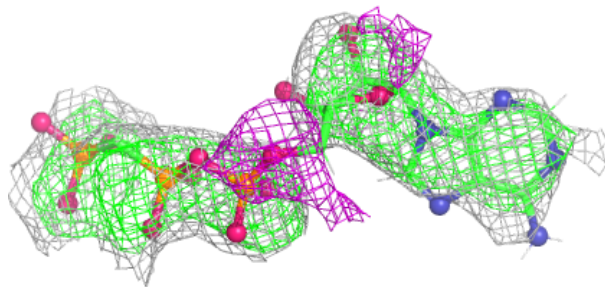
Electron density around A1D6D D 502:

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



Electron density around 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.