



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:37 PM UTC

PDB ID : 6LS4 / pdb_00006ls4
Title : A novel anti-tumor agent S-40 in complex with tubulin
Authors : Du, T.; Lin, S.; Ji, M.; Xue, N.; Liu, Y.; Zhang, K.; Lu, D.; Chen, X.; Xu, H.
Deposited on : 2020-01-17
Resolution : 2.40 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

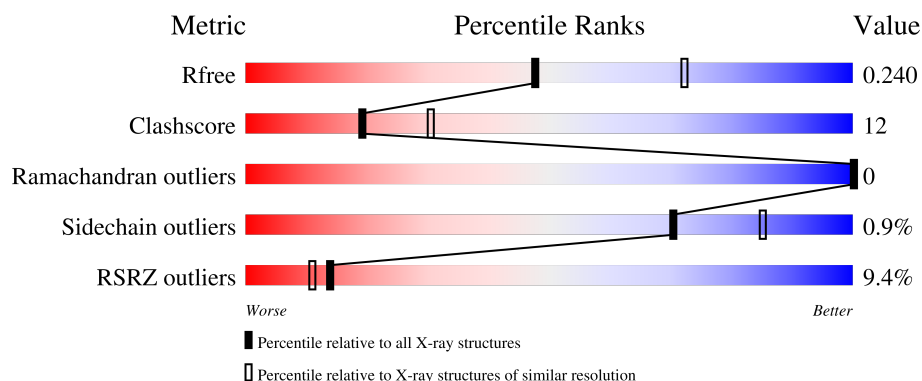
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	13% 66% 29% • 5%
1	C	451	8% 75% 22% •
2	B	445	6% 73% 21% 5%
2	D	445	8% 69% 27% •
3	E	152	11% 68% 12% • 18%

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
8	GOL	B	503	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 14402 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-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3255	2063	555	616	21			
1	C	439	Total	C	N	O	S	0	0	0
			3397	2150	574	651	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3239	2043	536	635	25			
2	D	428	Total	C	N	O	S	0	0	0
			3305	2080	558	641	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	55	THR	ALA	conflict	UNP P02554
B	170	MET	VAL	conflict	UNP P02554
B	296	SER	ALA	conflict	UNP P02554
B	316	ILE	VAL	conflict	UNP P02554
D	55	THR	ALA	conflict	UNP P02554
D	170	MET	VAL	conflict	UNP P02554
D	296	SER	ALA	conflict	UNP P02554
D	316	ILE	VAL	conflict	UNP P02554

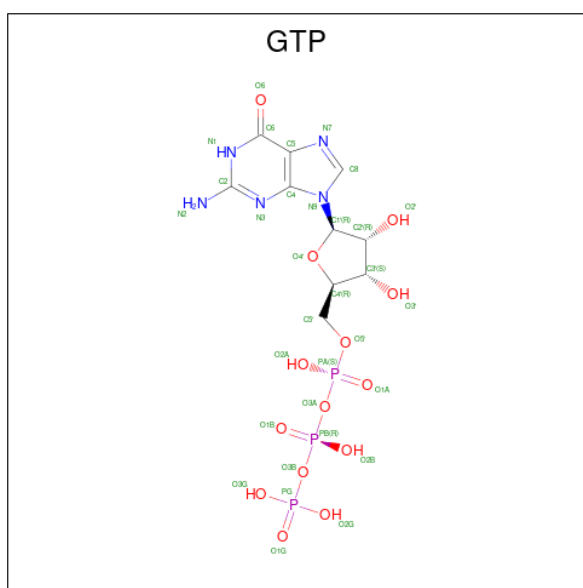
- Molecule 3 is a protein called Stathmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			978	606	175	192	5			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	ALA	-	expression tag	UNP F2Z508
E	143	LEU	-	expression tag	UNP F2Z508
E	144	GLU	-	expression tag	UNP F2Z508
E	145	HIS	-	expression tag	UNP F2Z508
E	146	HIS	-	expression tag	UNP F2Z508
E	147	HIS	-	expression tag	UNP F2Z508
E	148	HIS	-	expression tag	UNP F2Z508
E	149	HIS	-	expression tag	UNP F2Z508
E	150	HIS	-	expression tag	UNP F2Z508
E	151	HIS	-	expression tag	UNP F2Z508
E	152	HIS	-	expression tag	UNP F2Z508

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

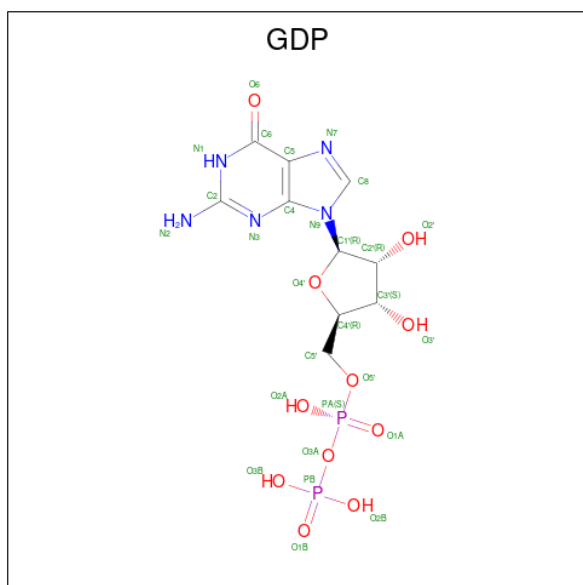
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	3	Total	Mg	0	0
			3	3		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



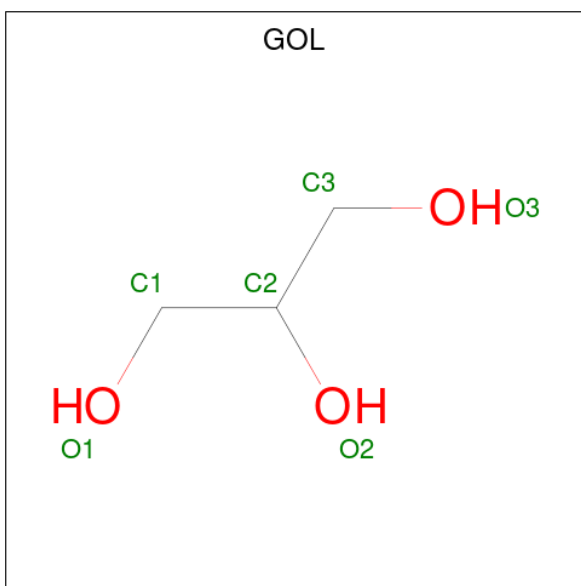
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



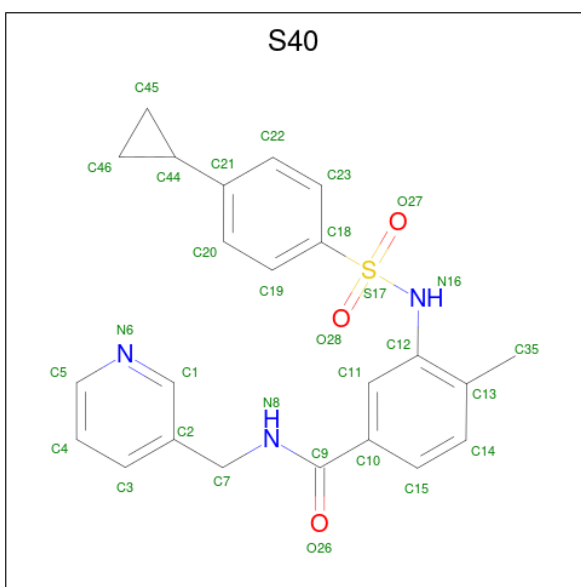
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 3-[(4-cyclopropylphenyl)sulfonylamino]-4-methyl-N-(pyridin-3-ylmethyl)benzamide (CCD ID: S40) (formula: $C_{23}H_{23}N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			30	23	3	3	1		
9	D	1	Total	C	N	O	S	0	0
			30	23	3	3	1		

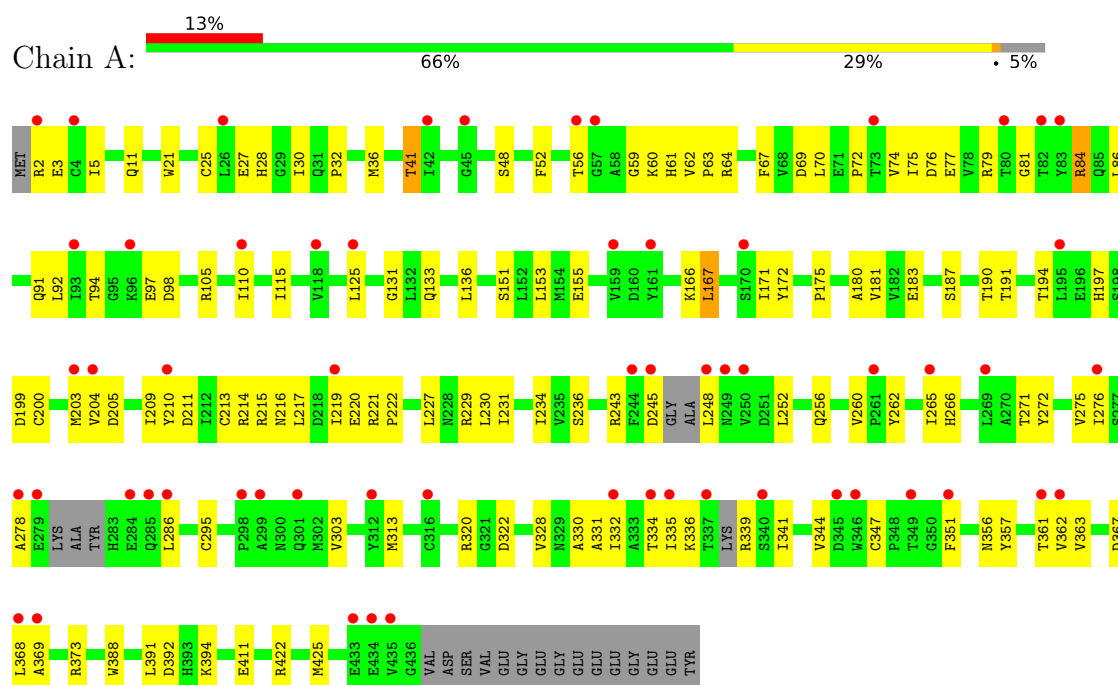
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total	O	0	0
			4	4		
10	B	7	Total	O	0	0
			7	7		
10	C	5	Total	O	0	0
			5	5		
10	D	4	Total	O	0	0
			4	4		

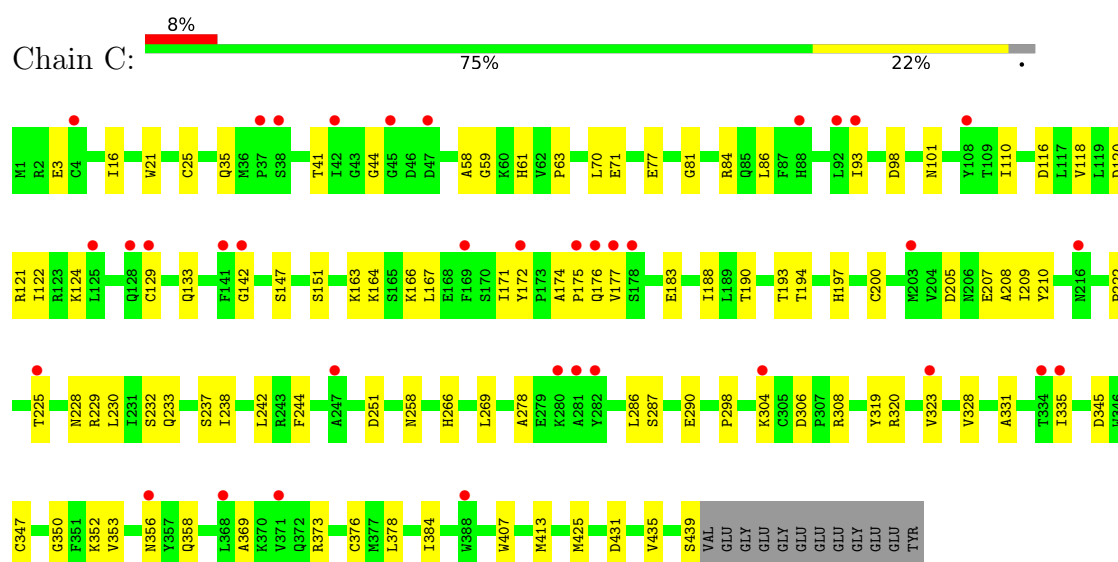
3 Residue-property plots [i](#)

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

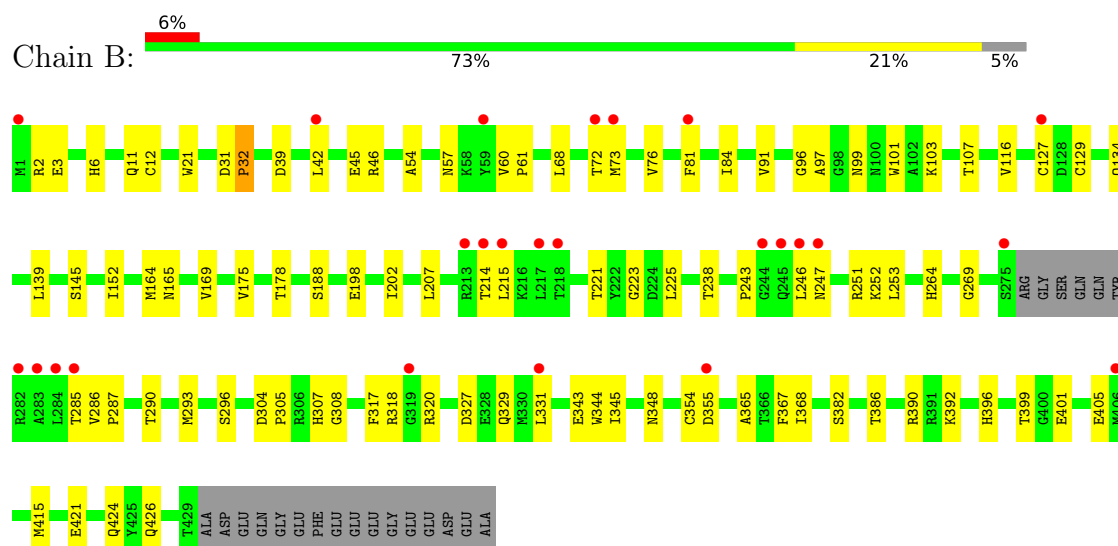
• Molecule 1: Tubulin alpha-1B chain



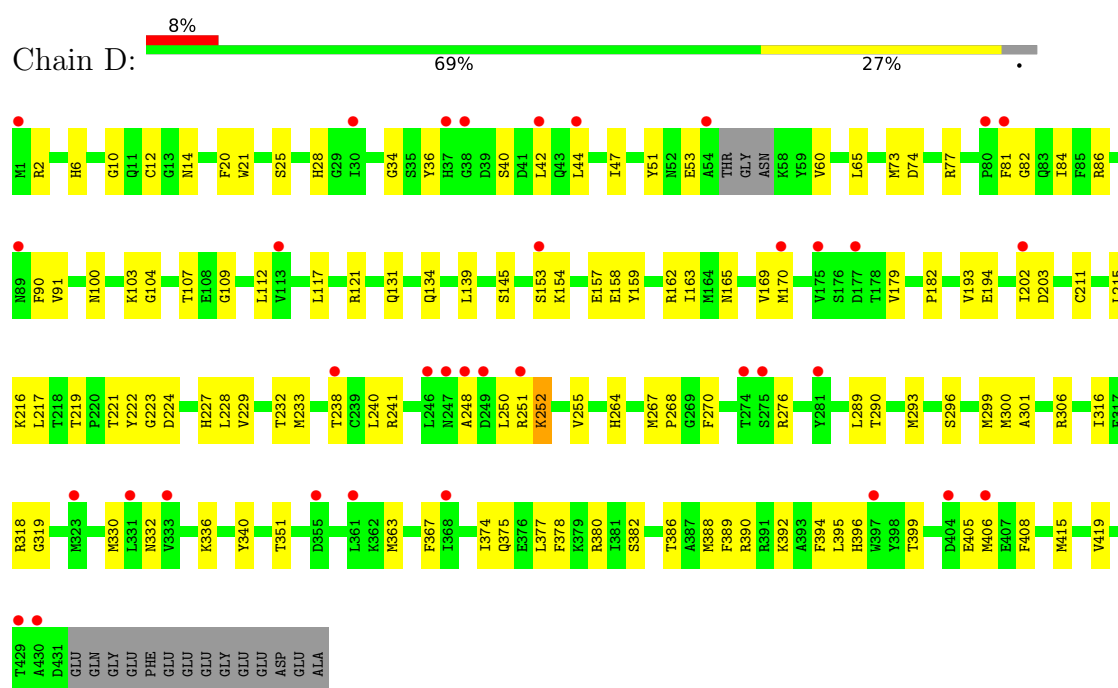
• Molecule 1: Tubulin alpha-1B chain



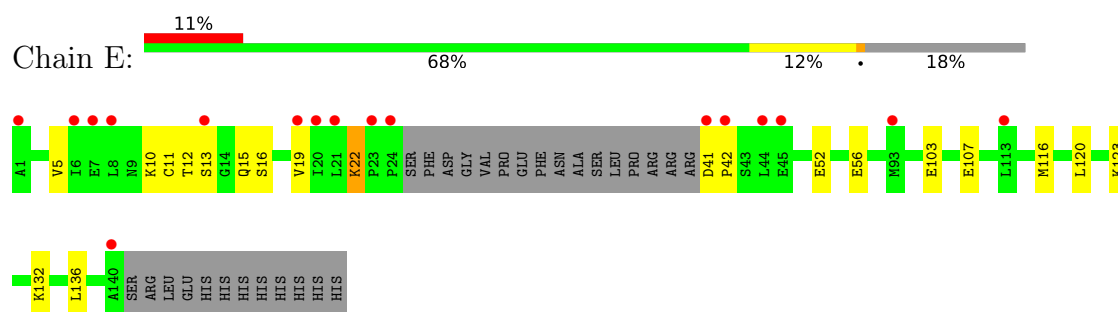
● Molecule 2: Tubulin beta chain



● Molecule 2: Tubulin beta chain



● Molecule 3: Stathmin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.68Å 102.20Å 131.50Å 90.00° 107.42° 90.00°	Depositor
Resolution (Å)	62.73 – 2.40 62.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (62.73-2.40) 99.3 (62.73-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.222 , 0.240 0.221 , 0.240	Depositor DCC
R_{free} test set	3935 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14402	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, GOL, MG, GDP, S40, GTP

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	0.36	0/3328	0.58	0/4532
1	C	0.24	0/3475	0.43	0/4726
2	B	0.41	1/3311 (0.0%)	0.58	0/4500
2	D	0.37	0/3378	0.52	0/4586
3	E	0.39	0/986	0.59	0/1315
All	All	0.35	1/14478 (0.0%)	0.53	0/19659

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	368	ILE	C-O	-5.05	1.18	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3255	0	3078	100	0
1	C	3397	0	3264	60	0
2	B	3239	0	3049	72	0
2	D	3305	0	3123	91	0
3	E	978	0	968	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	32	0	12	0	0
4	C	32	0	12	0	0
4	D	32	0	12	1	0
5	A	2	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
6	B	28	0	12	3	0
7	B	12	0	13	1	0
8	B	6	0	8	4	0
9	B	30	0	0	3	0
9	D	30	0	0	2	0
10	A	4	0	0	0	0
10	B	7	0	0	0	0
10	C	5	0	0	0	0
10	D	4	0	0	0	0
All	All	14402	0	13551	327	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 12.

All (327) 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:97:ALA:H	8:B:503:GOL:H2	1.17	1.06
2:D:157:GLU:HG3	3:E:120:LEU:HD13	1.39	1.02
1:A:70:LEU:HD13	1:A:110:ILE:HD13	1.43	0.99
1:A:70:LEU:HD13	1:A:110:ILE:CD1	1.92	0.99
2:D:157:GLU:CG	3:E:120:LEU:HD13	1.98	0.93
2:D:60:VAL:HG11	2:D:86:ARG:HG3	1.53	0.90
3:E:41:ASP:CB	3:E:42:PRO:CD	2.61	0.77
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.65	0.77
2:B:296:SER:OG	2:B:305:PRO:HD2	1.85	0.77
2:B:293:MET:HE2	2:B:365:ALA:HB1	1.66	0.75
1:A:70:LEU:CD1	1:A:110:ILE:HD11	2.17	0.74
1:A:70:LEU:CD1	1:A:110:ILE:CD1	2.66	0.73
1:A:27:GLU:OE2	1:A:243:ARG:NH1	2.24	0.71
1:A:79:ARG:HG3	1:A:92:LEU:HD12	1.72	0.71
2:D:53:GLU:O	2:D:53:GLU:HG3	1.89	0.71
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.73	0.71
3:E:41:ASP:CB	3:E:42:PRO:HD3	2.21	0.70
2:B:246:LEU:HD13	2:B:247:ASN:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD13	1:A:110:ILE:HD11	1.74	0.69
2:B:290:THR:HG21	2:B:329:GLN:HB3	1.75	0.69
2:D:229:VAL:HG12	2:D:233:MET:HE2	1.74	0.68
2:D:163:ILE:HD11	2:D:251:ARG:HG2	1.75	0.68
2:D:268:PRO:HG2	2:D:300:MET:HB2	1.75	0.68
2:B:238:THR:HG21	2:B:318:ARG:HD2	1.77	0.67
1:C:172:TYR:HB3	1:C:205:ASP:HB3	1.77	0.67
1:A:204:VAL:HG12	1:A:209:ILE:HD11	1.76	0.66
1:A:341:ILE:HD12	1:A:341:ILE:O	1.95	0.66
2:B:221:THR:HG22	2:B:223:GLY:H	1.59	0.66
1:A:77:GLU:O	1:A:81:GLY:N	2.29	0.66
2:B:97:ALA:N	8:B:503:GOL:H2	2.02	0.66
1:A:48:SER:HB2	1:A:245:ASP:H	1.61	0.65
2:B:293:MET:HE2	2:B:365:ALA:CB	2.26	0.65
1:A:11:GLN:HG3	1:A:74:VAL:HG11	1.78	0.65
2:D:139:LEU:HA	2:D:145:SER:HB2	1.77	0.65
3:E:5:VAL:HG22	3:E:19:VAL:HG12	1.79	0.65
1:A:265:ILE:HD12	1:A:313:MET:HE1	1.78	0.64
2:B:139:LEU:HA	2:B:145:SER:HB2	1.80	0.64
1:A:59:GLY:O	1:A:61:HIS:CE1	2.51	0.62
2:D:375:GLN:HB2	2:D:419:VAL:HG23	1.81	0.62
1:C:81:GLY:O	1:C:84:ARG:NH2	2.32	0.62
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.82	0.61
2:D:221:THR:O	2:D:224:ASP:N	2.34	0.61
2:B:2:ARG:HA	2:B:129:CYS:O	2.00	0.61
1:C:93:ILE:HG12	1:C:121:ARG:HH11	1.66	0.60
1:A:5:ILE:HG12	1:A:125:LEU:HD22	1.83	0.59
1:A:357:TYR:HD1	3:E:13:SER:HA	1.67	0.59
1:A:64:ARG:HB3	1:A:125:LEU:HD21	1.85	0.59
1:C:176:GLN:CB	1:C:207:GLU:OE1	2.51	0.59
2:D:44:LEU:HA	2:D:47:ILE:HB	1.84	0.59
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.83	0.59
2:B:221:THR:HG22	2:B:223:GLY:N	2.17	0.59
1:A:41:THR:O	1:A:41:THR:OG1	2.21	0.58
1:A:70:LEU:HD11	1:A:110:ILE:HD11	1.85	0.58
1:A:216:ASN:HD22	1:A:275:VAL:HG23	1.67	0.58
2:B:246:LEU:HD13	2:B:247:ASN:C	2.28	0.58
2:D:131:GLN:HB3	2:D:250:LEU:HD12	1.86	0.58
2:D:238:THR:HG21	2:D:318:ARG:HD2	1.86	0.58
2:B:285:THR:OG1	2:B:287:PRO:HD2	2.03	0.57
1:C:70:LEU:HD22	1:C:110:ILE:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:TYR:HB3	2:D:162:ARG:HG2	1.86	0.57
1:A:3:GLU:N	1:A:131:GLY:O	2.34	0.57
2:B:3:GLU:OE1	2:B:127:CYS:HB3	2.05	0.57
2:D:211:CYS:O	2:D:217:LEU:HB2	2.05	0.57
2:D:34:GLY:HA3	2:D:84:ILE:HD13	1.85	0.57
2:B:293:MET:CG	2:B:367:PHE:HB2	2.35	0.57
2:B:11:GLN:NE2	6:B:501:GDP:O1A	2.33	0.56
2:D:330:MET:HG3	2:D:351:THR:HG21	1.86	0.56
1:C:319:TYR:HB3	1:C:323:VAL:HG11	1.87	0.56
2:D:36:TYR:OH	2:D:40:SER:O	2.23	0.56
2:D:193:VAL:HG13	2:D:194:GLU:HG2	1.86	0.56
2:B:293:MET:HG3	2:B:367:PHE:HB2	1.88	0.56
2:D:10:GLY:O	2:D:14:ASN:ND2	2.25	0.55
1:A:320:ARG:HG2	1:A:356:ASN:HB3	1.88	0.55
1:C:133:GLN:HE22	1:C:242:LEU:HD22	1.72	0.55
1:A:332:ILE:HD11	1:A:351:PHE:CD1	2.41	0.55
2:B:421:GLU:HA	2:B:424:GLN:HB2	1.88	0.55
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.88	0.55
1:C:358:GLN:CD	1:C:358:GLN:H	2.15	0.55
1:A:56:THR:OG1	1:A:60:LYS:N	2.40	0.55
2:D:378:PHE:HD1	2:D:415:MET:HE2	1.72	0.55
2:D:134:GLN:HA	2:D:165:ASN:O	2.08	0.54
2:D:211:CYS:HB3	2:D:217:LEU:HD12	1.89	0.54
1:C:208:ALA:HB2	1:C:304:LYS:HG2	1.88	0.54
2:D:157:GLU:HG2	3:E:120:LEU:HD13	1.86	0.54
1:A:97:GLU:HA	2:B:2:ARG:HH11	1.73	0.54
2:D:228:LEU:O	2:D:232:THR:HG23	2.08	0.54
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.89	0.54
2:D:40:SER:OG	2:D:42:LEU:HD12	2.08	0.54
1:A:98:ASP:H	2:B:2:ARG:NH1	2.05	0.53
2:B:3:GLU:CD	2:B:127:CYS:HB3	2.33	0.53
2:D:77:ARG:O	2:D:82:GLY:HA3	2.08	0.53
1:A:98:ASP:H	2:B:2:ARG:HH11	1.56	0.53
1:A:236:SER:OG	1:A:320:ARG:NH1	2.41	0.53
2:D:219:THR:O	2:D:219:THR:OG1	2.25	0.53
1:A:187:SER:O	1:A:191:THR:HG23	2.09	0.53
1:A:204:VAL:HG11	1:A:231:ILE:HD12	1.91	0.53
2:B:293:MET:CE	2:B:365:ALA:HB1	2.38	0.53
1:A:166:LYS:NZ	1:A:197:HIS:O	2.42	0.52
1:A:278:ALA:N	1:A:367:ASP:O	2.40	0.52
1:C:269:LEU:HD23	1:C:384:ILE:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:MET:HE3	2:D:90:PHE:HB3	1.91	0.52
1:C:177:VAL:HG12	1:C:177:VAL:O	2.07	0.52
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.38	0.52
2:B:46:ARG:NH2	2:B:243:PRO:HA	2.24	0.52
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.91	0.52
2:B:308:GLY:HA2	2:B:426:GLN:HE21	1.75	0.52
3:E:11:CYS:SG	3:E:12:THR:N	2.82	0.52
1:A:229:ARG:HD3	1:A:363:VAL:HG11	1.91	0.52
2:B:253:LEU:HD22	9:B:504:S40:C4	2.39	0.51
1:C:233:GLN:OE1	1:C:320:ARG:NH2	2.43	0.51
2:D:296:SER:HA	2:D:299:MET:HG2	1.91	0.51
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.92	0.51
2:D:25:SER:OG	2:D:51:TYR:OH	2.28	0.51
2:D:44:LEU:C	2:D:44:LEU:HD12	2.35	0.51
1:A:171:ILE:HD13	1:A:204:VAL:HB	1.91	0.51
1:A:200:CYS:HA	1:A:266:HIS:HB2	1.91	0.51
1:A:260:VAL:HG12	1:A:262:TYR:O	2.11	0.51
1:A:213:CYS:O	1:A:217:LEU:HB2	2.11	0.51
2:B:72:THR:O	2:B:76:VAL:HG13	2.11	0.51
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.93	0.51
1:C:286:LEU:O	1:C:373:ARG:HD2	2.11	0.51
2:B:81:PHE:O	2:B:84:ILE:HG22	2.11	0.50
1:A:276:ILE:O	1:A:368:LEU:HD12	2.11	0.50
1:A:203:MET:HE1	1:A:388:TRP:CH2	2.47	0.50
1:C:237:SER:OG	1:C:376:CYS:HB3	2.11	0.50
1:C:133:GLN:OE1	1:C:251:ASP:HB2	2.12	0.50
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.30	0.50
2:D:170:MET:HG3	2:D:377:LEU:HD21	1.93	0.49
3:E:22:LYS:HB3	3:E:22:LYS:HZ2	1.76	0.49
2:B:343:GLU:H	2:B:343:GLU:CD	2.21	0.49
1:C:190:THR:O	1:C:194:THR:HG23	2.12	0.49
2:D:169:VAL:HA	2:D:202:ILE:O	2.13	0.49
1:A:115:ILE:HD11	1:A:153:LEU:HA	1.95	0.49
1:A:227:LEU:O	1:A:231:ILE:HG12	2.13	0.49
2:B:327:ASP:O	2:B:331:LEU:HD12	2.13	0.49
2:B:39:ASP:OD1	2:B:39:ASP:N	2.46	0.48
1:A:175:PRO:HG3	1:A:394:LYS:HZ1	1.79	0.48
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.49	0.48
2:D:227:HIS:HB2	2:D:276:ARG:HH12	1.78	0.48
1:C:41:THR:OG1	1:C:44:GLY:O	2.32	0.48
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:386:THR:O	2:D:390:ARG:HB2	2.14	0.48
1:A:190:THR:O	1:A:194:THR:HG23	2.12	0.48
1:C:101:ASN:ND2	2:D:252:LYS:HE2	2.28	0.48
2:D:221:THR:O	2:D:222:TYR:C	2.56	0.48
1:A:214:ARG:HA	1:A:219:ILE:HG22	1.96	0.48
2:D:28:HIS:NE2	2:D:241:ARG:HB3	2.29	0.48
1:A:344:VAL:HG13	1:A:347:CYS:HB2	1.96	0.48
2:B:54:ALA:HB2	2:B:60:VAL:HG23	1.96	0.48
2:D:117:LEU:HD11	2:D:154:LYS:HB3	1.96	0.47
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.48	0.47
2:D:240:LEU:HA	2:D:248:ALA:HB1	1.95	0.47
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.96	0.47
2:B:175:VAL:HG21	2:B:225:LEU:HD11	1.96	0.47
1:C:16:ILE:HD11	1:C:171:ILE:HD11	1.97	0.47
1:C:118:VAL:O	1:C:122:ILE:HG12	2.15	0.47
1:C:298:PRO:HG2	1:C:308:ARG:HH11	1.79	0.47
2:D:12:CYS:HB2	4:D:501:GTP:C8	2.50	0.47
2:D:267:MET:HG3	2:D:374:ILE:HD12	1.96	0.47
1:A:332:ILE:HG13	1:A:335:ILE:HD11	1.97	0.47
2:B:42:LEU:HA	2:B:45:GLU:HG3	1.96	0.47
1:C:287:SER:HG	1:C:290:GLU:H	1.58	0.47
2:B:91:VAL:HG11	2:B:116:VAL:HG22	1.97	0.47
2:D:290:THR:HA	2:D:293:MET:HE2	1.97	0.47
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.29	0.46
1:C:147:SER:O	1:C:151:SER:OG	2.26	0.46
1:A:136:LEU:HD23	1:A:167:LEU:HB3	1.97	0.46
1:C:258:ASN:ND2	1:C:352:LYS:HD3	2.30	0.46
1:C:304:LYS:HA	1:C:304:LYS:HD3	1.53	0.46
1:C:306:ASP:OD1	1:C:308:ARG:HB2	2.15	0.46
2:D:396:HIS:HA	2:D:399:THR:OG1	2.14	0.46
2:D:406:MET:HE2	2:D:406:MET:HB3	1.78	0.46
1:A:28:HIS:O	1:A:36:MET:HE3	2.15	0.46
1:A:204:VAL:CG1	1:A:209:ILE:HD11	2.44	0.46
1:A:271:THR:HG21	1:A:295:CYS:HA	1.96	0.46
2:B:286:VAL:O	2:B:290:THR:HG22	2.16	0.46
2:D:74:ASP:N	2:D:74:ASP:OD2	2.47	0.46
1:A:262:TYR:H	1:A:265:ILE:HD11	1.80	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.34	0.46
1:A:234:ILE:HG12	1:A:272:TYR:HB2	1.98	0.46
2:B:344:TRP:CD1	2:B:344:TRP:H	2.32	0.46
2:D:104:GLY:O	2:D:109:GLY:HA3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLU:OE2	1:A:220:GLU:N	2.40	0.46
1:A:330:ALA:O	1:A:334:THR:HG23	2.16	0.46
1:C:331:ALA:O	1:C:335:ILE:HD13	2.16	0.46
2:D:179:VAL:HG11	2:D:394:PHE:CE2	2.51	0.46
2:B:396:HIS:HA	2:B:399:THR:OG1	2.16	0.46
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.97	0.45
1:C:320:ARG:HA	1:C:356:ASN:O	2.15	0.45
1:A:203:MET:HE1	1:A:388:TRP:CZ2	2.51	0.45
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.98	0.45
1:A:335:ILE:HD12	1:A:336:LYS:N	2.31	0.45
1:C:120:ASP:O	1:C:124:LYS:HG3	2.17	0.45
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.51	0.45
2:D:232:THR:HG22	2:D:270:PHE:HB2	1.98	0.45
1:A:214:ARG:CZ	1:A:215:ARG:HG2	2.46	0.45
1:A:328:VAL:HA	1:A:331:ALA:HB3	1.97	0.45
2:B:73:MET:O	2:B:76:VAL:HG22	2.17	0.45
2:B:101:TRP:HE1	2:B:188:SER:HB3	1.82	0.45
1:C:225:THR:HA	1:C:228:ASN:HB2	1.99	0.45
3:E:10:LYS:HA	3:E:15:GLN:HA	1.97	0.45
2:B:269:GLY:HA3	2:B:367:PHE:HB3	1.97	0.45
2:B:198:GLU:HA	2:B:264:HIS:HB2	1.99	0.45
2:D:306:ARG:HD2	2:D:340:TYR:CE2	2.52	0.45
2:B:96:GLY:HA3	8:B:503:GOL:H12	1.99	0.45
1:C:41:THR:OG1	1:C:41:THR:O	2.35	0.45
2:D:34:GLY:HA3	2:D:84:ILE:CD1	2.47	0.44
2:D:221:THR:HG23	2:D:224:ASP:H	1.81	0.44
1:A:69:ASP:O	1:A:94:THR:HA	2.16	0.44
2:B:99:ASN:HB3	2:B:178:THR:HG21	1.99	0.44
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.53	0.44
1:C:35:GLN:NE2	1:C:58:ALA:O	2.51	0.44
1:A:221:ARG:NH1	2:B:327:ASP:OD2	2.50	0.44
1:C:25:CYS:SG	1:C:86:LEU:HD21	2.58	0.44
1:A:213:CYS:HB3	1:A:217:LEU:HD22	2.00	0.44
2:D:154:LYS:HA	2:D:154:LYS:HD2	1.66	0.44
1:A:81:GLY:O	1:A:84:ARG:HB3	2.16	0.44
2:B:61:PRO:HD3	2:B:84:ILE:HG12	1.98	0.44
1:C:347:CYS:SG	1:C:350:GLY:HA2	2.58	0.44
2:D:250:LEU:HD23	9:D:503:S40:C4	2.47	0.44
1:A:322:ASP:O	1:A:373:ARG:HD3	2.18	0.44
2:B:214:THR:C	2:B:215:LEU:HD12	2.42	0.44
2:B:68:LEU:HD12	2:B:97:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:ASP:OD1	1:C:439:SER:OG	2.32	0.43
3:E:103:GLU:O	3:E:107:GLU:HG3	2.18	0.43
1:A:216:ASN:HD22	1:A:275:VAL:CG2	2.30	0.43
2:D:2:ARG:HB3	2:D:131:GLN:NE2	2.33	0.43
1:A:362:VAL:HG21	1:A:368:LEU:O	2.18	0.43
1:C:229:ARG:O	1:C:232:SER:OG	2.34	0.43
2:D:182:PRO:HG2	2:D:388:MET:HE1	1.99	0.43
2:D:221:THR:C	2:D:223:GLY:N	2.76	0.43
2:D:389:PHE:HE1	2:D:395:LEU:HD11	1.83	0.43
1:A:392:ASP:HB3	1:A:422:ARG:NH2	2.33	0.43
1:C:151:SER:HB3	1:C:193:THR:OG1	2.19	0.43
1:A:203:MET:HG3	1:A:303:VAL:HG21	2.00	0.43
2:B:318:ARG:HA	2:B:354:CYS:O	2.18	0.43
2:B:392:LYS:HE3	2:B:405:GLU:CD	2.43	0.43
2:D:91:VAL:HG12	2:D:112:LEU:HD12	2.00	0.43
1:A:32:PRO:O	1:A:86:LEU:CD1	2.66	0.43
1:A:72:PRO:HA	1:A:94:THR:HG21	1.99	0.43
1:A:181:VAL:HG11	9:B:504:S40:C45	2.49	0.43
2:B:320:ARG:HA	2:B:355:ASP:OD1	2.18	0.43
2:D:238:THR:OG1	2:D:316:ILE:HG21	2.19	0.43
1:A:2:ARG:O	1:A:133:GLN:NE2	2.38	0.43
2:B:345:ILE:HG22	2:B:348:ASN:HB3	2.01	0.43
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.18	0.43
2:D:389:PHE:CE1	2:D:395:LEU:HD11	2.54	0.43
2:B:11:GLN:HB3	6:B:501:GDP:O1A	2.18	0.43
2:D:100:ASN:HB3	2:D:103:LYS:HD2	2.00	0.43
2:D:382:SER:O	2:D:386:THR:HG23	2.18	0.43
1:A:84:ARG:HB3	1:A:84:ARG:HE	1.65	0.42
1:A:175:PRO:HG3	1:A:394:LYS:NZ	2.34	0.42
1:C:166:LYS:HE2	1:C:197:HIS:O	2.19	0.42
1:A:62:VAL:HG13	1:A:86:LEU:O	2.19	0.42
1:A:151:SER:O	1:A:155:GLU:HG2	2.18	0.42
2:B:107:THR:OG1	2:B:401:GLU:OE1	2.23	0.42
2:B:202:ILE:HG22	2:B:207:LEU:HD11	2.02	0.42
2:B:382:SER:HB2	2:B:415:MET:HE3	2.01	0.42
2:D:216:LYS:HD3	2:D:216:LYS:HA	1.93	0.42
1:A:52:PHE:C	1:A:64:ARG:HG3	2.45	0.42
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.81	0.42
2:B:152:ILE:HG13	2:B:164:MET:SD	2.59	0.42
2:B:293:MET:HE1	2:B:317:PHE:CZ	2.55	0.42
2:D:153:SER:OG	3:E:120:LEU:CD2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASP:HA	1:A:79:ARG:HB2	2.02	0.42
3:E:132:LYS:HZ2	3:E:136:LEU:HD11	1.84	0.42
2:B:253:LEU:HD22	9:B:504:S40:C5	2.49	0.42
1:C:238:ILE:HG12	1:C:378:LEU:HD11	2.01	0.42
2:D:203:ASP:CG	2:D:380:ARG:HH22	2.27	0.42
3:E:10:LYS:HB3	3:E:10:LYS:HE3	1.67	0.42
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.54	0.42
2:B:386:THR:O	2:B:390:ARG:HB2	2.20	0.42
1:C:358:GLN:CD	1:C:358:GLN:N	2.78	0.42
1:C:431:ASP:O	1:C:435:VAL:HG13	2.20	0.42
2:D:332:ASN:O	2:D:336:LYS:HG3	2.19	0.42
3:E:52:GLU:O	3:E:56:GLU:HG2	2.19	0.42
1:A:25:CYS:O	1:A:30:ILE:N	2.41	0.42
1:A:52:PHE:O	1:A:64:ARG:HG3	2.20	0.42
1:A:388:TRP:CE3	1:A:425:MET:HE1	2.55	0.42
1:C:174:ALA:HA	1:C:175:PRO:HD2	1.81	0.42
1:A:67:PHE:HB3	1:A:75:ILE:CD1	2.50	0.41
1:A:204:VAL:HG11	1:A:231:ILE:CD1	2.50	0.41
2:D:193:VAL:O	2:D:264:HIS:HE1	2.03	0.41
2:D:139:LEU:HD12	2:D:170:MET:SD	2.60	0.41
2:D:81:PHE:O	2:D:84:ILE:HG22	2.20	0.41
1:C:77:GLU:O	1:C:81:GLY:N	2.54	0.41
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.56	0.41
1:A:286:LEU:O	1:A:373:ARG:NH2	2.54	0.41
1:A:361:THR:HG22	1:A:362:VAL:H	1.86	0.41
2:D:240:LEU:HG	9:D:503:S40:C7	2.50	0.41
2:D:319:GLY:HA3	2:D:363:MET:HE2	2.02	0.41
1:A:151:SER:HA	1:A:194:THR:HG22	2.03	0.41
1:A:248:LEU:HB2	3:E:16:SER:HB2	2.03	0.41
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.03	0.41
2:B:134:GLN:HA	2:B:165:ASN:O	2.20	0.41
1:C:163:LYS:O	1:C:164:LYS:C	2.64	0.41
2:D:293:MET:CG	2:D:367:PHE:HB2	2.47	0.41
2:D:299:MET:HE1	2:D:367:PHE:CE1	2.56	0.41
1:A:63:PRO:O	1:A:91:GLN:NE2	2.52	0.41
1:A:105:ARG:NH1	1:A:411:GLU:OE2	2.52	0.41
1:C:200:CYS:HA	1:C:266:HIS:HB2	2.02	0.41
2:D:221:THR:O	2:D:223:GLY:N	2.54	0.41
2:B:169:VAL:HA	2:B:202:ILE:O	2.21	0.41
2:B:251:ARG:NH1	7:B:502:MES:O3S	2.47	0.41
1:C:147:SER:HB2	1:C:190:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:TRP:CD2	2:D:255:VAL:HG22	2.56	0.41
2:D:121:ARG:HE	2:D:158:GLU:CD	2.28	0.41
2:D:202:ILE:HG21	2:D:229:VAL:HG22	2.03	0.41
2:D:268:PRO:HA	2:D:367:PHE:O	2.21	0.41
2:D:289:LEU:O	2:D:293:MET:HB2	2.20	0.41
1:A:199:ASP:HB3	1:A:256:GLN:CD	2.46	0.41
1:A:211:ASP:O	1:A:215:ARG:HG3	2.21	0.41
1:A:248:LEU:HB2	3:E:16:SER:CB	2.50	0.41
2:B:61:PRO:CD	2:B:84:ILE:HG12	2.51	0.40
2:D:20:PHE:HB2	2:D:233:MET:HE3	2.03	0.40
2:D:65:LEU:O	2:D:73:MET:HE1	2.21	0.40
2:D:203:ASP:HB2	2:D:301:ALA:HA	2.03	0.40
2:D:392:LYS:HB2	2:D:392:LYS:HE3	1.92	0.40
2:B:96:GLY:CA	8:B:503:GOL:H12	2.51	0.40
1:C:3:GLU:CD	1:C:129:CYS:HB3	2.46	0.40
1:C:59:GLY:O	1:C:61:HIS:ND1	2.54	0.40
2:B:12:CYS:HB2	6:B:501:GDP:C8	2.56	0.40
2:D:103:LYS:HA	2:D:107:THR:OG1	2.21	0.40
2:D:162:ARG:HA	2:D:162:ARG:HD2	1.95	0.40
1:A:214:ARG:HG3	1:A:215:ARG:N	2.36	0.40
1:C:413:MET:HB3	1:C:413:MET:HE2	1.87	0.40
2:D:405:GLU:O	2:D:408:PHE:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	421/451 (93%)	402 (96%)	19 (4%)	0	100	100
1	C	437/451 (97%)	417 (95%)	20 (5%)	0	100	100
2	B	419/445 (94%)	401 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
3	E	120/152 (79%)	117 (98%)	3 (2%)	0	100	100
All	All	1821/1944 (94%)	1751 (96%)	70 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/379 (89%)	332 (99%)	4 (1%)	63	81
1	C	361/379 (95%)	360 (100%)	1 (0%)	86	93
2	B	347/383 (91%)	343 (99%)	4 (1%)	63	81
2	D	351/383 (92%)	350 (100%)	1 (0%)	86	93
3	E	100/136 (74%)	97 (97%)	3 (3%)	36	58
All	All	1495/1660 (90%)	1482 (99%)	13 (1%)	70	85

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	84	ARG
1	A	167	LEU
1	A	339	ARG
2	B	32	PRO
2	B	57	ASN
2	B	103	LYS
2	B	252	LYS
1	C	116	ASP
2	D	252	LYS
3	E	22	LYS
3	E	116	MET
3	E	123	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	ASN
1	C	50	ASN
1	C	329	ASN
2	D	15	GLN
2	D	99	ASN
2	D	329	GLN
2	D	337	ASN
3	E	15	GLN
3	E	61	GLN
3	E	75	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GTP	C	501	5	33,34,34	1.18	3 (9%)	50,54,54	1.59	9 (18%)
8	GOL	B	503	-	5,5,5	0.13	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GTP	D	501	5	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
9	S40	B	504	-	33,33,33	2.18	8 (24%)	47,47,47	2.93	7 (14%)
6	GDP	B	501	-	29,30,30	1.39	5 (17%)	45,47,47	1.89	8 (17%)
9	S40	D	503	-	33,33,33	2.18	8 (24%)	47,47,47	2.93	7 (14%)
4	GTP	A	501	5	33,34,34	1.08	4 (12%)	50,54,54	1.56	8 (16%)
7	MES	B	502	-	12,12,12	0.71	0	15,16,16	0.29	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
4	GTP	C	501	5	-	7/22/38/38	0/3/3/3
8	GOL	B	503	-	-	2/4/4/4	-
4	GTP	D	501	5	-	9/22/38/38	0/3/3/3
9	S40	B	504	-	-	0/24/26/26	0/4/4/4
6	GDP	B	501	-	-	5/16/32/32	0/3/3/3
9	S40	D	503	-	-	2/24/26/26	0/4/4/4
4	GTP	A	501	5	-	8/22/38/38	0/3/3/3
7	MES	B	502	-	-	5/6/14/14	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	503	S40	C9-N8	6.15	1.47	1.33
9	B	504	S40	C9-N8	6.15	1.47	1.33
9	B	504	S40	S17-N16	5.77	1.72	1.63
9	D	503	S40	S17-N16	5.76	1.72	1.63
9	D	503	S40	C18-S17	4.75	1.83	1.76
9	B	504	S40	C18-S17	4.75	1.83	1.76
9	B	504	S40	O27-S17	3.22	1.47	1.43
9	D	503	S40	O28-S17	3.21	1.47	1.43
4	C	501	GTP	PB-O3A	-3.20	1.56	1.59
9	D	503	S40	O27-S17	3.18	1.47	1.43
9	B	504	S40	O28-S17	3.14	1.47	1.43
9	B	504	S40	C12-N16	2.94	1.47	1.42
9	D	503	S40	C12-N16	2.90	1.47	1.42
6	B	501	GDP	PA-O3A	2.87	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	501	GDP	C6-N1	-2.82	1.33	1.38
4	C	501	GTP	C2-N3	2.73	1.39	1.33
6	B	501	GDP	C5-C4	2.67	1.46	1.38
4	A	501	GTP	PB-O3B	2.59	1.62	1.59
4	A	501	GTP	PA-O3A	2.58	1.62	1.59
4	C	501	GTP	PA-O3A	2.56	1.62	1.59
6	B	501	GDP	PB-O2B	-2.54	1.45	1.54
6	B	501	GDP	C5-N7	-2.53	1.34	1.39
4	A	501	GTP	PB-O3A	2.27	1.62	1.59
4	A	501	GTP	C2-N3	2.21	1.38	1.33
9	D	503	S40	C10-C9	2.17	1.55	1.50
4	D	501	GTP	C2-N3	2.16	1.38	1.33
9	B	504	S40	C10-C9	2.14	1.54	1.50
9	D	503	S40	C46-C44	2.10	1.56	1.49
9	B	504	S40	C46-C44	2.09	1.56	1.49

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	503	S40	O28-S17-O27	-15.08	101.21	119.52
9	B	504	S40	O28-S17-O27	-15.05	101.25	119.52
9	B	504	S40	C46-C44-C21	7.68	131.78	121.28
9	D	503	S40	C46-C44-C21	7.66	131.75	121.28
9	B	504	S40	C45-C44-C21	6.84	130.63	121.28
9	D	503	S40	C45-C44-C21	6.81	130.58	121.28
6	B	501	GDP	C5-C4-N3	-6.19	118.53	128.39
6	B	501	GDP	C2-N3-C4	5.36	121.53	112.30
4	D	501	GTP	C5-C4-N3	-4.97	120.49	128.39
4	C	501	GTP	C5-C4-N3	-4.88	120.62	128.39
6	B	501	GDP	N9-C4-N3	4.74	135.44	125.95
4	A	501	GTP	C5-C4-N3	-4.67	120.96	128.39
4	D	501	GTP	C2-N3-C4	4.66	120.33	112.30
4	A	501	GTP	C2-N3-C4	4.61	120.25	112.30
4	C	501	GTP	C2-N3-C4	4.37	119.82	112.30
4	D	501	GTP	N9-C4-N3	3.11	132.17	125.95
6	B	501	GDP	C6-C5-N7	3.10	135.94	130.29
6	B	501	GDP	O6-C6-C5	-3.02	118.55	126.53
4	C	501	GTP	N9-C4-N3	2.94	131.83	125.95
4	C	501	GTP	N9-C8-N7	-2.93	107.97	113.40
4	A	501	GTP	N9-C4-N3	2.90	131.75	125.95
4	C	501	GTP	C8-N7-C5	2.83	109.30	104.26
4	D	501	GTP	C2-N1-C6	-2.82	120.00	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GTP	N9-C8-N7	-2.75	108.30	113.40
4	A	501	GTP	C2-N1-C6	-2.71	120.19	125.11
9	B	504	S40	C18-S17-N16	2.71	110.24	106.88
9	D	503	S40	C18-S17-N16	2.71	110.24	106.88
4	D	501	GTP	N9-C8-N7	-2.70	108.39	113.40
9	D	503	S40	O27-S17-C18	2.68	111.36	107.98
9	B	504	S40	C14-C13-C12	2.65	119.98	117.50
4	C	501	GTP	C2-N1-C6	-2.64	120.33	125.11
9	B	504	S40	O27-S17-C18	2.64	111.31	107.98
9	D	503	S40	C14-C13-C12	2.63	119.96	117.50
4	C	501	GTP	C5-C6-N1	2.62	119.92	113.25
9	B	504	S40	O28-S17-C18	2.62	111.28	107.98
4	D	501	GTP	C8-N7-C5	2.58	108.86	104.26
9	D	503	S40	O28-S17-C18	2.57	111.23	107.98
4	A	501	GTP	C8-N7-C5	2.53	108.76	104.26
4	D	501	GTP	C5-C6-N1	2.49	119.58	113.25
4	A	501	GTP	C5-C6-N1	2.45	119.50	113.25
6	B	501	GDP	C4-C5-N7	-2.39	106.88	110.67
4	A	501	GTP	O6-C6-C5	-2.34	120.36	126.53
4	D	501	GTP	O6-C6-C5	-2.33	120.38	126.53
4	C	501	GTP	O2B-PB-O3A	2.12	113.01	107.27
6	B	501	GDP	C8-N7-C5	2.10	108.00	104.26
6	B	501	GDP	C5-C6-N1	2.09	118.56	113.25
4	C	501	GTP	O6-C6-C5	-2.04	121.16	126.53

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	C	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	C5'-O5'-PA-O3A
4	C	501	GTP	C5'-O5'-PA-O1A
4	C	501	GTP	C5'-O5'-PA-O2A
4	D	501	GTP	PB-O3B-PG-O3G
4	D	501	GTP	C5'-O5'-PA-O3A
4	D	501	GTP	C5'-O5'-PA-O1A
4	D	501	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O1A
7	B	502	MES	C7-C8-S-O2S

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Mol	Chain	Res	Type	Atoms
7	B	502	MES	C7-C8-S-O3S
8	B	503	GOL	O1-C1-C2-C3
7	B	502	MES	C8-C7-N4-C3
7	B	502	MES	C8-C7-N4-C5
7	B	502	MES	C7-C8-S-O1S
4	A	501	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O2A
8	B	503	GOL	O1-C1-C2-O2
9	D	503	S40	C20-C21-C44-C45
9	D	503	S40	C22-C21-C44-C45
4	A	501	GTP	PB-O3A-PA-O2A
4	D	501	GTP	PB-O3A-PA-O2A
4	A	501	GTP	C4'-C5'-O5'-PA
4	C	501	GTP	C4'-C5'-O5'-PA
6	B	501	GDP	PB-O3A-PA-O2A
4	D	501	GTP	C4'-C5'-O5'-PA
4	A	501	GTP	PB-O3B-PG-O2G
4	D	501	GTP	PB-O3B-PG-O2G
4	C	501	GTP	PB-O3A-PA-O1A
4	C	501	GTP	PB-O3A-PA-O2A
4	D	501	GTP	PB-O3A-PA-O1A
4	D	501	GTP	PB-O3B-PG-O1G
4	A	501	GTP	C3'-C4'-C5'-O5'
4	A	501	GTP	PB-O3A-PA-O1A
6	B	501	GDP	PB-O3A-PA-O1A

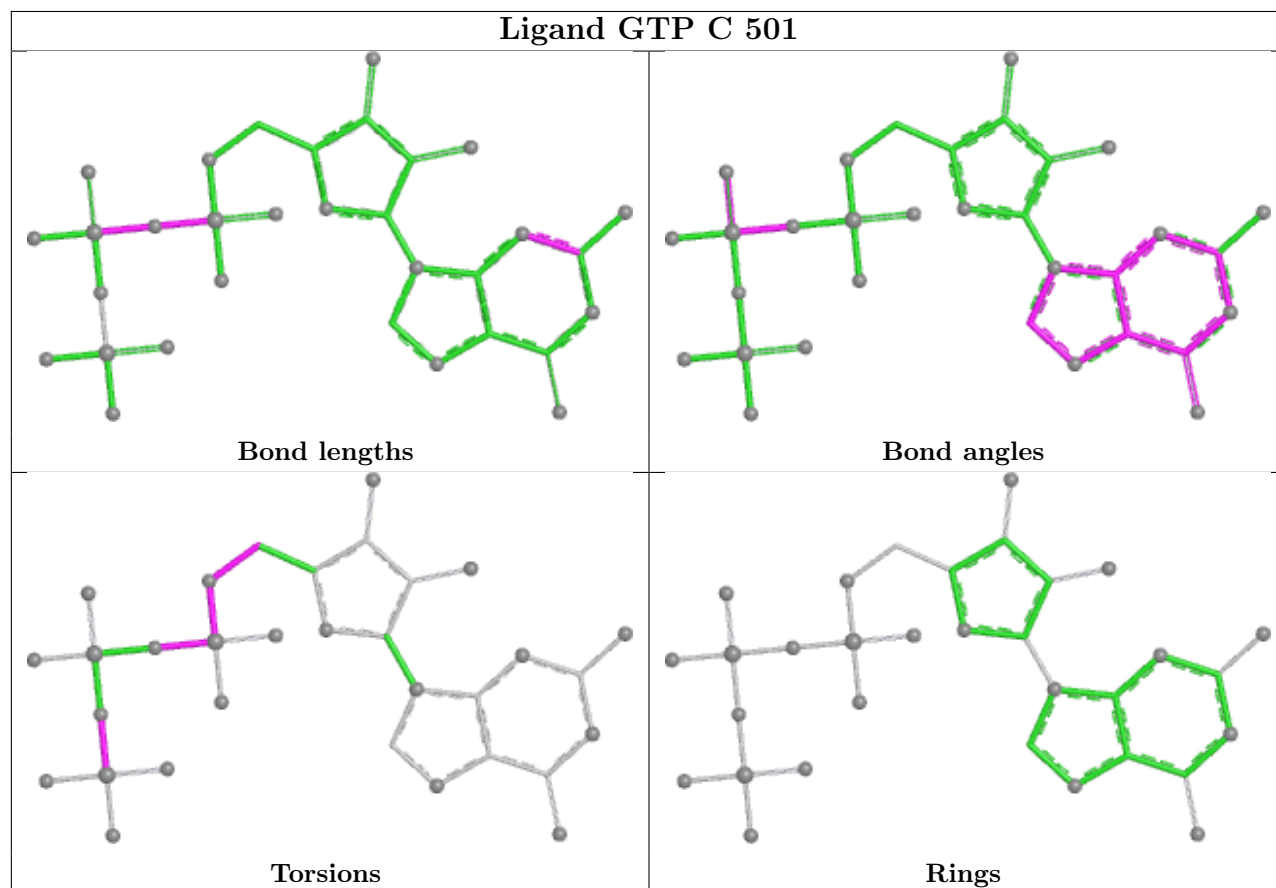
There are no ring outliers.

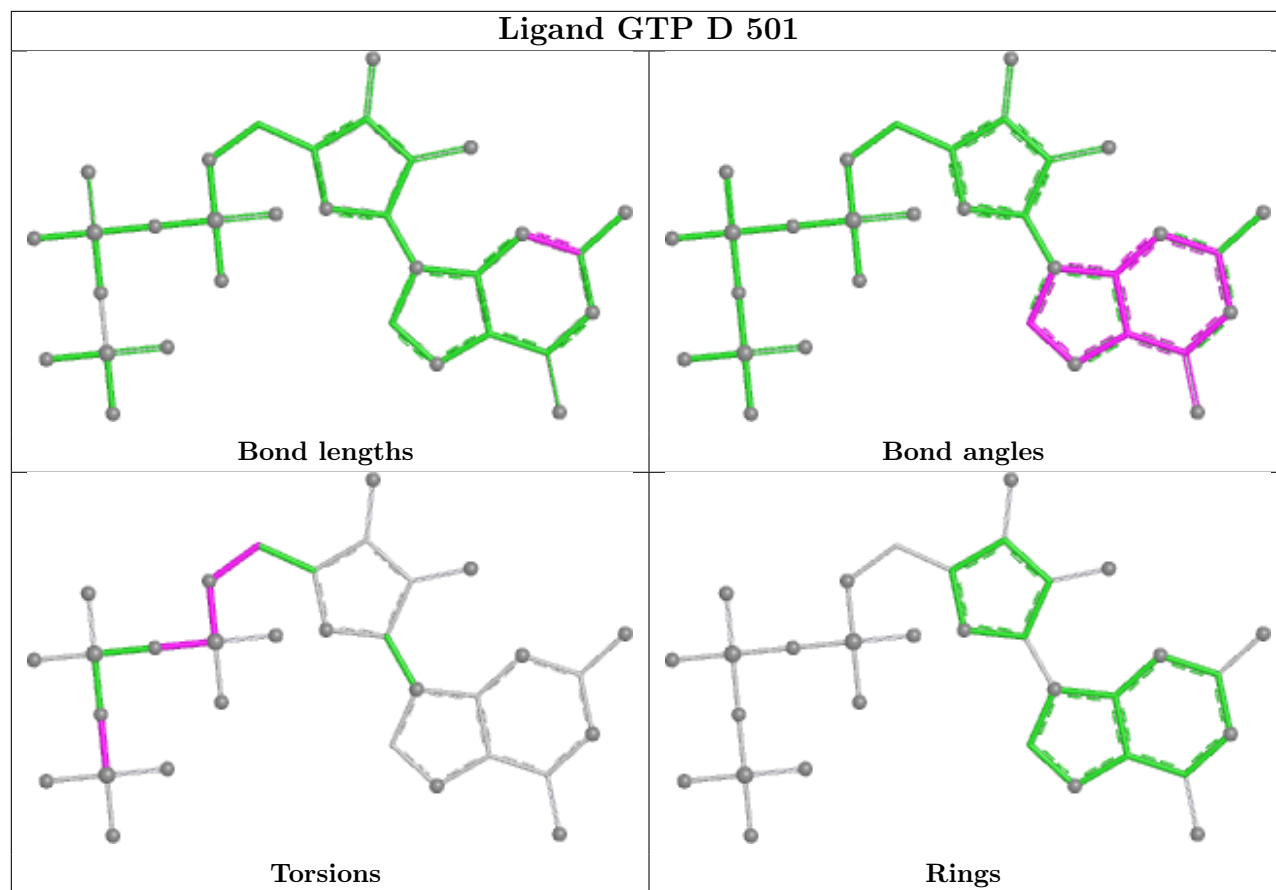
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	503	GOL	4	0
4	D	501	GTP	1	0
9	B	504	S40	3	0
6	B	501	GDP	3	0
9	D	503	S40	2	0
7	B	502	MES	1	0

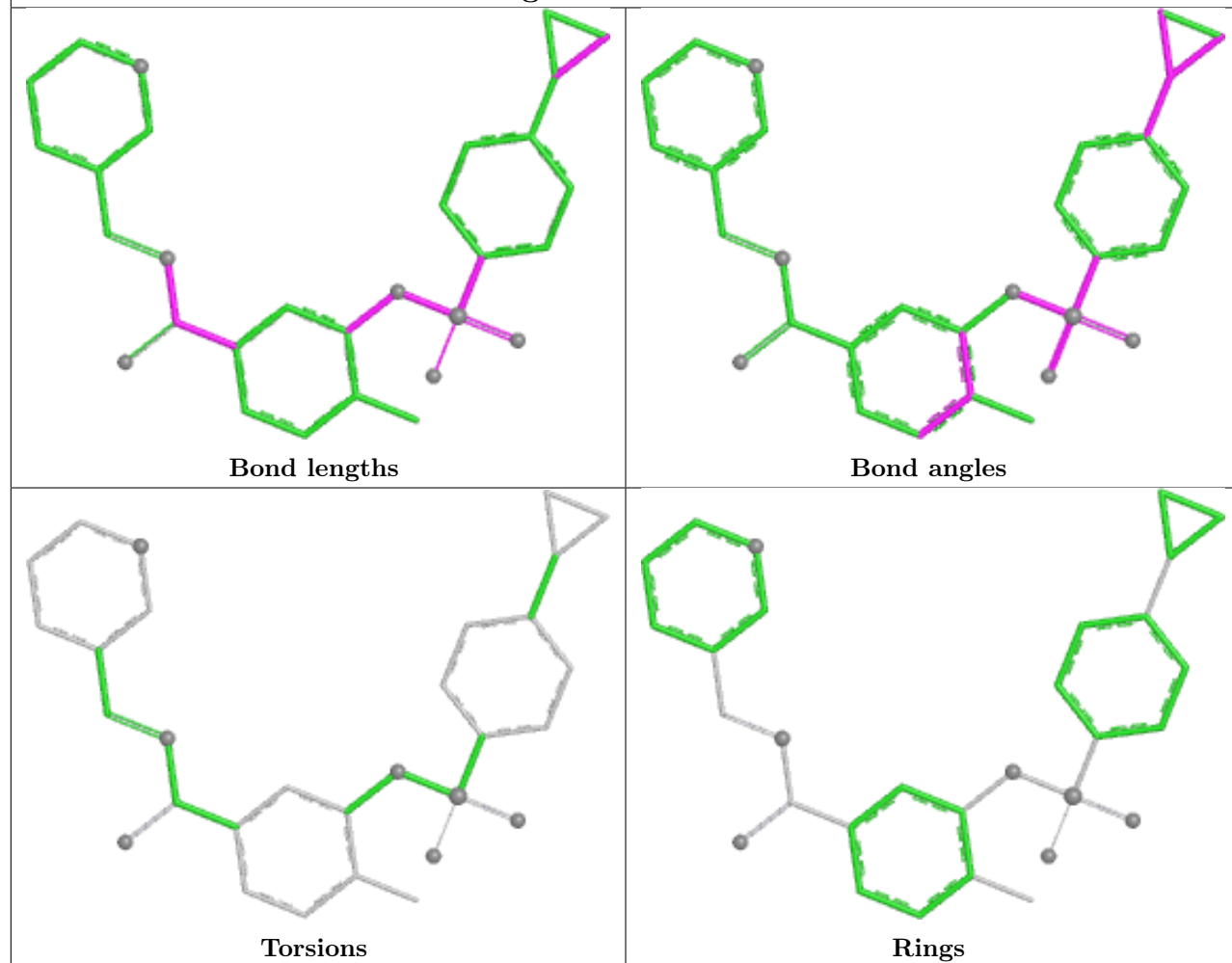
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

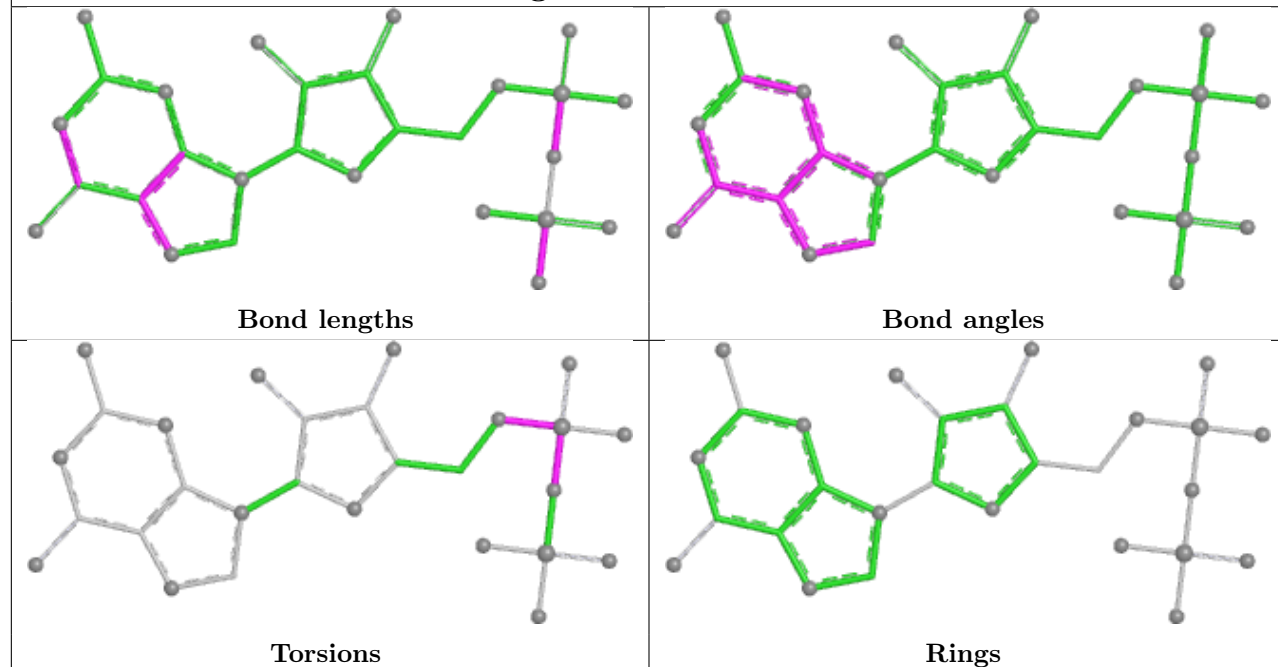




Ligand S40 B 504



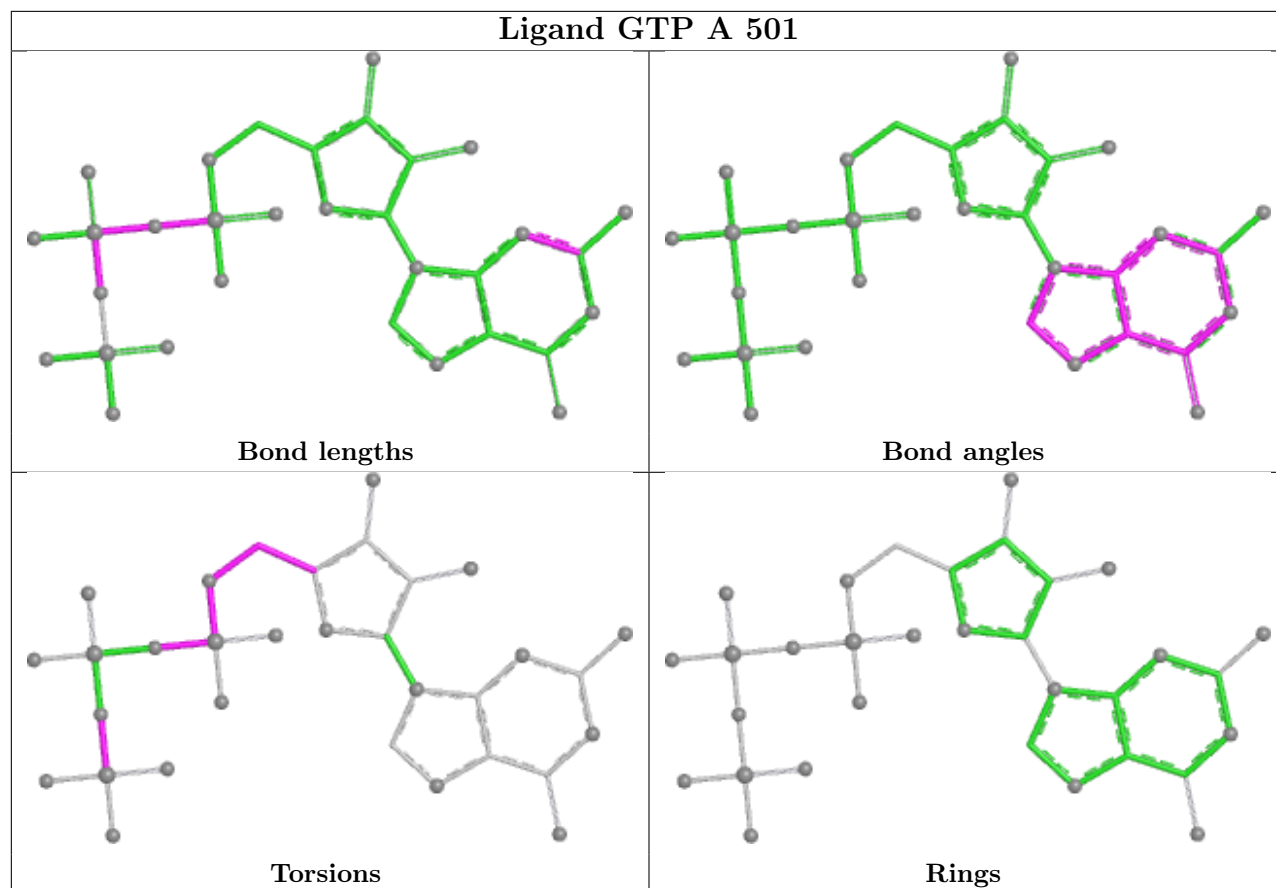
Ligand GDP B 501



Ligand S40 D 503

The figure displays four panels of structural data for Ligand S40 D 503, which is a complex organic molecule featuring a central benzene ring substituted with a cyclopropylmethyl group, a 2-(cyclohexylmethyl)ethyl group, and a 2-(cyclohexylmethyl)ethyl group. The panels are:

- Bond lengths:** A 3D ball-and-stick model where bond lengths are highlighted in green.
- Bond angles:** A 3D ball-and-stick model where bond angles are highlighted in green.
- Torsions:** A 3D ball-and-stick model where torsion angles are highlighted in green.
- Rings:** A 3D ball-and-stick model where the rings are highlighted in green.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	429/451 (95%)	1.18	59 (13%) 6 5	64, 93, 114, 136	0
1	C	439/451 (97%)	0.89	36 (8%) 17 14	55, 74, 100, 126	0
2	B	423/445 (95%)	0.84	25 (5%) 28 24	57, 75, 99, 121	0
2	D	428/445 (96%)	0.90	36 (8%) 17 14	57, 79, 105, 119	0
3	E	124/152 (81%)	1.00	17 (13%) 6 5	67, 84, 116, 129	0
All	All	1843/1944 (94%)	0.96	173 (9%) 14 11	55, 80, 109, 136	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	177	VAL	6.0
1	A	245	ASP	5.1
2	B	214	THR	5.0
3	E	1	ALA	4.9
3	E	41	ASP	4.9
2	D	247	ASN	4.8
1	A	82	THR	4.6
2	D	54	ALA	4.5
2	D	248	ALA	4.3
2	B	319	GLY	4.2
2	B	217	LEU	4.1
1	A	337	THR	4.1
2	D	246	LEU	3.9
1	A	351	PHE	3.6
1	C	172	TYR	3.6
3	E	24	PRO	3.5
1	A	4	CYS	3.4
2	B	246	LEU	3.4
1	A	57	GLY	3.3
1	A	244	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	178	SER	3.2
1	A	26	LEU	3.2
1	C	280	LYS	3.2
2	D	406	MET	3.2
1	A	249	ASN	3.2
2	B	275	SER	3.1
1	A	118	VAL	3.1
2	B	244	GLY	3.1
1	C	4	CYS	3.0
2	D	397	TRP	3.0
1	A	2	ARG	3.0
2	B	245	GLN	3.0
1	A	250	VAL	3.0
1	A	279	GLU	3.0
2	B	215	LEU	3.0
2	D	44	LEU	3.0
1	A	362	VAL	2.9
2	B	1	MET	2.9
2	B	72	THR	2.9
1	C	42	ILE	2.9
1	C	247	ALA	2.9
2	D	81	PHE	2.9
2	B	284	LEU	2.8
1	C	47	ASP	2.8
2	B	283	ALA	2.7
2	D	1	MET	2.7
1	C	141	PHE	2.7
1	A	83	TYR	2.7
1	C	128	GLN	2.7
1	C	88	HIS	2.7
1	C	334	THR	2.7
3	E	140	ALA	2.7
3	E	44	LEU	2.7
1	A	269	LEU	2.6
1	A	369	ALA	2.6
2	D	249	ASP	2.6
1	A	335	ILE	2.6
2	B	218	THR	2.6
2	D	404	ASP	2.6
1	C	368	LEU	2.6
3	E	8	LEU	2.6
2	D	38	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	170	MET	2.5
1	A	332	ILE	2.5
1	A	368	LEU	2.5
2	D	361	LEU	2.5
1	C	142	GLY	2.5
1	A	265	ILE	2.5
1	C	304	LYS	2.5
2	B	213	ARG	2.5
2	D	30	ILE	2.5
1	C	282	TYR	2.5
3	E	21	LEU	2.5
1	A	346	TRP	2.5
2	B	282	ARG	2.5
1	A	361	THR	2.5
1	A	345	ASP	2.4
2	B	355	ASP	2.4
2	D	175	VAL	2.4
2	D	333	VAL	2.4
1	C	175	PRO	2.4
1	A	93	ILE	2.4
1	A	110	ILE	2.4
1	A	161	TYR	2.4
1	C	216	ASN	2.4
1	A	278	ALA	2.4
1	C	281	ALA	2.4
1	A	349	THR	2.4
3	E	42	PRO	2.4
1	A	219	ILE	2.4
2	B	331	LEU	2.4
1	C	388	TRP	2.4
1	A	285	GLN	2.4
2	D	355	ASP	2.4
1	A	316	CYS	2.4
2	D	429	THR	2.3
1	C	45	GLY	2.3
1	A	248	LEU	2.3
1	C	129	CYS	2.3
2	B	127	CYS	2.3
2	B	406	MET	2.3
1	C	108	TYR	2.3
1	A	284	GLU	2.3
1	C	38	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	275	SER	2.3
1	A	433	GLU	2.3
3	E	20	ILE	2.3
1	A	204	VAL	2.3
1	C	323	VAL	2.3
3	E	7	GLU	2.3
2	B	42	LEU	2.3
1	A	203	MET	2.3
2	B	81	PHE	2.3
1	A	159	VAL	2.3
1	A	435	VAL	2.3
1	A	261	PRO	2.3
1	A	73	THR	2.2
1	A	45	GLY	2.2
2	D	430	ALA	2.2
1	A	80	THR	2.2
1	A	125	LEU	2.2
1	C	125	LEU	2.2
1	C	203	MET	2.2
2	B	73	MET	2.2
2	D	368	ILE	2.2
3	E	6	ILE	2.2
3	E	13	SER	2.2
2	B	247	ASN	2.2
1	A	210	TYR	2.2
1	C	176	GLN	2.2
3	E	93	MET	2.2
2	D	113	VAL	2.2
3	E	19	VAL	2.2
1	A	96	LYS	2.2
2	D	274	THR	2.2
1	A	286	LEU	2.2
1	A	340	SER	2.2
1	A	434	GLU	2.2
2	D	177	ASP	2.2
1	C	37	PRO	2.2
2	D	80	PRO	2.2
1	A	276	ILE	2.1
3	E	23	PRO	2.1
1	A	301	GLN	2.1
2	D	323	MET	2.1
1	A	56	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	42	ILE	2.1
1	C	335	ILE	2.1
2	D	281	TYR	2.1
3	E	45	GLU	2.1
1	C	371	VAL	2.1
1	A	299	ALA	2.1
3	E	113	LEU	2.1
1	A	334	THR	2.1
2	D	238	THR	2.1
2	D	251	ARG	2.1
2	B	59	TYR	2.1
1	A	298	PRO	2.1
2	D	37	HIS	2.1
1	C	169	PHE	2.0
1	A	195	LEU	2.0
1	C	92	LEU	2.0
1	C	356	ASN	2.0
2	D	42	LEU	2.0
2	D	89	ASN	2.0
2	D	331	LEU	2.0
1	C	93	ILE	2.0
1	C	225	THR	2.0
2	B	285	THR	2.0
2	D	202	ILE	2.0
1	A	312	TYR	2.0
1	A	170	SER	2.0
2	D	153	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,

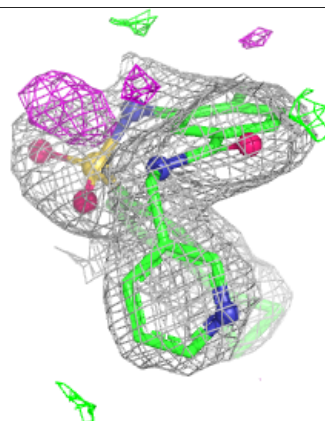
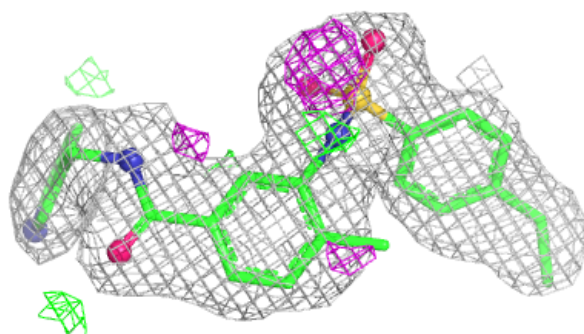
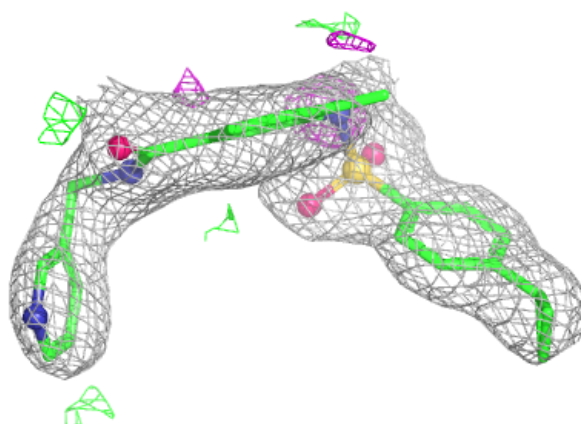
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	B	503	6/6	0.84	0.16	66,72,75,90	0
9	S40	D	503	30/30	0.90	0.15	70,82,88,92	0
5	MG	A	503	1/1	0.91	0.13	92,92,92,92	0
5	MG	C	504	1/1	0.91	0.19	63,63,63,63	0
5	MG	D	502	1/1	0.92	0.10	77,77,77,77	0
4	GTP	C	501	32/32	0.93	0.11	56,73,81,84	0
7	MES	B	502	12/12	0.93	0.12	66,68,76,79	0
9	S40	B	504	30/30	0.94	0.11	66,77,84,84	0
4	GTP	D	501	32/32	0.94	0.10	61,70,76,79	0
5	MG	C	502	1/1	0.95	0.14	68,68,68,68	0
6	GDP	B	501	28/28	0.95	0.09	56,66,72,75	0
5	MG	A	502	1/1	0.96	0.07	78,78,78,78	0
4	GTP	A	501	32/32	0.96	0.10	64,72,80,81	0
5	MG	C	503	1/1	0.98	0.07	83,83,83,83	0

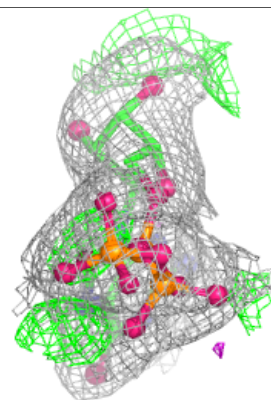
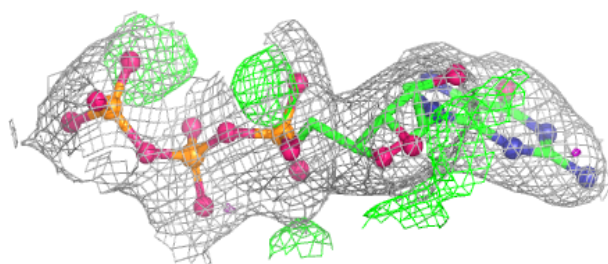
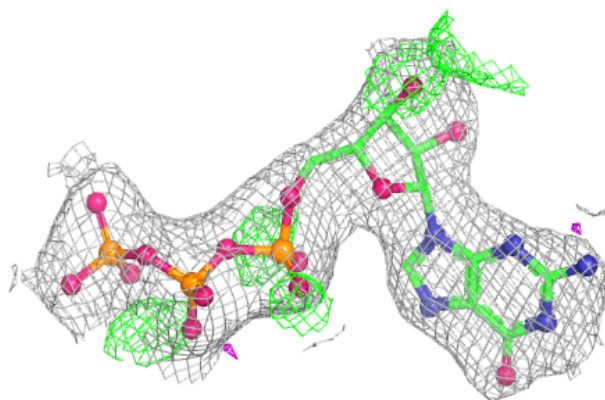
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around S40 D 503:

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

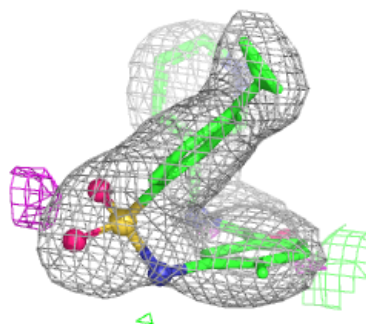
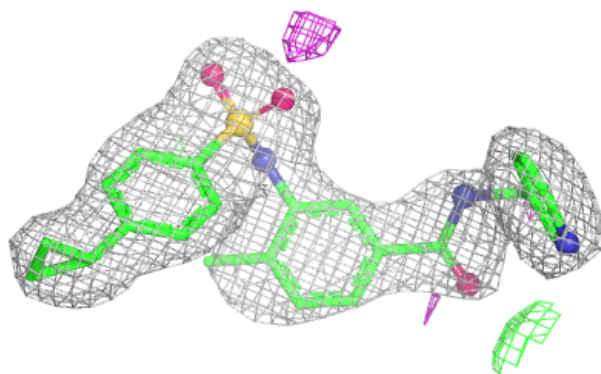
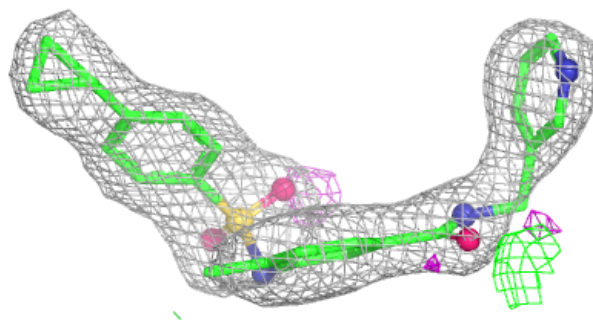
**Electron density around GTP C 501:**

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

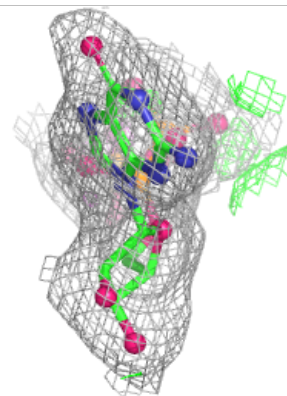
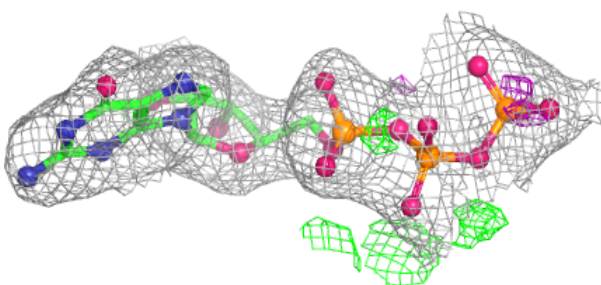
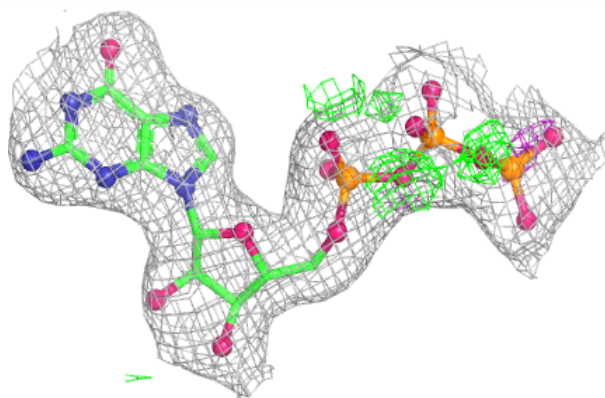


Electron density around S40 B 504:

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

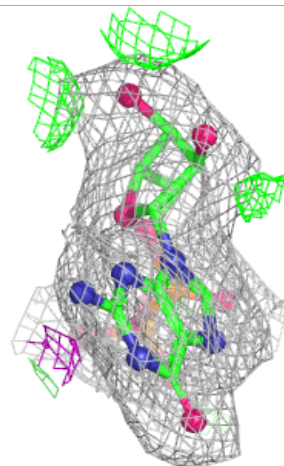
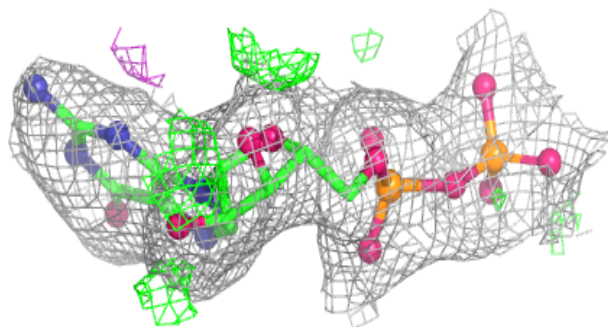
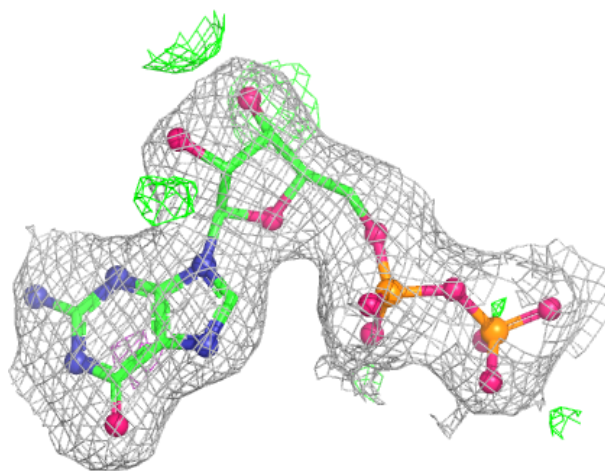
**Electron density around GTP D 501:**

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



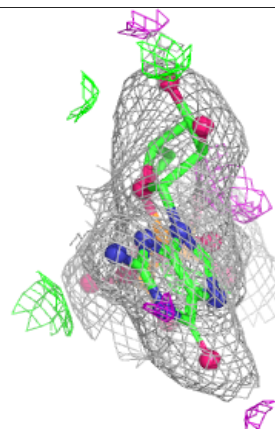
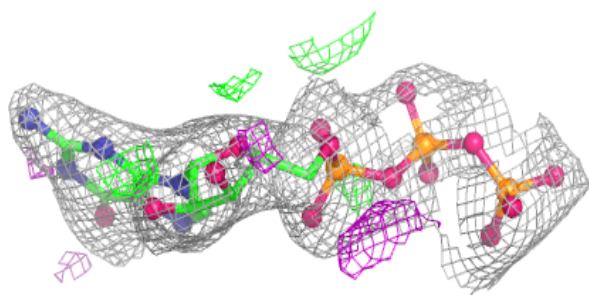
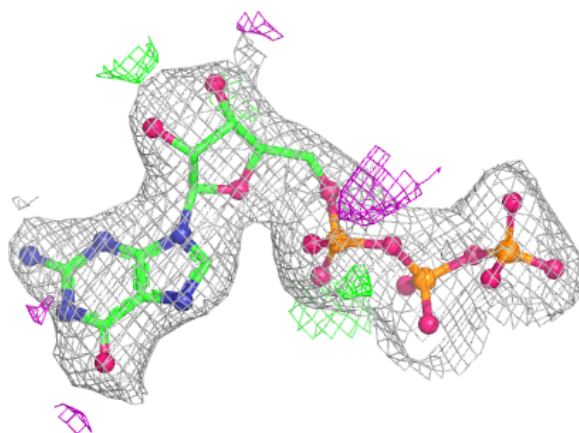
Electron density around GDP B 501:

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



Electron density around GTP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.