



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:20 PM UTC

PDB ID : 5LXT / pdb_00005lxt
Title : Tubulin-Discodermolide complex
Authors : Prota, A.E.; Steinmetz, M.O.
Deposited on : 2016-09-22
Resolution : 1.90 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

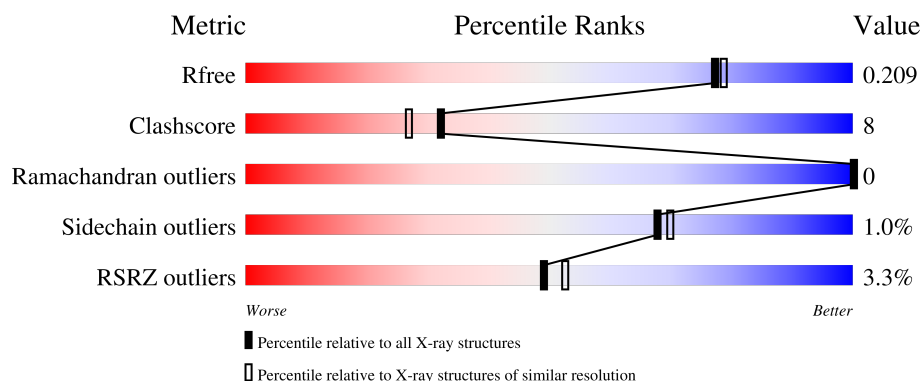
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



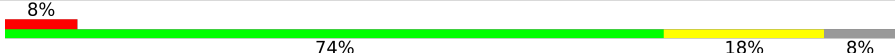
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	451	2% 83% 14% ..
1	C	451	2% 84% 13% .
2	B	445	2% 79% 17% .
2	D	445	2% 78% 18% .
3	E	143	3% 69% 17% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	

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
9	MES	B	504	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19693 atoms, of which 108 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	14	0
			3513	2230	589	669	25			
1	C	440	Total	C	N	O	S	0	14	0
			3499	2219	587	668	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	10	0
			3398	2137	579	654	28			
2	D	426	Total	C	N	O	S	0	6	0
			3366	2116	570	651	29			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	6	0
			1044	646	187	205	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called TUBULIN-TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	354	Total	C	N	O	S	0	8	0
			2942	1890	508	529	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



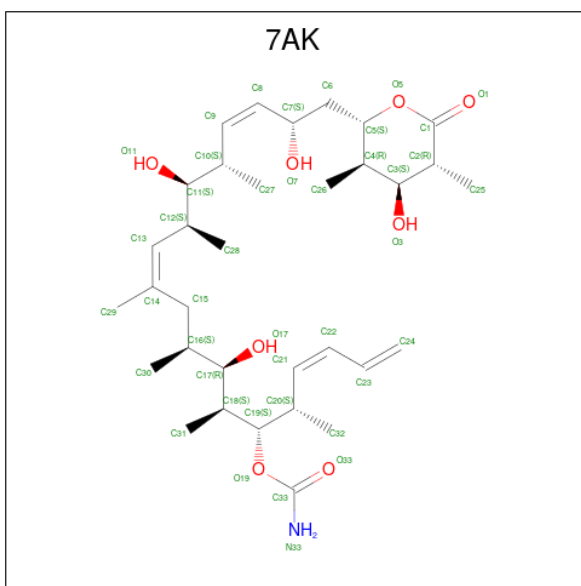
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- 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	0	0
			12	6	1	4	1		

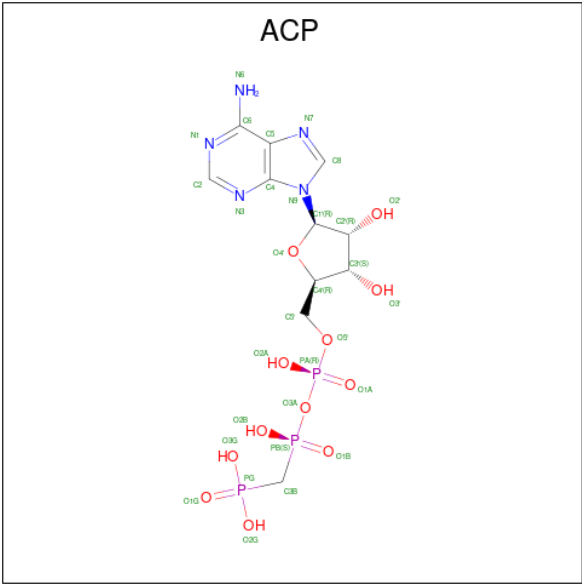
- Molecule 10 is (+)-Discodermolide (CCD ID: 7AK) (formula: $C_{33}H_{55}NO_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			96	33	54	1	8		
10	D	1	Total	C	H	N	O	0	0
			96	33	54	1	8		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD

ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

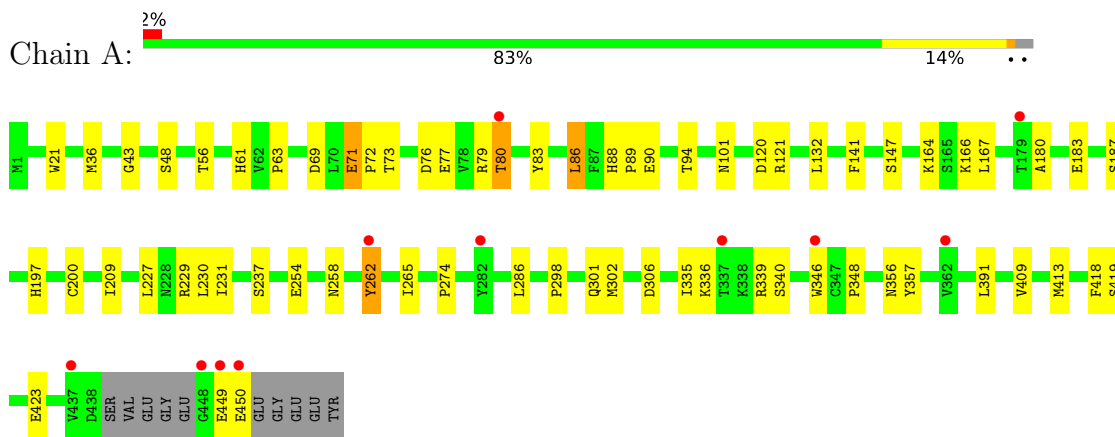
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	313	Total	O	0	0
			313	313		
12	B	307	Total	O	0	0
			307	307		
12	C	477	Total	O	0	0
			477	477		
12	D	226	Total	O	0	0
			226	226		
12	E	108	Total	O	0	0
			108	108		
12	F	136	Total	O	0	0
			136	136		

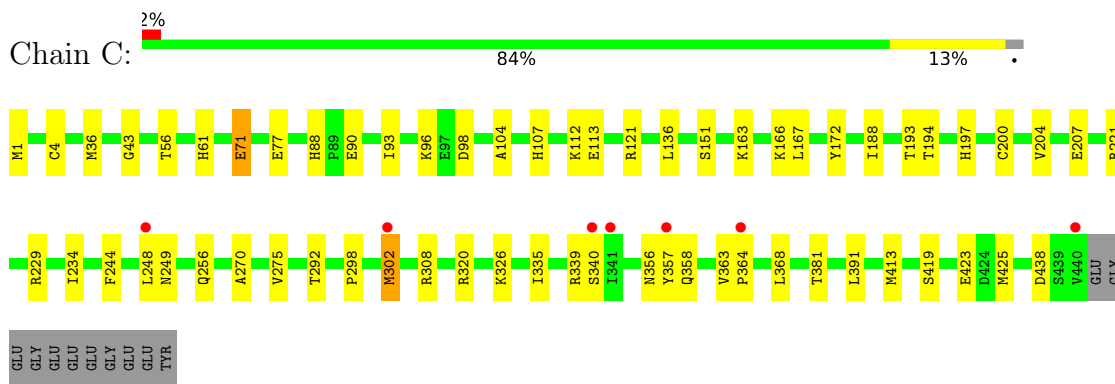
3 Residue-property plots [i](#)

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.

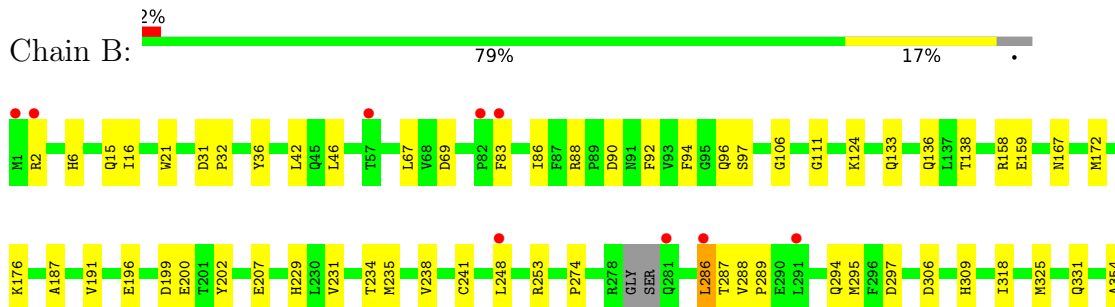
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain

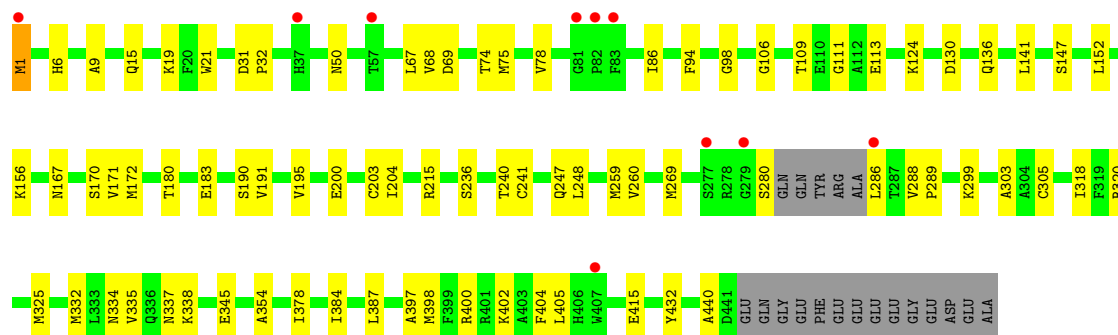
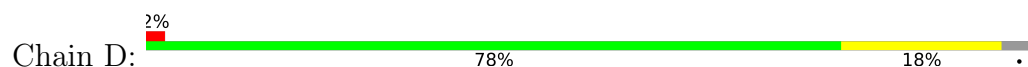


- Molecule 2: Tubulin beta-2B chain

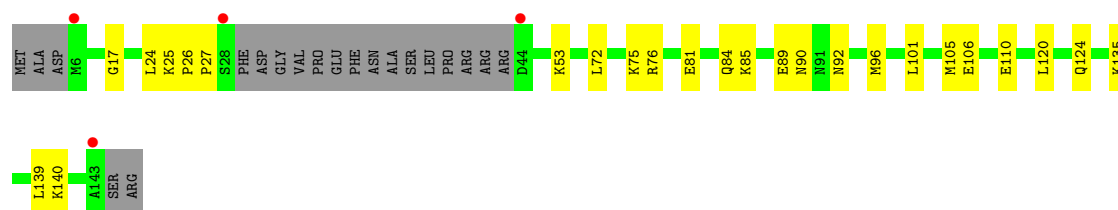




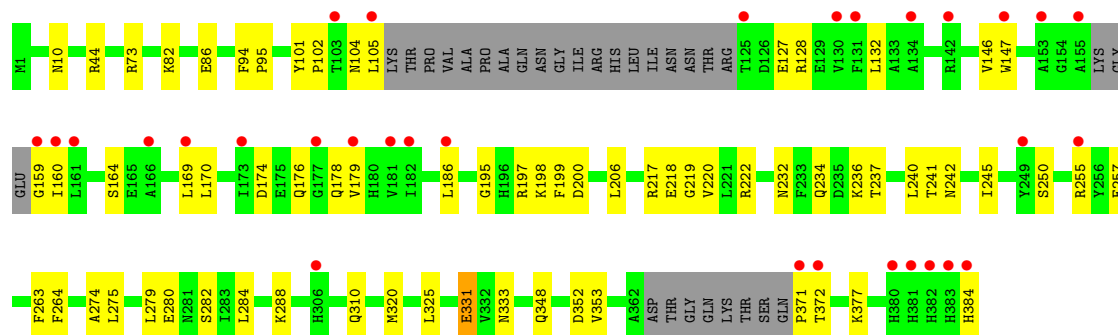
• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: TUBULIN-TYROSINE LIGASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.50Å 157.79Å 180.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.25 – 1.90 52.25 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.25-1.90) 100.0 (52.25-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.173 , 0.208 0.176 , 0.209	Depositor DCC
R_{free} test set	11713 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19693	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, CA, MES, 7AK, GDP, ACP, 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	0.39	0/3626	0.71	4/4921 (0.1%)
1	C	0.44	0/3622	0.73	0/4921
2	B	0.40	0/3502	0.69	0/4741
2	D	0.36	0/3457	0.71	2/4682 (0.0%)
3	E	0.34	0/1071	0.62	0/1422
4	F	0.29	0/3032	0.69	0/4096
All	All	0.38	0/18310	0.70	6/24783 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	TYR	CA-C-N	5.71	125.18	119.24
1	A	262	TYR	C-N-CA	5.71	125.18	119.24
2	D	98	GLY	N-CA-C	-5.41	106.24	112.29
2	D	260	VAL	N-CA-C	5.33	113.43	108.15
1	A	306	ASP	CA-C-N	5.01	124.67	119.56
1	A	306	ASP	C-N-CA	5.01	124.67	119.56

There are no chirality outliers.

There are no planarity outliers.

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	3513	0	3453	51	0
1	C	3499	0	3442	53	0
2	B	3398	0	3306	62	0
2	D	3366	0	3264	60	1
3	E	1044	0	1071	19	0
4	F	2942	0	2932	51	1
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	1	0
9	B	12	0	13	6	0
10	B	42	54	0	1	0
10	D	42	54	0	0	0
11	F	31	0	14	4	0
12	A	313	0	0	8	0
12	B	307	0	0	9	0
12	C	477	0	0	10	0
12	D	226	0	0	11	0
12	E	108	0	0	3	0
12	F	136	0	0	4	0
All	All	19585	108	17543	286	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 8.

All (286) 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:C:270:ALA:HB3	1:C:302:MET:HE2	1.36	1.08
11:F:401:ACP:H3B2	11:F:401:ACP:H5'2	1.39	1.02
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.38	1.01
1:A:450:GLU:HG3	4:F:333:ASN:HB3	1.51	0.90
1:C:256:GLN:NE2	12:C:601:HOH:O	2.09	0.86
2:D:241[B]:CYS:SG	12:D:632:HOH:O	2.33	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147[B]:SER:HG	2:D:190:SER:HG	1.25	0.83
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.61	0.83
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.44	0.81
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.65	0.79
2:B:294:GLN:NE2	12:B:601:HOH:O	2.16	0.77
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.50	0.77
2:B:241[A]:CYS:SG	12:B:857:HOH:O	2.42	0.76
2:D:241[B]:CYS:SG	12:D:780:HOH:O	2.44	0.76
2:D:1:MET:HA	2:D:1:MET:HE2	1.68	0.76
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.67	0.75
2:B:158:ARG:CZ	9:B:504:MES:H21	2.16	0.75
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.69	0.75
2:B:199:ASP:OD2	9:B:504:MES:H52	1.88	0.73
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.08	0.71
1:C:356[B]:ASN:ND2	1:C:358[B]:GLN:OE1	2.24	0.71
4:F:198:LYS:HE3	4:F:320:MET:HE1	1.73	0.71
1:C:221:ARG:CG	2:D:325:MET:HG2	2.18	0.70
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.72	0.70
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.32	0.69
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.25	0.68
2:D:247:GLN:OE1	12:D:601:HOH:O	2.11	0.68
1:A:336:LYS:HG3	3:E:24:LEU:CD1	2.24	0.67
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.11	0.67
1:C:204:VAL:HG22	1:C:302:MET:SD	2.36	0.66
2:B:97:SER:HB2	12:B:700:HOH:O	1.96	0.65
1:C:438:ASP:OD1	12:C:602:HOH:O	2.14	0.65
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.37	0.64
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.27	0.64
2:D:215:ARG:NH1	12:D:605:HOH:O	2.30	0.64
2:B:424:ASN:HB3	12:B:613:HOH:O	1.97	0.64
2:D:106:GLY:O	2:D:111:GLY:HA3	1.99	0.63
2:D:269[A]:MET:HG3	2:D:303:ALA:HB3	1.79	0.63
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.99	0.63
1:C:358[B]:GLN:NE2	12:C:613:HOH:O	2.31	0.62
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.30	0.62
4:F:331:GLU:OE2	11:F:401:ACP:O1B	2.18	0.62
1:A:101:ASN:ND2	1:A:180:ALA:HB2	2.13	0.62
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.81	0.62
2:D:269[B]:MET:CE	2:D:305:CYS:HB2	2.29	0.62
2:B:124:LYS:HD3	2:B:124:LYS:C	2.25	0.62
1:C:270:ALA:HB3	1:C:302:MET:CE	2.23	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.14	0.61
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.31	0.60
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.84	0.60
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.36	0.60
1:A:132:LEU:O	1:A:164:LYS:NZ	2.34	0.59
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.85	0.58
1:C:1:MET:O	12:C:603:HOH:O	2.17	0.58
2:B:414:ASP:HB2	12:B:676:HOH:O	2.03	0.58
1:C:229:ARG:NE	1:C:363[B]:VAL:HG21	2.18	0.58
4:F:73:ARG:NH1	12:F:503:HOH:O	2.36	0.58
2:B:199:ASP:OD1	9:B:504:MES:H32	2.03	0.58
2:D:432:TYR:OH	12:D:602:HOH:O	2.16	0.58
2:D:1:MET:N	2:D:130:ASP:OD2	2.36	0.58
2:D:1:MET:HA	2:D:1:MET:CE	2.34	0.58
2:B:431:GLU:O	2:B:434:GLN:HG2	2.04	0.58
2:B:369:ARG:O	10:B:505:7AK:O3	2.22	0.57
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.69	0.57
1:C:339:ARG:O	12:C:604:HOH:O	2.18	0.57
4:F:159:GLY:C	4:F:160:ILE:HD12	2.29	0.57
2:B:199:ASP:OD1	9:B:504:MES:H72	2.04	0.57
4:F:371:PRO:CA	4:F:372:THR:HB	2.34	0.57
4:F:288:LYS:NZ	12:F:502:HOH:O	2.36	0.57
4:F:371:PRO:HA	4:F:372:THR:O	2.05	0.57
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.37	0.57
3:E:72:LEU:O	3:E:76:ARG:HG2	2.04	0.56
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.36	0.56
3:E:92:ASN:O	3:E:96:MET:HG2	2.06	0.56
12:B:602:HOH:O	3:E:76:ARG:HG3	2.06	0.56
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.71	0.55
4:F:371:PRO:HA	4:F:372:THR:HB	1.89	0.55
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.36	0.55
2:B:253[A]:ARG:NH2	9:B:504:MES:O2S	2.34	0.55
2:D:1:MET:SD	2:D:50:ASN:HB2	2.47	0.54
3:E:120:LEU:O	3:E:124:GLN:HG3	2.08	0.54
2:D:1:MET:HE1	12:D:759:HOH:O	2.07	0.54
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.40	0.54
4:F:371:PRO:HA	4:F:372:THR:C	2.31	0.54
1:C:96:LYS:NZ	2:D:130:ASP:OD1	2.36	0.54
1:C:308:ARG:HG2	1:C:340:SER:HB2	1.90	0.54
4:F:102:PRO:HB2	4:F:104:ASN:OD1	2.08	0.54
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:85:LYS:O	3:E:89:GLU:HG3	2.07	0.53
2:B:274:PRO:HB3	2:B:286:LEU:HD11	1.90	0.53
1:A:166:LYS:HE2	1:A:197:HIS:O	2.09	0.53
1:C:207:GLU:OE2	12:C:605:HOH:O	2.19	0.53
2:B:96:GLN:CB	1:C:1:MET:HE2	2.39	0.53
2:D:124:LYS:C	2:D:124:LYS:HD3	2.33	0.53
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.91	0.52
2:B:106:GLY:O	2:B:111:GLY:HA3	2.09	0.52
1:C:43:GLY:HA2	1:C:56:THR:O	2.09	0.52
2:B:15:GLN:NE2	8:B:501:GDP:O6	2.42	0.52
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.39	0.52
8:D:501:GDP:O3B	12:D:603:HOH:O	2.19	0.52
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.91	0.52
1:A:180:ALA:O	1:A:183:GLU:HG3	2.10	0.52
2:D:180:THR:O	2:D:183:GLU:HG3	2.10	0.52
2:D:240[B]:THR:HG21	2:D:320:ARG:HD2	1.91	0.52
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.45	0.52
1:C:229:ARG:CD	1:C:363[B]:VAL:HG21	2.40	0.51
2:D:259:MET:HE2	2:D:378:ILE:HG22	1.93	0.51
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.92	0.51
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.25	0.51
4:F:176:GLN:HB3	4:F:178:GLN:NE2	2.26	0.51
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.34	0.51
1:C:229:ARG:HD3	1:C:363[B]:VAL:HG21	1.91	0.51
1:A:69:ASP:O	1:A:94:THR:HA	2.10	0.51
1:A:48:SER:HB2	12:A:705:HOH:O	2.11	0.51
3:E:101:LEU:O	3:E:105[A]:MET:HG2	2.10	0.51
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.26	0.51
2:B:297:ASP:HA	12:B:695:HOH:O	2.10	0.51
1:A:209[A]:ILE:HG22	1:A:227:LEU:HD22	1.93	0.50
1:C:112:LYS:NZ	12:C:626:HOH:O	2.44	0.50
2:D:191:VAL:O	2:D:195:VAL:HG23	2.11	0.50
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.29	0.50
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.43	0.50
2:D:136:GLN:HA	2:D:167:ASN:O	2.10	0.50
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.94	0.50
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.92	0.50
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.94	0.49
2:D:109:THR:O	2:D:113:GLU:HG2	2.12	0.49
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.47	0.49
1:A:301:GLN:C	1:A:302[B]:MET:HE3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLN:HA	2:B:167:ASN:O	2.13	0.49
1:A:419:SER:O	1:A:423:GLU:HG3	2.13	0.48
3:E:81:GLU:HA	3:E:84[B]:GLN:HG2	1.93	0.48
1:A:77:GLU:HB2	12:A:670:HOH:O	2.13	0.48
1:A:237[B]:SER:HB2	12:A:656:HOH:O	2.14	0.48
1:C:163:LYS:HG3	3:E:90[A]:ASN:OD1	2.12	0.48
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.20	0.48
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.96	0.48
2:B:295:MET:CG	2:B:377:PHE:HB2	2.39	0.48
1:A:450:GLU:HB2	4:F:333:ASN:OD1	2.14	0.48
2:D:269[B]:MET:HE3	2:D:305:CYS:HB2	1.96	0.48
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.49	0.48
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE1	2.48	0.48
1:A:262:TYR:HD2	1:A:265:ILE:HG13	1.79	0.48
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.95	0.47
2:B:248:LEU:HD23	2:B:354:ALA:HB2	1.96	0.47
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.95	0.47
4:F:10:ASN:HB2	4:F:44:ARG:NH2	2.25	0.47
2:B:2:ARG:HB3	2:B:133:GLN:HG2	1.95	0.47
2:B:318:ILE:N	2:B:318:ILE:HD12	2.29	0.47
2:D:387:LEU:HD23	2:D:387:LEU:C	2.39	0.47
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.30	0.47
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.14	0.47
11:F:401:ACP:O5'	11:F:401:ACP:H8	2.14	0.47
2:B:274:PRO:HB3	2:B:286:LEU:CD1	2.44	0.47
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.96	0.47
2:B:234:THR:O	2:B:238[A]:VAL:HG13	2.15	0.47
3:E:25:LYS:HG2	3:E:26:PRO:HD2	1.97	0.47
2:B:96:GLN:HB2	1:C:1:MET:HE2	1.97	0.47
2:B:176:LYS:HG3	2:B:207:GLU:OE1	2.15	0.47
2:D:318:ILE:N	2:D:318:ILE:HD12	2.29	0.47
3:E:81:GLU:OE2	12:E:201:HOH:O	2.21	0.47
1:C:363[A]:VAL:HG13	1:C:364:PRO:HD2	1.97	0.47
1:C:77:GLU:OE2	12:C:606:HOH:O	2.20	0.46
3:E:135:LYS:HZ2	3:E:139:LEU:HD11	1.79	0.46
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.97	0.46
4:F:82:LYS:NZ	4:F:127:GLU:OE2	2.46	0.46
1:A:90:GLU:O	1:A:121:ARG:HD2	2.14	0.46
2:D:172:MET:HE3	2:D:203:CYS:SG	2.56	0.46
3:E:84[A]:GLN:HG3	12:E:210:HOH:O	2.15	0.46
2:B:158:ARG:NE	9:B:504:MES:H21	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.97	0.46
12:B:705:HOH:O	3:E:75:LYS:HD2	2.15	0.46
2:D:236:SER:O	2:D:240[B]:THR:HG23	2.16	0.46
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.98	0.46
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.46	0.46
1:C:151[B]:SER:HA	1:C:194[B]:THR:HG22	1.97	0.45
2:B:42:LEU:H	2:B:42:LEU:HD12	1.81	0.45
4:F:237:THR:HG21	4:F:250:SER:HB2	1.98	0.45
1:A:340:SER:O	12:A:601:HOH:O	2.21	0.45
1:C:270:ALA:CB	1:C:302:MET:HE2	2.27	0.45
1:A:43:GLY:HA2	1:A:56:THR:O	2.17	0.45
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.99	0.45
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.97	0.45
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.52	0.45
1:A:356:ASN:ND2	12:A:617:HOH:O	2.48	0.45
2:B:288:VAL:HG12	2:B:331:GLN:HG3	1.98	0.45
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.98	0.45
4:F:237:THR:CG2	4:F:250:SER:HB2	2.47	0.45
2:B:69:ASP:O	2:B:94:PHE:HA	2.17	0.45
2:B:386:GLU:O	2:B:390:ARG:HG3	2.16	0.45
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.98	0.45
1:C:229:ARG:HD3	1:C:363[B]:VAL:CG2	2.46	0.45
2:D:19:LYS:HE2	12:D:784:HOH:O	2.16	0.45
2:D:171:VAL:HA	2:D:204:ILE:O	2.17	0.45
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.98	0.44
1:C:104:ALA:HB2	1:C:413:MET:SD	2.58	0.44
2:D:152:LEU:O	2:D:156:LYS:HG2	2.17	0.44
1:C:244:PHE:CD1	1:C:358[B]:GLN:HG2	2.53	0.44
1:C:221:ARG:HG3	2:D:325:MET:CG	2.28	0.44
1:A:298:PRO:HA	1:A:301:GLN:CD	2.43	0.44
2:B:83:PHE:O	2:B:86:ILE:HG22	2.18	0.43
1:C:308:ARG:HD2	12:C:821:HOH:O	2.18	0.43
2:B:138[A]:THR:HG21	2:B:235:MET:HE1	1.99	0.43
3:E:140:LYS:HB3	3:E:140:LYS:HE2	1.82	0.43
2:B:159:GLU:OE2	12:B:602:HOH:O	2.21	0.43
1:A:348:PRO:HG3	3:E:27:PRO:HD3	2.00	0.43
1:C:107:HIS:HD2	1:C:151[A]:SER:OG	2.01	0.43
1:A:83:TYR:O	1:A:86:LEU:HB2	2.18	0.43
2:B:202:TYR:CZ	2:B:238[B]:VAL:HG11	2.53	0.43
1:C:234:ILE:HG21	1:C:302:MET:SD	2.59	0.43
4:F:240:LEU:HD12	4:F:240:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.51	0.43
2:B:306:ASP:O	2:B:309:HIS:HB2	2.18	0.43
4:F:280:GLU:HB2	12:F:560:HOH:O	2.17	0.43
2:D:167:ASN:ND2	12:D:622:HOH:O	2.51	0.42
2:D:345:GLU:HG3	2:D:440:ALA:HB2	2.00	0.42
2:B:373:MET:HE2	2:B:373:MET:HB3	1.91	0.42
1:C:166:LYS:HE2	1:C:197:HIS:O	2.19	0.42
2:D:398:MET:HE3	2:D:404:PHE:CD2	2.54	0.42
4:F:101:TYR:CE2	4:F:179:VAL:HG22	2.54	0.42
3:E:106:GLU:O	3:E:110:GLU:HG3	2.19	0.42
1:A:77:GLU:O	1:A:80:THR:HG22	2.19	0.42
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.01	0.42
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.84	0.42
2:D:74:THR:O	2:D:78:VAL:HG23	2.19	0.42
4:F:232:ASN:OD1	4:F:234:GLN:HB3	2.20	0.42
2:D:147[B]:SER:OG	2:D:190:SER:OG	2.08	0.42
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.02	0.42
1:A:302[A]:MET:HA	1:A:302[A]:MET:HE2	2.01	0.42
1:A:339:ARG:HD3	12:A:730:HOH:O	2.19	0.42
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.54	0.42
2:D:141:LEU:HD21	2:D:170:SER:HB3	2.01	0.42
1:A:409:VAL:HA	1:A:413:MET:O	2.20	0.42
1:A:71:GLU:HG2	1:A:72:PRO:N	2.33	0.42
1:A:413:MET:CE	1:A:418:PHE:CE2	3.03	0.42
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.55	0.42
2:B:287:THR:HB	2:B:289:PRO:HD2	2.02	0.42
1:C:419:SER:O	1:C:423:GLU:HG3	2.20	0.42
2:D:203:CYS:SG	2:D:384[B]:ILE:HD11	2.60	0.42
2:D:299:LYS:NZ	12:D:608:HOH:O	2.39	0.42
4:F:199:PHE:HA	4:F:241:THR:HG21	2.01	0.42
2:B:187:ALA:O	2:B:191:VAL:HG23	2.20	0.42
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.35	0.42
1:C:356[B]:ASN:ND2	12:C:636:HOH:O	2.50	0.42
4:F:279:LEU:HG	4:F:284[B]:LEU:HG	2.01	0.42
2:B:325:MET:HE2	2:B:355:VAL:HG21	2.02	0.42
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.02	0.42
2:D:9:ALA:HA	2:D:68:VAL:O	2.19	0.42
2:B:196:GLU:HG3	12:E:263:HOH:O	2.20	0.41
2:B:405:LEU:HD23	2:B:405:LEU:HA	1.89	0.41
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.54	0.41
4:F:94:PHE:HA	4:F:95:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238[B]:VAL:HG22	2:B:378:ILE:HD11	2.01	0.41
2:D:74:THR:HB	12:D:671:HOH:O	2.19	0.41
2:D:248:LEU:HD23	2:D:354:ALA:HB2	2.02	0.41
2:B:42:LEU:HD12	2:B:42:LEU:N	2.36	0.41
2:D:15:GLN:O	2:D:19:LYS:HG2	2.20	0.41
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.02	0.41
1:A:449:GLU:OE2	12:A:602:HOH:O	2.22	0.41
4:F:371:PRO:N	4:F:372:THR:HB	2.35	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.39	0.41
4:F:377:LYS:NZ	12:F:511:HOH:O	2.53	0.41
1:C:151[A]:SER:HB2	1:C:193:THR:CG2	2.50	0.41
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.55	0.41
1:A:229:ARG:NH1	12:A:611:HOH:O	2.40	0.41
2:B:325:MET:HE2	2:B:355:VAL:HB	2.03	0.41
2:B:387:LEU:HD23	2:B:387:LEU:C	2.46	0.41
4:F:206:LEU:HD23	4:F:353[A]:VAL:CG2	2.50	0.41
2:B:67:LEU:HD12	2:B:67:LEU:N	2.36	0.41
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.56	0.41
2:D:332:MET:O	2:D:335:VAL:HG12	2.20	0.41
4:F:206:LEU:HD23	4:F:353[A]:VAL:HG21	2.03	0.41
2:B:199:ASP:C	2:B:200:GLU:HG3	2.45	0.40
2:D:67:LEU:N	2:D:67:LEU:HD12	2.36	0.40
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.20	0.40
4:F:274:ALA:C	4:F:275[A]:LEU:HD22	2.45	0.40
1:A:141:PHE:O	1:A:147:SER:HB3	2.22	0.40
1:A:346:TRP:CD1	1:A:346:TRP:H	2.39	0.40
2:D:69:ASP:O	2:D:94:PHE:HA	2.22	0.40
2:D:286:LEU:O	2:D:286:LEU:HG	2.22	0.40
2:D:75:MET:HE1	2:D:94:PHE:HD1	1.87	0.40
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.03	0.40
2:D:405:LEU:HD13	2:D:415:GLU:HG2	2.04	0.40
4:F:242:ASN:HD22	4:F:245:ILE:CD1	2.33	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:D:337:ASN:OD1	4:F:384:HIS:NE2[3_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	451/451 (100%)	445 (99%)	6 (1%)	0	100	100
1	C	453/451 (100%)	441 (97%)	12 (3%)	0	100	100
2	B	432/445 (97%)	425 (98%)	7 (2%)	0	100	100
2	D	428/445 (96%)	422 (99%)	6 (1%)	0	100	100
3	E	125/143 (87%)	122 (98%)	3 (2%)	0	100	100
4	F	354/384 (92%)	343 (97%)	11 (3%)	0	100	100
All	All	2243/2319 (97%)	2198 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	385/379 (102%)	381 (99%)	4 (1%)	68	70
1	C	386/379 (102%)	382 (99%)	4 (1%)	68	70
2	B	379/383 (99%)	377 (100%)	2 (0%)	81	84
2	D	374/383 (98%)	370 (99%)	4 (1%)	65	67
3	E	116/127 (91%)	115 (99%)	1 (1%)	70	73
4	F	325/342 (95%)	319 (98%)	6 (2%)	51	50
All	All	1965/1993 (99%)	1944 (99%)	21 (1%)	68	67

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

Mol	Chain	Res	Type
1	A	71	GLU
1	A	80	THR
1	A	86	LEU
1	A	120	ASP
2	B	229	HIS
2	B	286	LEU
1	C	71	GLU
1	C	302	MET
1	C	326	LYS
1	C	381	THR
2	D	1	MET
2	D	86	ILE
2	D	200	GLU
2	D	280	SER
3	E	53	LYS
4	F	86	GLU
4	F	186	LEU
4	F	255[A]	ARG
4	F	255[B]	ARG
4	F	310	GLN
4	F	331	GLU

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	15	GLN
1	A	285	GLN
1	A	301	GLN
1	A	393	HIS
2	B	193	GLN
2	B	229	HIS
2	B	247	GLN
2	B	349	ASN
1	C	107	HIS
1	C	133	GLN
2	D	8	GLN
2	D	14	ASN
2	D	136	GLN
2	D	167	ASN
2	D	331	GLN
2	D	436	GLN

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Mol	Chain	Res	Type
3	E	136	ASN
4	F	180	HIS

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 17 ligands modelled in this entry, 9 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
10	7AK	D	503	-	42,42,42	1.51	3 (7%)	49,58,58	1.72	9 (18%)
10	7AK	B	505	-	42,42,42	1.54	3 (7%)	49,58,58	1.55	7 (14%)
5	GTP	A	501	6	33,34,34	1.36	5 (15%)	50,54,54	1.57	6 (12%)
8	GDP	D	501	6	29,30,30	1.16	2 (6%)	45,47,47	1.67	6 (13%)
5	GTP	C	501	6	33,34,34	1.22	4 (12%)	50,54,54	1.65	6 (12%)
9	MES	B	504	-	12,12,12	2.18	1 (8%)	15,16,16	1.00	1 (6%)
11	ACP	F	401	6	31,33,33	2.14	11 (35%)	47,52,52	1.81	10 (21%)
8	GDP	B	501	6	29,30,30	1.30	5 (17%)	45,47,47	1.70	7 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	7AK	D	503	-	-	3/49/69/69	0/1/1/1
10	7AK	B	505	-	-	2/49/69/69	0/1/1/1
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
8	GDP	D	501	6	-	4/16/32/32	0/3/3/3
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
9	MES	B	504	-	-	1/6/14/14	0/1/1/1
11	ACP	F	401	6	-	7/19/38/38	0/3/3/3
8	GDP	B	501	6	-	4/16/32/32	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	7AK	O5-C1	7.61	1.45	1.34
9	B	504	MES	C8-S	-7.29	1.67	1.77
10	D	503	7AK	O5-C1	7.12	1.45	1.34
11	F	401	ACP	PG-O1G	5.59	1.61	1.50
10	D	503	7AK	O19-C33	5.17	1.45	1.35
10	B	505	7AK	O19-C33	4.96	1.45	1.35
11	F	401	ACP	C5-C4	4.71	1.47	1.39
11	F	401	ACP	PB-O1B	4.19	1.61	1.51
8	B	501	GDP	PA-O3A	3.74	1.63	1.59
5	A	501	GTP	PA-O3A	3.55	1.63	1.59
11	F	401	ACP	PB-O2B	-3.33	1.48	1.56
5	A	501	GTP	PB-O3B	3.23	1.63	1.59
11	F	401	ACP	PB-O3A	3.20	1.62	1.58
8	D	501	GDP	C5-C4	2.97	1.46	1.38
11	F	401	ACP	PG-O2G	-2.91	1.48	1.55
5	C	501	GTP	PB-O3B	2.84	1.62	1.59
5	C	501	GTP	C5-C4	2.80	1.46	1.38
5	A	501	GTP	C5-C4	2.78	1.46	1.38
5	C	501	GTP	PA-O3A	2.76	1.62	1.59
11	F	401	ACP	PG-O3G	2.75	1.61	1.55
11	F	401	ACP	C5-C6	2.70	1.48	1.41
8	D	501	GDP	PA-O3A	2.67	1.62	1.59
10	D	503	7AK	O5-C5	-2.66	1.42	1.46
8	B	501	GDP	C5-C4	2.59	1.45	1.38
11	F	401	ACP	PA-O3A	2.42	1.62	1.59
5	A	501	GTP	C6-N1	-2.40	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	GDP	C6-N1	-2.36	1.34	1.38
11	F	401	ACP	C5-N7	-2.33	1.34	1.39
10	B	505	7AK	O5-C5	-2.29	1.43	1.46
8	B	501	GDP	C4-N9	-2.22	1.32	1.38
11	F	401	ACP	C8-N7	2.13	1.35	1.31
5	C	501	GTP	C6-N1	-2.13	1.34	1.38
5	A	501	GTP	C4-N9	-2.10	1.32	1.38
8	B	501	GDP	C5-N7	-2.00	1.35	1.39

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	C5-C4-N3	-6.01	118.44	126.72
5	C	501	GTP	C5-C4-N3	-5.58	119.51	128.39
8	D	501	GDP	C5-C4-N3	-5.37	119.84	128.39
10	D	503	7AK	O19-C33-N33	5.34	119.19	110.92
5	A	501	GTP	C5-C4-N3	-5.16	120.18	128.39
8	B	501	GDP	C5-C4-N3	-5.06	120.33	128.39
11	F	401	ACP	N3-C4-N9	4.88	135.47	127.17
5	C	501	GTP	C2-N3-C4	4.86	120.68	112.30
10	B	505	7AK	O19-C33-N33	4.81	118.37	110.92
8	D	501	GDP	C2-N3-C4	4.78	120.53	112.30
10	D	503	7AK	C29-C14-C13	-4.76	114.86	123.85
5	C	501	GTP	N9-C4-N3	4.57	135.09	125.95
8	B	501	GDP	C2-N3-C4	4.56	120.16	112.30
5	A	501	GTP	C2-N3-C4	4.47	120.00	112.30
10	B	505	7AK	C29-C14-C13	-4.36	115.61	123.85
8	B	501	GDP	N9-C4-N3	4.14	134.24	125.95
8	D	501	GDP	N9-C4-N3	3.94	133.84	125.95
10	D	503	7AK	O33-C33-N33	-3.89	119.44	125.58
5	A	501	GTP	N9-C4-N3	3.88	133.71	125.95
11	F	401	ACP	C2-N3-C4	3.69	120.85	111.83
8	D	501	GDP	C6-C5-N7	3.50	136.66	130.29
5	A	501	GTP	C6-C5-N7	3.37	136.43	130.29
11	F	401	ACP	C4-C5-N7	-3.28	106.83	110.58
5	C	501	GTP	C6-C5-N7	3.19	136.09	130.29
10	B	505	7AK	O33-C33-N33	-3.18	120.56	125.58
11	F	401	ACP	N3-C2-N1	-3.06	123.94	128.58
8	B	501	GDP	C6-C5-N7	3.00	135.74	130.29
8	B	501	GDP	O6-C6-C5	-2.86	118.98	126.53
11	F	401	ACP	PB-O3A-PA	-2.85	123.07	132.37
10	B	505	7AK	C25-C2-C3	-2.73	108.11	112.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	7AK	C25-C2-C3	-2.64	108.27	112.95
10	D	503	7AK	C19-O19-C33	2.57	120.75	117.03
10	D	503	7AK	C15-C14-C13	2.55	126.93	121.24
11	F	401	ACP	C4-N9-C8	2.55	108.41	105.74
8	D	501	GDP	C4-C5-N7	-2.47	106.75	110.67
10	B	505	7AK	C19-O19-C33	2.45	120.58	117.03
11	F	401	ACP	C5-N7-C8	2.45	107.30	103.45
10	D	503	7AK	C28-C12-C13	-2.43	105.96	110.08
5	A	501	GTP	O6-C6-C5	-2.38	120.26	126.53
10	B	505	7AK	C6-C7-C8	-2.37	107.68	112.64
8	B	501	GDP	O4'-C1'-N9	-2.35	103.03	108.36
9	B	504	MES	O3S-S-C8	2.34	110.58	106.00
8	D	501	GDP	O6-C6-C5	-2.24	120.63	126.53
5	A	501	GTP	C4-C5-N7	-2.23	107.13	110.67
11	F	401	ACP	C2'-C1'-N9	-2.22	107.79	113.30
5	C	501	GTP	C4-C5-N7	-2.22	107.15	110.67
10	D	503	7AK	C6-C7-C8	-2.20	108.03	112.64
10	D	503	7AK	C26-C4-C3	-2.19	109.11	112.13
5	C	501	GTP	O6-C6-C5	-2.18	120.77	126.53
10	B	505	7AK	C17-C18-C19	2.15	114.69	110.58
11	F	401	ACP	C3'-C2'-C1'	2.09	105.41	101.46
8	B	501	GDP	C5-C6-N1	2.01	118.37	113.25

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
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
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O1A
10	D	503	7AK	C31-C18-C19-C20
10	D	503	7AK	C11-C10-C9-C8
10	B	505	7AK	C17-C18-C19-C20
10	B	505	7AK	C31-C18-C19-C20
10	D	503	7AK	C17-C18-C19-C20
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O1A
8	D	501	GDP	PB-O3A-PA-O1A

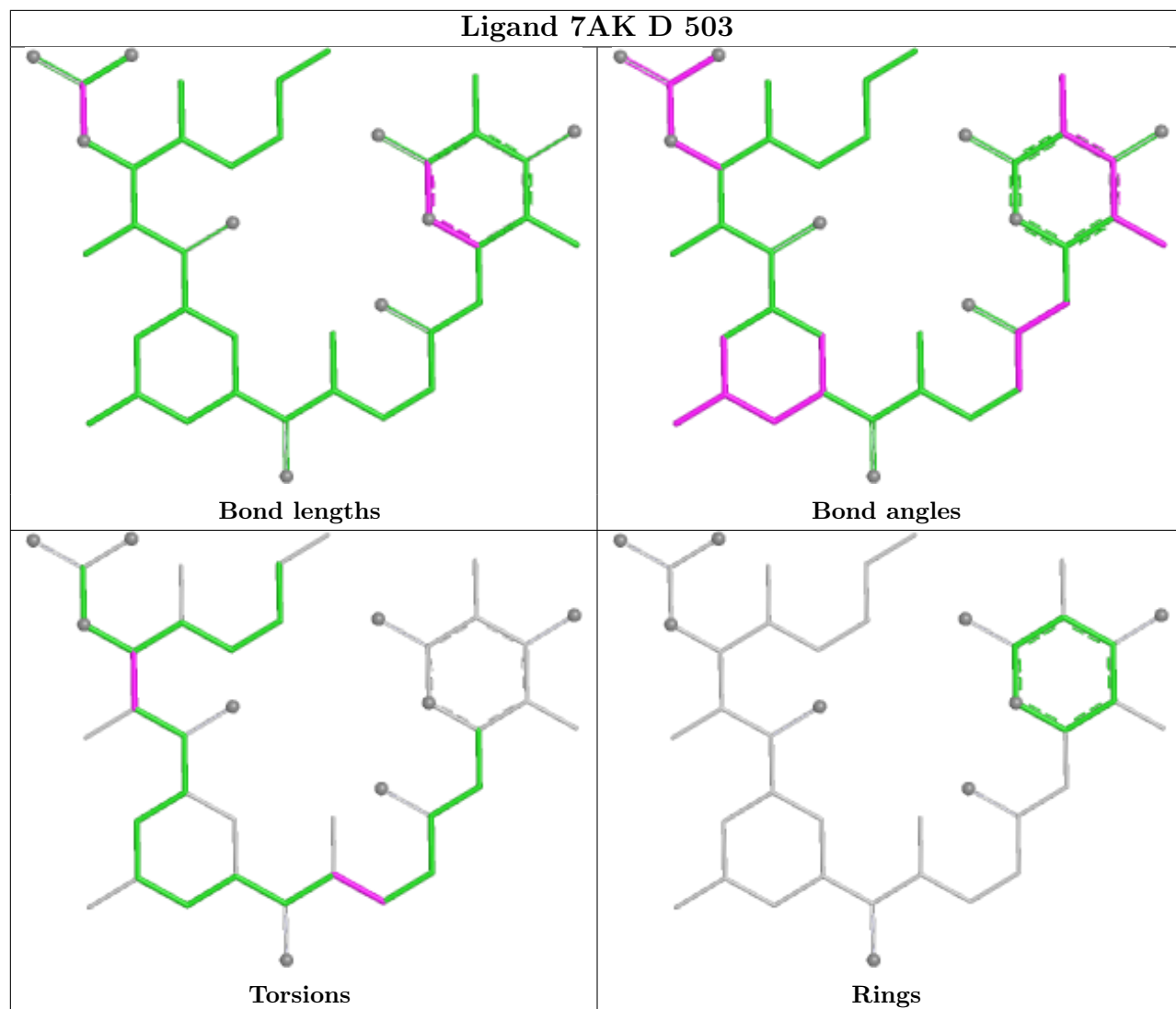
There are no ring outliers.

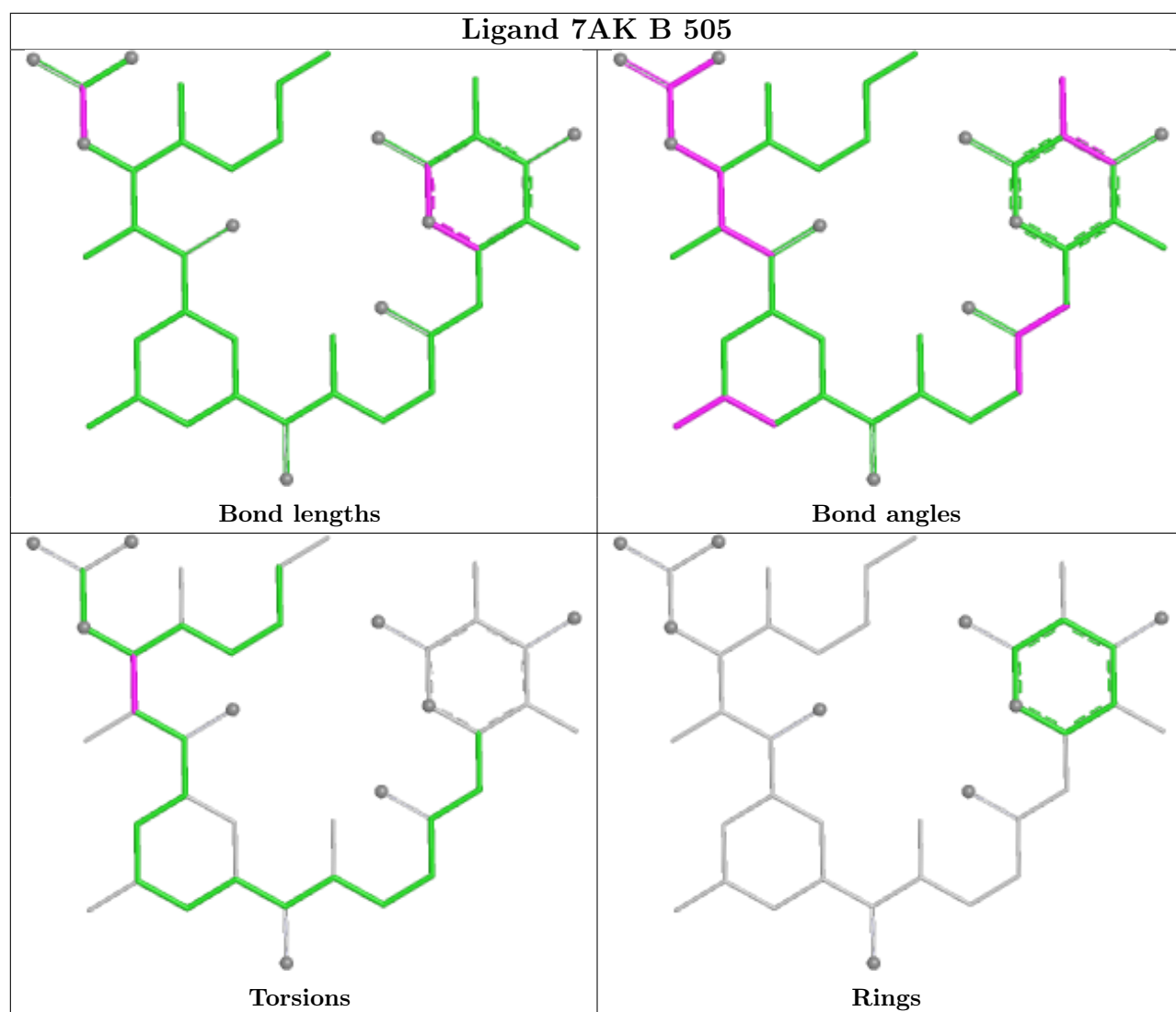
5 monomers are involved in 13 short contacts:

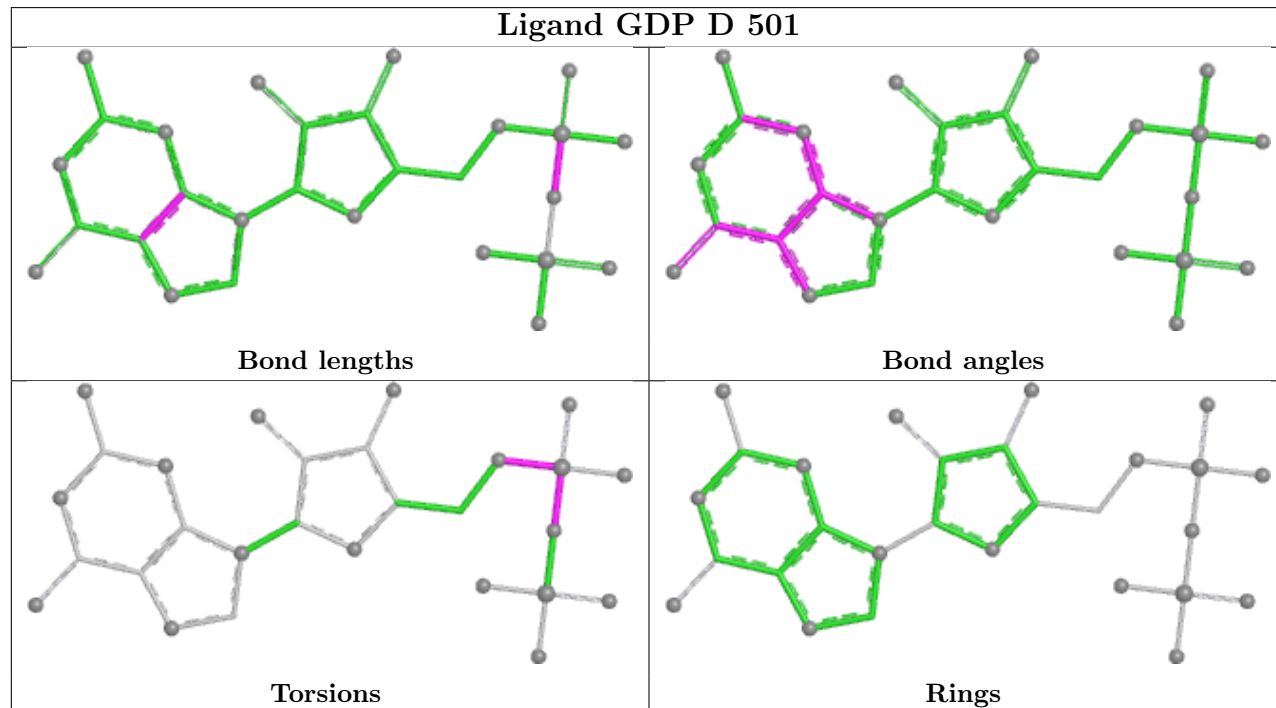
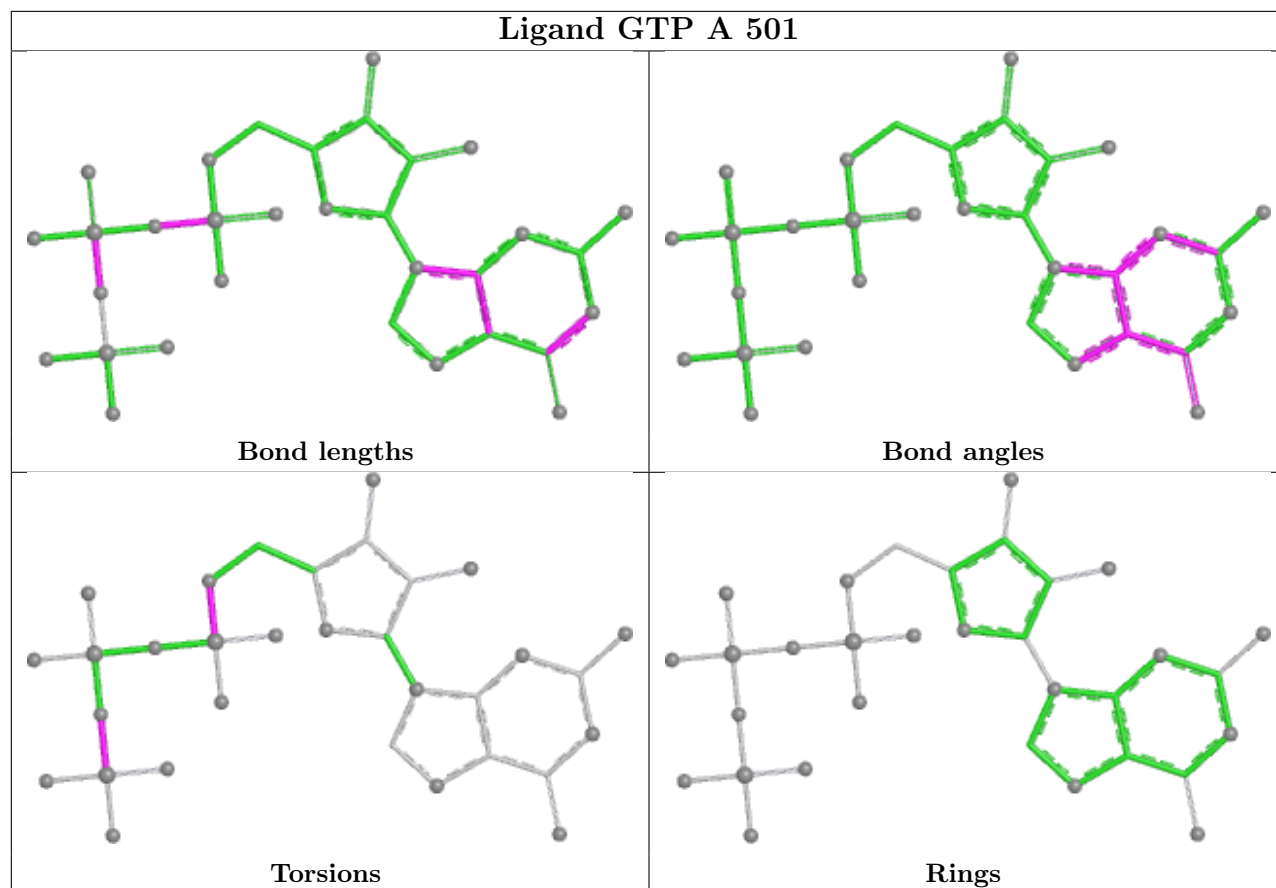
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	7AK	1	0
8	D	501	GDP	1	0
9	B	504	MES	6	0
11	F	401	ACP	4	0
8	B	501	GDP	1	0

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.

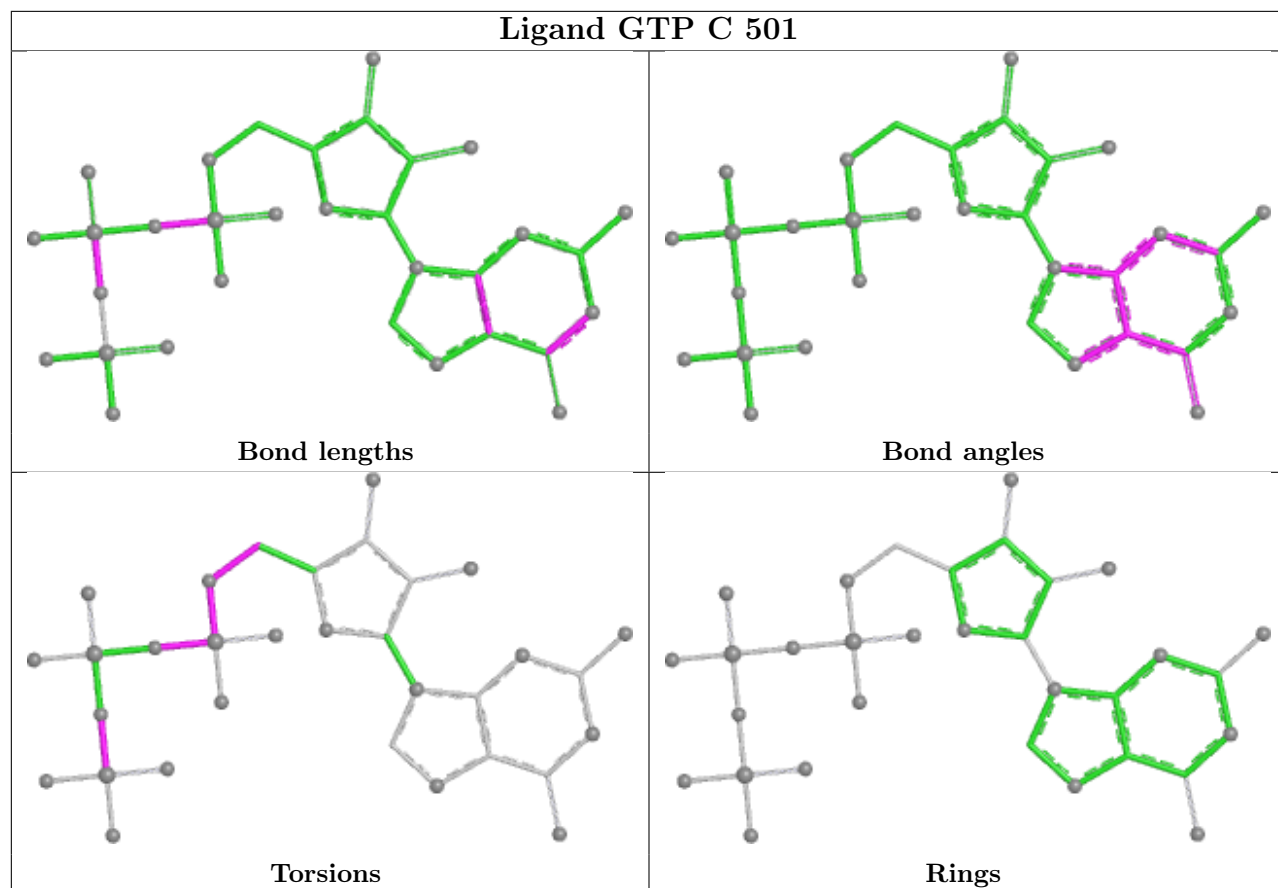
Ligand 7AK D 503



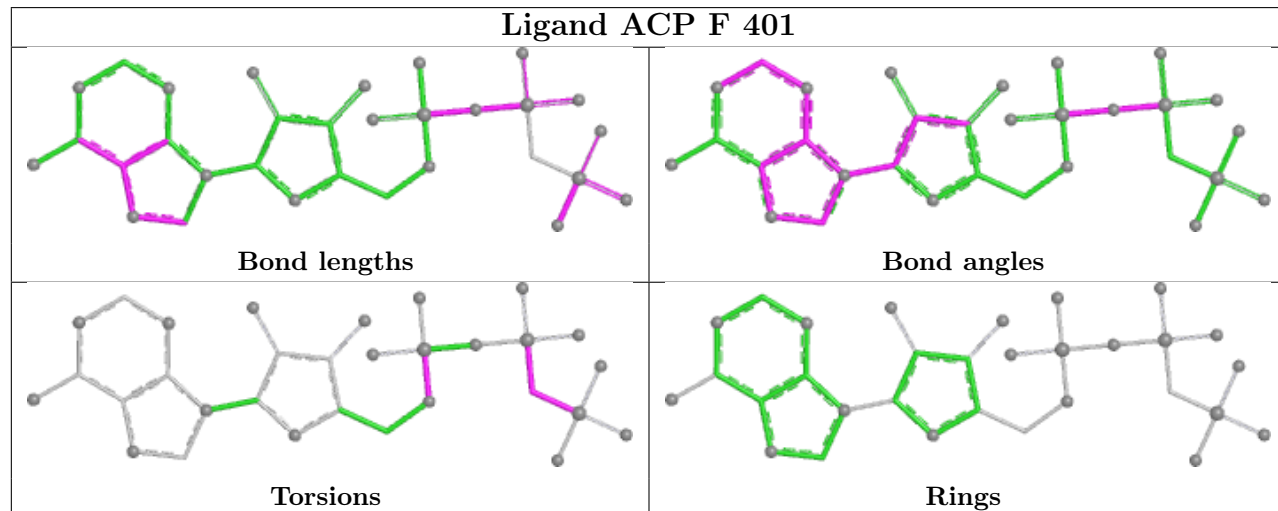


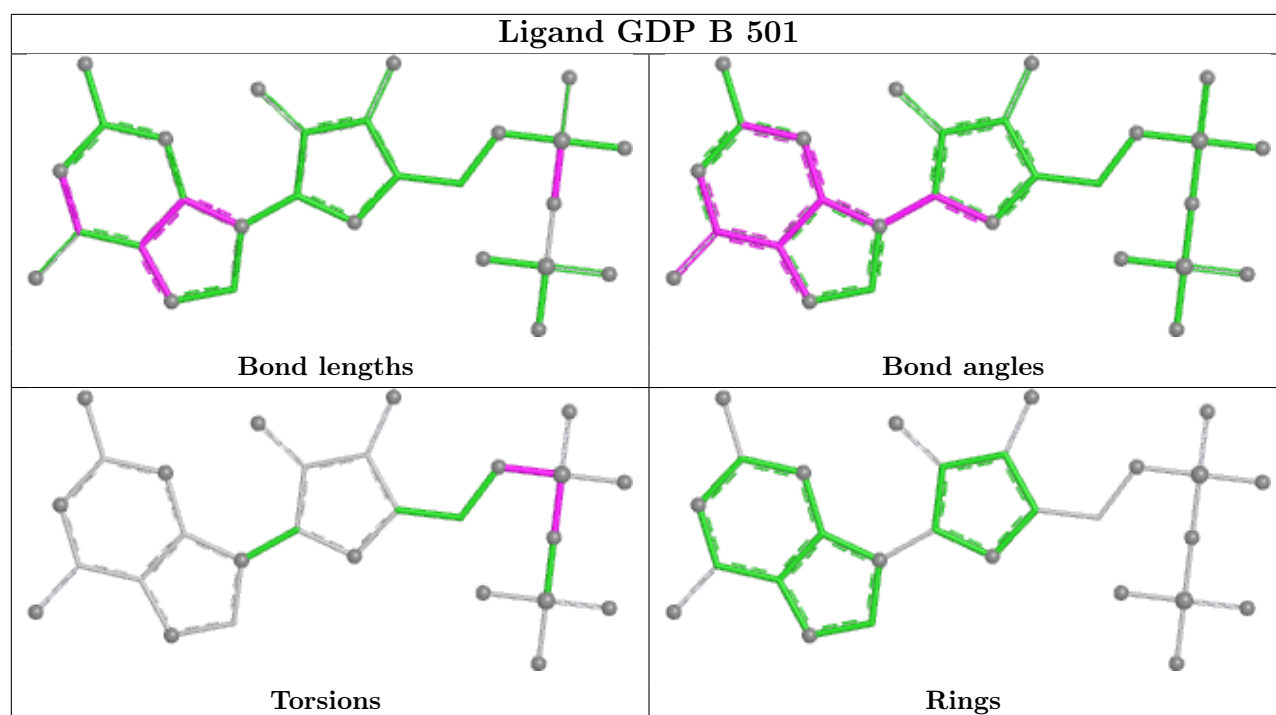


Ligand GTP C 501



Ligand ACP F 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	441/451 (97%)	-0.04	11 (2%) 58 62	17, 41, 69, 134	14 (3%)
1	C	440/451 (97%)	-0.30	7 (1%) 70 74	13, 32, 54, 89	14 (3%)
2	B	426/445 (95%)	0.06	10 (2%) 61 65	16, 41, 73, 116	12 (2%)
2	D	426/445 (95%)	0.09	10 (2%) 61 65	21, 46, 77, 103	12 (2%)
3	E	123/143 (86%)	0.47	4 (3%) 49 52	22, 53, 91, 115	6 (4%)
4	F	354/384 (92%)	0.63	31 (8%) 15 16	20, 63, 123, 158	8 (2%)
All	All	2210/2319 (95%)	0.09	73 (3%) 49 52	13, 43, 89, 158	66 (2%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	155	ALA	5.5
2	D	286	LEU	5.1
1	C	340	SER	4.4
2	B	438	ALA	4.3
2	D	279	GLY	4.2
1	A	262	TYR	4.1
4	F	384	HIS	4.0
4	F	382	HIS	4.0
2	B	1	MET	4.0
2	D	407	TRP	3.9
2	D	1	MET	3.9
3	E	143	ALA	3.8
1	A	450	GLU	3.5
4	F	383	HIS	3.5
4	F	179	VAL	3.5
1	A	179	THR	3.4
4	F	125	THR	3.4
4	F	161	LEU	3.4
1	A	282	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	437	VAL	3.3
4	F	159	GLY	3.3
4	F	169	LEU	3.2
2	B	248	LEU	3.2
4	F	371	PRO	3.1
2	B	2	ARG	3.0
2	B	57	THR	3.0
4	F	147	TRP	3.0
2	D	83	PHE	2.9
1	A	346	TRP	2.9
1	A	448	GLY	2.9
4	F	134	ALA	2.8
4	F	160	ILE	2.8
4	F	173	ILE	2.8
4	F	130	VAL	2.8
4	F	153	ALA	2.8
4	F	380	HIS	2.7
4	F	381	HIS	2.7
2	D	82	PRO	2.7
1	A	449	GLU	2.7
1	C	440	VAL	2.7
2	B	286	LEU	2.5
1	C	302	MET	2.5
2	D	277	SER	2.5
3	E	6	MET	2.5
2	B	281	GLN	2.4
4	F	182	ILE	2.4
1	A	337	THR	2.4
3	E	28	SER	2.4
1	C	357	TYR	2.4
4	F	181	VAL	2.3
4	F	103	THR	2.3
4	F	249	TYR	2.3
1	C	248	LEU	2.3
2	D	37	HIS	2.3
4	F	131	PHE	2.2
4	F	105	LEU	2.2
4	F	177	GLY	2.2
1	A	80	THR	2.2
2	D	81	GLY	2.2
4	F	186	LEU	2.2
4	F	166	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	341	ILE	2.1
3	E	44	ASP	2.1
1	A	362	VAL	2.1
2	B	82	PRO	2.1
2	B	83	PHE	2.1
2	B	291	LEU	2.1
4	F	255[A]	ARG	2.1
2	D	57	THR	2.1
4	F	372	THR	2.1
4	F	142	ARG	2.0
4	F	306	HIS	2.0
1	C	364	PRO	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
6	MG	F	402	1/1	0.82	0.12	65,65,65,65	0
10	7AK	B	505	42/42	0.84	0.12	45,65,83,90	0
6	MG	D	502	1/1	0.88	0.09	59,59,59,59	0
11	ACP	F	401	31/31	0.91	0.10	53,58,105,124	0
10	7AK	D	503	42/42	0.92	0.08	44,57,69,74	0
9	MES	B	504	12/12	0.93	0.10	32,51,57,63	0
7	CA	B	503	1/1	0.93	0.07	75,75,75,75	0
8	GDP	D	501	28/28	0.95	0.08	33,40,47,48	0
7	CA	A	503	1/1	0.97	0.05	51,51,51,51	0
7	CA	A	504	1/1	0.97	0.07	80,80,80,80	0
7	CA	C	503	1/1	0.98	0.04	41,41,41,41	0

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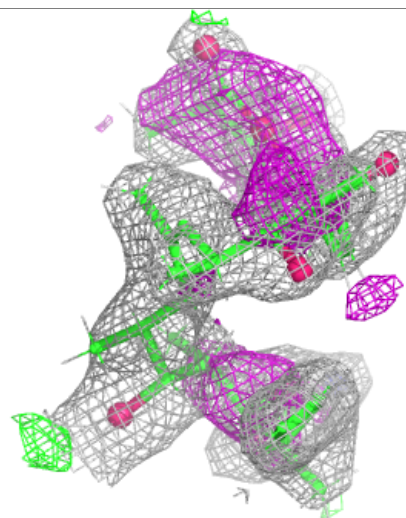
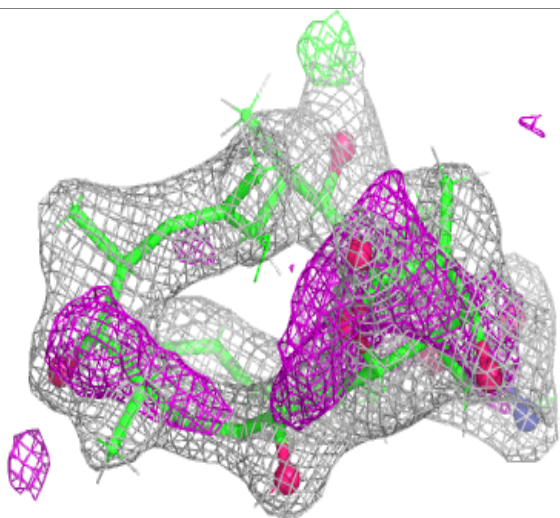
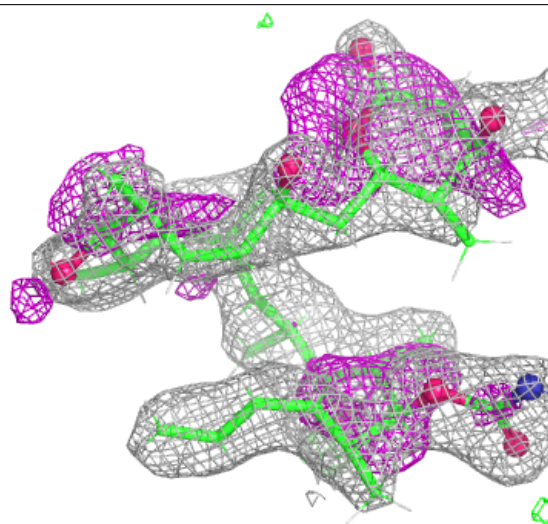
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	A	502	1/1	0.99	0.03	28,28,28,28	0
6	MG	B	502	1/1	0.99	0.04	20,20,20,20	0
5	GTP	A	501	32/32	0.99	0.04	23,28,32,33	0
5	GTP	C	501	32/32	0.99	0.04	19,23,25,26	0
8	GDP	B	501	28/28	0.99	0.04	21,26,30,32	0
6	MG	C	502	1/1	1.00	0.06	24,24,24,24	0

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

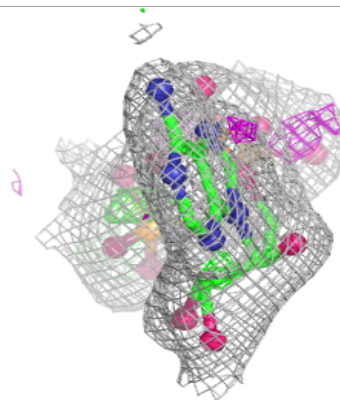
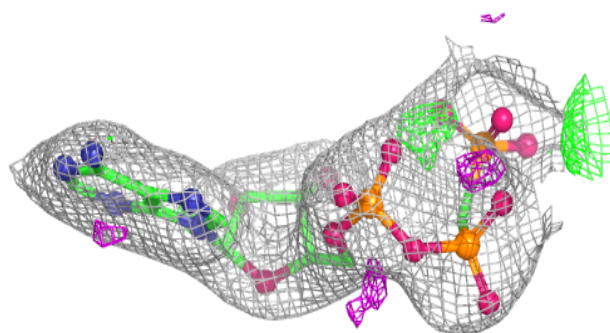
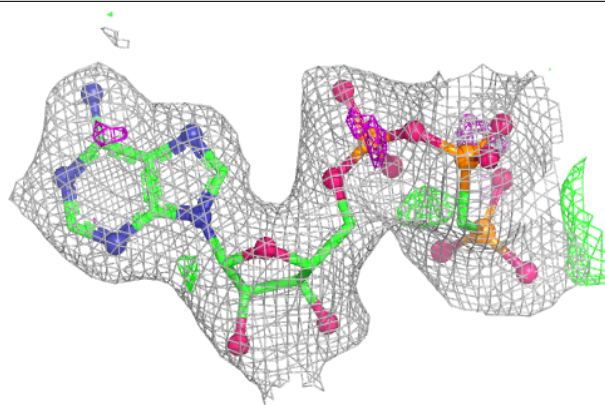
Electron density around 7AK B 505:

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



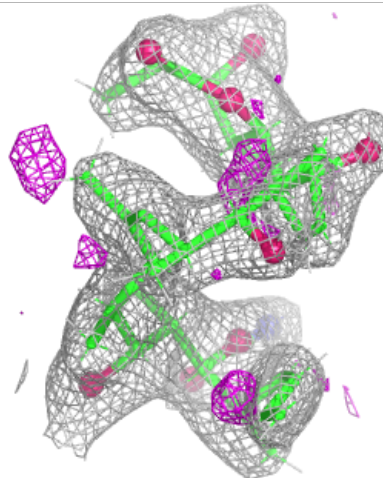
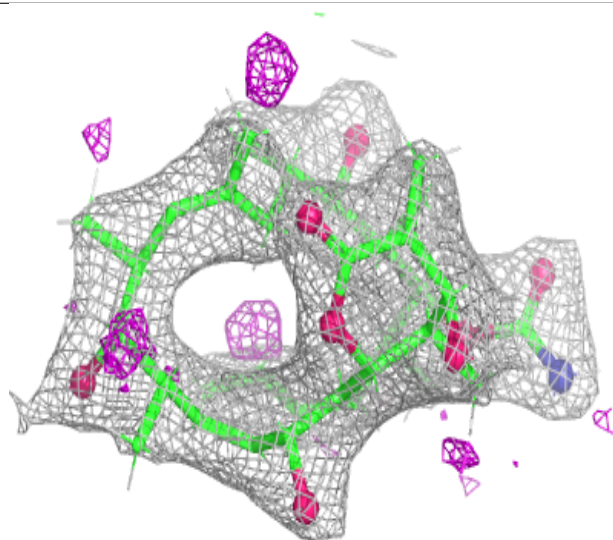
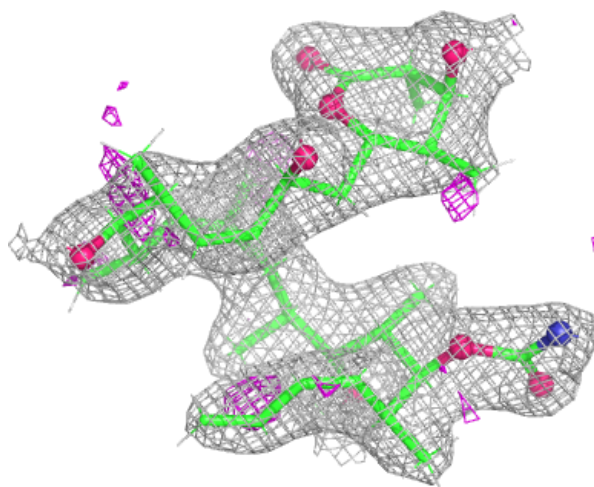
Electron density around ACP F 401:

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



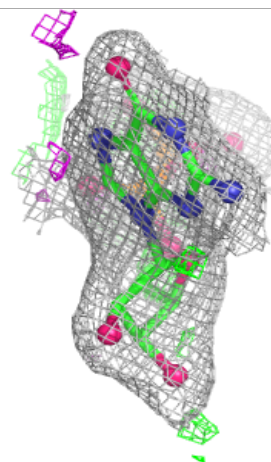
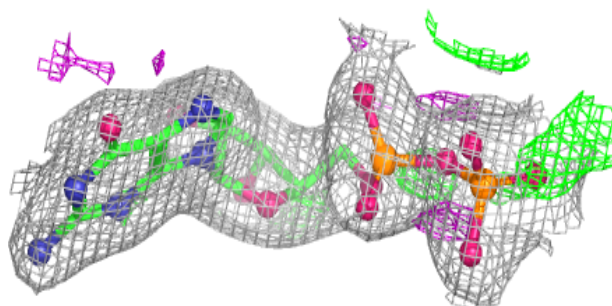
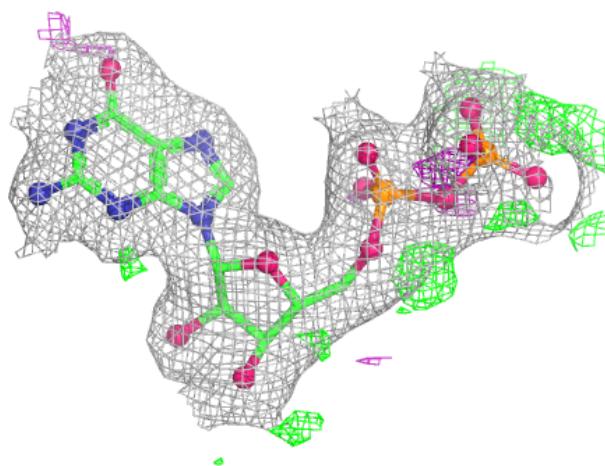
Electron density around 7AK D 503:

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



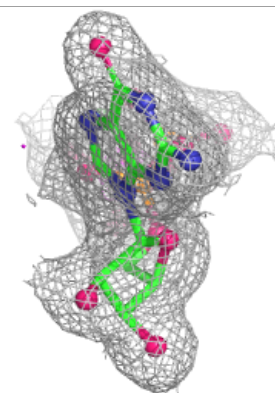
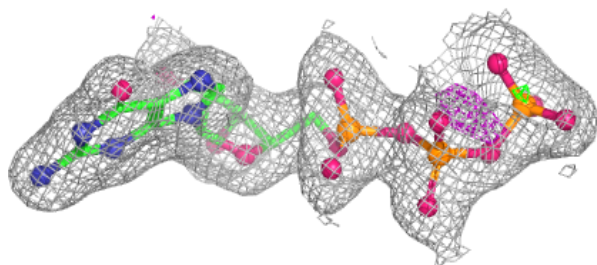
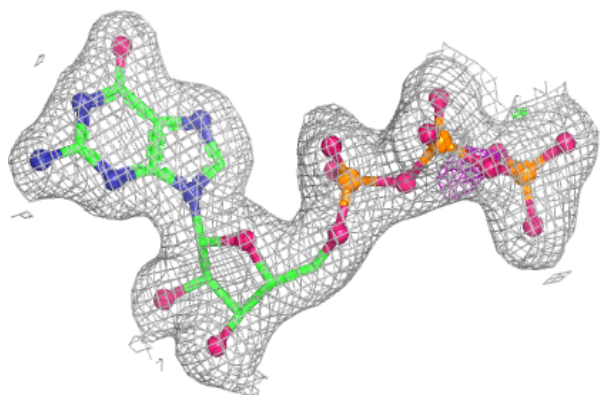
Electron density around GDP D 501:

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

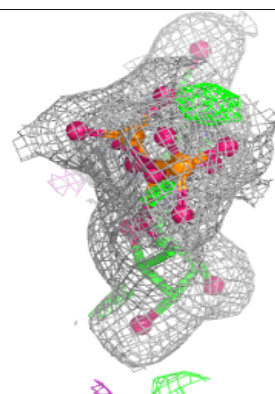
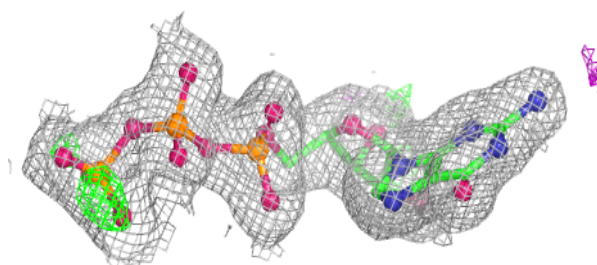
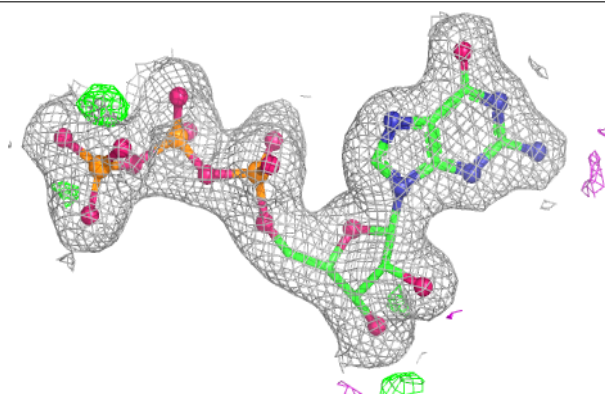


Electron density around GTP A 501:

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

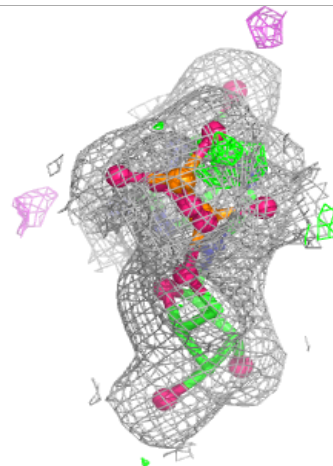
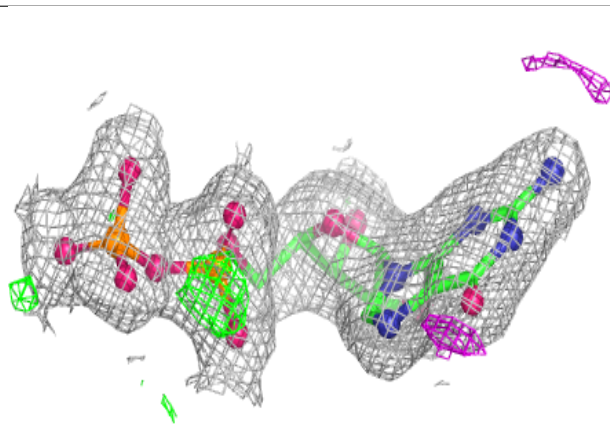
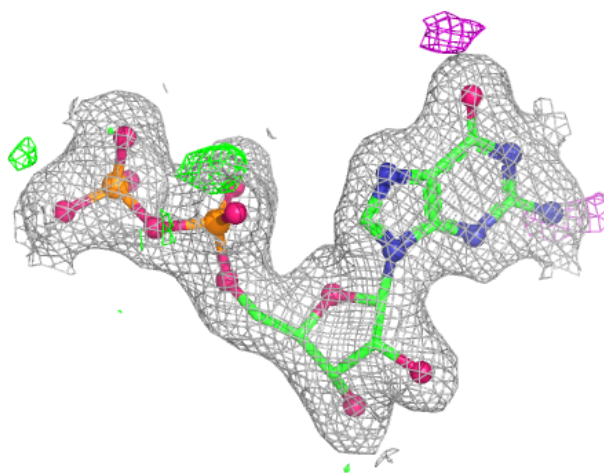
**Electron density around GTP C 501:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.