



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:48 PM UTC

PDB ID : 8CLF / pdb_00008clf
Title : Z-SolQ2Br bound to tubulin (T2R-TTL) complex
Authors : Wranik, M.; Bertrand, Q.; Kepa, M.; Weinert, T.; Steinmetz, M.; Standfuss, J.
Deposited on : 2023-02-16
Resolution : 2.70 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

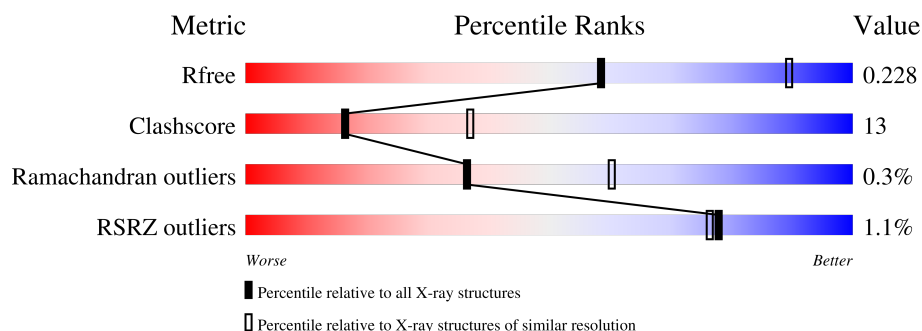
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	73%26%
1	C	440	84%16%
2	B	431	71%28%
2	D	431	2% 68%31%
3	E	121	2% 79%21%
4	F	320	70%30%

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	V1O	B	503	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 34805 atoms, of which 17172 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	439	Total	C	H	N	O	S	0	10	0
			6888	2204	3414	585	661	24			
1	C	440	Total	C	H	N	O	S	0	10	0
			6884	2203	3405	586	666	24			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	428	Total	C	H	N	O	S	2	11	0
			6733	2148	3317	581	660	27			
2	D	431	Total	C	H	N	O	S	0	4	0
			6705	2140	3299	580	658	28			

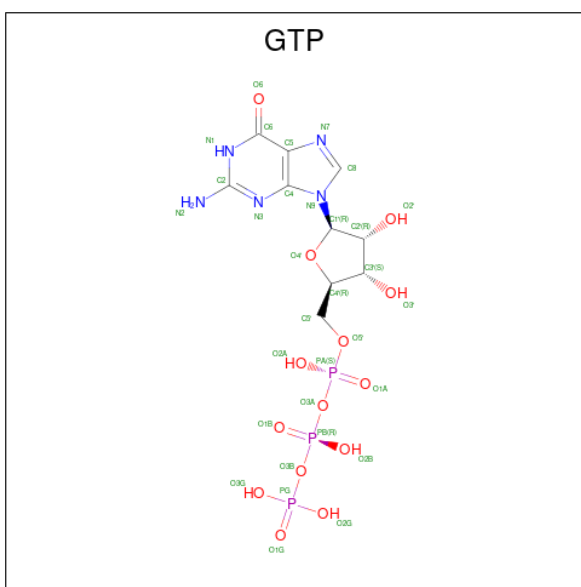
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	2	0
			2046	625	1035	182	198	6			

- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	320	Total	C	H	N	O	S	0	4	0
			5269	1707	2633	437	478	14			

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		

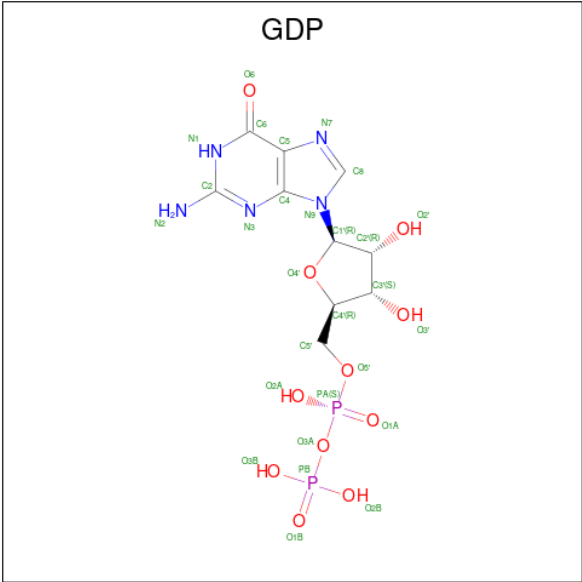
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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		

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

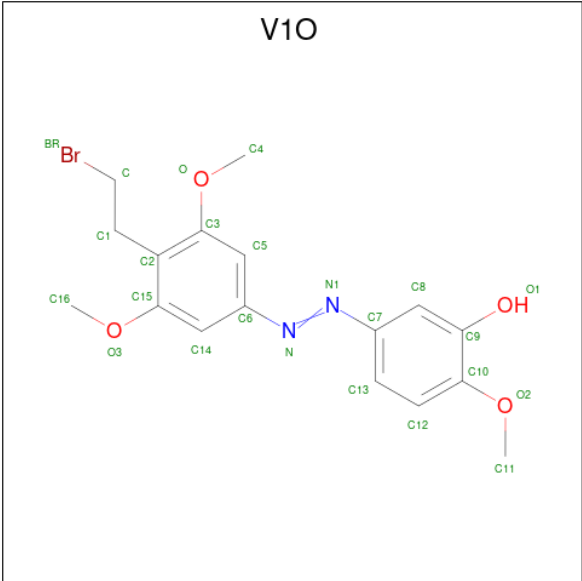
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



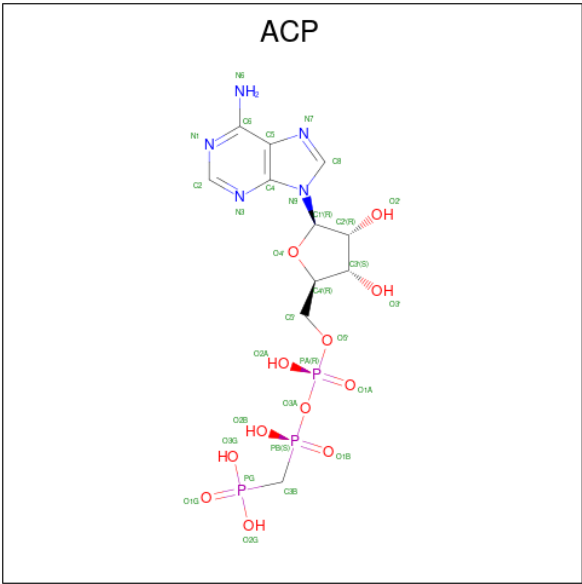
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		
8	D	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		

- Molecule 9 is 5-[[4-(2-bromoethyl)-3,5-dimethoxy-phenyl]diazenyl]-2-methoxy-phenol (CCD ID: V1O) (formula: C₁₇H₁₉BrN₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	Br	C	H	N	O	0	0
			31	1	17	7	2	4		

- Molecule 10 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	F	1	Total	C	H	N	O	0	0
			45	11	14	5	12		

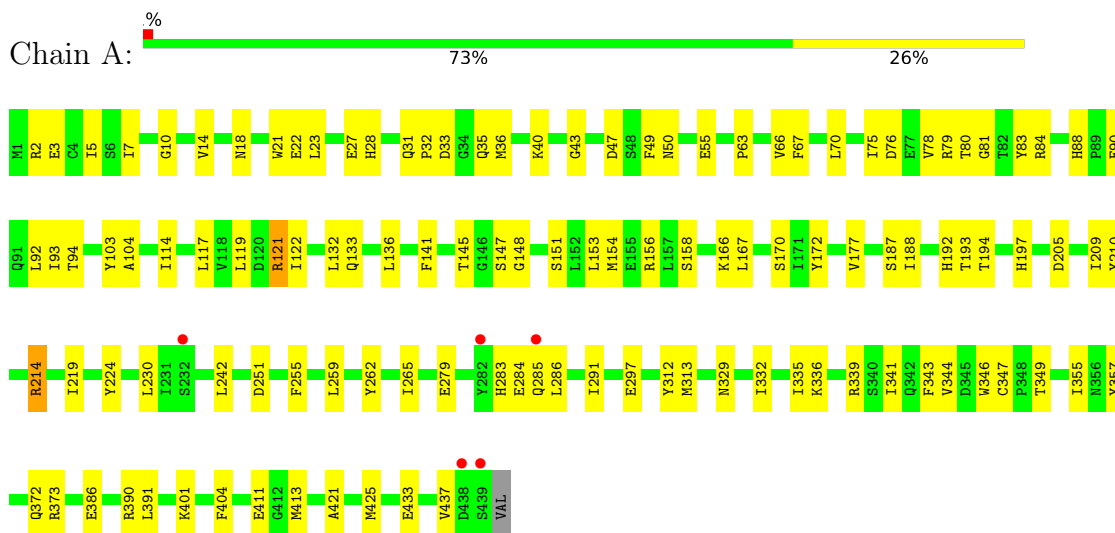
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	4	Total	O	0	0
			4	4		
11	B	6	Total	O	0	0
			6	6		
11	C	18	Total	O	0	0
			18	18		
11	D	1	Total	O	0	0
			1	1		
11	F	1	Total	O	0	0
			1	1		

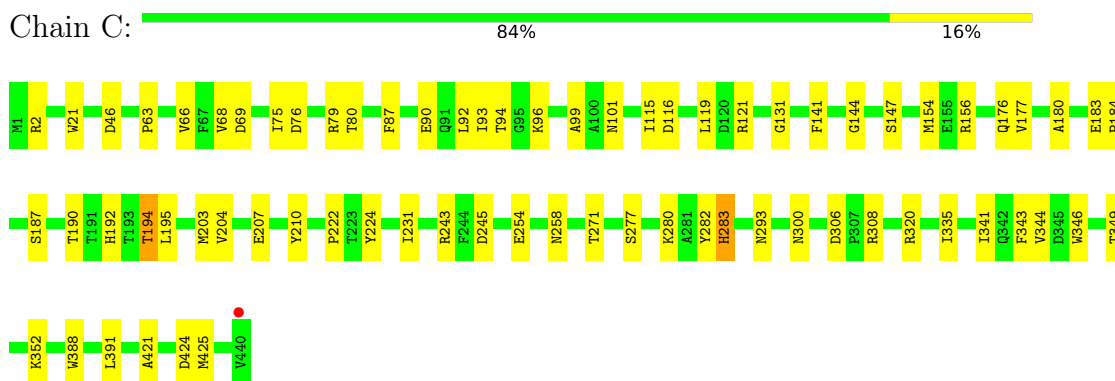
3 Residue-property plots

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

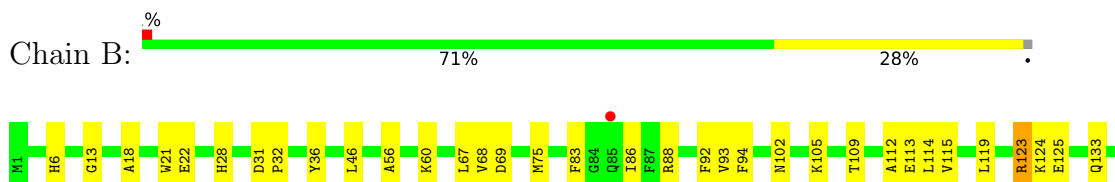
• Molecule 1: Tubulin alpha-1B chain

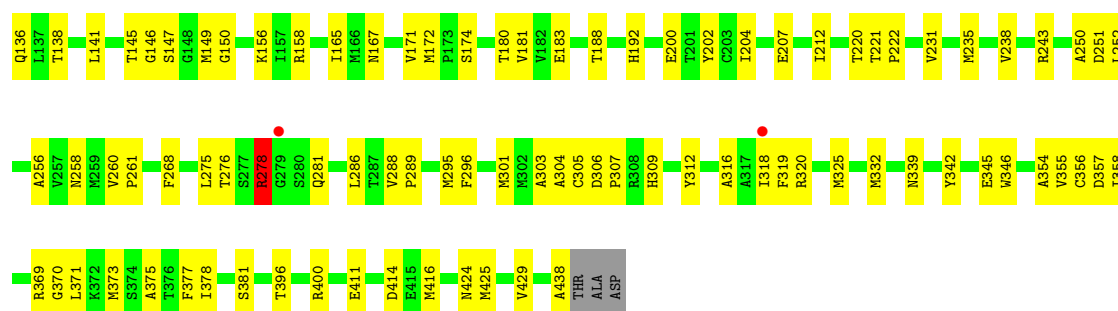


• Molecule 1: Tubulin alpha-1B chain

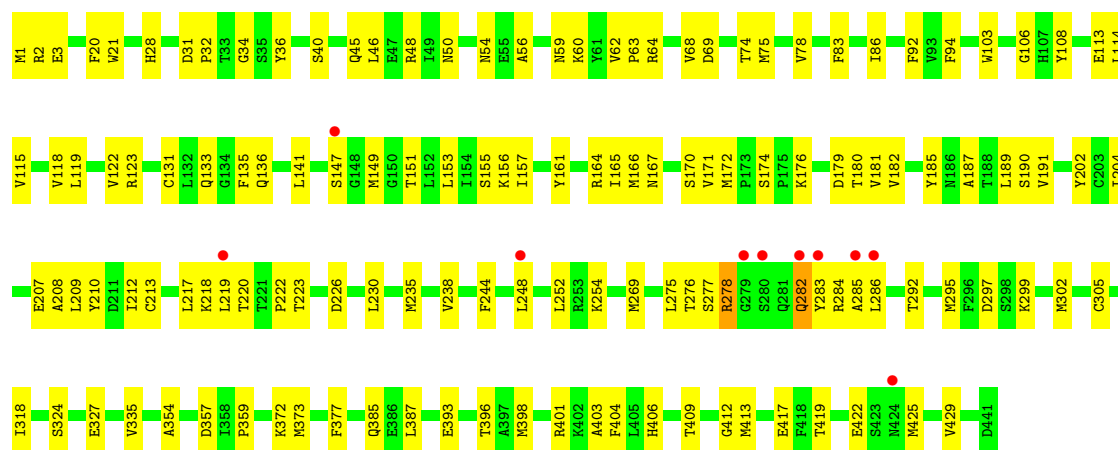


• Molecule 2: Tubulin beta-2B chain

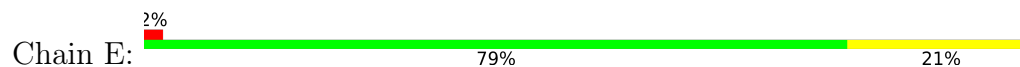




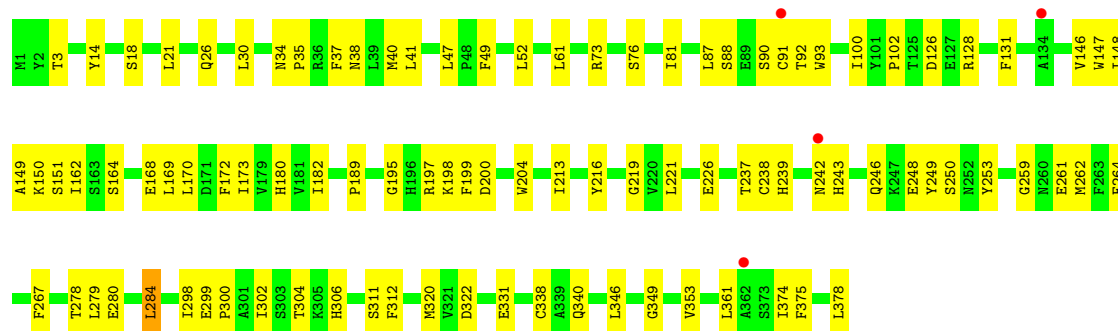
• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.65Å 160.33Å 180.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.35 – 2.70 15.35 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.35-2.70) 99.3 (15.35-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1764.17 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.20_4487	Depositor
R, R_{free}	0.168 , 0.217 (Not available) , 0.228	Depositor DCC
R_{free} test set	1974 reflections (1.71%)	wwPDB-VP
Wilson B-factor (Å ²)	-9.9	Xtriage
Anisotropy	-0.596	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 112.3	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	0.94	EDS
Total number of atoms	34805	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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, V1O, GTP, CA, MG, ACP

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	0.24	0/3582	0.41	0/4864
1	C	0.32	2/3593 (0.1%)	0.50	2/4878 (0.0%)
2	B	0.41	2/3527 (0.1%)	0.56	2/4776 (0.0%)
2	D	0.33	0/3493	0.50	2/4733 (0.0%)
3	E	0.11	0/1025	0.23	0/1359
4	F	0.36	2/2705 (0.1%)	0.55	4/3653 (0.1%)
All	All	0.33	6/17925 (0.0%)	0.49	10/24263 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
2	B	0	2
2	D	0	1
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	147[A]	SER	C-O	6.91	1.32	1.24
2	B	147[B]	SER	C-O	6.91	1.32	1.24
4	F	284[A]	LEU	C-O	6.85	1.32	1.24
4	F	284[B]	LEU	C-O	6.85	1.32	1.24
1	C	194[A]	THR	C-O	6.14	1.32	1.24
1	C	194[B]	THR	C-O	6.14	1.32	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	147[A]	SER	CA-C-O	7.57	128.70	120.90
2	B	147[B]	SER	CA-C-O	7.57	128.70	120.90
1	C	194[A]	THR	CA-C-O	7.48	128.02	119.27
1	C	194[B]	THR	CA-C-O	7.48	128.02	119.27
4	F	284[A]	LEU	CA-C-O	7.43	128.42	120.55
4	F	284[B]	LEU	CA-C-O	7.43	128.42	120.55
2	D	155[A]	SER	CA-C-O	6.19	127.11	120.55
2	D	155[B]	SER	CA-C-O	6.19	127.11	120.55
4	F	284[A]	LEU	N-CA-C	5.45	117.22	111.28
4	F	284[B]	LEU	N-CA-C	5.45	117.22	111.28

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ARG	Sidechain
1	A	214	ARG	Sidechain
2	B	123	ARG	Sidechain
2	B	278	ARG	Sidechain
1	C	243	ARG	Sidechain
1	C	320	ARG	Sidechain
2	D	278	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	3474	3414	3412	99	0
1	C	3479	3405	3392	50	0
2	B	3416	3317	3309	100	0
2	D	3406	3299	3298	118	0
3	E	1011	1035	1035	26	0
4	F	2636	2633	2632	72	0
5	A	32	12	12	1	0
5	C	32	12	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	12	12	0	0
8	D	28	12	12	1	0
9	B	24	7	0	9	0
10	F	31	14	14	3	0
11	A	4	0	0	0	0
11	B	6	0	0	0	0
11	C	18	0	0	0	0
11	D	1	0	0	1	0
11	F	1	0	0	0	0
All	All	17633	17172	17140	450	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 13.

All (450) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	1.47	0.93
2:B:256:ALA:O	2:B:260:VAL:HG13	1.85	0.76
4:F:248:GLU:HG2	4:F:249:TYR:CD1	2.19	0.76
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.68	0.75
2:D:20:PHE:HB2	2:D:235:MET:HE2	1.67	0.75
1:A:79:ARG:HH22	1:A:94:THR:HG21	1.50	0.75
1:C:293[B]:ASN:OD1	1:C:335:ILE:HD11	1.87	0.75
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.69	0.74
2:D:181:VAL:O	2:D:398:MET:HE1	1.88	0.74
2:B:83:PHE:O	2:B:86:ILE:HG22	1.87	0.74
4:F:3:THR:HG23	4:F:38:ASN:H	1.53	0.73
2:B:156:LYS:HE2	3:E:76:ARG:NE	2.03	0.73
2:D:180:THR:HG22	2:D:182:VAL:H	1.52	0.73
4:F:278:THR:HG22	4:F:280:GLU:H	1.53	0.72
2:B:268:PHE:HB3	2:B:378:ILE:CG2	2.19	0.72
2:D:133:GLN:HE21	2:D:252:LEU:H	1.36	0.72
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.08	0.72
1:A:343:PHE:HB2	1:A:349:THR:HG22	1.72	0.72
1:A:70:LEU:HD23	1:A:145:THR:OG1	1.90	0.71
2:B:378:ILE:N	2:B:378:ILE:HD12	2.05	0.71
2:D:180:THR:CG2	2:D:182:VAL:HG22	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ALA:HB2	1:A:413:MET:HE3	1.74	0.70
2:B:325:MET:HG3	2:B:355:VAL:HG21	1.74	0.69
2:B:370:GLY:O	2:B:371:LEU:HD12	1.92	0.69
2:D:147:SER:O	2:D:151:THR:HG23	1.92	0.69
2:B:221:THR:HG23	2:B:221:THR:O	1.92	0.69
2:D:324:SER:OG	2:D:327:GLU:HB2	1.92	0.68
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.74	0.68
2:D:75:MET:HG2	2:D:92:PHE:HD2	1.58	0.68
2:D:118:VAL:HG11	2:D:153:LEU:HD21	1.75	0.67
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.77	0.67
4:F:100:ILE:HD13	4:F:173:ILE:HD13	1.76	0.67
2:D:286:LEU:HD13	2:D:373:MET:HG2	1.77	0.66
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.78	0.65
4:F:248:GLU:HG2	4:F:249:TYR:CE1	2.30	0.65
1:A:40:LYS:HE3	1:A:40:LYS:CA	2.26	0.65
1:A:104:ALA:HB2	1:A:413:MET:CE	2.27	0.65
1:A:386:GLU:O	1:A:390:ARG:HG3	1.97	0.65
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.78	0.65
2:B:378:ILE:HD12	2:B:378:ILE:H	1.61	0.64
4:F:149:ALA:O	4:F:150:LYS:HD2	1.97	0.63
1:A:286:LEU:HD22	1:A:286:LEU:H	1.63	0.63
1:A:339:ARG:HB2	1:A:341:ILE:HD11	1.80	0.63
2:D:174:SER:HB2	2:D:207:GLU:HB2	1.80	0.63
2:B:268:PHE:HB3	2:B:378:ILE:HG23	1.81	0.63
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.80	0.63
1:A:81:GLY:O	1:A:84:ARG:HG2	1.99	0.63
2:D:172:MET:HE2	2:D:172:MET:N	2.13	0.63
3:E:57:ALA:HA	3:E:60:ARG:NH1	2.12	0.63
1:A:336:LYS:C	1:A:336:LYS:HD3	2.23	0.62
1:A:344:VAL:HG22	1:A:347:CYS:HB2	1.82	0.62
2:D:56:ALA:HB3	2:D:60:LYS:HB2	1.81	0.62
4:F:149:ALA:HB2	4:F:182:ILE:HG12	1.82	0.62
1:A:285:GLN:HG3	1:A:372[B]:GLN:OE1	1.99	0.62
2:D:59:ASN:O	2:D:59:ASN:ND2	2.28	0.61
2:D:136:GLN:HA	2:D:167:ASN:O	2.00	0.61
2:B:295:MET:HE3	2:B:296:PHE:CE1	2.36	0.61
1:A:40:LYS:HE3	1:A:40:LYS:HA	1.82	0.61
2:D:118:VAL:CG1	2:D:153:LEU:HD21	2.31	0.61
1:A:177:VAL:HG12	5:A:501:GTP:O2'	2.01	0.61
2:B:316:ALA:HB1	9:B:503:V1O:C16	2.31	0.61
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:ILE:HD11	9:B:503:V1O:BR	2.57	0.60
2:D:403:ALA:HB1	2:D:404:PHE:HD1	1.66	0.60
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.82	0.60
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.83	0.60
4:F:148:ILE:HB	4:F:162:ILE:HG23	1.82	0.60
4:F:237:THR:HG21	4:F:249:TYR:O	2.01	0.60
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.82	0.60
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.84	0.60
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.36	0.60
1:C:96:LYS:HZ3	1:C:96:LYS:HB2	1.67	0.59
2:D:230:LEU:HB3	2:D:302:MET:HE3	1.82	0.59
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG13	1.84	0.59
1:A:279:GLU:HA	1:A:279:GLU:OE1	2.02	0.59
2:B:69:ASP:O	2:B:94:PHE:HA	2.03	0.59
2:D:171:VAL:HA	2:D:204:ILE:O	2.03	0.59
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.83	0.59
1:A:136[A]:LEU:HD23	1:A:167:LEU:HB2	1.84	0.59
2:B:301:MET:HE1	2:B:377:PHE:CE2	2.38	0.59
2:D:36:TYR:CE2	2:D:46:LEU:HD11	2.37	0.58
2:D:393:GLU:O	2:D:396:THR:HG22	2.02	0.58
2:D:179:ASP:HB2	8:D:501:GDP:H3'	1.85	0.58
1:A:36:MET:HE1	1:A:49:PHE:CE1	2.38	0.58
1:A:166:LYS:HE2	1:A:197:HIS:O	2.03	0.58
4:F:3:THR:HG23	4:F:38:ASN:N	2.17	0.58
1:A:2:ARG:CB	1:A:133:GLN:HG2	2.33	0.58
4:F:100:ILE:HD11	4:F:180:HIS:HB2	1.84	0.58
2:B:318:ILE:HG12	9:B:503:V1O:BR	2.59	0.58
3:E:6:MET:HG2	3:E:24:LEU:CD2	2.34	0.58
2:D:223:THR:HG22	2:D:226:ASP:OD2	2.04	0.57
4:F:213:ILE:HG22	4:F:378[B]:LEU:HD12	1.84	0.57
1:A:336:LYS:HD3	1:A:336:LYS:O	2.04	0.57
4:F:374:ILE:HD11	4:F:375:PHE:CE2	2.40	0.57
2:D:164:ARG:HG2	2:D:164:ARG:HH11	1.67	0.57
2:D:209:LEU:HD21	2:D:302:MET:HG3	1.87	0.57
1:A:151:SER:HB2	1:A:193:THR:CG2	2.35	0.57
2:D:269[B]:MET:CE	2:D:305:CYS:HB2	2.35	0.57
2:D:180:THR:HG21	2:D:182:VAL:HG22	1.87	0.57
4:F:3:THR:OG1	4:F:30:LEU:HD11	2.04	0.57
2:B:13:GLY:CA	2:B:138[B]:THR:HG22	2.27	0.56
4:F:259:GLY:O	4:F:261:GLU:HG3	2.05	0.56
1:A:344:VAL:CG2	1:A:347:CYS:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:LEU:HD23	2:D:149:MET:HE1	1.87	0.56
1:C:277:SER:OG	1:C:280:LYS:HG3	2.05	0.56
2:D:212:ILE:HG22	2:D:217:LEU:HD23	1.86	0.56
1:A:344:VAL:HG21	1:A:346:TRP:CE2	2.41	0.56
2:D:141:LEU:HD22	2:D:190:SER:HB3	1.87	0.56
3:E:9:ILE:HD13	3:E:23:ILE:HD12	1.87	0.56
4:F:278:THR:HG22	4:F:280:GLU:N	2.19	0.56
2:D:113:GLU:OE2	2:D:113:GLU:HA	2.06	0.56
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.41	0.55
4:F:40:MET:HE2	4:F:47:LEU:HD21	1.87	0.55
2:D:74:THR:O	2:D:78:VAL:HG13	2.06	0.55
4:F:304:THR:HG21	4:F:311:SER:HB2	1.87	0.55
2:B:102:ASN:HB3	2:B:105[A]:LYS:HG3	1.88	0.55
2:D:133:GLN:NE2	2:D:252:LEU:H	2.04	0.55
4:F:146:VAL:HG22	4:F:164:SER:OG	2.06	0.55
2:D:161:TYR:HB3	2:D:164:ARG:HG3	1.88	0.55
2:D:269[B]:MET:HE3	2:D:305:CYS:HB2	1.89	0.55
2:D:284:ARG:NH2	2:D:285:ALA:H	2.04	0.55
2:D:180:THR:HG22	2:D:182:VAL:HG22	1.88	0.55
2:B:202:TYR:CE1	2:B:238:VAL:HG21	2.42	0.55
4:F:280:GLU:HA	4:F:284[A]:LEU:HB2	1.89	0.55
2:D:75:MET:HG2	2:D:92:PHE:CD2	2.40	0.54
4:F:100:ILE:HD12	4:F:100:ILE:O	2.07	0.54
1:A:31:GLN:HB3	1:A:32:PRO:HD2	1.89	0.54
4:F:213:ILE:CG2	4:F:378[B]:LEU:HD12	2.38	0.54
2:B:86:ILE:HG12	2:B:86:ILE:O	2.08	0.54
2:D:413:MET:HE3	2:D:417:GLU:CD	2.31	0.54
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.37	0.54
2:B:295:MET:SD	2:B:375:ALA:HB1	2.48	0.54
1:A:33:ASP:OD1	1:A:35:GLN:HG2	2.08	0.54
4:F:374:ILE:HD11	4:F:375:PHE:CZ	2.43	0.54
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.90	0.53
3:E:6:MET:HG2	3:E:24:LEU:HD22	1.90	0.53
2:B:319:PHE:HB2	2:B:355:VAL:HG12	1.90	0.53
4:F:49:PHE:HA	4:F:52:LEU:HD12	1.89	0.53
2:B:318:ILE:HA	2:B:354:ALA:O	2.09	0.53
1:C:154:MET:HG3	1:C:194[A]:THR:HG23	1.90	0.53
2:B:56:ALA:HB3	2:B:60:LYS:HG2	1.91	0.53
4:F:91:CYS:C	4:F:93:TRP:H	2.16	0.53
1:A:433:GLU:O	1:A:437:VAL:HB	2.08	0.53
2:B:67:LEU:N	2:B:67:LEU:HD12	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:218:LYS:O	2:D:219:LEU:HD23	2.09	0.53
2:D:164:ARG:HG2	2:D:164:ARG:NH1	2.24	0.53
2:B:75:MET:HG3	2:B:94:PHE:HD1	1.75	0.53
2:B:158[B]:ARG:CZ	3:E:68:LEU:HD11	2.38	0.52
2:B:316:ALA:HB1	9:B:503:V1O:O3	2.08	0.52
4:F:61:LEU:HD11	4:F:312:PHE:HD1	1.74	0.52
2:D:34:GLY:CA	2:D:86:ILE:HD11	2.38	0.52
2:D:50:ASN:H	2:D:50:ASN:ND2	2.06	0.52
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.90	0.52
1:A:283:HIS:HD2	1:A:284:GLU:O	1.92	0.52
1:C:271:THR:HG23	1:C:300:ASN:O	2.10	0.52
2:D:286:LEU:HD12	2:D:286:LEU:O	2.09	0.52
4:F:128:ARG:CZ	4:F:170:LEU:HD22	2.40	0.52
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.45	0.52
1:C:147:SER:HB2	1:C:190:THR:HB	1.91	0.52
2:D:218:LYS:C	2:D:219:LEU:HD23	2.34	0.52
4:F:100:ILE:HA	4:F:126:ASP:HB2	1.90	0.52
1:C:99:ALA:HB3	1:C:144:GLY:HA3	1.92	0.52
2:D:220:THR:O	2:D:222:PRO:HD3	2.09	0.52
2:B:124:LYS:HD3	2:B:125:GLU:HG2	1.92	0.51
2:B:200:GLU:OE2	2:B:256:ALA:HB2	2.10	0.51
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.44	0.51
4:F:204:TRP:CZ2	4:F:338:CYS:HA	2.45	0.51
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.10	0.51
3:E:57:ALA:HA	3:E:60:ARG:HH11	1.75	0.51
4:F:242:ASN:O	4:F:246:GLN:HG2	2.11	0.51
1:C:96:LYS:HB2	1:C:96:LYS:NZ	2.25	0.51
2:D:181:VAL:HG22	2:D:398:MET:HE1	1.93	0.51
2:B:22[A]:GLU:HG2	2:B:83:PHE:CD1	2.46	0.51
1:C:79:ARG:HG2	1:C:92:LEU:HD12	1.92	0.51
4:F:102:PRO:HB3	4:F:173:ILE:CG2	2.40	0.51
2:B:220:THR:O	2:B:222:PRO:HD3	2.11	0.51
2:D:20:PHE:HB2	2:D:235:MET:CE	2.41	0.51
2:D:75:MET:SD	2:D:94:PHE:HB3	2.51	0.51
2:D:248:LEU:HD12	2:D:354:ALA:HB2	1.93	0.51
4:F:168:GLU:O	4:F:172:PHE:HB2	2.11	0.51
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.46	0.50
2:B:105[A]:LYS:HA	2:B:109:THR:OG1	2.11	0.50
2:D:403:ALA:HB1	2:D:404:PHE:CD1	2.45	0.50
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.12	0.50
1:A:335:ILE:C	1:A:335:ILE:HD12	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LYS:HE3	2:B:438:ALA:HB1	1.93	0.50
2:B:141:LEU:HD12	2:B:172:MET:SD	2.52	0.50
2:D:282:GLN:C	2:D:284:ARG:H	2.19	0.50
2:D:387:LEU:HD23	2:D:387:LEU:C	2.36	0.50
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.47	0.50
2:B:301:MET:HE1	2:B:377:PHE:HE2	1.77	0.50
2:B:276:THR:HG21	2:B:371:LEU:HD11	1.93	0.50
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.25	0.50
3:E:9:ILE:HD13	3:E:23:ILE:CD1	2.40	0.50
4:F:131:PHE:C	4:F:131:PHE:CD2	2.89	0.50
2:B:180:THR:O	2:B:183:GLU:HG3	2.12	0.50
2:D:176:LYS:HD3	2:D:210:TYR:CD2	2.46	0.50
2:D:191:VAL:HG11	2:D:425:MET:HE2	1.94	0.50
2:B:112:ALA:O	2:B:115:VAL:HG12	2.12	0.50
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.93	0.50
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.93	0.50
1:C:245:ASP:N	1:C:245:ASP:OD1	2.42	0.50
1:C:176:GLN:HE22	1:C:207:GLU:HG3	1.77	0.50
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.94	0.50
1:A:297:GLU:OE2	4:F:306:HIS:ND1	2.44	0.49
1:C:177:VAL:HG12	1:C:177:VAL:O	2.12	0.49
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.93	0.49
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.42	0.49
3:E:81:GLU:O	3:E:84[B]:GLN:HG2	2.12	0.49
3:E:135:LYS:HE2	3:E:139:LEU:HD11	1.94	0.49
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.48	0.49
4:F:246:GLN:O	4:F:250:SER:OG	2.30	0.49
1:A:40:LYS:HE3	1:A:40:LYS:O	2.11	0.49
1:A:265:ILE:O	1:A:265:ILE:HG22	2.12	0.49
4:F:198:LYS:HG2	4:F:199:PHE:H	1.77	0.49
1:A:103:TYR:CD2	1:A:148:GLY:HA2	2.48	0.49
2:B:425:MET:O	2:B:429:VAL:HG23	2.12	0.49
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.47	0.49
2:B:318:ILE:CG1	9:B:503:V1O:BR	3.16	0.49
2:D:372:LYS:HD3	2:D:373:MET:HE3	1.93	0.49
1:A:283:HIS:CD2	1:A:284:GLU:O	2.65	0.49
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.95	0.48
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.95	0.48
4:F:49:PHE:HA	4:F:52:LEU:CD1	2.43	0.48
2:B:105[B]:LYS:HA	2:B:109:THR:OG1	2.13	0.48
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLU:N	1:C:184:PRO:CD	2.77	0.48
2:D:119:LEU:O	2:D:123:ARG:HG3	2.12	0.48
2:D:318:ILE:HG22	11:D:601:HOH:O	2.13	0.48
4:F:102:PRO:HB3	4:F:173:ILE:HG22	1.93	0.48
2:B:75:MET:HG3	2:B:94:PHE:CD1	2.48	0.48
2:B:105[A]:LYS:HE2	2:B:411:GLU:OE2	2.13	0.48
2:B:346:TRP:HE1	2:B:438:ALA:HB3	1.78	0.48
2:D:278:ARG:CZ	2:D:278:ARG:HB3	2.43	0.48
2:D:282:GLN:C	2:D:284:ARG:N	2.70	0.48
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.48	0.48
2:B:320:ARG:HA	2:B:356:CYS:O	2.13	0.48
2:B:378:ILE:CD1	9:B:503:V1O:BR	3.17	0.48
2:B:28:HIS:NE2	2:B:243:ARG:HD2	2.29	0.48
4:F:331:GLU:CD	10:F:401:ACP:H3B1	2.39	0.48
4:F:128:ARG:NH2	4:F:170:LEU:HD22	2.29	0.48
1:A:28:HIS:O	1:A:36:MET:HE3	2.12	0.48
2:D:153:LEU:O	2:D:157:ILE:HD12	2.14	0.48
2:D:286:LEU:HD13	2:D:373:MET:CG	2.41	0.48
4:F:26:GLN:NE2	4:F:361:LEU:HD22	2.27	0.48
1:A:67:PHE:HB2	1:A:92:LEU:HD12	1.96	0.48
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.94	0.48
2:B:156:LYS:HE2	3:E:76:ARG:HE	1.75	0.48
2:B:369:ARG:HD2	2:B:370:GLY:N	2.29	0.48
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.96	0.48
1:A:210:TYR:CE2	1:A:214:ARG:HD3	2.49	0.47
4:F:243:HIS:NE2	4:F:253:TYR:OH	2.46	0.47
1:A:355:ILE:O	3:E:17:GLY:HA3	2.13	0.47
1:C:282:TYR:O	1:C:283:HIS:CB	2.62	0.47
2:D:275:LEU:O	2:D:277:SER:N	2.47	0.47
3:E:130:ALA:C	3:E:134:ARG:HH21	2.22	0.47
1:A:114:ILE:HD12	1:A:117:LEU:HB3	1.96	0.47
1:A:329:ASN:HD21	3:E:8:VAL:HG21	1.80	0.47
1:C:90:GLU:CD	1:C:90:GLU:H	2.23	0.47
4:F:320:MET:HE2	10:F:401:ACP:H2'	1.95	0.47
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.95	0.47
2:B:318:ILE:HG23	9:B:503:V1O:BR	2.69	0.47
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.14	0.47
1:A:23:LEU:O	1:A:27:GLU:HG3	2.14	0.47
1:C:141:PHE:HE2	1:C:203:MET:HE3	1.79	0.47
2:D:103:TRP:HD1	2:D:147:SER:OG	1.98	0.47
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:ALA:HB1	9:B:503:V1O:C5	2.45	0.47
2:B:258:ASN:HB3	9:B:503:V1O:C11	2.43	0.47
2:B:260:VAL:O	2:B:260:VAL:HG22	2.14	0.47
1:C:192:HIS:CG	1:C:421:ALA:HA	2.50	0.47
1:C:343:PHE:HB2	1:C:349:THR:HG22	1.95	0.47
2:D:413:MET:HE3	2:D:417:GLU:OE2	2.14	0.47
4:F:238:CYS:SG	4:F:239:HIS:CD2	3.08	0.47
1:A:347:CYS:C	3:E:27:PRO:HB3	2.40	0.47
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.47	0.47
2:B:133:GLN:OE1	2:B:251:ASP:HB2	2.14	0.47
2:B:221:THR:O	2:B:221:THR:CG2	2.61	0.47
2:B:286:LEU:N	2:B:286:LEU:HD12	2.29	0.47
2:D:69:ASP:N	2:D:75:MET:HE1	2.29	0.47
1:A:187:SER:CB	1:A:391:LEU:HD21	2.45	0.46
2:D:406:HIS:HA	2:D:409:THR:OG1	2.15	0.46
3:E:6:MET:HE3	3:E:22:VAL:HG21	1.97	0.46
1:A:177:VAL:HG11	1:A:224:TYR:HE1	1.80	0.46
1:A:404:PHE:CD1	2:B:261:PRO:HA	2.50	0.46
2:B:88:ARG:HH11	2:B:88:ARG:HG2	1.79	0.46
2:B:123:ARG:O	2:B:124:LYS:C	2.58	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.97	0.46
1:C:177:VAL:HG11	1:C:224:TYR:CE1	2.51	0.46
2:D:108:TYR:O	3:E:134:ARG:HD3	2.14	0.46
2:D:185:TYR:OH	2:D:398:MET:HB3	2.15	0.46
2:B:146:GLY:O	2:B:150:GLY:HA3	2.16	0.46
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	1.98	0.46
1:A:154:MET:HG3	1:A:194:THR:HG23	1.98	0.46
4:F:88:SER:C	4:F:90:SER:N	2.72	0.46
4:F:91:CYS:O	4:F:93:TRP:N	2.47	0.46
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.81	0.46
4:F:267:PHE:CD2	4:F:279:LEU:HD13	2.51	0.46
1:A:40:LYS:HA	1:A:40:LYS:CE	2.43	0.46
1:A:151:SER:HB2	1:A:193:THR:HG22	1.97	0.46
1:A:158:SER:OG	1:A:166:LYS:HE3	2.16	0.46
1:A:285:GLN:HE21	1:A:373:ARG:NH1	2.13	0.46
2:B:181:VAL:HG13	1:C:258:ASN:ND2	2.31	0.46
2:B:318:ILE:O	2:B:318:ILE:HD12	2.16	0.46
4:F:216:TYR:CE1	4:F:374:ILE:HD13	2.51	0.46
2:B:305:CYS:O	2:B:307:PRO:HD3	2.15	0.45
2:D:297:ASP:OD2	2:D:299:LYS:HB2	2.16	0.45
4:F:189:PRO:HA	4:F:322:ASP:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ARG:HG2	1:A:219:ILE:O	2.16	0.45
1:A:117:LEU:HD11	1:A:121:ARG:HH11	1.81	0.45
2:B:332:MET:HE3	2:B:332:MET:CA	2.46	0.45
2:D:106:GLY:O	2:D:149:MET:HB2	2.17	0.45
2:B:212:ILE:HG23	2:B:275:LEU:HD13	1.98	0.45
2:D:180:THR:CG2	2:D:181:VAL:N	2.79	0.45
1:A:411:GLU:OE1	1:A:411:GLU:HA	2.17	0.45
2:B:18:ALA:O	2:B:22[A]:GLU:HG3	2.17	0.45
1:C:76:ASP:O	1:C:80:THR:HG23	2.16	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.52	0.45
2:D:141:LEU:HD12	2:D:172:MET:SD	2.56	0.45
2:D:401:ARG:O	2:D:401:ARG:HG3	2.15	0.45
2:B:171:VAL:HA	2:B:204:ILE:O	2.17	0.45
1:C:69:ASP:O	1:C:94:THR:HA	2.17	0.45
1:C:282:TYR:O	1:C:283:HIS:HB2	2.17	0.45
2:D:357:ASP:O	2:D:359:PRO:HD3	2.17	0.45
2:D:48:ARG:NH1	2:D:244:PHE:O	2.50	0.45
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.99	0.45
1:A:5:ILE:HD12	1:A:132:LEU:HD11	1.99	0.44
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.51	0.44
1:C:2:ARG:HA	1:C:131:GLY:O	2.17	0.44
4:F:151:SER:HB2	4:F:180:HIS:CD2	2.52	0.44
1:C:388:TRP:CE3	1:C:425:MET:HE1	2.51	0.44
4:F:18:SER:HA	4:F:21:LEU:HD12	1.99	0.44
2:B:358:ILE:HD13	2:B:358:ILE:N	2.32	0.44
2:B:303:ALA:O	2:B:305:CYS:N	2.50	0.44
2:B:414[A]:ASP:OD1	2:B:416:MET:HB2	2.18	0.44
1:A:3:GLU:O	1:A:133:GLN:HG3	2.17	0.44
1:A:114:ILE:HD12	1:A:114:ILE:O	2.18	0.44
1:A:312:TYR:O	1:A:344:VAL:HG13	2.16	0.44
1:A:332:ILE:HD13	3:E:22:VAL:HG11	2.00	0.44
2:B:278:ARG:H	2:B:278:ARG:HG2	1.52	0.44
2:D:292:THR:CG2	2:D:335:VAL:HG21	2.44	0.44
2:D:3:GLU:O	2:D:133:GLN:HB3	2.17	0.44
2:D:220:THR:C	2:D:222:PRO:HD3	2.42	0.44
1:A:188:ILE:HG13	1:A:425:MET:HG3	2.00	0.44
4:F:299:GLU:N	4:F:300:PRO:HD2	2.33	0.44
2:B:88:ARG:HG2	2:B:88:ARG:NH1	2.33	0.43
2:B:396:THR:O	2:B:400:ARG:HB2	2.18	0.43
1:C:115:ILE:HG23	1:C:116:ASP:N	2.33	0.43
1:C:177:VAL:HG12	5:C:501:GTP:O2'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:340:GLN:OE1	4:F:340:GLN:HA	2.17	0.43
1:A:262:TYR:CE1	1:A:346:TRP:CH2	3.06	0.43
3:E:6:MET:HE3	3:E:6:MET:HB3	1.90	0.43
2:B:400:ARG:HA	2:B:400:ARG:NE	2.34	0.43
2:D:56:ALA:HB2	2:D:62:VAL:HG23	2.01	0.43
2:D:283:TYR:O	2:D:284:ARG:C	2.60	0.43
4:F:81:ILE:O	4:F:87:LEU:O	2.35	0.43
1:C:204:VAL:HG11	1:C:231:ILE:HG12	2.00	0.43
3:E:14:CYS:SG	3:E:15:THR:N	2.91	0.43
1:A:329:ASN:OD1	1:A:329:ASN:N	2.51	0.43
2:D:1:MET:O	2:D:131:CYS:HB3	2.18	0.43
2:D:68:VAL:HG13	2:D:149:MET:HE2	2.01	0.43
4:F:200:ASP:C	4:F:200:ASP:OD2	2.62	0.43
2:B:136:GLN:HA	2:B:167:ASN:O	2.19	0.43
2:D:118:VAL:O	2:D:122:VAL:HG23	2.19	0.43
2:B:188:THR:HA	2:B:425:MET:HE3	2.00	0.43
2:D:295:MET:HG2	2:D:377:PHE:HB2	2.01	0.43
1:C:119:LEU:HD11	1:C:156:ARG:CB	2.47	0.42
2:D:28:HIS:HA	2:D:45:GLN:HB3	2.00	0.42
2:D:135:PHE:HB2	2:D:166:MET:HE1	2.00	0.42
4:F:226:GLU:HB2	4:F:238:CYS:HB3	2.00	0.42
1:A:2:ARG:HB2	1:A:133:GLN:HG2	2.01	0.42
1:A:262:TYR:HE1	1:A:346:TRP:CH2	2.38	0.42
2:B:357:ASP:C	2:B:358:ILE:HD13	2.44	0.42
3:E:9:ILE:HG13	3:E:10:GLU:HG3	2.00	0.42
1:A:70:LEU:CD2	1:A:145:THR:HG23	2.49	0.42
1:A:153:LEU:HD12	1:A:153:LEU:O	2.19	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.42
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.89	0.42
2:B:113:GLU:H	2:B:113:GLU:HG2	1.47	0.42
2:B:288:VAL:N	2:B:289:PRO:CD	2.82	0.42
2:D:170:SER:O	2:D:172:MET:HE1	2.20	0.42
4:F:100:ILE:CD1	4:F:173:ILE:HD13	2.47	0.42
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.55	0.42
2:D:34:GLY:HA2	2:D:86:ILE:HD11	2.01	0.42
2:D:208:ALA:O	2:D:212:ILE:HG13	2.19	0.42
4:F:102:PRO:HA	4:F:173:ILE:HG22	2.00	0.42
1:A:255:PHE:O	1:A:259:LEU:HB2	2.19	0.42
2:B:68:VAL:HA	2:B:93:VAL:O	2.19	0.42
2:D:48:ARG:HG3	2:D:48:ARG:HH11	1.84	0.42
2:D:187:ALA:O	2:D:191:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:349:GLY:O	4:F:353:VAL:HG13	2.19	0.42
1:A:141:PHE:O	1:A:147:SER:HB3	2.19	0.42
3:E:76:ARG:NH1	3:E:76:ARG:HG2	2.35	0.42
1:A:7:ILE:HG23	1:A:66[B]:VAL:CG1	2.50	0.42
1:A:7:ILE:HD13	1:A:122:ILE:HD11	2.02	0.42
1:A:75:ILE:HD12	1:A:94:THR:HG22	2.01	0.42
1:A:313:MET:HG2	1:A:346:TRP:CH2	2.55	0.42
2:B:345:GLU:OE2	2:B:345:GLU:N	2.48	0.42
1:A:31:GLN:HB3	1:A:32:PRO:CD	2.48	0.41
2:B:268:PHE:HB3	2:B:378:ILE:HG22	2.01	0.41
1:C:192:HIS:ND1	1:C:424:ASP:OD2	2.53	0.41
1:C:306:ASP:OD1	1:C:308:ARG:HG2	2.20	0.41
4:F:37:PHE:CE1	4:F:40:MET:HB2	2.55	0.41
1:C:101:ASN:HD21	2:D:254:LYS:HE2	1.84	0.41
2:D:48:ARG:NH1	2:D:48:ARG:HG3	2.35	0.41
2:D:68:VAL:C	2:D:75:MET:HE1	2.45	0.41
2:D:202:TYR:CZ	2:D:238:VAL:CG1	3.03	0.41
2:B:231:VAL:O	2:B:235:MET:HG3	2.20	0.41
1:C:277:SER:HG	1:C:280:LYS:HG3	1.84	0.41
1:C:343:PHE:CB	1:C:349:THR:HG22	2.51	0.41
4:F:216:TYR:CD2	4:F:346:LEU:HD13	2.55	0.41
1:A:43:GLY:HA2	1:A:55:GLU:HB3	2.02	0.41
1:A:76:ASP:O	1:A:80[A]:THR:HG22	2.20	0.41
2:D:2:ARG:NE	2:D:2:ARG:HA	2.36	0.41
2:D:40:SER:O	2:D:45:GLN:HG3	2.20	0.41
2:D:54:ASN:OD1	2:D:64:ARG:NE	2.53	0.41
2:B:312:TYR:CD1	2:B:381:SER:HB2	2.55	0.41
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	2.03	0.41
2:D:282:GLN:HB2	2:D:283:TYR:H	1.58	0.41
1:A:119:LEU:HD12	1:A:156:ARG:NH2	2.35	0.41
1:C:177:VAL:O	1:C:177:VAL:CG1	2.69	0.41
4:F:242:ASN:ND2	10:F:401:ACP:O2B	2.51	0.41
1:A:49:PHE:C	1:A:49:PHE:CD2	2.99	0.41
2:D:377:PHE:CD1	2:D:377:PHE:C	2.98	0.41
3:E:90:ASN:O	3:E:94:ILE:HG13	2.21	0.41
1:C:46:ASP:OD1	1:C:46:ASP:N	2.53	0.41
2:D:156:LYS:HD3	2:D:156:LYS:HA	1.90	0.41
2:D:419:THR:HA	2:D:422:GLU:HB3	2.03	0.41
4:F:73:ARG:HB2	4:F:76[B]:SER:OG	2.21	0.41
1:A:47:ASP:O	1:A:50:ASN:HB2	2.21	0.40
2:D:282:GLN:O	2:D:284:ARG:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLY:O	1:A:14:VAL:HG23	2.21	0.40
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.56	0.40
2:B:145:THR:O	2:B:149:MET:HB3	2.21	0.40
2:B:320:ARG:O	2:B:373:MET:HA	2.21	0.40
2:B:56:ALA:HB3	2:B:60:LYS:HD3	2.03	0.40
2:B:114:LEU:HB3	2:B:149:MET:HE1	2.03	0.40
2:B:192:HIS:CE1	2:B:424[A]:ASN:OD1	2.75	0.40
1:C:335:ILE:HG22	1:C:341:ILE:HD11	2.04	0.40
2:D:412:GLY:O	3:E:136:ASN:ND2	2.50	0.40
4:F:149:ALA:CB	4:F:182:ILE:HG12	2.51	0.40
1:C:195:LEU:HD12	1:C:195:LEU:HA	1.78	0.40
2:D:86:ILE:HD12	2:D:86:ILE:HA	1.81	0.40
2:D:113:GLU:OE2	2:D:113:GLU:CA	2.68	0.40
2:D:115:VAL:O	2:D:119:LEU:HG	2.21	0.40
2:D:136:GLN:O	2:D:136:GLN:HG3	2.21	0.40
4:F:147:TRP:HB2	4:F:169:LEU:HD11	2.03	0.40
2:D:32:PRO:HA	2:D:83:PHE:CD1	2.56	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	447/440 (102%)	439 (98%)	8 (2%)	0	100	100
1	C	448/440 (102%)	433 (97%)	14 (3%)	1 (0%)	43	68
2	B	437/431 (101%)	421 (96%)	13 (3%)	3 (1%)	18	41
2	D	433/431 (100%)	403 (93%)	28 (6%)	2 (0%)	24	48
3	E	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
4	F	309/320 (97%)	294 (95%)	14 (4%)	1 (0%)	36	60
All	All	2193/2183 (100%)	2107 (96%)	79 (4%)	7 (0%)	36	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	283	HIS
2	D	276	THR
2	B	278	ARG
2	B	281	GLN
2	B	304	ALA
2	D	282	GLN
4	F	92	THR

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	GDP	D	501	6	29,30,30	0.51	0	45,47,47	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GDP	B	501	6	29,30,30	0.54	0	45,47,47	0.43	0
5	GTP	A	501	6	33,34,34	0.58	0	50,54,54	0.49	0
9	V1O	B	503	-	25,25,25	0.35	0	32,33,33	1.88	2 (6%)
5	GTP	C	501	-	33,34,34	0.60	0	50,54,54	0.48	0
10	ACP	F	401	-	31,33,33	0.76	1 (3%)	47,52,52	0.61	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	D	501	6	-	5/16/32/32	0/3/3/3
8	GDP	B	501	6	-	4/16/32/32	0/3/3/3
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
9	V1O	B	503	-	-	12/14/14/14	0/2/2/2
5	GTP	C	501	-	-	5/22/38/38	0/3/3/3
10	ACP	F	401	-	-	5/19/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	401	ACP	PB-O2B	-2.41	1.50	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	V1O	C1-C2-C15	-7.37	111.03	121.44
9	B	503	V1O	C1-C2-C3	6.76	130.99	121.44
10	F	401	ACP	O1G-PG-C3B	-2.36	106.22	111.37

There are no chirality outliers.

All (36) 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	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A

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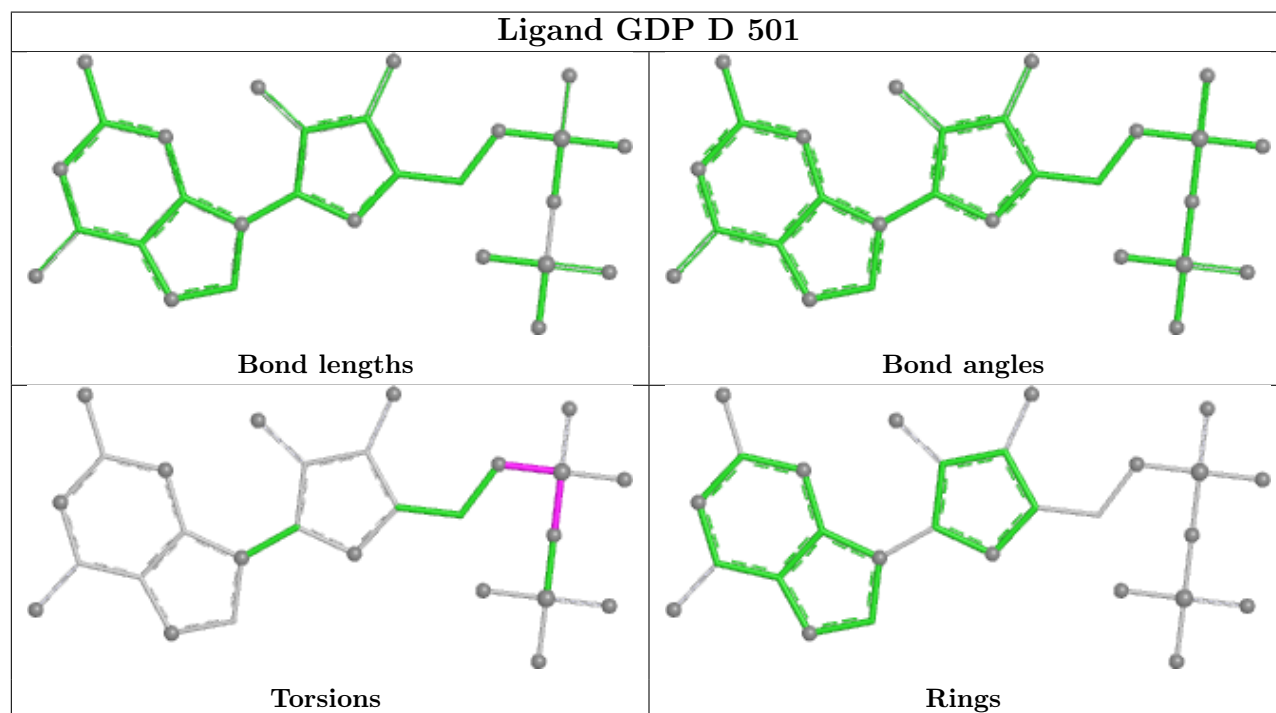
Mol	Chain	Res	Type	Atoms
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
9	B	503	V1O	BR-C-C1-C2
10	F	401	ACP	PG-C3B-PB-O1B
10	F	401	ACP	PG-C3B-PB-O2B
10	F	401	ACP	PG-C3B-PB-O3A
9	B	503	V1O	C6-N-N1-C7
9	B	503	V1O	C2-C3-O-C4
9	B	503	V1O	C14-C6-N-N1
10	F	401	ACP	O4'-C4'-C5'-O5'
9	B	503	V1O	C13-C7-N1-N
9	B	503	V1O	C5-C6-N-N1
9	B	503	V1O	C8-C7-N1-N
9	B	503	V1O	C14-C15-O3-C16
9	B	503	V1O	C12-C10-O2-C11
9	B	503	V1O	C5-C3-O-C4
9	B	503	V1O	C2-C15-O3-C16
10	F	401	ACP	C3'-C4'-C5'-O5'
9	B	503	V1O	C9-C10-O2-C11
8	D	501	GDP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O2A
8	B	501	GDP	PB-O3A-PA-O2A
8	D	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O1A

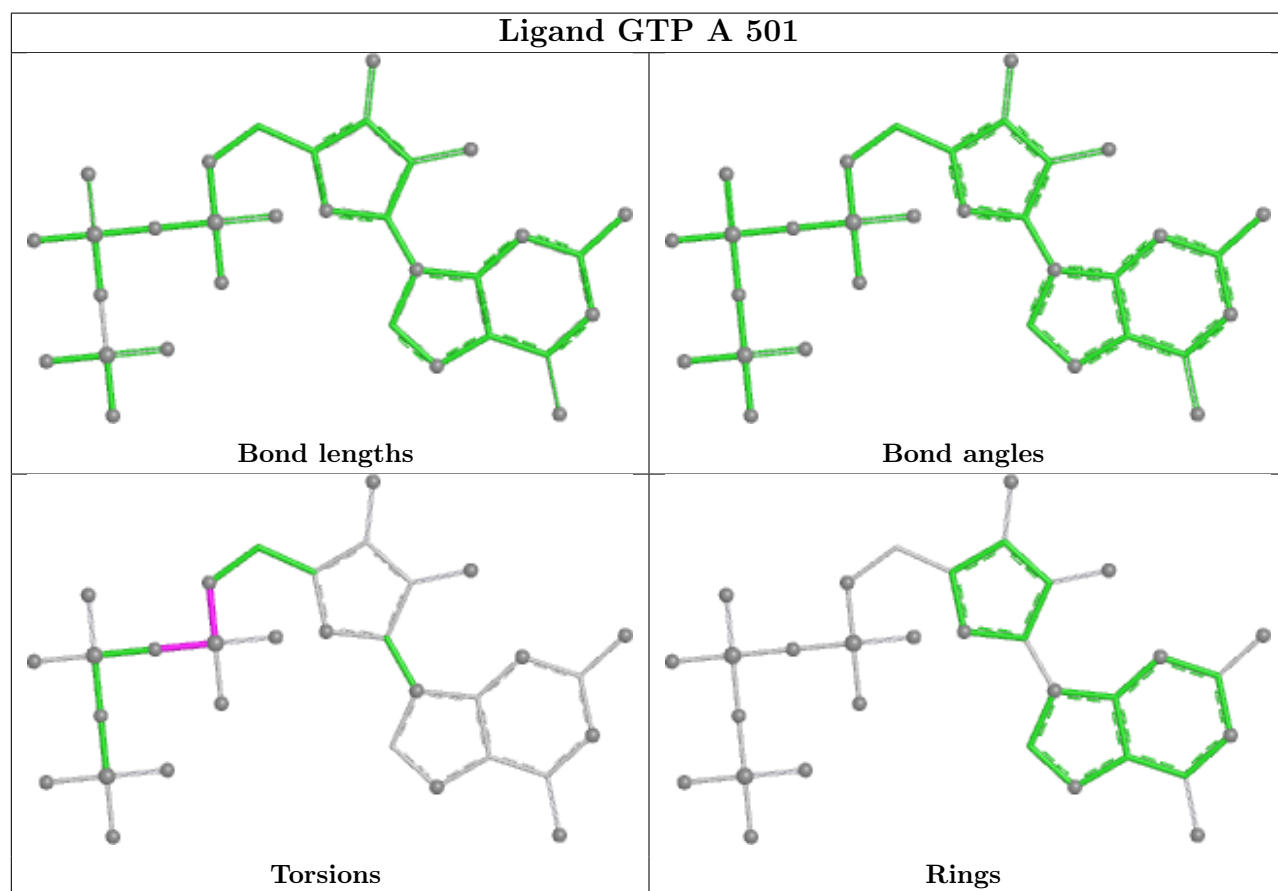
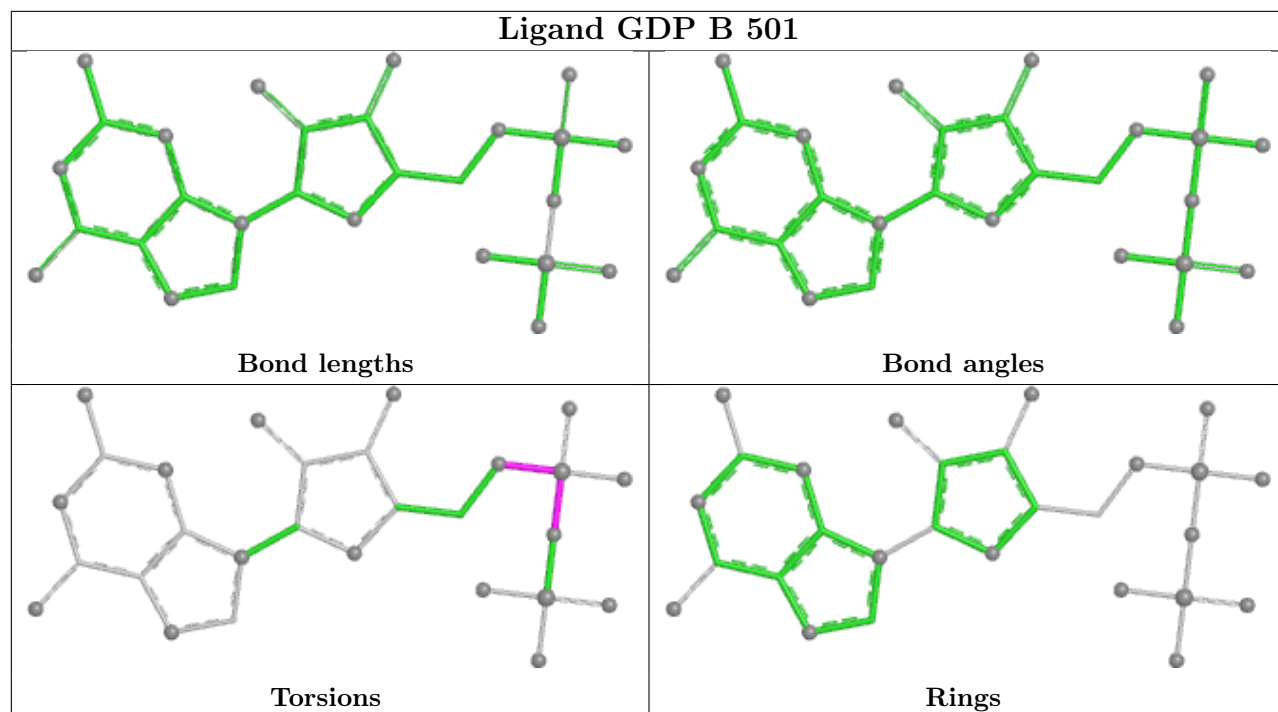
There are no ring outliers.

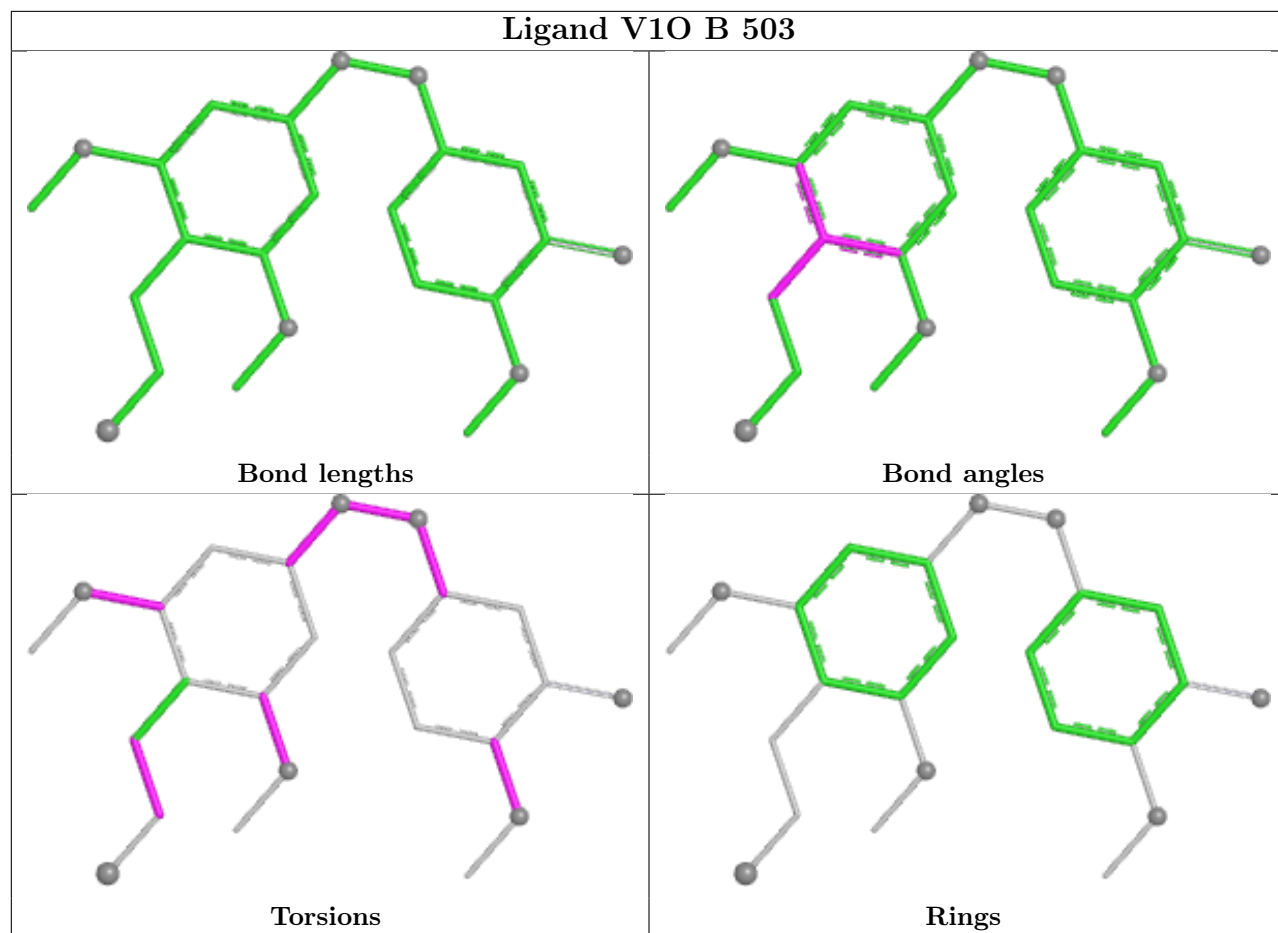
5 monomers are involved in 15 short contacts:

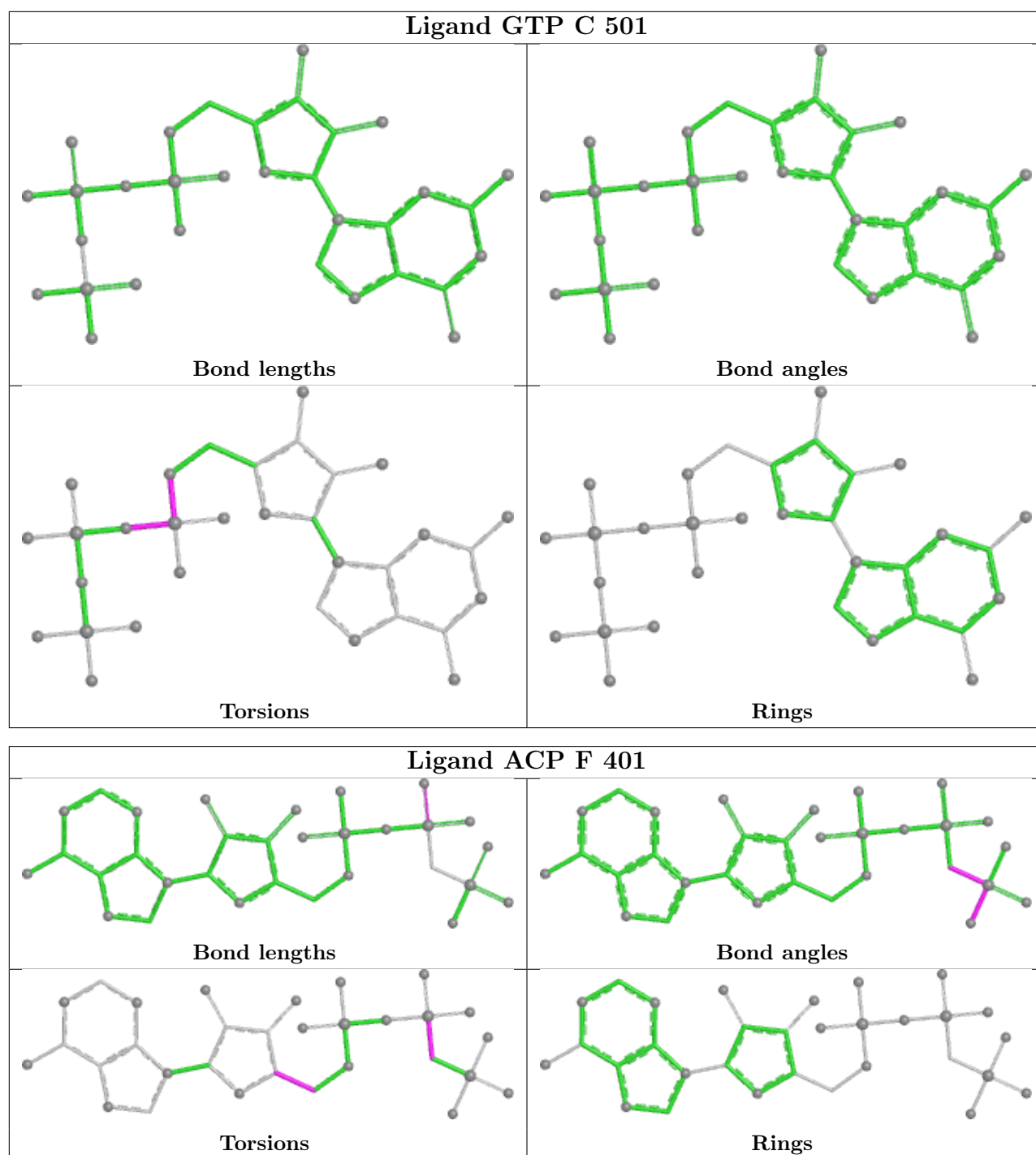
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	1	0
5	A	501	GTP	1	0
9	B	503	V1O	9	0
5	C	501	GTP	1	0
10	F	401	ACP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	F	6
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	31.51
1	F	362:ALA	C	373:SER	N	19.14
1	F	102:PRO	C	125:THR	N	12.94
1	F	151:SER	C	162:ILE	N	12.03
1	F	136:ASN	C	144:GLY	N	10.25
1	F	173:ILE	C	179:VAL	N	8.39
1	F	231:ALA	C	235:ASP	N	6.80

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/440 (99%)	-0.21	5 (1%) 78 76	34, 76, 125, 210	10 (2%)
1	C	440/440 (100%)	-0.37	1 (0%) 91 90	27, 61, 99, 147	9 (2%)
2	B	428/431 (99%)	-0.25	3 (0%) 84 83	28, 70, 121, 178	13 (3%)
2	D	431/431 (100%)	-0.06	10 (2%) 61 58	37, 89, 142, 218	6 (1%)
3	E	121/121 (100%)	-0.10	2 (1%) 69 67	34, 88, 145, 192	2 (1%)
4	F	320/320 (100%)	0.01	4 (1%) 75 73	41, 103, 179, 247	4 (1%)
All	All	2179/2183 (99%)	-0.18	25 (1%) 78 76	27, 79, 144, 247	44 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	248	LEU	4.6
2	B	318	ILE	3.8
1	A	282	TYR	3.4
4	F	362	ALA	3.3
1	A	232	SER	3.2
2	D	280	SER	3.1
2	D	219	LEU	3.0
2	D	282	GLN	2.8
2	B	279	GLY	2.8
2	D	279	GLY	2.6
1	A	285	GLN	2.5
2	D	424	ASN	2.5
3	E	133	VAL	2.5
3	E	28	SER	2.4
1	A	438	ASP	2.4
2	D	283	TYR	2.3
4	F	91	CYS	2.3
4	F	242	ASN	2.3
2	D	147	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	85	GLN	2.2
1	C	440	VAL	2.2
4	F	134	ALA	2.1
2	D	285	ALA	2.1
2	D	286	LEU	2.1
1	A	439	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

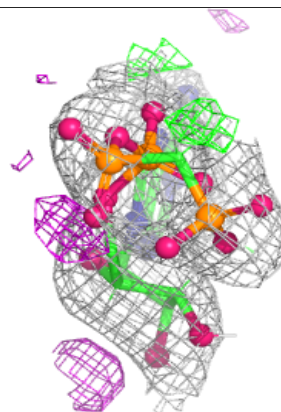
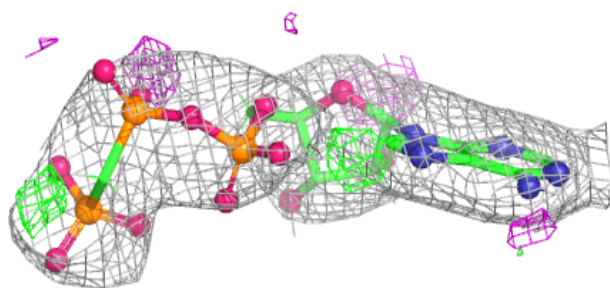
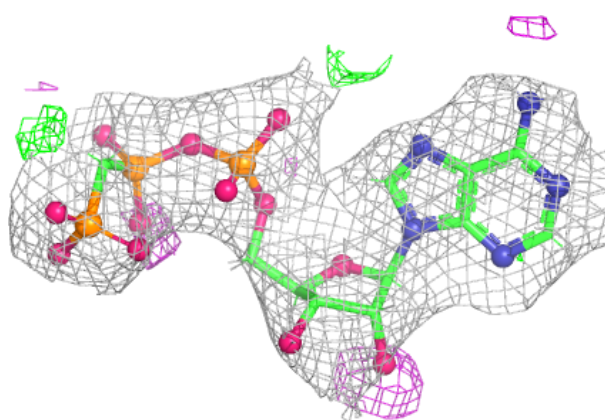
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	502	1/1	0.75	0.11	98,98,98,98	0
10	ACP	F	401	31/31	0.79	0.12	98,135,159,180	0
9	V1O	B	503	24/24	0.86	0.17	72,90,109,125	0
6	MG	A	502	1/1	0.92	0.21	71,71,71,71	0
8	GDP	D	501	28/28	0.93	0.10	71,88,104,121	0
5	GTP	A	501	32/32	0.95	0.08	46,58,67,79	0
8	GDP	B	501	28/28	0.96	0.09	42,56,67,76	0
5	GTP	C	501	32/32	0.97	0.06	45,52,62,71	0
7	CA	C	503	1/1	0.97	0.04	94,94,94,94	0
6	MG	B	502	1/1	0.97	0.24	65,65,65,65	0
7	CA	A	503	1/1	0.99	0.03	109,109,109,109	0
6	MG	C	502	1/1	0.99	0.08	61,61,61,61	0

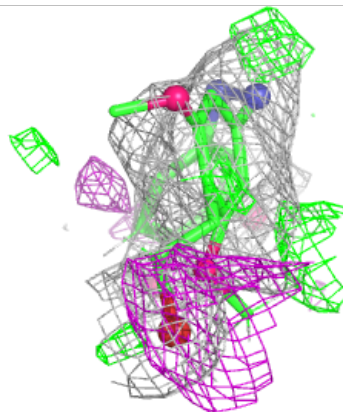
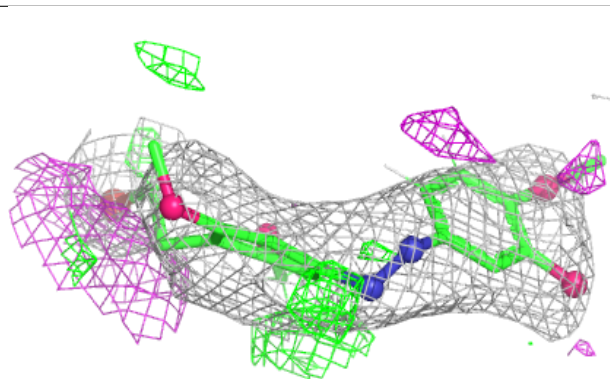
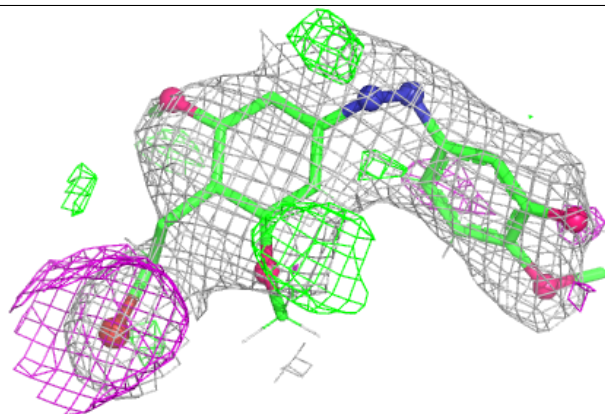
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

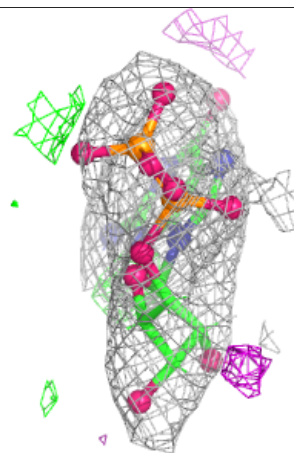
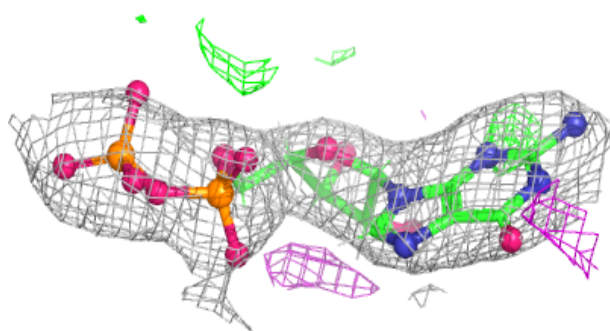
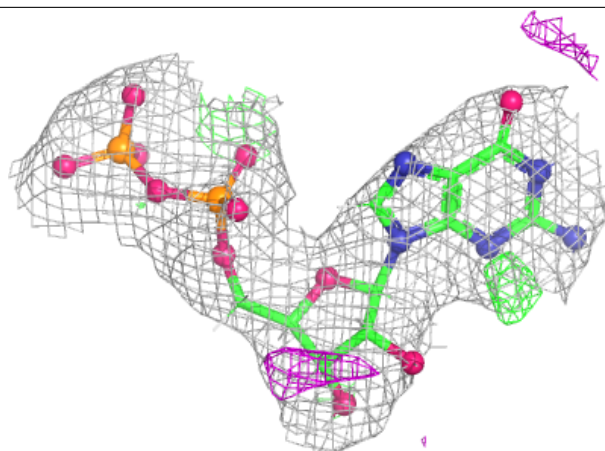
**Electron density around V1O B 503:**

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

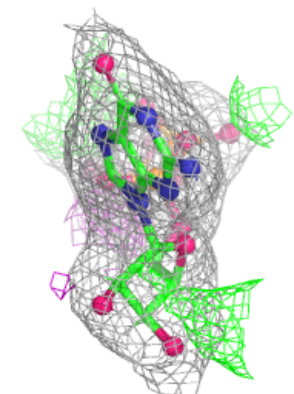
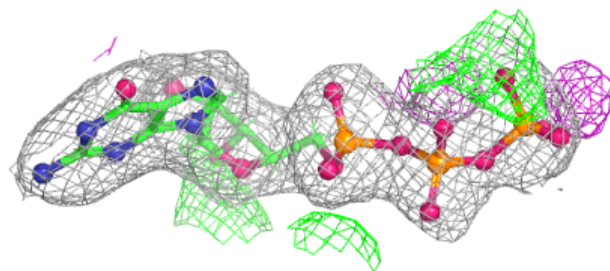
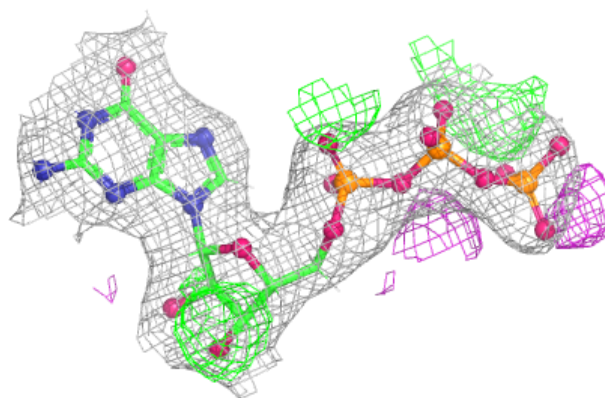


Electron density around GDP D 501:

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

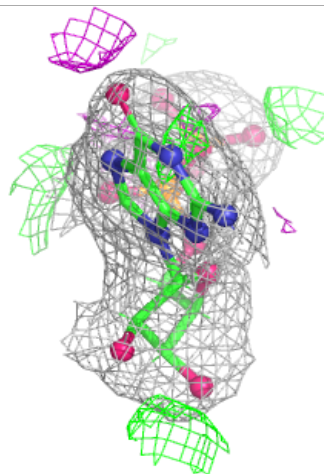
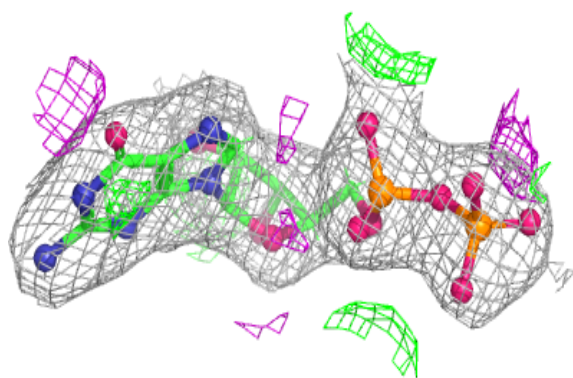
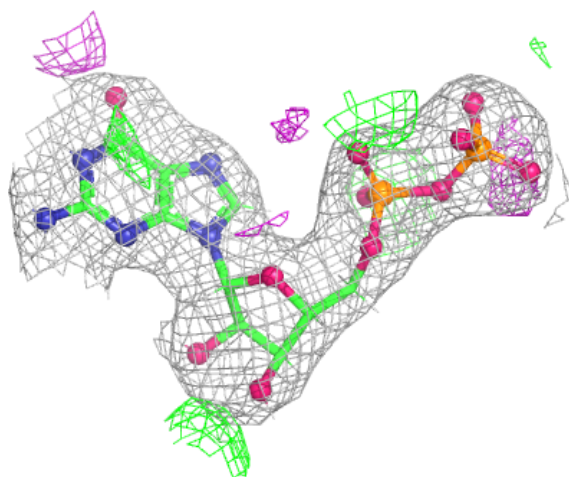
**Electron density around GTP A 501:**

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



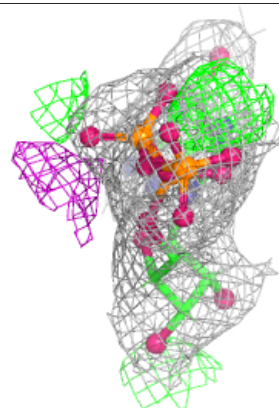
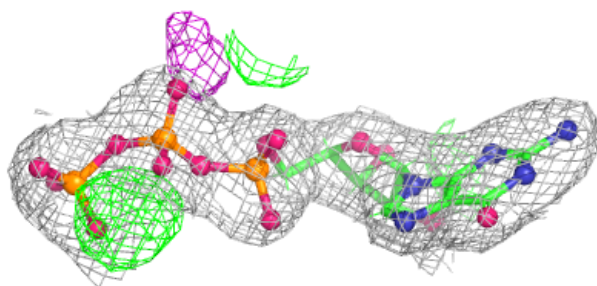
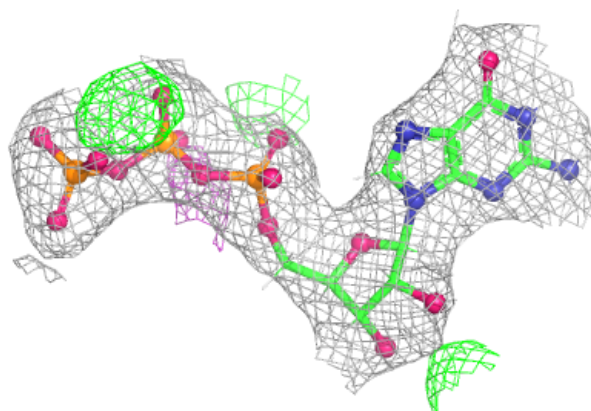
Electron density around GDP B 501:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.