



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:14 AM UTC

PDB ID : 3UT5 / pdb_00003ut5
Title : Tubulin-Colchicine-Ustiloxin: Stathmin-like domain complex
Authors : Ranaivoson, F.M.; Gigant, B.; Knossow, M.
Deposited on : 2011-11-25
Resolution : 2.73 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

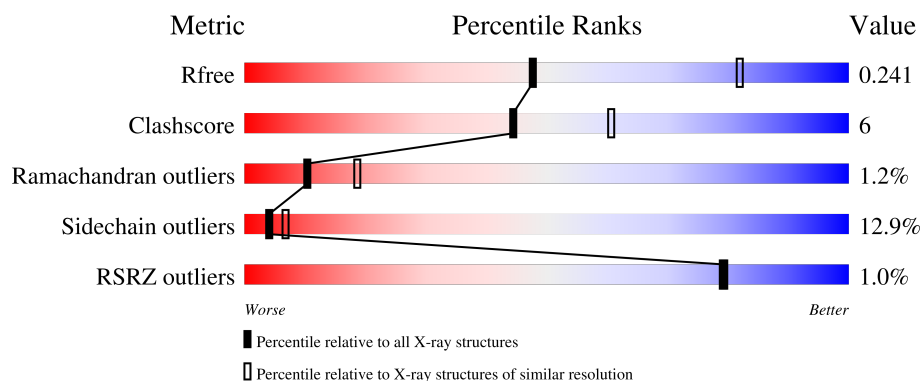
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
2	B	445	
2	D	445	
3	E	142	

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Mol	Chain	Length	Quality of chain
4	F	4	

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
4	0E5	F	3	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15107 atoms, of which 0 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	1	0
			3399	2153	577	647	22			
1	C	432	Total	C	N	O	S	0	4	0
			3404	2158	575	648	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
A	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
C	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
C	340	SER	THR	SEE REMARK 999	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	3	0
			3417	2141	584	665	27			
2	D	432	Total	C	N	O	S	0	5	0
			3433	2153	584	670	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
B	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	375	SER	ALA	SEE REMARK 999	UNP D0VWY9
D	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
D	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	375	SER	ALA	SEE REMARK 999	UNP D0VWY9

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	132	Total	C	N	O	S	0	1	0
			1077	666	195	212	4			

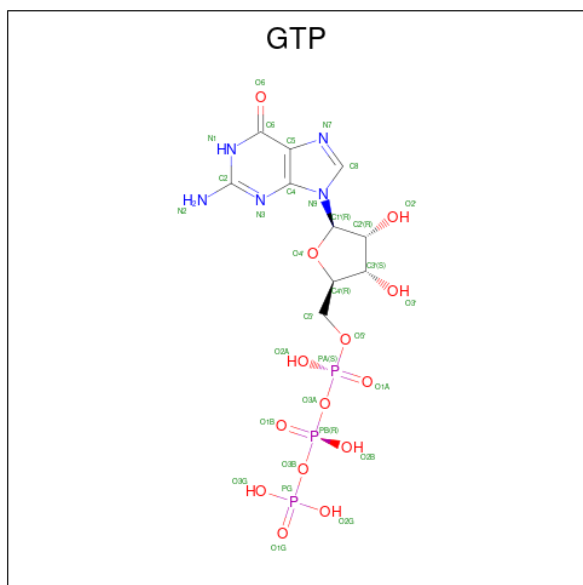
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is a protein called Vinca tetrapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	4	Total	C	N	O	0	0	0
			35	23	4	8			

- 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).

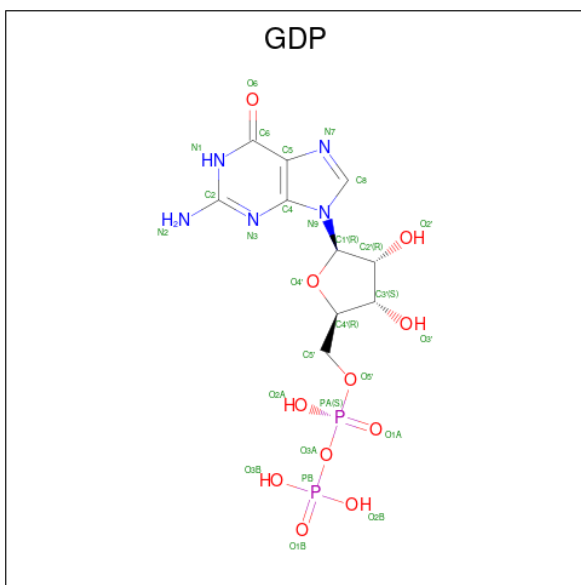
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



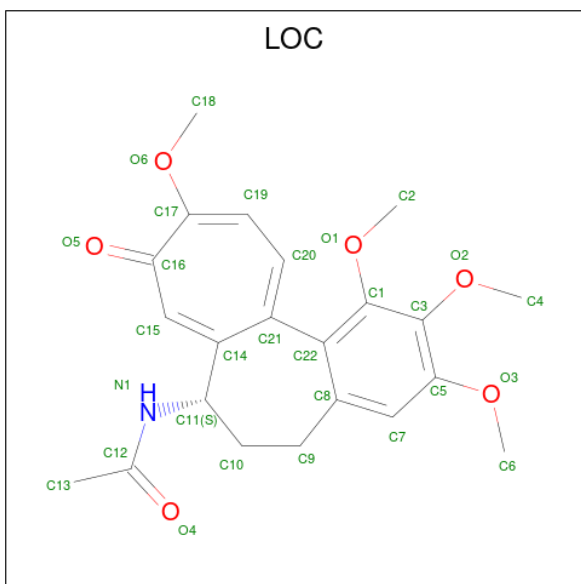
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		

- 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 N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]ethanamide (CCD ID: LOC) (formula: C₂₂H₂₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			29	22	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	1	Total	C	N	O	0	0
			29	22	1	6		

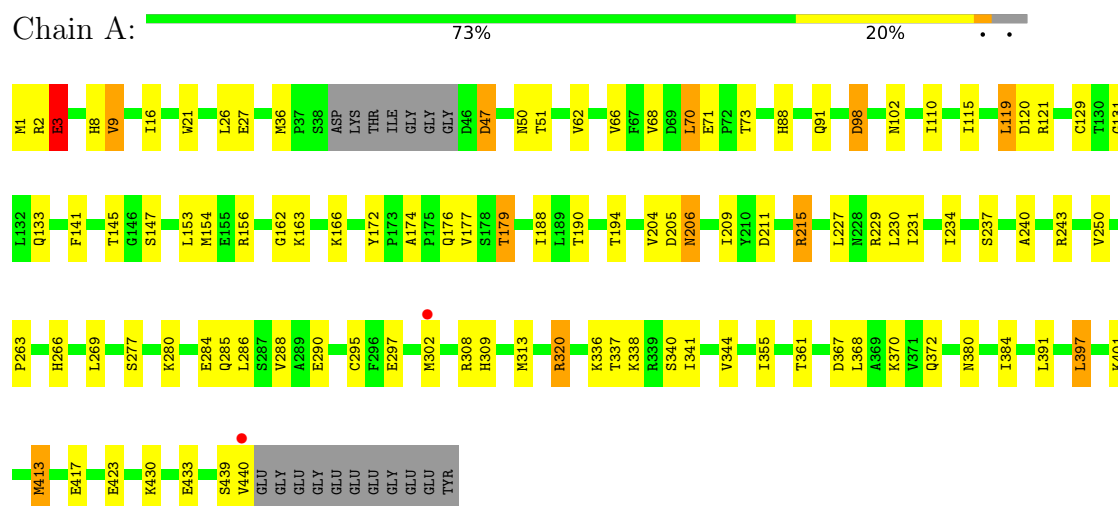
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	27	Total	O	0	0
			27	27		
10	B	28	Total	O	0	0
			28	28		
10	C	43	Total	O	0	0
			43	43		
10	D	36	Total	O	0	0
			36	36		
10	E	3	Total	O	0	0
			3	3		

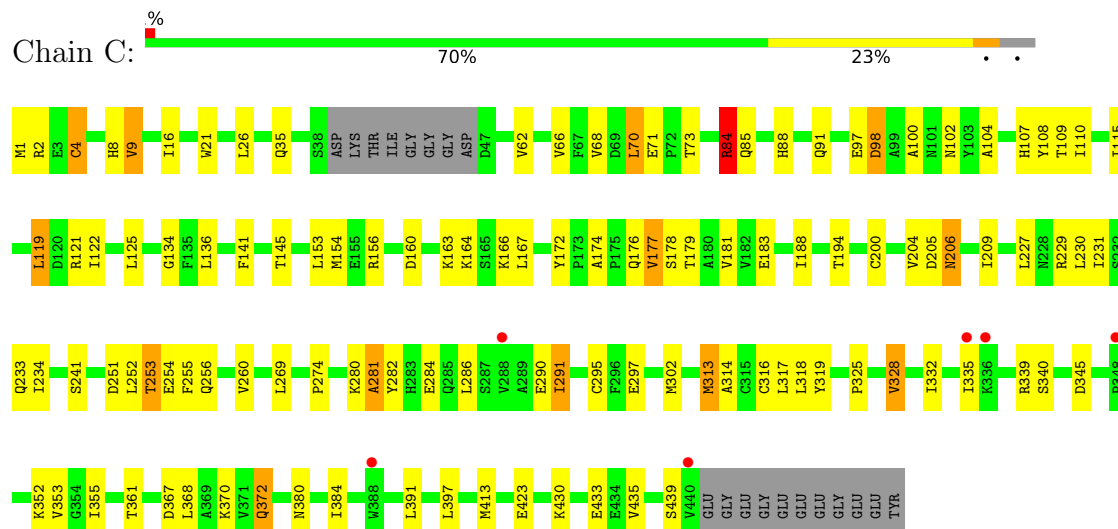
3 Residue-property plots [i](#)

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

• Molecule 1: Tubulin alpha chain

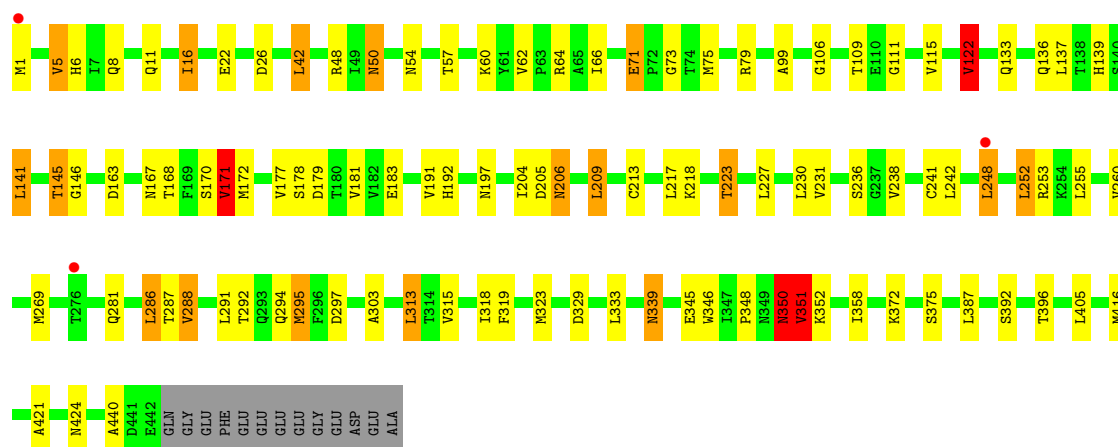


• Molecule 1: Tubulin alpha chain

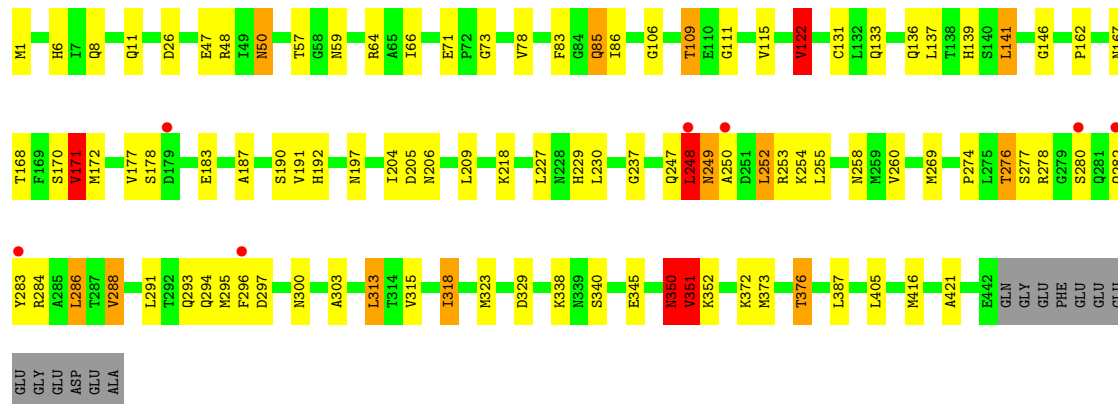
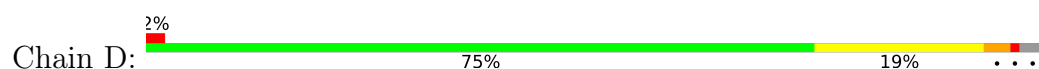


• Molecule 2: Tubulin beta chain

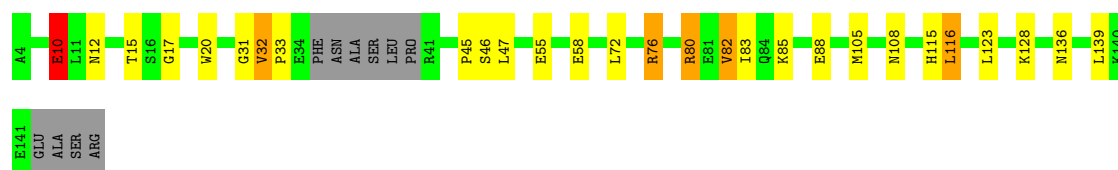




• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4



• Molecule 4: Vinca tetrapeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.81Å 128.87Å 254.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.26 – 2.73 38.26 – 2.73	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.26-2.73) 97.6 (38.26-2.73)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.72Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.184 , 0.222 0.201 , 0.241	Depositor DCC
R_{free} test set	2872 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15107	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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, SO4, GDP, MG, 0EA, 0E5, LOC

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	0.76	0/3479	1.39	13/4723 (0.3%)
1	C	0.77	0/3491	1.41	17/4741 (0.4%)
2	B	0.74	0/3503	1.39	24/4744 (0.5%)
2	D	0.74	1/3516 (0.0%)	1.36	17/4762 (0.4%)
3	E	0.82	0/1092	1.54	2/1455 (0.1%)
4	F	1.24	0/10	0.43	0/9
All	All	0.76	1/15091 (0.0%)	1.40	73/20434 (0.4%)

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
4	F	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	288	VAL	CA-CB	5.70	1.56	1.54

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	288	VAL	N-CA-CB	9.88	116.72	110.50
2	D	288	VAL	N-CA-CB	8.30	116.08	110.52
2	B	181	VAL	N-CA-C	8.03	118.81	110.62
1	C	281	ALA	CA-C-N	7.21	130.91	120.38
1	C	281	ALA	C-N-CA	7.21	130.91	120.38
1	C	84	ARG	N-CA-C	-7.06	100.54	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	171	VAL	N-CA-CB	6.80	118.75	111.00
2	B	297	ASP	CA-CB-CG	6.74	119.34	112.60
2	D	171	VAL	N-CA-CB	6.74	118.69	111.00
2	B	5	VAL	N-CA-CB	6.28	118.55	111.21
2	B	115	VAL	N-CA-C	6.20	116.86	110.36
1	C	345	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	115	ILE	N-CA-C	6.05	116.71	110.36
2	D	115	VAL	N-CA-C	6.04	116.70	110.36
2	D	248	LEU	CA-C-N	5.99	132.98	121.54
2	D	248	LEU	C-N-CA	5.99	132.98	121.54
1	C	178	SER	N-CA-C	5.95	118.45	111.02
1	C	115	ILE	N-CA-C	5.89	116.55	110.36
1	C	284	GLU	N-CA-C	5.82	119.20	111.75
1	A	433	GLU	CA-C-N	5.82	128.35	120.38
1	A	433	GLU	C-N-CA	5.82	128.35	120.38
2	B	73	GLY	CA-C-N	5.78	128.02	120.28
2	B	73	GLY	C-N-CA	5.78	128.02	120.28
2	B	339	ASN	CA-CB-CG	5.77	118.37	112.60
2	B	350	ASN	CA-CB-CG	5.74	118.34	112.60
2	B	351	VAL	CB-CA-C	5.69	118.39	110.99
1	C	134	GLY	N-CA-C	5.64	117.78	110.45
1	A	120	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	3	GLU	N-CA-C	5.57	118.52	110.28
3	E	82	VAL	N-CA-CB	5.55	118.91	110.58
2	D	350	ASN	CA-CB-CG	5.50	118.10	112.60
1	C	62	VAL	N-CA-C	5.45	113.88	107.77
1	C	433	GLU	CA-C-N	5.45	128.33	120.38
1	C	433	GLU	C-N-CA	5.45	128.33	120.38
2	B	248	LEU	CA-C-N	5.42	130.11	122.46
2	B	248	LEU	C-N-CA	5.42	130.11	122.46
2	D	313	LEU	N-CA-C	-5.42	104.25	111.24
2	B	236	SER	CA-C-N	5.40	125.97	119.98
2	B	236	SER	C-N-CA	5.40	125.97	119.98
2	D	205	ASP	CA-CB-CG	5.40	118.00	112.60
2	D	191	VAL	CA-C-N	5.38	127.81	120.54
2	D	191	VAL	C-N-CA	5.38	127.81	120.54
1	C	160	ASP	CA-CB-CG	5.36	117.96	112.60
2	D	351	VAL	CB-CA-C	5.36	117.96	110.99
1	C	141	PHE	CA-CB-CG	5.36	119.16	113.80
3	E	31	GLY	N-CA-C	5.36	118.95	111.19
1	A	141	PHE	CA-CB-CG	5.30	119.10	113.80
1	A	62	VAL	N-CA-C	5.28	113.69	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	205	ASP	CA-CB-CG	5.28	117.88	112.60
2	D	197	ASN	N-CA-C	5.27	120.57	113.72
1	C	313	MET	CA-C-N	5.26	131.59	121.54
1	C	313	MET	C-N-CA	5.26	131.59	121.54
1	C	102	ASN	CA-CB-CG	5.26	117.86	112.60
2	B	197	ASN	N-CA-C	5.25	120.55	113.72
2	B	62	VAL	N-CA-C	5.24	113.71	107.73
1	A	98	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	240	ALA	CA-C-N	5.15	128.13	120.31
1	A	240	ALA	C-N-CA	5.15	128.13	120.31
2	D	109	THR	CA-C-N	5.07	127.33	120.38
2	D	109	THR	C-N-CA	5.07	127.33	120.38
2	D	122	VAL	N-CA-CB	5.06	117.43	110.54
2	B	191	VAL	CA-C-N	5.05	127.36	120.54
2	B	191	VAL	C-N-CA	5.05	127.36	120.54
2	B	313	LEU	N-CA-C	-5.05	104.72	111.24
2	B	22	GLU	CA-C-N	5.05	127.02	120.70
2	B	22	GLU	C-N-CA	5.05	127.02	120.70
2	B	122	VAL	N-CA-CB	5.05	117.41	110.54
2	D	78	VAL	CA-C-N	5.04	127.28	120.38
2	D	78	VAL	C-N-CA	5.04	127.28	120.38
1	A	237	SER	CA-C-N	5.02	127.34	120.46
1	A	237	SER	C-N-CA	5.02	127.34	120.46
1	A	102	ASN	CA-CB-CG	5.01	117.61	112.60
1	C	98	ASP	CA-CB-CG	5.00	117.60	112.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	3	0E5	C3

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3399	0	3312	35	0
1	C	3404	0	3311	41	0
2	B	3417	0	3283	48	0
2	D	3433	0	3301	53	0
3	E	1077	0	1068	7	0
4	F	35	0	24	1	0
5	A	32	0	12	1	0
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	10	0	0	0	0
7	B	5	0	0	0	0
7	D	10	0	0	0	0
8	B	28	0	12	3	0
8	D	28	0	12	2	0
9	B	29	0	25	4	0
9	D	29	0	25	3	0
10	A	27	0	0	0	0
10	B	28	0	0	1	0
10	C	43	0	0	0	0
10	D	36	0	0	1	0
10	E	3	0	0	0	0
All	All	15107	0	14397	175	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 6.

All (175) 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:206:ASN:HD21	8:B:501:GDP:HN22	1.24	0.86
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.59	0.85
1:C:206:ASN:HD21	5:C:600:GTP:HN22	1.24	0.83
1:A:206:ASN:HD21	5:A:501:GTP:HN22	1.26	0.82
2:D:206:ASN:HD21	8:D:501:GDP:HN22	1.25	0.82
2:D:6:HIS:HE1	2:D:8:GLN:HG3	1.51	0.76
2:D:237:GLY:CA	2:D:376:THR:HG21	2.17	0.74
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.37	0.72
2:D:318:ILE:HG23	2:D:376:THR:HG23	1.71	0.71
2:B:350:ASN:HD22	2:B:350:ASN:H	1.40	0.68
2:D:6:HIS:CE1	2:D:8:GLN:HG3	2.28	0.68
2:D:350:ASN:H	2:D:350:ASN:HD22	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:ILE:HD11	9:B:502:LOC:H4	1.76	0.68
2:D:172:MET:HG3	2:D:387:LEU:HD21	1.75	0.68
2:D:50:ASN:O	2:D:64:ARG:NH2	2.27	0.68
2:B:50:ASN:O	2:B:64:ARG:NH2	2.21	0.68
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.76	0.68
2:D:141:LEU:HD21	2:D:170:SER:HB3	1.77	0.66
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.76	0.66
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.78	0.66
1:C:84:ARG:O	1:C:85:GLN:HB2	1.96	0.66
2:B:141:LEU:HD21	2:B:170:SER:HB3	1.78	0.65
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.79	0.64
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.79	0.64
2:B:71[B]:GLU:HG2	1:C:2:ARG:HH22	1.61	0.63
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.80	0.63
2:B:295:MET:HE3	2:B:375:SER:HB2	1.81	0.62
2:D:133:GLN:HE21	2:D:252:LEU:H	1.45	0.62
2:D:209:LEU:HB3	2:D:227:LEU:HG	1.83	0.60
2:D:352:LYS:HB2	9:D:502:LOC:H18B	1.84	0.59
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.83	0.59
2:D:66:ILE:HD13	2:D:122:VAL:HG12	1.84	0.59
2:D:83:PHE:O	2:D:86:ILE:HG22	2.03	0.59
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.86	0.57
1:A:1:MET:HE3	1:A:51:THR:HG23	1.86	0.57
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.87	0.57
1:C:70:LEU:HG	1:C:110:ILE:HG22	1.87	0.57
3:E:32:VAL:HB	3:E:33:PRO:HD3	1.86	0.57
1:C:313:MET:HE3	1:C:380:ASN:HD22	1.70	0.56
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.24	0.56
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.71	0.56
1:A:313:MET:HE3	1:A:380:ASN:HD22	1.69	0.56
1:A:3:GLU:HG3	1:A:129:CYS:SG	2.46	0.56
2:D:278:ARG:C	2:D:280:SER:H	2.14	0.56
1:A:70:LEU:HG	1:A:110:ILE:HG22	1.88	0.56
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.88	0.55
2:D:229:HIS:NE2	2:D:276:THR:HG22	2.21	0.55
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.53	0.55
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.88	0.55
3:E:10:GLU:HA	3:E:20:TRP:HB2	1.89	0.55
2:B:133:GLN:HE21	2:B:252:LEU:H	1.55	0.55
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.71	0.55
2:B:136:GLN:HA	2:B:167:ASN:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:TYR:HB2	1:C:355:ILE:HG12	1.89	0.54
1:A:285:GLN:HE22	1:A:372:GLN:H	1.57	0.53
1:A:397:LEU:HD23	2:B:348:PRO:HG3	1.90	0.53
2:D:136:GLN:HA	2:D:167:ASN:O	2.08	0.53
2:B:315:VAL:HB	2:B:351:VAL:HB	1.92	0.52
2:B:106:GLY:O	2:B:111:GLY:HA3	2.09	0.52
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.58	0.52
2:B:392:SER:O	2:B:396:THR:HG23	2.09	0.52
2:D:133:GLN:NE2	2:D:252:LEU:H	2.08	0.52
1:A:308:ARG:HH21	1:A:309:HIS:HD2	1.57	0.52
2:B:424:ASN:HB2	10:B:619:HOH:O	2.08	0.52
1:C:97:GLU:HB2	2:D:1:MET:HG2	1.91	0.52
2:B:209:LEU:HB3	2:B:227:LEU:HG	1.92	0.51
2:D:248:LEU:HD13	2:D:249:ASN:H	1.75	0.51
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.24	0.51
1:C:8:HIS:HE1	1:C:21:TRP:HE1	1.57	0.51
2:D:323:MET:HE2	2:D:373:MET:HG2	1.93	0.51
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.43	0.51
1:C:241:SER:HB2	1:C:251:ASP:HA	1.93	0.50
1:A:211:ASP:O	1:A:215:ARG:HD2	2.11	0.50
2:B:99:ALA:HB2	2:B:145:THR:HG22	1.93	0.50
2:B:286:LEU:HD21	2:B:291:LEU:HD13	1.94	0.50
2:D:315:VAL:HB	2:D:351:VAL:HB	1.92	0.50
2:D:85:GLN:H	2:D:85:GLN:CD	2.19	0.50
1:A:263:PRO:O	1:A:266:HIS:HD2	1.94	0.50
2:B:171:VAL:HA	2:B:204:ILE:O	2.11	0.50
2:B:42:LEU:HD12	2:B:358:ILE:HD11	1.94	0.50
2:D:171:VAL:HA	2:D:204:ILE:O	2.12	0.49
1:C:325:PRO:HA	1:C:328:VAL:CG2	2.42	0.49
1:C:100:ALA:HA	2:D:254:LYS:HG2	1.93	0.49
3:E:115:HIS:HD2	3:E:116:LEU:HD22	1.77	0.49
2:D:350:ASN:H	2:D:350:ASN:ND2	2.09	0.49
2:B:223:THR:HA	4:F:3:OE5:H5	1.95	0.49
1:A:154:MET:HG3	1:A:194:THR:HG23	1.96	0.48
2:D:106:GLY:O	2:D:111:GLY:HA3	2.14	0.48
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.95	0.48
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.95	0.47
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.96	0.47
1:A:174:ALA:HB1	1:A:176:GLN:HE21	1.80	0.47
2:B:318:ILE:HD11	9:B:502:LOC:C4	2.45	0.47
1:C:174:ALA:HB1	1:C:176:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:HB3	1:A:133[A]:GLN:NE2	2.30	0.47
1:C:154:MET:HG3	1:C:194:THR:HG23	1.97	0.47
2:B:141:LEU:HD23	2:B:172:MET:SD	2.56	0.46
1:A:355:ILE:O	3:E:17:GLY:HA2	2.15	0.46
2:B:183:GLU:OE2	8:B:501:GDP:H3'	2.16	0.46
2:D:183:GLU:OE2	8:D:501:GDP:H3'	2.16	0.46
1:A:1:MET:HE2	1:A:50:ASN:HB2	1.98	0.46
1:C:179:THR:HG22	1:C:183:GLU:OE2	2.15	0.46
2:B:163:ASP:O	2:B:253[B]:ARG:NH2	2.48	0.45
1:A:9:VAL:HG23	1:A:145:THR:HG22	1.98	0.45
1:C:181:VAL:HG22	2:D:258:ASN:HD22	1.80	0.45
2:B:16:ILE:HG12	2:B:231:VAL:HG11	1.98	0.45
2:D:141:LEU:HD23	2:D:172:MET:SD	2.56	0.45
2:B:346:TRP:HB3	2:B:440:ALA:HB2	1.99	0.45
2:D:253:ARG:NH2	10:D:633:HOH:O	2.49	0.45
2:B:99:ALA:CB	2:B:145:THR:HG22	2.46	0.45
2:D:139:HIS:HD2	2:D:146:GLY:O	2.00	0.45
2:D:350:ASN:HD22	2:D:350:ASN:N	2.10	0.45
2:B:350:ASN:H	2:B:350:ASN:ND2	2.09	0.44
1:C:9:VAL:HG23	1:C:145:THR:HG22	1.99	0.44
1:C:286:LEU:HD21	1:C:291:ILE:HG23	1.99	0.44
2:B:352:LYS:HE3	9:B:502:LOC:O5	2.18	0.44
1:C:8:HIS:CE1	1:C:21:TRP:HE1	2.35	0.44
1:A:147:SER:HB2	1:A:190:THR:HB	1.99	0.44
1:A:230:LEU:O	1:A:234:ILE:HD12	2.17	0.44
1:C:230:LEU:O	1:C:234:ILE:HD12	2.18	0.44
2:D:294:GLN:HA	2:D:297:ASP:HB2	2.00	0.44
1:C:84:ARG:O	1:C:85:GLN:CB	2.66	0.44
2:D:162:PRO:HB2	3:E:116:LEU:HD12	2.00	0.43
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.58	0.43
1:A:2:ARG:HB3	1:A:133[A]:GLN:HE21	1.83	0.43
2:D:133:GLN:HE21	2:D:252:LEU:HB2	1.83	0.43
3:E:76:ARG:HG3	3:E:80:ARG:HH21	1.83	0.43
2:B:139:HIS:HD2	2:B:146:GLY:O	2.01	0.43
1:A:401:LYS:HD3	2:B:346:TRP:CG	2.53	0.43
1:C:251:ASP:OD2	1:C:253:THR:OG1	2.37	0.43
1:C:119:LEU:HD21	1:C:156:ARG:HB3	2.01	0.42
1:C:204:VAL:HG11	1:C:231:ILE:HG12	2.00	0.42
1:C:255:PHE:CD2	1:C:316:CYS:HB3	2.54	0.42
1:C:255:PHE:CE1	1:C:318:LEU:HD21	2.54	0.42
2:D:1:MET:N	2:D:131:CYS:SG	2.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:VAL:HG11	1:A:231:ILE:HG12	2.01	0.42
2:B:133:GLN:HE21	2:B:252:LEU:HB2	1.84	0.42
2:D:352:LYS:HE3	9:D:502:LOC:O5	2.20	0.42
1:C:313:MET:HE3	1:C:380:ASN:ND2	2.35	0.42
2:D:192:HIS:CD2	2:D:421:ALA:HA	2.55	0.42
2:B:241[A]:CYS:SG	9:B:502:LOC:O3	2.77	0.42
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.37	0.42
2:D:141:LEU:HB3	2:D:187:ALA:HA	2.02	0.42
1:A:206:ASN:HD22	1:A:206:ASN:HA	1.67	0.41
2:B:206:ASN:HD22	2:B:206:ASN:HA	1.72	0.41
2:B:133:GLN:NE2	2:B:252:LEU:H	2.18	0.41
2:D:1:MET:HE3	2:D:133:GLN:HG3	2.02	0.41
1:A:286:LEU:HD23	1:A:290:GLU:HG2	2.03	0.41
1:A:27:GLU:OE2	1:A:320:ARG:NH2	2.53	0.41
1:A:71:GLU:OE2	1:A:73:THR:HB	2.20	0.41
2:B:192:HIS:CD2	2:B:421:ALA:HA	2.55	0.41
2:D:237:GLY:C	2:D:376:THR:HG21	2.45	0.41
2:D:229:HIS:HB2	2:D:278:ARG:HB3	2.02	0.41
2:B:292:THR:HG22	2:B:319:PHE:HZ	1.84	0.41
2:D:297:ASP:HB3	2:D:300:ASN:HD22	1.85	0.41
2:B:213:CYS:HA	2:B:217:LEU:HD12	2.03	0.41
1:C:286:LEU:HD11	1:C:291:ILE:CG2	2.51	0.41
1:C:317:LEU:HB2	1:C:353:VAL:HG22	2.03	0.41
1:A:440:VAL:CG2	3:E:33:PRO:HD2	2.51	0.41
2:D:250:ALA:HB1	9:D:502:LOC:H6B	2.02	0.41
2:D:274:PRO:HB3	2:D:286:LEU:HG	2.03	0.41
1:A:119:LEU:HD21	1:A:156:ARG:HB3	2.03	0.41
2:B:133:GLN:HE22	2:B:242:LEU:HD22	1.86	0.41
1:C:177:VAL:HG22	1:C:177:VAL:O	2.22	0.41
1:C:107:HIS:HD2	1:C:108[A]:TYR:CE2	2.39	0.40
1:C:274:PRO:HG3	1:C:286:LEU:HG	2.03	0.40
1:C:104:ALA:HB2	1:C:413:MET:SD	2.61	0.40
2:D:48:ARG:HE	2:D:248:LEU:HD11	1.87	0.40
2:B:1:MET:HE3	2:B:133:GLN:HG3	2.03	0.40
1:C:372:GLN:H	1:C:372:GLN:HG3	1.73	0.40
2:B:206:ASN:HD21	8:B:501:GDP:N2	2.05	0.40
2:D:139:HIS:HE1	2:D:170:SER:OG	2.05	0.40
2:B:350:ASN:HD22	2:B:350:ASN:N	2.10	0.40
1:C:71:GLU:OE2	1:C:73:THR:HB	2.21	0.40
1:C:122:ILE:HA	1:C:125:LEU:HD12	2.04	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	430/451 (95%)	404 (94%)	21 (5%)	5 (1%)	10	19
1	C	432/451 (96%)	406 (94%)	23 (5%)	3 (1%)	18	32
2	B	433/445 (97%)	411 (95%)	18 (4%)	4 (1%)	14	26
2	D	435/445 (98%)	411 (94%)	17 (4%)	7 (2%)	7	13
3	E	129/142 (91%)	118 (92%)	7 (5%)	4 (3%)	3	5
4	F	1/4 (25%)	0	1 (100%)	0	100	100
All	All	1860/1938 (96%)	1750 (94%)	87 (5%)	23 (1%)	10	19

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	178[A]	SER
2	D	178[B]	SER
2	D	248	LEU
2	B	178	SER
2	B	248	LEU
1	C	281	ALA
2	D	249	ASN
1	A	179	THR
1	A	340	SER
2	B	109	THR
2	D	109	THR
2	D	283	TYR
1	A	162	GLY
1	C	109	THR
3	E	45	PRO
2	B	286	LEU
1	C	314	ALA
3	E	10	GLU
3	E	32	VAL
3	E	46	SER

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Mol	Chain	Res	Type
1	A	47	ASP
2	D	73	GLY
1	A	131	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/379 (97%)	321 (87%)	47 (13%)	4	7
1	C	369/379 (97%)	315 (85%)	54 (15%)	3	4
2	B	378/385 (98%)	333 (88%)	45 (12%)	5	9
2	D	380/385 (99%)	338 (89%)	42 (11%)	6	11
3	E	113/125 (90%)	93 (82%)	20 (18%)	2	2
4	F	1/1 (100%)	1 (100%)	0	100	100
All	All	1609/1654 (97%)	1401 (87%)	208 (13%)	4	7

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	9	VAL
1	A	16	ILE
1	A	26	LEU
1	A	36	MET
1	A	47	ASP
1	A	66	VAL
1	A	68	VAL
1	A	70	LEU
1	A	119	LEU
1	A	121	ARG
1	A	153	LEU
1	A	163	LYS
1	A	166	LYS
1	A	177	VAL

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Mol	Chain	Res	Type
1	A	179	THR
1	A	188	ILE
1	A	206	ASN
1	A	215	ARG
1	A	227	LEU
1	A	229	ARG
1	A	250	VAL
1	A	269	LEU
1	A	277	SER
1	A	280	LYS
1	A	284	GLU
1	A	288	VAL
1	A	295	CYS
1	A	297	GLU
1	A	302	MET
1	A	320	ARG
1	A	336	LYS
1	A	337	THR
1	A	338	LYS
1	A	341	ILE
1	A	344	VAL
1	A	361	THR
1	A	367	ASP
1	A	368	LEU
1	A	370	LYS
1	A	384	ILE
1	A	391	LEU
1	A	397	LEU
1	A	413	MET
1	A	423	GLU
1	A	430	LYS
1	A	439	SER
2	B	5	VAL
2	B	11	GLN
2	B	16	ILE
2	B	26	ASP
2	B	42	LEU
2	B	48	ARG
2	B	50	ASN
2	B	54	ASN
2	B	57	THR
2	B	60	LYS

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Mol	Chain	Res	Type
2	B	71[A]	GLU
2	B	71[B]	GLU
2	B	75	MET
2	B	79	ARG
2	B	122	VAL
2	B	141	LEU
2	B	145	THR
2	B	171	VAL
2	B	177	VAL
2	B	179	ASP
2	B	206	ASN
2	B	209	LEU
2	B	218	LYS
2	B	223	THR
2	B	230	LEU
2	B	238	VAL
2	B	252	LEU
2	B	255	LEU
2	B	260	VAL
2	B	281	GLN
2	B	287	THR
2	B	288	VAL
2	B	294	GLN
2	B	295	MET
2	B	313	LEU
2	B	323	MET
2	B	329	ASP
2	B	333	LEU
2	B	339	ASN
2	B	345	GLU
2	B	350	ASN
2	B	351	VAL
2	B	372	LYS
2	B	405	LEU
2	B	416	MET
1	C	1	MET
1	C	4[A]	CYS
1	C	4[B]	CYS
1	C	9	VAL
1	C	16	ILE
1	C	26	LEU
1	C	35	GLN

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Mol	Chain	Res	Type
1	C	66	VAL
1	C	68	VAL
1	C	70	LEU
1	C	84	ARG
1	C	119	LEU
1	C	121	ARG
1	C	153	LEU
1	C	163	LYS
1	C	164	LYS
1	C	166	LYS
1	C	177	VAL
1	C	188	ILE
1	C	206	ASN
1	C	227	LEU
1	C	229	ARG
1	C	233	GLN
1	C	252	LEU
1	C	253	THR
1	C	254	GLU
1	C	256	GLN
1	C	260	VAL
1	C	269	LEU
1	C	280	LYS
1	C	282	TYR
1	C	290	GLU
1	C	291	ILE
1	C	295	CYS
1	C	297	GLU
1	C	302	MET
1	C	328	VAL
1	C	332	ILE
1	C	335	ILE
1	C	339	ARG
1	C	340	SER
1	C	352	LYS
1	C	361	THR
1	C	367	ASP
1	C	368	LEU
1	C	370	LYS
1	C	372	GLN
1	C	384	ILE
1	C	391	LEU

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Mol	Chain	Res	Type
1	C	397	LEU
1	C	423	GLU
1	C	430	LYS
1	C	435	VAL
1	C	439	SER
2	D	11	GLN
2	D	26	ASP
2	D	47	GLU
2	D	50	ASN
2	D	57	THR
2	D	59	ASN
2	D	71	GLU
2	D	85	GLN
2	D	122	VAL
2	D	141	LEU
2	D	171	VAL
2	D	177	VAL
2	D	190	SER
2	D	218	LYS
2	D	230	LEU
2	D	247	GLN
2	D	248	LEU
2	D	252	LEU
2	D	255	LEU
2	D	260	VAL
2	D	276	THR
2	D	277	SER
2	D	282	GLN
2	D	284	ARG
2	D	286	LEU
2	D	288	VAL
2	D	291	LEU
2	D	293	GLN
2	D	295	MET
2	D	296	PHE
2	D	313	LEU
2	D	318	ILE
2	D	329	ASP
2	D	338	LYS
2	D	340	SER
2	D	345	GLU
2	D	350	ASN

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Mol	Chain	Res	Type
2	D	351	VAL
2	D	372	LYS
2	D	376	THR
2	D	405	LEU
2	D	416	MET
3	E	10	GLU
3	E	12	ASN
3	E	15	THR
3	E	47	LEU
3	E	55	GLU
3	E	58	GLU
3	E	72	LEU
3	E	76	ARG
3	E	80	ARG
3	E	82	VAL
3	E	83	ILE
3	E	85	LYS
3	E	88	GLU
3	E	105	MET
3	E	108	ASN
3	E	116	LEU
3	E	123	LEU
3	E	128	LYS
3	E	136	ASN
3	E	139	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	11	GLN
1	A	15	GLN
1	A	35	GLN
1	A	91	GLN
1	A	101	ASN
1	A	102	ASN
1	A	176	GLN
1	A	197	HIS
1	A	206	ASN
1	A	216	ASN
1	A	249	ASN
1	A	258	ASN

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Mol	Chain	Res	Type
1	A	285	GLN
1	A	301	GLN
1	A	309	HIS
1	A	380	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	85	GLN
2	B	96	GLN
2	B	101	ASN
2	B	133	GLN
2	B	136	GLN
2	B	139	HIS
2	B	206	ASN
2	B	281	GLN
2	B	339	ASN
2	B	350	ASN
2	B	380	ASN
2	B	385	GLN
2	B	406	HIS
2	B	433	GLN
1	C	8	HIS
1	C	11	GLN
1	C	15	GLN
1	C	50	ASN
1	C	91	GLN
1	C	101	ASN
1	C	102	ASN
1	C	107	HIS
1	C	176	GLN
1	C	197	HIS
1	C	206	ASN
1	C	216	ASN
1	C	301	GLN
1	C	380	ASN
2	D	6	HIS
2	D	133	GLN
2	D	139	HIS
2	D	197	ASN
2	D	206	ASN
2	D	247	GLN
2	D	258	ASN

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Mol	Chain	Res	Type
2	D	300	ASN
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
2	D	433	GLN
2	D	436	GLN
3	E	18	GLN
3	E	78	HIS
3	E	84	GLN
3	E	91	ASN
3	E	111	ASN
3	E	115	HIS
3	E	124	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
4	0E5	F	3	4	6,7,9	1.27	0	4,8,13	2.53	3 (75%)
4	0EA	F	1	4	13,15,16	2.76	8 (61%)	16,20,22	2.99	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	0E5	F	3	4	1/1/2/3	5/7/8/13	-
4	0EA	F	1	4	-	0/10/12/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	0EA	O5-C7	-4.93	1.26	1.36
4	F	1	0EA	O1-C5	4.00	1.44	1.36
4	F	1	0EA	C6-C5	3.96	1.44	1.38
4	F	1	0EA	C6-C10	3.85	1.44	1.39
4	F	1	0EA	O8-C11	2.79	1.48	1.42
4	F	1	0EA	C9-C10	2.43	1.43	1.39
4	F	1	0EA	O-C	2.37	1.29	1.20
4	F	1	0EA	C10-C11	2.15	1.55	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	0EA	C10-C11-CA	-7.44	102.82	112.06
4	F	1	0EA	C6-C5-C7	-5.87	114.46	119.89
4	F	1	0EA	C8-C7-C5	5.73	125.77	119.66
4	F	3	0E5	O-C-CA	-3.59	115.54	124.77
4	F	3	0E5	C2-C3-CA	-2.87	103.90	111.19
4	F	3	0E5	C4-C3-C2	-2.11	106.50	111.81

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	3	0E5	C3

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	3	0E5	C2-C3-CA-C
4	F	3	0E5	C4-C3-CA-C
4	F	3	0E5	C4-C3-CA-N
4	F	3	0E5	C1-C2-C3-C4
4	F	3	0E5	C1-C2-C3-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	3	0E5	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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$
5	GTP	A	501	6	33,34,34	1.56	3 (9%)	50,54,54	1.70	13 (26%)
7	SO4	A	503	-	4,4,4	0.40	0	6,6,6	0.12	0
9	LOC	D	502	-	31,31,31	2.81	7 (22%)	44,44,44	3.34	21 (47%)
8	GDP	B	501	-	29,30,30	1.26	3 (10%)	45,47,47	1.64	8 (17%)
9	LOC	B	502	-	31,31,31	2.53	8 (25%)	44,44,44	2.85	20 (45%)
5	GTP	C	600	6	33,34,34	1.92	3 (9%)	50,54,54	1.65	12 (24%)
7	SO4	D	503	-	4,4,4	0.40	0	6,6,6	0.10	0
8	GDP	D	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.35	8 (17%)
7	SO4	A	504	-	4,4,4	0.24	0	6,6,6	0.13	0
7	SO4	B	503	-	4,4,4	0.28	0	6,6,6	0.10	0
7	SO4	D	504	-	4,4,4	0.28	0	6,6,6	0.13	0

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
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
9	LOC	D	502	-	-	2/12/25/25	0/3/3/3
8	GDP	B	501	-	-	5/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	LOC	B	502	-	-	2/12/25/25	0/3/3/3
5	GTP	C	600	6	-	5/22/38/38	0/3/3/3
8	GDP	D	501	-	-	5/16/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	502	LOC	C11-C14	-10.57	1.38	1.53
9	B	502	LOC	C11-C14	-7.46	1.42	1.53
9	B	502	LOC	C22-C21	-7.44	1.41	1.50
5	C	600	GTP	PB-O3A	6.64	1.66	1.59
5	A	501	GTP	PB-O3B	5.91	1.65	1.59
9	D	502	LOC	C22-C21	-5.60	1.43	1.50
9	D	502	LOC	O6-C18	-5.43	1.33	1.45
9	D	502	LOC	C9-C8	-5.42	1.39	1.51
9	B	502	LOC	C9-C8	-5.40	1.39	1.51
5	C	600	GTP	PA-O3A	4.96	1.64	1.59
5	C	600	GTP	PB-O3B	4.91	1.64	1.59
8	B	501	GDP	PA-O3A	4.07	1.63	1.59
9	B	502	LOC	O6-C18	-3.30	1.37	1.45
5	A	501	GTP	PB-O3A	3.30	1.63	1.59
5	A	501	GTP	PA-O3A	3.22	1.63	1.59
9	B	502	LOC	C20-C21	2.93	1.42	1.37
8	D	501	GDP	PA-O3A	2.90	1.62	1.59
9	B	502	LOC	O2-C3	-2.73	1.33	1.38
9	D	502	LOC	C15-C14	2.69	1.41	1.36
9	D	502	LOC	C22-C8	2.65	1.46	1.41
9	D	502	LOC	O2-C3	-2.54	1.33	1.38
8	D	501	GDP	C5-C4	2.42	1.45	1.38
8	B	501	GDP	C5-C4	2.36	1.45	1.38
8	D	501	GDP	PB-O2B	2.34	1.63	1.54
9	B	502	LOC	C22-C8	2.28	1.45	1.41
8	B	501	GDP	PB-O3B	2.25	1.63	1.54
9	B	502	LOC	C15-C14	2.12	1.40	1.36

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	502	LOC	C11-C14-C15	-7.01	110.88	117.06
9	D	502	LOC	O6-C17-C16	6.97	116.01	109.60
9	D	502	LOC	C1-C22-C21	6.88	128.59	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	502	LOC	C22-C21-C14	6.36	123.83	118.62
9	B	502	LOC	C14-C11-N1	6.11	119.13	114.31
9	B	502	LOC	C9-C8-C22	6.02	129.77	119.88
9	D	502	LOC	C10-C11-N1	5.95	120.65	109.76
9	D	502	LOC	C15-C16-C17	5.94	129.68	121.86
9	D	502	LOC	C22-C21-C20	-5.45	108.11	116.95
9	B	502	LOC	C9-C8-C7	-5.37	107.70	119.35
9	B	502	LOC	C20-C21-C14	5.30	130.04	124.67
9	D	502	LOC	C8-C22-C21	-5.16	114.47	120.20
9	B	502	LOC	O6-C17-C16	5.09	114.28	109.60
5	A	501	GTP	C2-N3-C4	4.95	120.83	112.30
9	B	502	LOC	C15-C16-C17	4.95	128.38	121.86
9	B	502	LOC	C22-C21-C20	-4.87	109.05	116.95
9	D	502	LOC	C11-C14-C21	4.77	119.73	115.37
5	C	600	GTP	C2-N3-C4	4.69	120.38	112.30
8	B	501	GDP	C5-C4-N3	-4.61	121.06	128.39
5	A	501	GTP	C5-C4-N3	-4.48	121.26	128.39
9	D	502	LOC	C9-C10-C11	4.47	117.54	112.13
8	B	501	GDP	C2-N3-C4	4.44	119.95	112.30
9	D	502	LOC	C9-C8-C22	4.37	127.05	119.88
9	D	502	LOC	C9-C8-C7	-4.20	110.24	119.35
5	C	600	GTP	C5-C4-N3	-4.15	121.78	128.39
9	B	502	LOC	C11-C14-C21	4.10	119.11	115.37
9	B	502	LOC	C10-C11-N1	3.98	117.05	109.76
9	D	502	LOC	C14-C15-C16	-3.87	127.31	134.20
9	B	502	LOC	C4-O2-C3	-3.79	104.44	114.74
5	A	501	GTP	N9-C4-N3	3.70	133.35	125.95
8	D	501	GDP	C2-N3-C4	3.67	118.62	112.30
8	B	501	GDP	C6-C5-N7	3.65	136.93	130.29
5	C	600	GTP	N9-C4-N3	3.63	133.21	125.95
8	D	501	GDP	C5-C4-N3	-3.49	122.84	128.39
9	D	502	LOC	O6-C17-C19	-3.48	117.24	122.29
9	D	502	LOC	C20-C21-C14	3.31	128.03	124.67
8	B	501	GDP	C4-C5-N7	-3.26	105.51	110.67
9	D	502	LOC	O5-C16-C15	-3.25	110.30	119.02
9	B	502	LOC	C11-C14-C15	-3.20	114.24	117.06
9	B	502	LOC	C1-C22-C21	3.16	124.66	121.33
5	C	600	GTP	C6-C5-N7	3.14	136.00	130.29
9	B	502	LOC	C8-C22-C21	-3.07	116.79	120.20
8	B	501	GDP	N9-C4-N3	3.03	132.01	125.95
8	B	501	GDP	O2B-PB-O3A	3.02	114.75	104.64
5	A	501	GTP	C6-C5-N7	2.96	135.68	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	502	LOC	C6-O3-C5	-2.92	113.23	117.51
9	B	502	LOC	O5-C16-C15	-2.90	111.25	119.02
8	B	501	GDP	C8-N7-C5	2.86	109.35	104.26
9	B	502	LOC	O3-C5-C3	2.82	119.97	115.14
8	D	501	GDP	C6-C5-N7	2.81	135.41	130.29
9	B	502	LOC	C22-C21-C14	2.77	120.89	118.62
8	B	501	GDP	O2A-PA-O3A	2.76	114.74	107.27
5	A	501	GTP	C8-N7-C5	2.70	109.07	104.26
8	D	501	GDP	N9-C4-N3	2.67	131.28	125.95
9	B	502	LOC	C14-C15-C16	-2.63	129.52	134.20
5	C	600	GTP	C2-N1-C6	-2.58	120.44	125.11
9	D	502	LOC	C4-O2-C3	-2.57	107.77	114.74
5	C	600	GTP	C5-C6-N1	2.56	119.78	113.25
9	D	502	LOC	C7-C8-C22	2.48	122.70	119.54
8	D	501	GDP	O2B-PB-O3A	2.47	112.91	104.64
5	A	501	GTP	N9-C8-N7	-2.46	108.84	113.40
5	C	600	GTP	C8-N7-C5	2.43	108.59	104.26
8	D	501	GDP	O2A-PA-O3A	2.42	113.81	107.27
9	B	502	LOC	C7-C8-C22	2.34	122.52	119.54
9	B	502	LOC	O6-C17-C19	-2.31	118.93	122.29
5	A	501	GTP	O3G-PG-O3B	2.31	112.38	104.64
5	A	501	GTP	C4-C5-N7	-2.29	107.04	110.67
5	A	501	GTP	C2-N1-C6	-2.29	120.97	125.11
9	D	502	LOC	C5-C3-C1	2.27	122.31	119.58
5	A	501	GTP	C5-C6-N1	2.21	118.88	113.25
5	A	501	GTP	O2B-PB-O3A	2.19	113.19	107.27
8	D	501	GDP	C4-C5-N7	-2.18	107.21	110.67
5	C	600	GTP	O6-C6-C5	-2.17	120.81	126.53
9	D	502	LOC	C15-C14-C21	2.15	129.39	127.56
8	D	501	GDP	C8-N7-C5	2.15	108.10	104.26
5	C	600	GTP	N9-C8-N7	-2.12	109.48	113.40
5	A	501	GTP	O6-C6-C5	-2.12	120.95	126.53
5	A	501	GTP	O4'-C4'-C5'	-2.11	102.58	109.33
9	B	502	LOC	O4-C12-N1	2.06	125.63	121.98
5	C	600	GTP	C4-C5-N7	-2.05	107.42	110.67
5	C	600	GTP	O4'-C4'-C5'	-2.05	102.78	109.33
5	C	600	GTP	O3G-PG-O3B	2.04	111.49	104.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	600	GTP	PB-O3B-PG-O2G
5	C	600	GTP	C5'-O5'-PA-O3A
5	C	600	GTP	C5'-O5'-PA-O1A
5	C	600	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	502	LOC	C19-C17-O6-C18
9	B	502	LOC	C16-C17-O6-C18
9	D	502	LOC	C19-C17-O6-C18
9	D	502	LOC	C16-C17-O6-C18
8	B	501	GDP	PB-O3A-PA-O1A
8	D	501	GDP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3B-PG-O1G
5	C	600	GTP	PB-O3B-PG-O1G
8	B	501	GDP	PB-O3A-PA-O2A
8	D	501	GDP	PB-O3A-PA-O2A

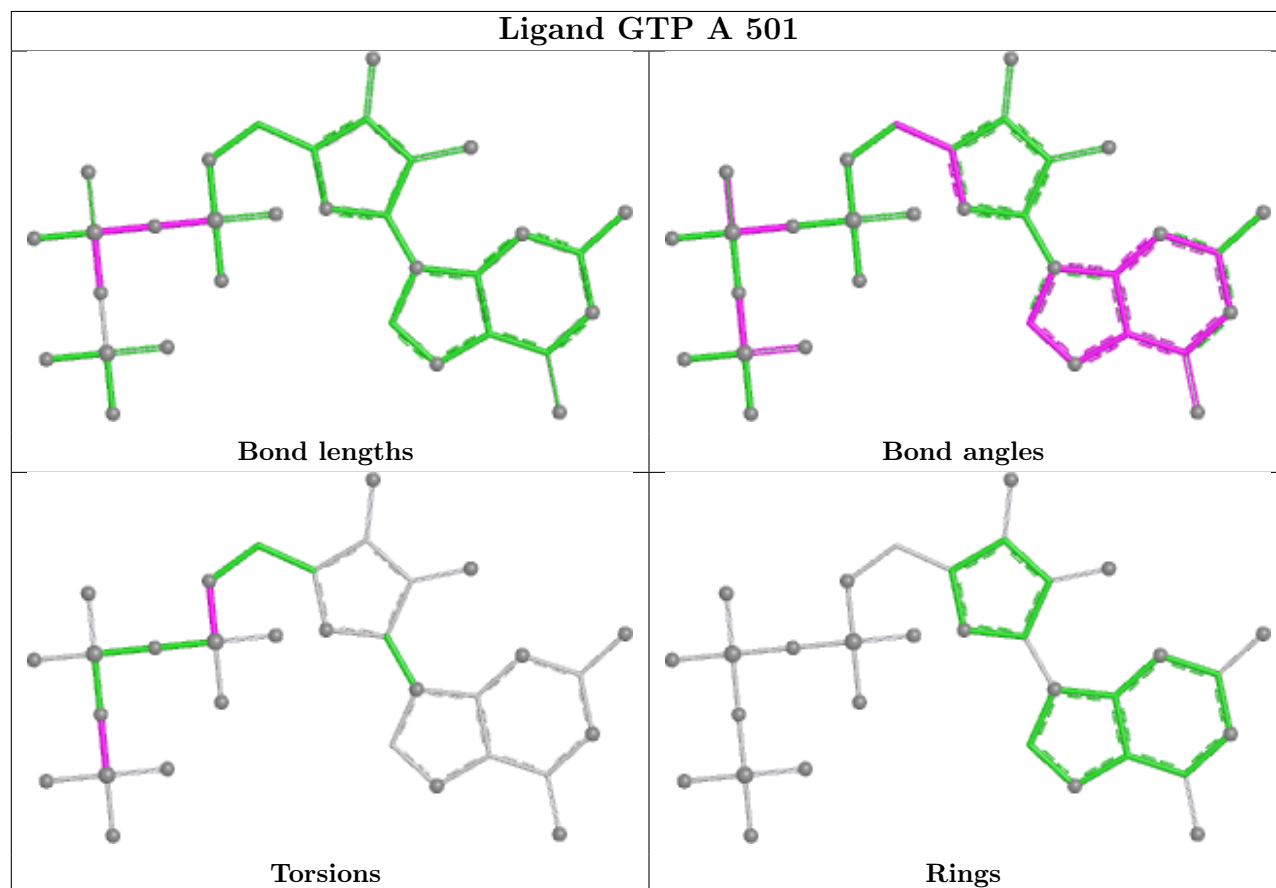
There are no ring outliers.

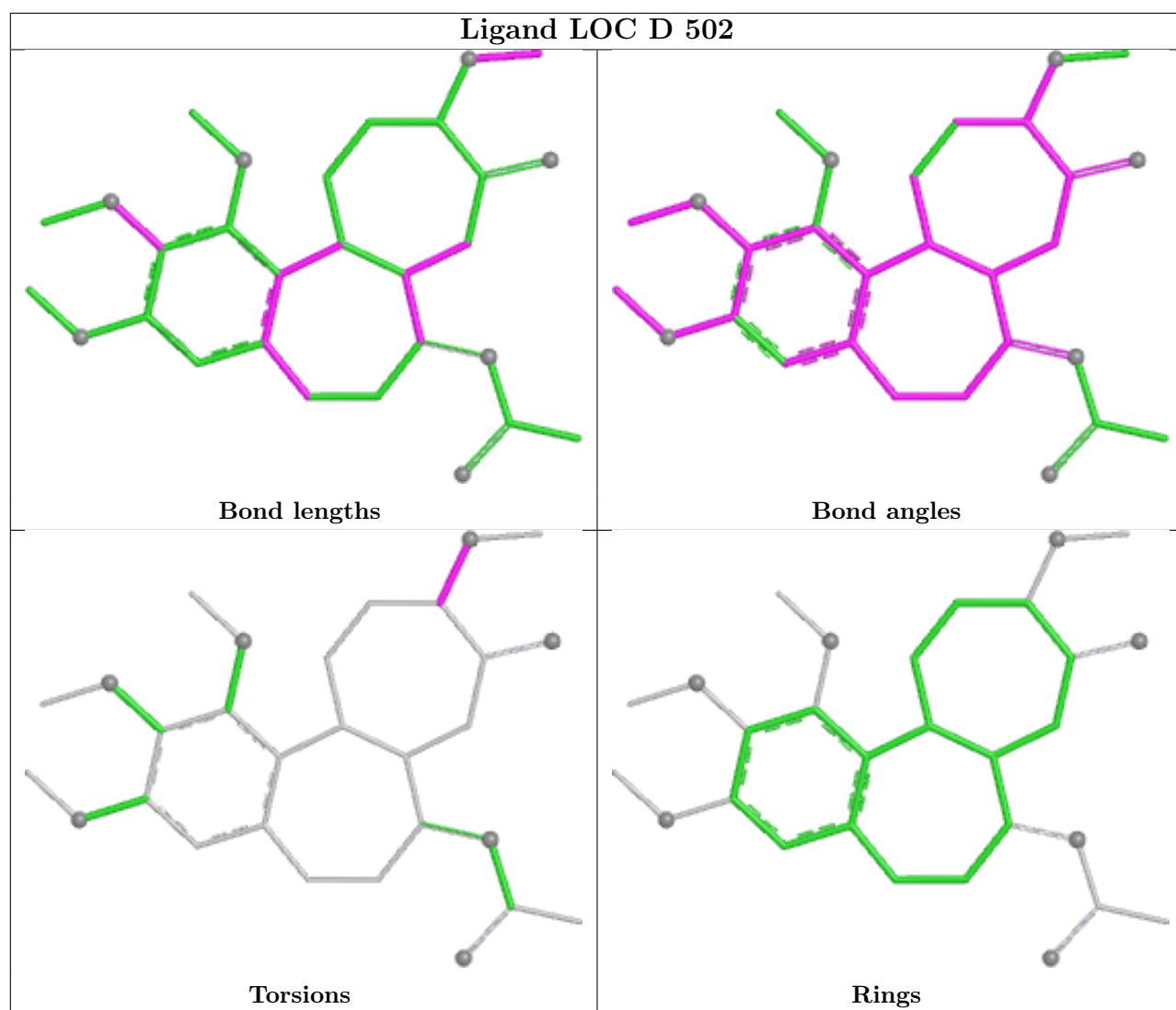
6 monomers are involved in 14 short contacts:

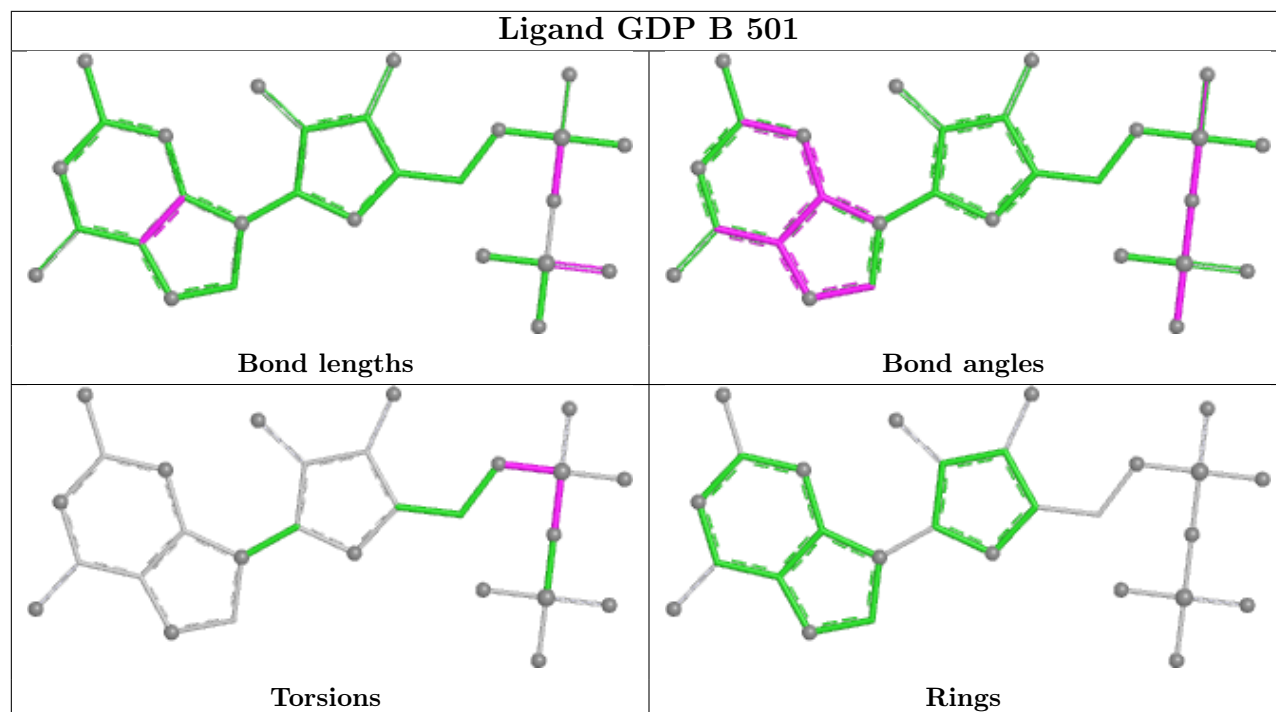
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
9	D	502	LOC	3	0
8	B	501	GDP	3	0
9	B	502	LOC	4	0
5	C	600	GTP	1	0
8	D	501	GDP	2	0

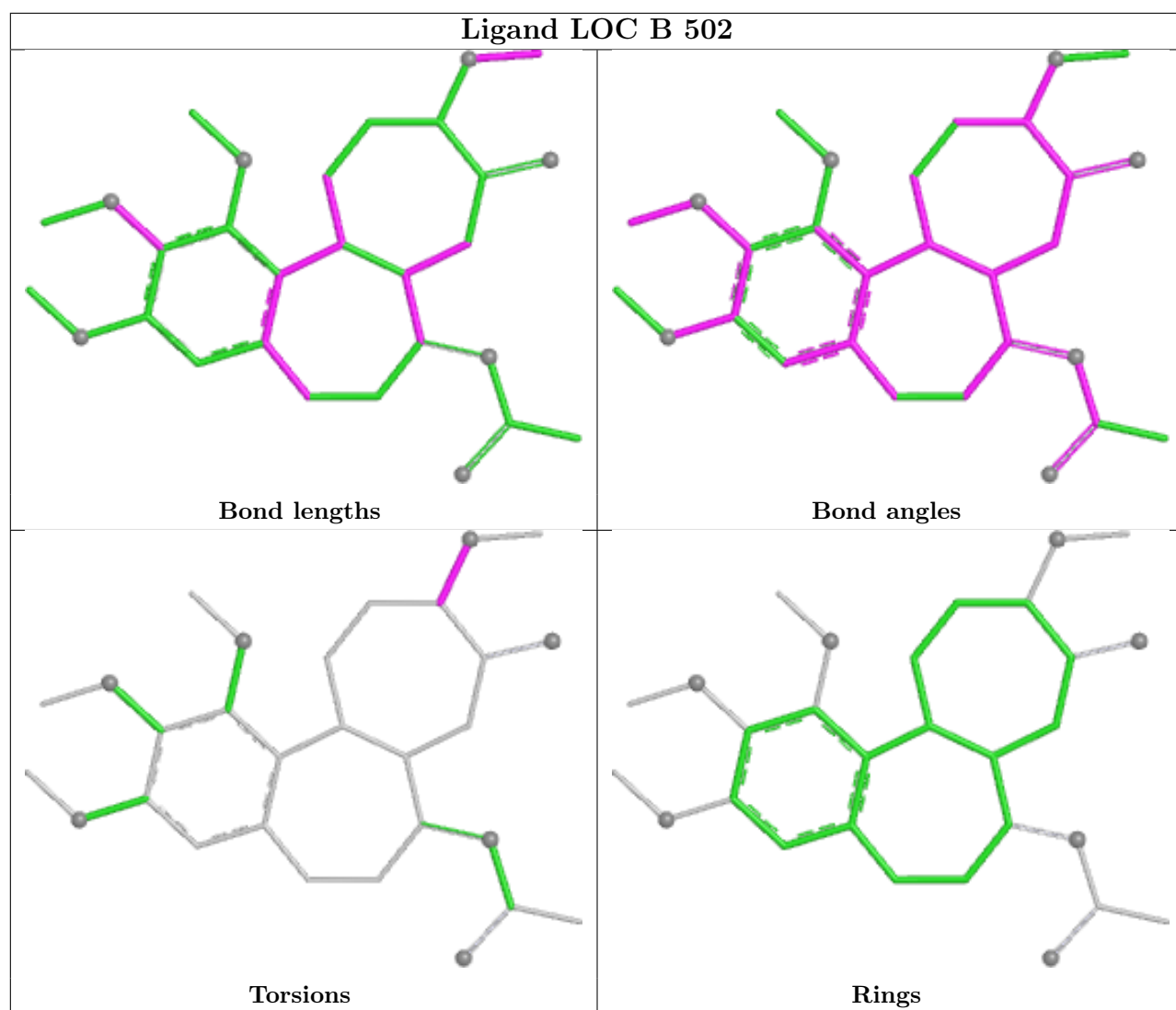
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

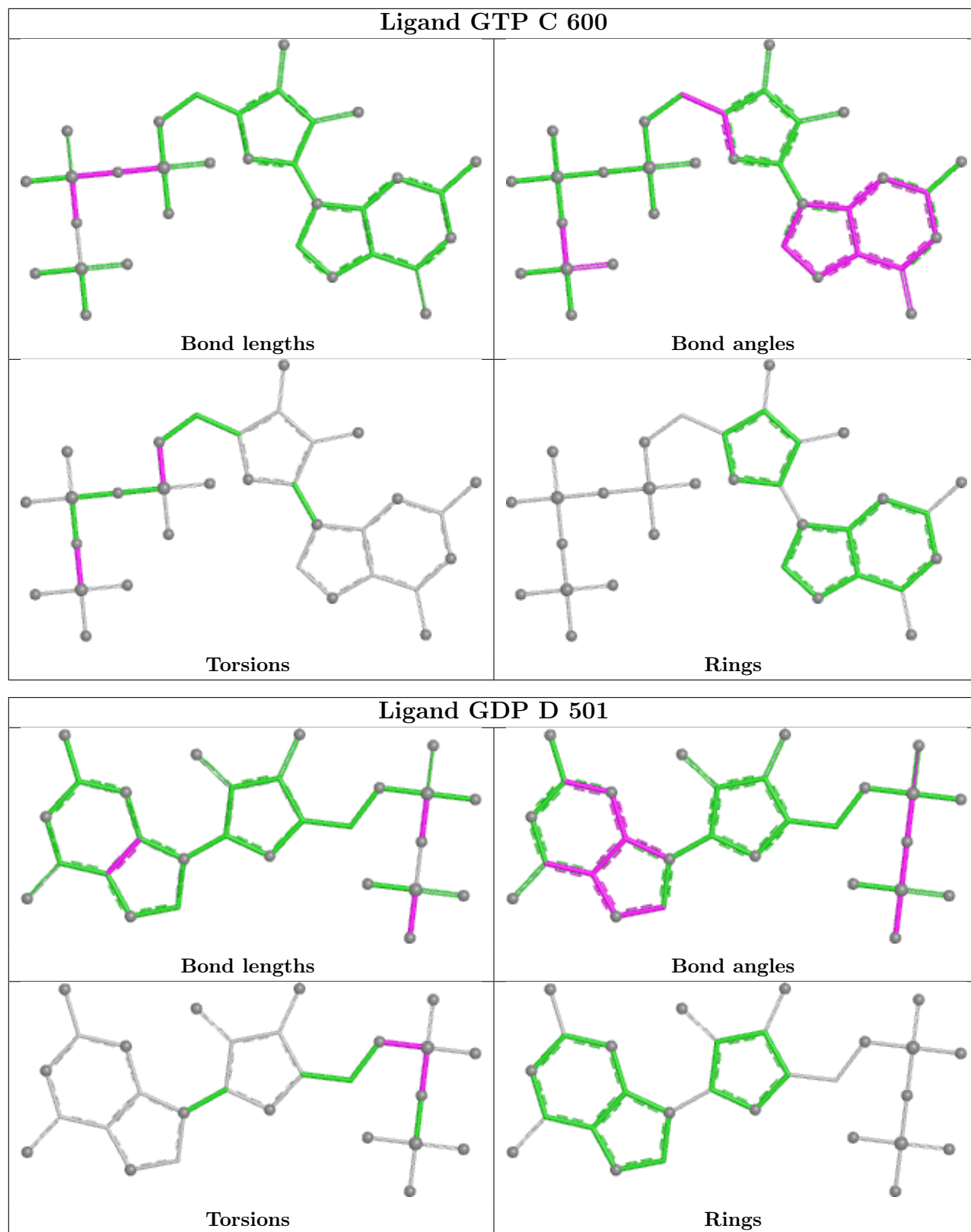
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers 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 ⓘ

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	433/451 (96%)	-0.11	2 (0%) 87 87	52, 97, 153, 198	1 (0%)
1	C	432/451 (95%)	-0.13	6 (1%) 73 72	32, 81, 133, 180	4 (0%)
2	B	432/445 (97%)	-0.14	3 (0%) 84 84	44, 90, 155, 215	5 (1%)
2	D	432/445 (97%)	-0.20	7 (1%) 70 68	33, 77, 122, 162	7 (1%)
3	E	132/142 (92%)	-0.17	0 100 100	58, 107, 176, 214	1 (0%)
4	F	2/4 (50%)	1.74	1 (50%) 0 0	117, 117, 117, 129	0
All	All	1863/1938 (96%)	-0.15	19 (1%) 79 79	32, 89, 145, 215	18 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	440	VAL	3.0
2	D	296	PHE	3.0
2	D	248	LEU	2.8
2	D	179[A]	ASP	2.7
2	D	282	GLN	2.7
1	C	336	LYS	2.7
2	D	250	ALA	2.5
2	D	283	TYR	2.5
2	B	276	THR	2.4
2	B	1	MET	2.4
2	D	280	SER	2.4
1	C	348	PRO	2.3
2	B	248	LEU	2.3
1	C	388	TRP	2.3
1	C	335	ILE	2.1
4	F	2	VAL	2.1
1	A	302	MET	2.0
1	A	440	VAL	2.0
1	C	288	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
4	0E5	F	3	8/10	0.80	0.14	110,113,121,122	0
4	0EA	F	1	15/16	0.89	0.10	113,115,118,119	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

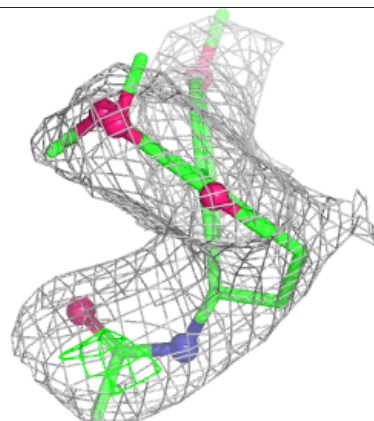
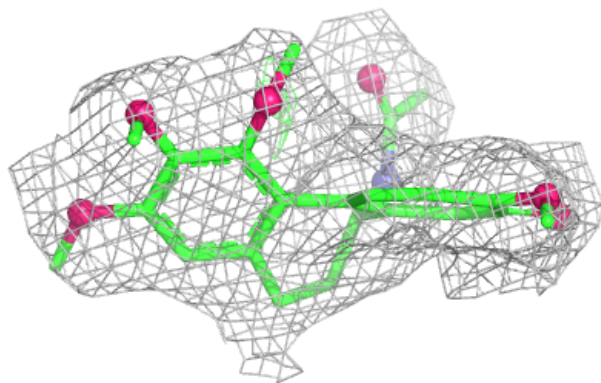
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SO4	D	504	5/5	0.75	0.14	141,143,147,149	0
7	SO4	B	503	5/5	0.82	0.06	157,160,165,165	0
7	SO4	A	503	5/5	0.83	0.07	127,130,133,134	0
7	SO4	D	503	5/5	0.85	0.10	142,143,148,149	0
7	SO4	A	504	5/5	0.92	0.07	140,143,147,147	0
9	LOC	B	502	29/29	0.93	0.09	75,79,83,85	0
9	LOC	D	502	29/29	0.96	0.07	51,63,67,67	0
8	GDP	D	501	28/28	0.97	0.06	62,66,70,73	0
5	GTP	C	600	32/32	0.97	0.05	57,59,66,68	0
8	GDP	B	501	28/28	0.97	0.05	69,71,76,76	0
5	GTP	A	501	32/32	0.98	0.06	63,70,76,76	0
6	MG	A	502	1/1	0.99	0.05	74,74,74,74	0
6	MG	C	601	1/1	1.00	0.02	56,56,56,56	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.

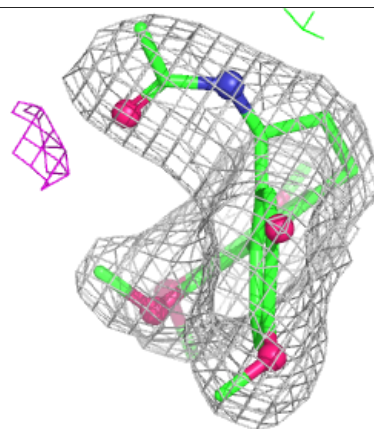
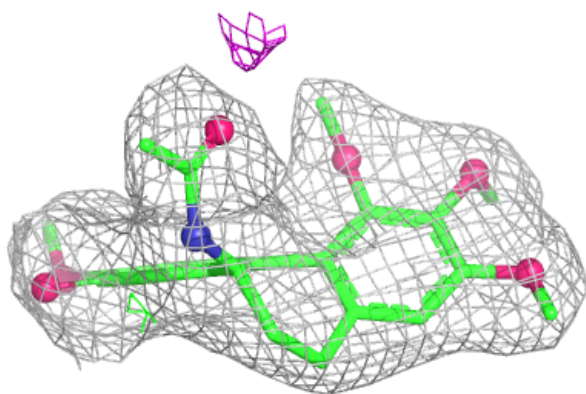
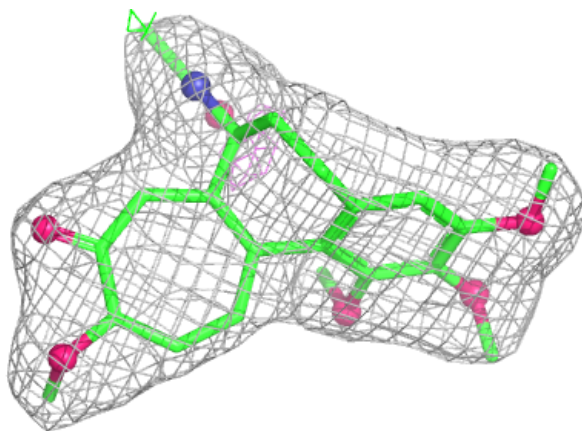
Electron density around LOC B 502:

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



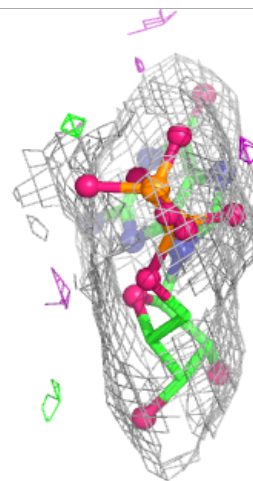
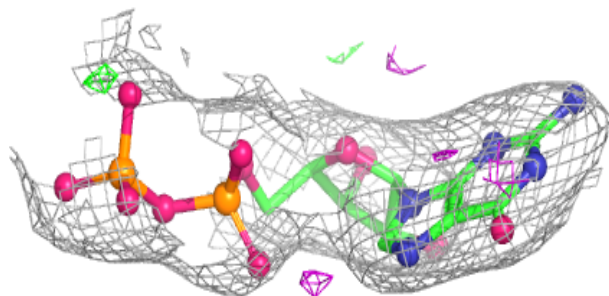
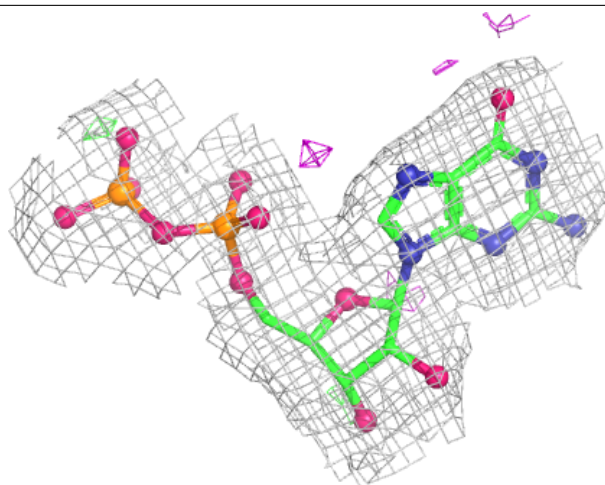
Electron density around LOC D 502:

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



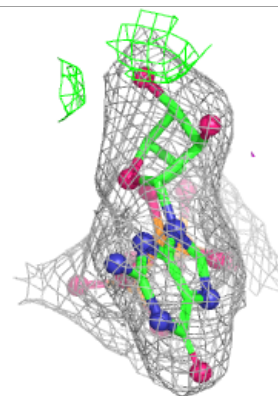
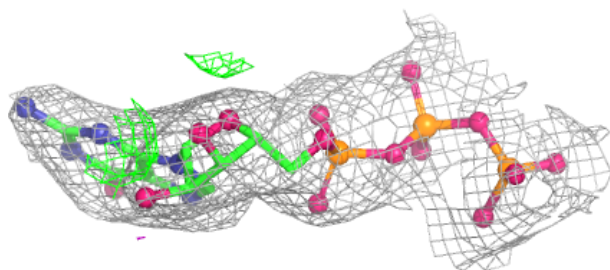
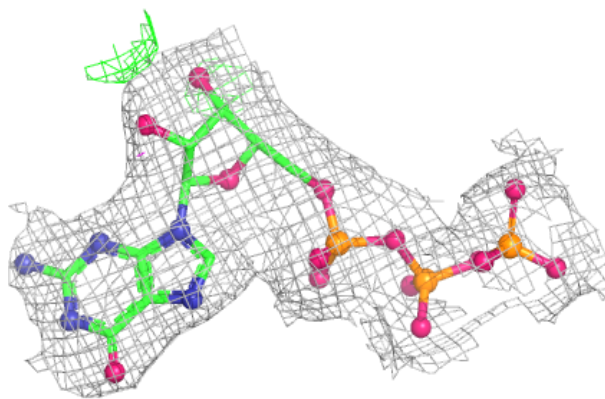
Electron density around GDP D 501:

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

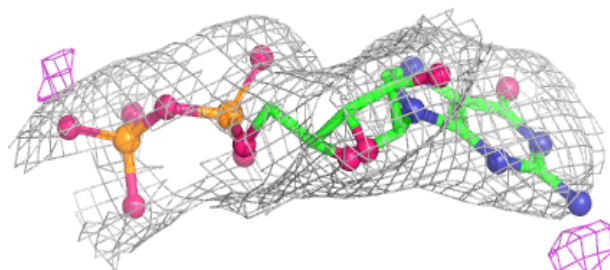
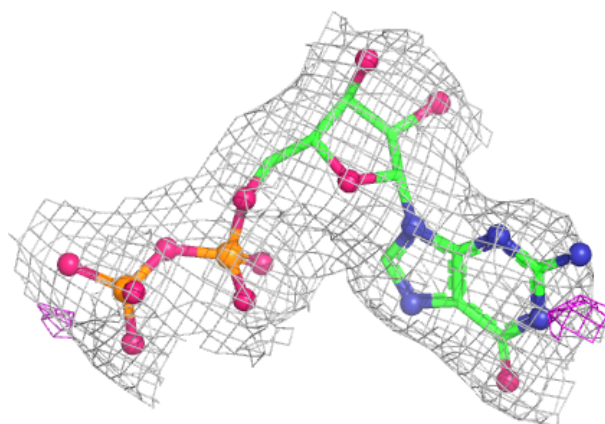


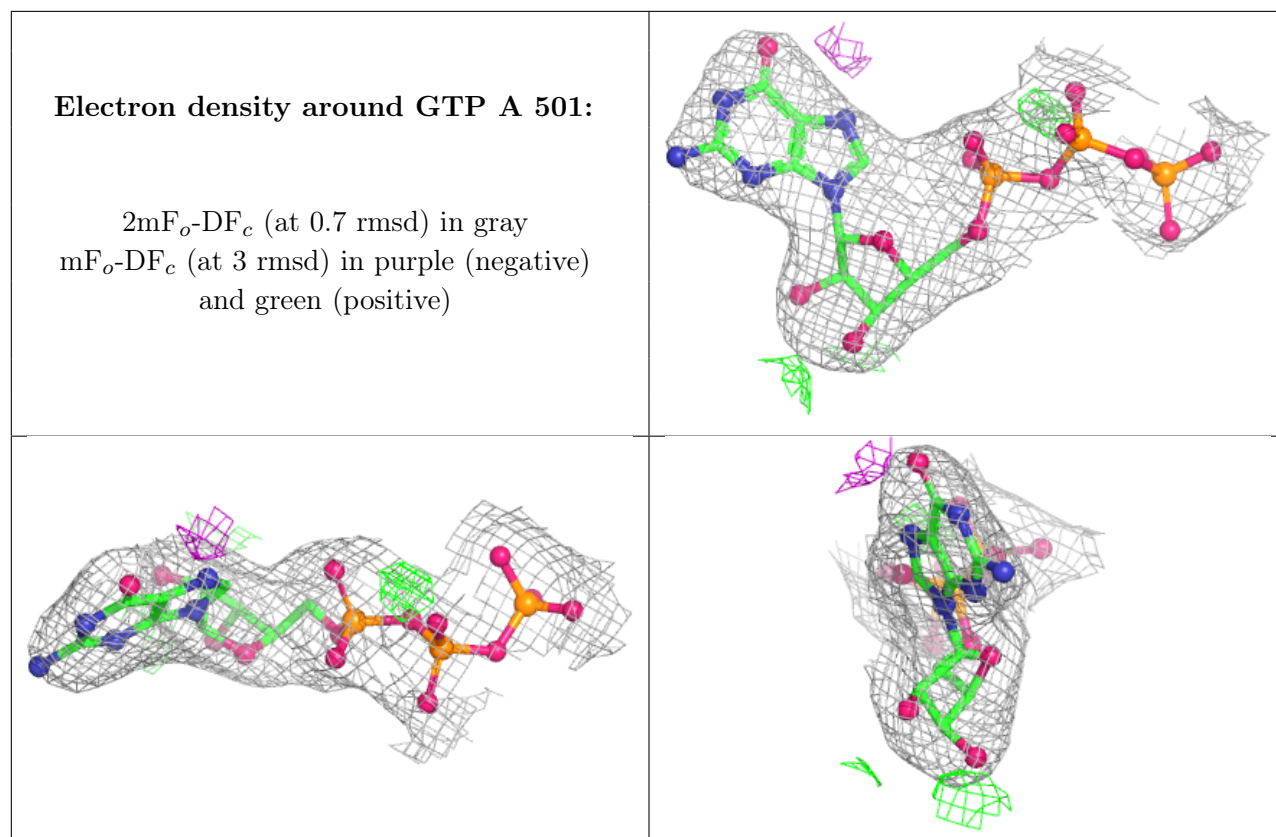
Electron density around GTP C 600:

$2mF_o-DF_c$ (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.