Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 02:21 PM EDT

PDB ID	:	6Y6D
Title	:	Tubulin-7-Aminonoscapine complex
Authors	:	Oliva, M.A.; Prota, A.E.; Rodriguez-Salarichs, J.; Gu, W.; Bennani, Y.L.; Jimenez-Barbero, J.; Canales, A.; Steinmetz, M.O.; Diaz, J.F.
Deposited on	:	2020-02-26
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

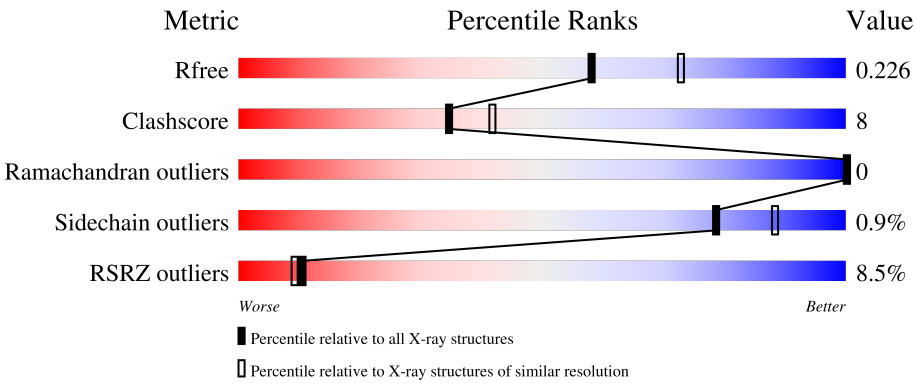
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	4%, 78%, 19%, •
1	C	451	%, 82%, 16%, •
2	B	445	4%, 78%, 17%, 5%
2	D	445	7%, 77%, 18%, 5%
3	E	143	8%, 76%, 10%, 15%

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Mol	Chain	Length	Quality of chain
4	F	384	26% 67% 19% • 13%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 18081 atoms, of which 52 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
			Total	C	N	O	S			
1	A	439	3436	2174	583	655	24	0	2	0
1	C	440	3443	2179	584	656	24	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	422	3330	2094	568	642	26	0	1	0
2	D	421	3339	2096	572	644	27	0	3	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	122	1008	622	182	199	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

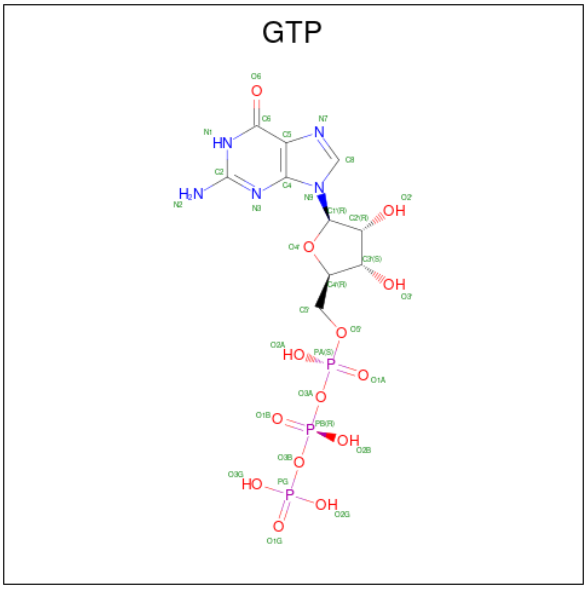
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	333	2733	1758	465	496	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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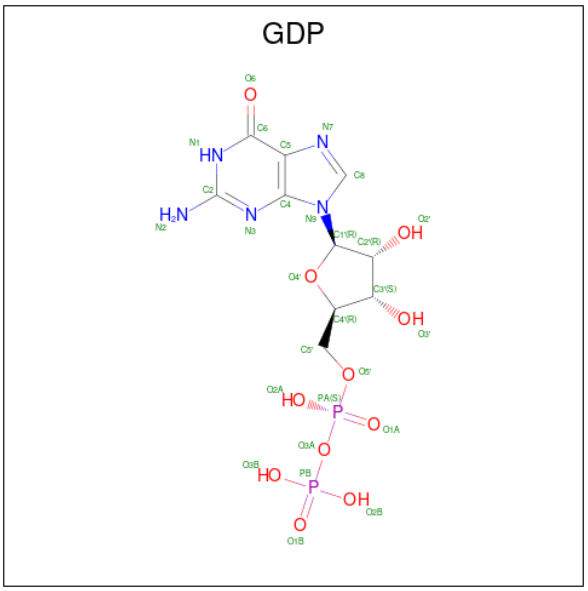
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	F	1	1	1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

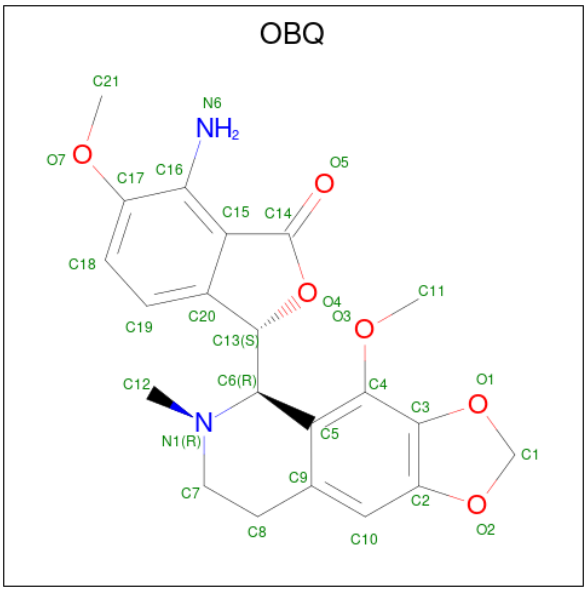
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
			Total	Ca		
7	C	1	1	1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



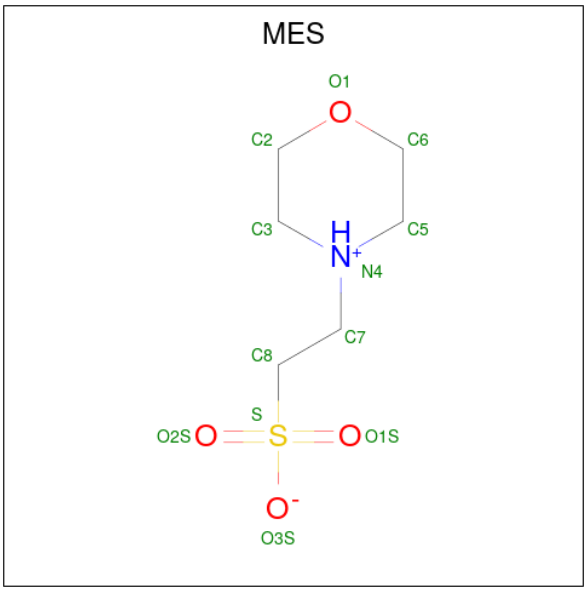
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
8	D	1	28	10	5	11	2	0	0

- Molecule 9 is (3 {S})-7-azanyl-6-methoxy-3-[(5 {R})-4-methoxy-6-methyl-7,8-dihydro-5 {H}-[1,3]dioxolo[4,5-g]isoquinolin-5-yl]-3 {H}-2-benzofuran-1-one (three-letter code: OBQ) (formula: $C_{21}H_{22}N_2O_6$) (labeled as "Ligand of Interest" by depositor).



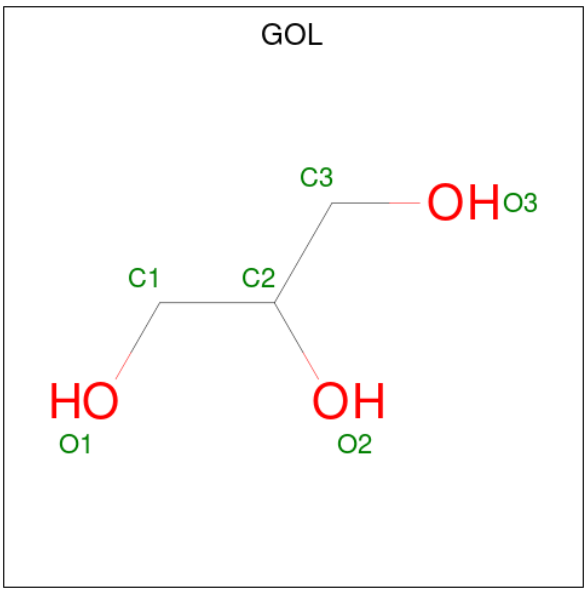
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
9	B	1	51	21	22	2	6	0	0
			Total	C	H	N	O		
9	D	1	51	21	22	2	6	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



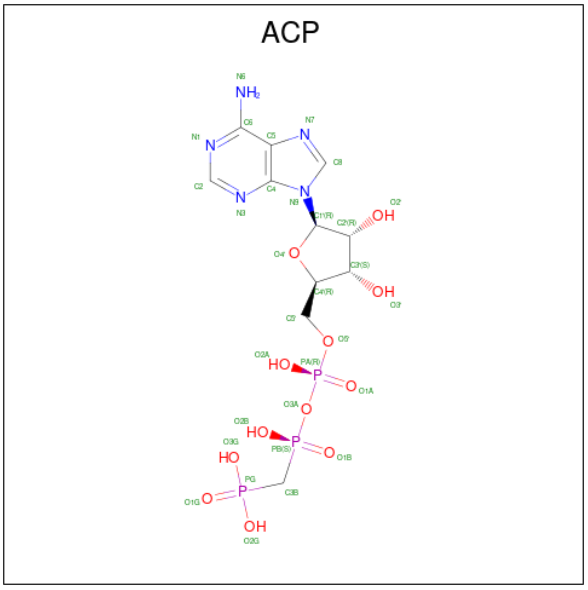
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
10	B	1	12	6	1	4	1	0	0

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
11	B	1	14	3	8	3	0	0

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

- Molecule 13 is water.

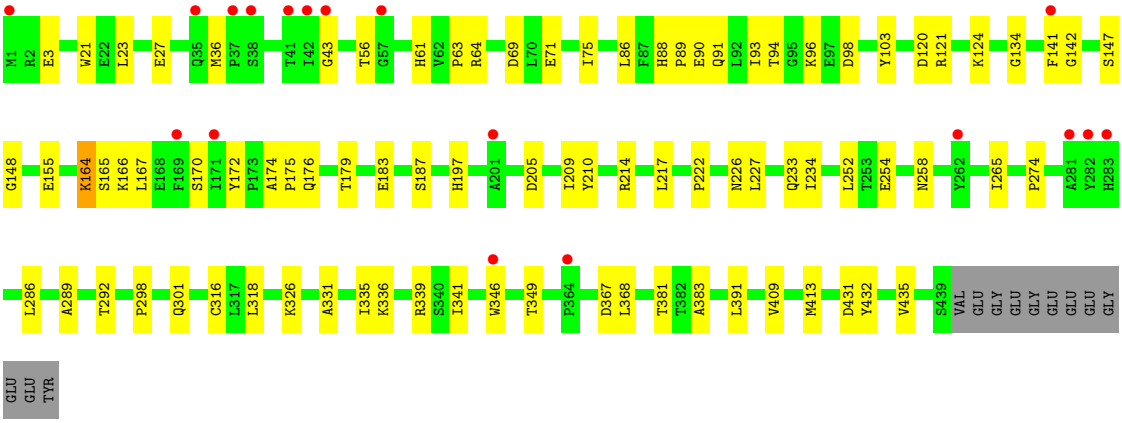
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	89	89	89	0	0
			Total	O		
13	B	87	87	87	0	0
			Total	O		
13	C	196	196	196	0	0
			Total	O		
13	D	70	70	70	0	0
			Total	O		
13	E	28	28	28	0	0
			Total	O		
13	F	36	36	36	0	0

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.

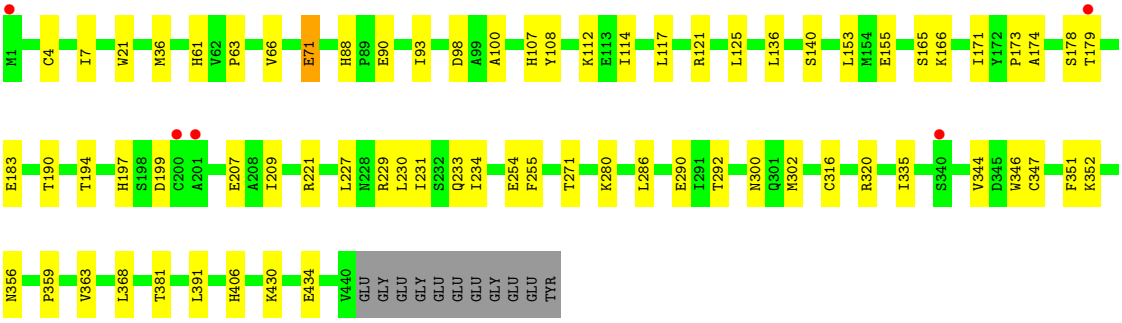
• Molecule 1: Tubulin alpha-1B chain

Chain A:



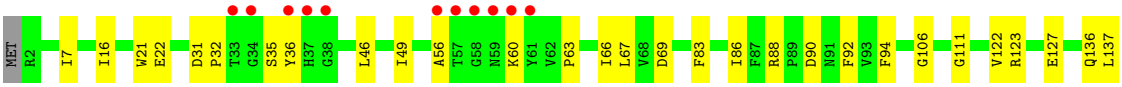
• Molecule 1: Tubulin alpha-1B chain

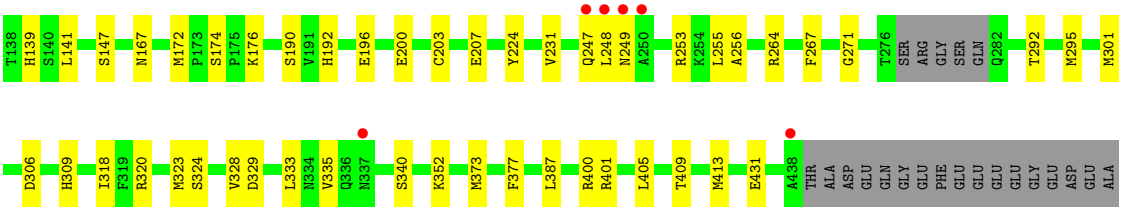
Chain C:



• Molecule 2: Tubulin beta-2B chain

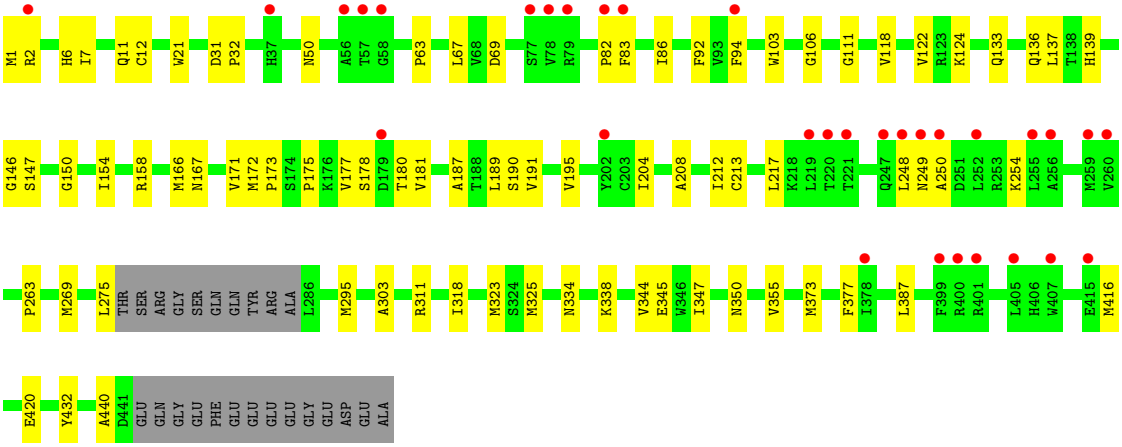
Chain B:





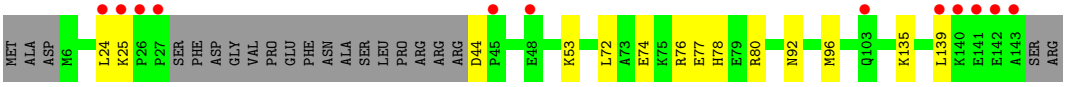
- Molecule 2: Tubulin beta-2B chain

Chain D:



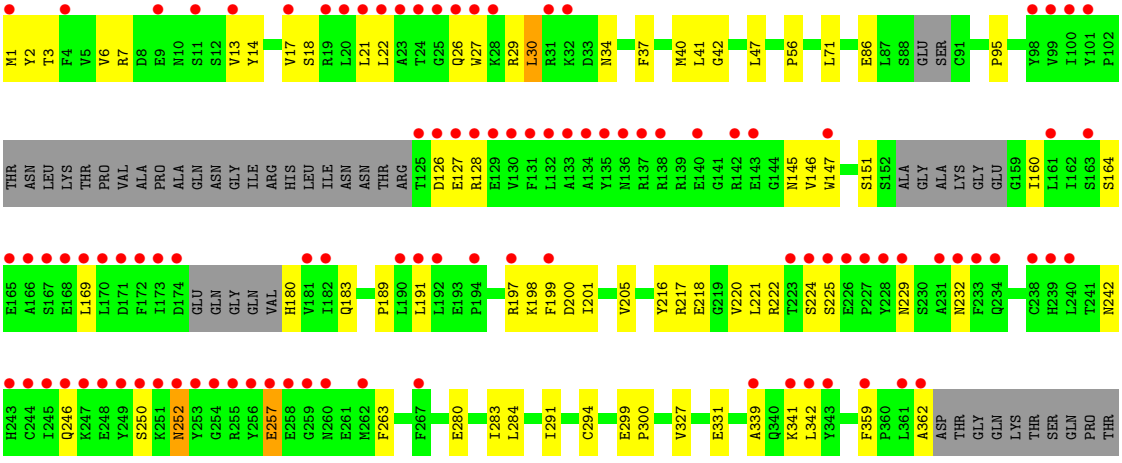
- Molecule 3: Stathmin-4

Chain E:



- Molecule 4: Tubulin-Tyrosine Ligase

Chain F:



S373
I374
L378
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.36Å 157.15Å 180.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.34 – 2.20 47.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.34-2.20) 100.0 (47.75-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.184 , 0.224 0.187 , 0.226	Depositor DCC
R_{free} test set	7566 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18081	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GTP, MG, ACP, GDP, CA, GOL, MES, OBQ

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	0.25	0/3520	0.42	0/4778
1	C	0.26	0/3527	0.43	0/4789
2	B	0.26	0/3404	0.42	0/4611
2	D	0.25	0/3412	0.42	0/4620
3	E	0.24	0/1016	0.35	0/1348
4	F	0.24	0/2793	0.40	0/3769
All	All	0.25	0/17672	0.42	0/23915

There are no bond length outliers.

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	3436	0	3349	67	0
1	C	3443	0	3358	50	0
2	B	3330	0	3204	54	0
2	D	3339	0	3218	63	0
3	E	1008	0	1024	11	0
4	F	2733	0	2712	54	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	1	0
9	B	29	22	0	3	0
9	D	29	22	0	3	0
10	B	12	0	12	1	0
11	B	6	8	8	1	0
12	F	31	0	14	2	0
13	A	89	0	0	4	0
13	B	87	0	0	2	0
13	C	196	0	0	2	0
13	D	70	0	0	4	1
13	E	28	0	0	4	0
13	F	36	0	0	1	1
All	All	18029	52	16947	287	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (287) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:HG22	1:A:383:ALA:H	1.33	0.91
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.54	0.88
2:D:50[B]:ASN:ND2	13:D:602:HOH:O	2.10	0.84
2:D:432:TYR:OH	13:D:601:HOH:O	2.03	0.77
2:B:340:SER:HB3	4:F:34:ASN:HD21	1.51	0.75
3:E:44:ASP:N	13:E:201:HOH:O	2.21	0.72
2:B:323:MET:HB3	2:B:373:MET:HE2	1.74	0.70
2:B:83:PHE:O	2:B:86:ILE:HG22	1.92	0.69
2:B:147:SER:HG	2:B:190:SER:HG	1.39	0.69
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.75	0.69
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.73	0.69
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.76	0.68
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.28	0.67
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.77	0.67
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.76	0.66
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.31	0.66
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.76	0.66
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.61	0.66
2:D:311[B]:ARG:HH21	2:D:344:VAL:HA	1.61	0.66
4:F:242:ASN:ND2	12:F:701:ACP:H3B2	2.11	0.65
2:D:2[B]:ARG:HH22	2:D:249:ASN:HB2	1.62	0.65
2:D:180:THR:HG22	2:D:181:VAL:H	1.61	0.65
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.79	0.65
1:C:320:ARG:HA	1:C:356:ASN:O	1.97	0.65
2:B:136:GLN:HA	2:B:167:ASN:O	1.97	0.64
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.61	0.64
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.27	0.64
3:E:80:ARG:HG3	13:E:209:HOH:O	1.99	0.63
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.34	0.63
2:B:323:MET:HB3	2:B:373:MET:CE	2.27	0.63
1:C:179:THR:HB	2:D:248:LEU:CD2	2.28	0.63
4:F:200:ASP:OD1	4:F:222:ARG:HB2	1.99	0.63
2:D:2[B]:ARG:HD3	13:D:607:HOH:O	1.99	0.63
2:D:250:ALA:HB1	9:D:503:OBQ:C11	2.28	0.62
2:D:323:MET:HB3	2:D:373:MET:HE2	1.82	0.62
2:B:248:LEU:HD23	9:B:503:OBQ:C12	2.30	0.62
2:D:83:PHE:O	2:D:86:ILE:HG22	1.99	0.62
4:F:246:GLN:O	4:F:250:SER:HB3	2.00	0.62
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.34	0.62
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.81	0.62
4:F:18:SER:O	4:F:22:LEU:HD22	1.99	0.62
2:B:264:ARG:NE	2:B:431:GLU:OE2	2.33	0.62
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.39	0.61
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.35	0.61
1:A:346:TRP:HH2	1:A:435:VAL:HG13	1.65	0.61
1:A:346:TRP:CH2	1:A:435:VAL:HG13	2.35	0.61
2:B:253[B]:ARG:NH1	10:B:504:MES:O2S	2.28	0.60
2:B:352:LYS:HG2	9:B:503:OBQ:C7	2.32	0.60
2:B:248:LEU:HD11	13:B:640:HOH:O	2.01	0.60
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.83	0.60
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.85	0.59
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.17	0.59
2:D:311[B]:ARG:NH2	2:D:345:GLU:OE1	2.34	0.59
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.38	0.59
1:A:381:THR:HG23	13:A:641:HOH:O	2.02	0.58
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.84	0.58
2:D:1:MET:HG2	2:D:50[B]:ASN:ND2	2.19	0.58
2:D:323:MET:HB3	2:D:373:MET:CE	2.33	0.58
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.38	0.58
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.36	0.58
2:B:69:ASP:O	2:B:94:PHE:HA	2.04	0.57
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.87	0.57
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.87	0.57
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.41	0.55
2:B:196:GLU:HG3	13:E:226:HOH:O	2.04	0.55
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.41	0.55
2:D:106:GLY:O	2:D:111:GLY:HA3	2.06	0.55
2:D:136:GLN:HA	2:D:167:ASN:O	2.07	0.55
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.42	0.54
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.06	0.54
2:B:329:ASP:O	2:B:333:LEU:HG	2.08	0.54
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.38	0.54
1:C:190:THR:O	1:C:194:THR:HG23	2.07	0.54
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.90	0.54
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.90	0.54
1:A:166:LYS:HE2	1:A:197:HIS:O	2.08	0.53
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.23	0.53
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.44	0.53
1:C:165:SER:HA	1:C:199:ASP:OD2	2.08	0.53
1:A:155:GLU:OE1	3:E:53:LYS:NZ	2.38	0.53
1:A:88:HIS:HD2	1:A:91:GLN:OE1	1.91	0.53
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.43	0.53
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.91	0.53
2:D:325:MET:SD	2:D:355:VAL:HG21	2.49	0.52
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.38	0.52
2:D:146:GLY:O	2:D:150:GLY:HA3	2.09	0.52
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.44	0.52
4:F:263:PHE:CE1	4:F:341:LYS:HE2	2.44	0.52
2:B:167:ASN:HD22	2:B:200:GLU:HB2	1.75	0.52
4:F:126:ASP:OD1	4:F:127:GLU:N	2.42	0.52
1:A:166:LYS:NZ	13:A:604:HOH:O	2.42	0.52
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.45	0.52
1:C:107:HIS:HE1	1:C:155:GLU:OE1	1.93	0.52
1:A:176:GLN:HG3	4:F:56:PRO:HB3	1.92	0.51
2:D:177:VAL:HG12	2:D:177:VAL:O	2.10	0.51
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.92	0.51
3:E:135:LYS:NZ	3:E:139:LEU:HD11	2.25	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.51
4:F:126:ASP:OD1	4:F:128:ARG:HG3	2.11	0.51
4:F:263:PHE:CE2	4:F:341:LYS:HE2	2.46	0.51
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.46	0.51
1:C:209:ILE:HD11	1:C:302:MET:SD	2.51	0.51
1:A:289:ALA:HA	1:A:331:ALA:CB	2.41	0.50
2:B:248:LEU:HD21	13:B:612:HOH:O	2.12	0.50
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.11	0.50
2:D:124:LYS:C	2:D:124:LYS:HD3	2.32	0.50
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.47	0.50
2:B:141:LEU:HD12	2:B:172:MET:SD	2.52	0.50
4:F:40:MET:HE2	4:F:47:LEU:HG	1.94	0.50
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.46	0.50
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.93	0.50
2:D:2[B]:ARG:HB3	2:D:133:GLN:CG	2.42	0.49
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.48	0.49
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.95	0.49
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.94	0.49
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.95	0.49
2:B:200:GLU:OE2	2:B:256:ALA:HB2	2.12	0.49
2:D:67:LEU:N	2:D:67:LEU:HD12	2.27	0.49
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.42	0.49
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.43	0.49
4:F:17:VAL:O	4:F:21:LEU:HG	2.13	0.49
1:C:166:LYS:HE2	1:C:197:HIS:O	2.13	0.49
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.94	0.49
4:F:37:PHE:CE1	4:F:40:MET:HB2	2.47	0.49
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.53	0.48
2:B:271:GLY:HA3	2:B:301:MET:HE2	1.94	0.48
1:C:179:THR:HB	2:D:248:LEU:HD21	1.94	0.48
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.94	0.48
1:C:174:ALA:O	1:C:178:SER:HB3	2.13	0.48
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.12	0.48
1:A:141:PHE:O	1:A:147:SER:HB3	2.13	0.48
2:D:171:VAL:HA	2:D:204:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:PRO:HA	2:D:178:SER:HB3	1.93	0.48
2:B:318:ILE:N	2:B:318:ILE:HD12	2.27	0.48
4:F:26:GLN:HE22	4:F:362:ALA:H	1.61	0.48
2:D:318:ILE:N	2:D:318:ILE:HD12	2.29	0.48
2:B:301:MET:HE2	2:B:301:MET:HA	1.96	0.48
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.96	0.48
4:F:225:SER:O	4:F:252:ASN:ND2	2.47	0.48
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.54	0.48
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.94	0.48
2:B:31:ASP:OD1	2:B:35:SER:N	2.44	0.48
1:C:179:THR:O	9:D:503:OBQ:N6	2.47	0.48
2:D:2[A]:ARG:HB3	2:D:133:GLN:CG	2.43	0.48
2:D:212:ILE:HG21	2:D:275:LEU:HD13	1.95	0.48
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.96	0.48
4:F:95:PRO:HB2	4:F:183:GLN:HG3	1.96	0.47
1:C:179:THR:HB	2:D:248:LEU:HD22	1.96	0.47
4:F:242:ASN:HD22	12:F:701:ACP:H3B2	1.79	0.47
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.97	0.47
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.96	0.47
4:F:197:ARG:HB2	4:F:224:SER:O	2.14	0.47
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.49	0.47
1:A:167:LEU:HD22	1:A:252:LEU:HD22	1.95	0.47
2:B:409:THR:HA	2:B:413:MET:O	2.15	0.47
2:D:2[A]:ARG:HB3	2:D:133:GLN:HG2	1.96	0.47
3:E:44:ASP:N	13:E:203:HOH:O	2.47	0.47
4:F:160:ILE:HD12	4:F:160:ILE:N	2.29	0.47
1:A:23:LEU:O	1:A:27:GLU:HG3	2.14	0.47
1:A:175:PRO:HA	1:A:179:THR:OG1	2.14	0.47
1:C:108:TYR:O	1:C:112:LYS:HG2	2.15	0.47
2:D:118:VAL:O	2:D:122:VAL:HG23	2.15	0.47
2:D:295:MET:HE2	2:D:295:MET:HB2	1.57	0.47
1:A:88:HIS:ND1	1:A:90:GLU:OE1	2.48	0.47
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.30	0.47
1:A:75:ILE:HB	1:A:94:THR:CG2	2.44	0.47
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.78	0.47
4:F:3:THR:HB	4:F:30:LEU:HD22	1.97	0.47
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.50	0.47
1:C:234:ILE:HD13	1:C:302:MET:SD	2.54	0.47
1:A:93:ILE:CD1	1:A:121:ARG:HG3	2.45	0.46
4:F:217:ARG:NH1	4:F:374:ILE:HB	2.30	0.46
4:F:189:PRO:HG2	4:F:191:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:VAL:HA	1:A:413:MET:O	2.16	0.46
1:A:134:GLY:HA3	1:A:165:SER:O	2.15	0.46
2:B:7:ILE:O	2:B:137:LEU:HA	2.15	0.46
2:B:67:LEU:N	2:B:67:LEU:HD12	2.31	0.46
2:D:69:ASP:O	2:D:94:PHE:HA	2.16	0.46
2:D:147:SER:HB2	2:D:190:SER:OG	2.16	0.46
1:A:298:PRO:HA	1:A:301:GLN:CD	2.37	0.46
1:A:71:GLU:OE1	2:B:249:ASN:ND2	2.48	0.46
4:F:339:ALA:HB3	4:F:342:LEU:HD12	1.98	0.46
1:C:227:LEU:O	1:C:231:ILE:HG13	2.16	0.45
4:F:14:TYR:HA	4:F:17:VAL:HB	1.98	0.45
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.51	0.45
4:F:198:LYS:HG2	4:F:199:PHE:H	1.82	0.45
2:D:387:LEU:HD23	2:D:387:LEU:C	2.36	0.45
1:C:93:ILE:CG2	1:C:114:ILE:HD11	2.45	0.45
2:D:11:GLN:OE1	13:D:603:HOH:O	2.21	0.45
4:F:220:VAL:HG11	4:F:339:ALA:HB2	1.98	0.45
1:A:431:ASP:O	1:A:435:VAL:HG23	2.17	0.45
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.52	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.45
1:C:229:ARG:NE	1:C:363:VAL:HG21	2.31	0.45
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.47	0.45
1:A:96:LYS:HB2	13:A:601:HOH:O	2.17	0.45
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.98	0.45
2:B:320:ARG:O	2:B:373:MET:HA	2.17	0.45
1:A:96:LYS:N	13:A:601:HOH:O	2.21	0.44
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.99	0.44
2:D:82:PRO:O	2:D:83:PHE:HB2	2.17	0.44
2:D:208:ALA:O	2:D:212:ILE:HG13	2.17	0.44
2:D:416:MET:O	2:D:420:GLU:HG3	2.16	0.44
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.99	0.44
3:E:92:ASN:O	3:E:96:MET:HG2	2.17	0.44
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.53	0.44
2:D:7:ILE:O	2:D:137:LEU:HA	2.17	0.44
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.99	0.44
4:F:225:SER:HB2	4:F:252:ASN:HD22	1.83	0.44
1:A:103:TYR:CD2	1:A:148:GLY:HA2	2.53	0.44
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.37	0.44
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.99	0.44
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.99	0.44
1:A:164:LYS:HD2	1:A:164:LYS:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:THR:HG22	2:D:181:VAL:N	2.30	0.43
2:D:2[B]:ARG:HB3	2:D:133:GLN:HG2	2.00	0.43
4:F:284:LEU:HD23	4:F:284:LEU:HA	1.80	0.43
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.49	0.43
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.53	0.43
4:F:283:ILE:HG23	4:F:327:VAL:CG2	2.47	0.43
1:A:336:LYS:HD2	1:A:341:ILE:HD12	2.00	0.43
2:D:295:MET:CE	2:D:377:PHE:HB2	2.48	0.43
2:D:345:GLU:HG2	2:D:440:ALA:HB2	2.01	0.43
1:C:173:PRO:HB3	1:C:183:GLU:OE2	2.19	0.43
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.53	0.43
4:F:13:VAL:HG23	13:F:804:HOH:O	2.19	0.43
4:F:126:ASP:OD1	4:F:128:ARG:N	2.51	0.43
1:C:406:HIS:CD2	2:D:263:PRO:HD3	2.53	0.43
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.49	0.43
1:A:174:ALA:O	1:A:179:THR:HG23	2.19	0.43
1:A:179:THR:HA	1:A:183:GLU:OE1	2.19	0.43
1:A:349:THR:HB	3:E:25:LYS:HB3	2.00	0.43
3:E:72:LEU:O	3:E:76:ARG:HG2	2.18	0.43
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.46	0.42
2:D:250:ALA:HB1	9:D:503:OBQ:O3	2.18	0.42
1:A:43:GLY:HA2	1:A:56:THR:O	2.19	0.42
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.55	0.42
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.34	0.42
4:F:7:ARG:HD3	4:F:40:MET:CE	2.46	0.42
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.50	0.42
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.49	0.42
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.55	0.42
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.00	0.42
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.02	0.42
1:A:292:THR:HG22	1:A:335:ILE:HD12	2.01	0.42
2:B:123:ARG:O	2:B:127:GLU:HG3	2.19	0.42
4:F:40:MET:HE3	4:F:42:GLY:HA2	2.02	0.42
1:A:234:ILE:HD12	1:A:234:ILE:N	2.35	0.41
1:C:271:THR:HG23	1:C:300:ASN:O	2.20	0.41
4:F:71:LEU:HD11	4:F:294:CYS:HB3	2.02	0.41
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.36	0.41
2:B:224:TYR:CE2	11:B:505:GOL:H2	2.56	0.41
2:D:248:LEU:HD12	2:D:249:ASN:N	2.35	0.41
1:A:289:ALA:HA	1:A:331:ALA:HB2	2.02	0.41
2:B:106:GLY:O	2:B:111:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:SER:O	2:B:328:VAL:HG23	2.19	0.41
2:D:191:VAL:O	2:D:195:VAL:HG23	2.21	0.41
4:F:299:GLU:N	4:F:300:PRO:HD2	2.35	0.41
1:C:255:PHE:CD1	1:C:316:CYS:HB3	2.55	0.41
1:C:280:LYS:HG3	13:C:620:HOH:O	2.20	0.41
4:F:201:ILE:HG12	4:F:221:LEU:HG	2.03	0.41
1:A:326:LYS:HE2	1:A:326:LYS:HB3	1.86	0.41
2:B:249:ASN:OD1	2:B:249:ASN:N	2.44	0.41
2:B:301:MET:HA	2:B:301:MET:CE	2.50	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD12	2.03	0.41
1:A:120:ASP:O	1:A:124:LYS:HG3	2.21	0.41
1:C:359:PRO:HB3	13:C:709:HOH:O	2.19	0.41
2:D:173:PRO:HG3	2:D:187:ALA:HB2	2.01	0.41
1:A:69:ASP:O	1:A:94:THR:HA	2.21	0.41
1:C:140:SER:HA	1:C:171:ILE:HB	2.03	0.41
3:E:77:GLU:HG3	3:E:78:HIS:N	2.36	0.41
1:C:351:PHE:N	1:C:351:PHE:CD1	2.89	0.40
3:E:74:GLU:O	3:E:77:GLU:HG2	2.22	0.40
2:B:46:LEU:HA	2:B:49:ILE:HB	2.02	0.40
2:B:405:LEU:HD23	2:B:405:LEU:HA	1.91	0.40
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.57	0.40
4:F:6:VAL:HB	4:F:29:ARG:NH2	2.36	0.40
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.47	0.40
1:A:289:ALA:HA	1:A:331:ALA:HB1	2.01	0.40
1:C:391:LEU:HD23	1:C:391:LEU:HA	1.97	0.40
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.03	0.40
4:F:229:ASN:ND2	4:F:232:ASN:HB3	2.36	0.40
2:B:255:LEU:HD13	9:B:503:OBQ:C3	2.52	0.40
1:C:430:LYS:HE2	1:C:434:GLU:OE1	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:665:HOH:O	13:F:836:HOH:O[3_545]	2.15	0.05

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	439/451 (97%)	428 (98%)	11 (2%)	0	100	100
1	C	440/451 (98%)	431 (98%)	9 (2%)	0	100	100
2	B	419/445 (94%)	411 (98%)	8 (2%)	0	100	100
2	D	420/445 (94%)	414 (99%)	6 (1%)	0	100	100
3	E	118/143 (82%)	116 (98%)	2 (2%)	0	100	100
4	F	321/384 (84%)	308 (96%)	13 (4%)	0	100	100
All	All	2157/2319 (93%)	2108 (98%)	49 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	372/379 (98%)	371 (100%)	1 (0%)	92	97
1	C	373/379 (98%)	368 (99%)	5 (1%)	69	81
2	B	365/383 (95%)	362 (99%)	3 (1%)	81	90
2	D	367/383 (96%)	365 (100%)	2 (0%)	88	94
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	300/342 (88%)	293 (98%)	7 (2%)	50	63
All	All	1886/1993 (95%)	1868 (99%)	18 (1%)	78	86

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	LYS
2	B	139	HIS
2	B	192	HIS
2	B	247	GLN
1	C	71	GLU
1	C	221	ARG
1	C	347[A]	CYS
1	C	347[B]	CYS
1	C	381	THR
2	D	139	HIS
2	D	158	ARG
4	F	1	MET
4	F	30	LEU
4	F	86	GLU
4	F	145	ASN
4	F	252	ASN
4	F	257	GLU
4	F	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	301	GLN
2	B	167	ASN
2	B	247	GLN
1	C	107	HIS
1	C	356	ASN
2	D	334	ASN
4	F	252	ASN
4	F	269	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	OBQ	B	503	-	33,33,33	0.81	0	48,50,50	2.40	10 (20%)
8	GDP	D	501	6	25,30,30	1.04	2 (8%)	30,47,47	1.09	1 (3%)
5	GTP	A	501	6	29,34,34	1.27	4 (13%)	35,54,54	1.29	4 (11%)
11	GOL	B	505	-	5,5,5	1.31	0	5,5,5	1.56	1 (20%)
5	GTP	C	501	6	29,34,34	1.23	3 (10%)	35,54,54	1.30	5 (14%)
8	GDP	B	501	6	25,30,30	1.02	2 (8%)	30,47,47	1.13	3 (10%)
9	OBQ	D	503	-	33,33,33	0.79	0	48,50,50	2.38	8 (16%)
10	MES	B	504	-	12,12,12	2.36	1 (8%)	15,16,16	2.05	5 (33%)
12	ACP	F	701	6	27,33,33	1.60	7 (25%)	33,52,52	1.64	3 (9%)

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
9	OBQ	B	503	-	-	3/8/39/39	0/5/5/5
8	GDP	D	501	6	-	4/12/32/32	0/3/3/3
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
11	GOL	B	505	-	-	0/4/4/4	-
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
8	GDP	B	501	6	-	5/12/32/32	0/3/3/3
9	OBQ	D	503	-	-	2/8/39/39	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
12	ACP	F	701	6	-	6/15/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-7.92	1.66	1.77
5	A	501	GTP	C5-C6	-4.17	1.39	1.47
5	C	501	GTP	C5-C6	-3.96	1.39	1.47
12	F	701	ACP	O4'-C1'	3.33	1.45	1.40
12	F	701	ACP	PB-O3A	3.29	1.62	1.58
12	F	701	ACP	PG-O2G	2.96	1.61	1.55
12	F	701	ACP	PG-O3G	2.85	1.61	1.55
8	D	501	GDP	PA-O3A	2.41	1.62	1.59
5	A	501	GTP	PA-O3A	2.30	1.62	1.59
12	F	701	ACP	PA-O3A	2.28	1.62	1.59
12	F	701	ACP	C8-N7	-2.28	1.30	1.34
8	B	501	GDP	C6-N1	-2.26	1.34	1.37
8	D	501	GDP	C6-N1	-2.18	1.34	1.37
8	B	501	GDP	PA-O3A	2.18	1.61	1.59
5	A	501	GTP	C2-N3	2.07	1.38	1.33
5	C	501	GTP	PA-O3A	2.06	1.61	1.59
12	F	701	ACP	PB-O2B	2.05	1.61	1.56
5	C	501	GTP	C2-N3	2.01	1.38	1.33
5	A	501	GTP	PB-O3A	2.00	1.61	1.59

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	503	OBQ	C5-C6-N1	-8.81	108.28	115.03
9	D	503	OBQ	C13-C6-N1	8.72	121.25	109.61
9	D	503	OBQ	C5-C6-N1	-8.36	108.62	115.03
9	B	503	OBQ	C13-C6-N1	8.00	120.29	109.61
9	D	503	OBQ	C12-N1-C6	6.52	119.64	111.72
12	F	701	ACP	PB-O3A-PA	-6.40	111.47	132.37
9	B	503	OBQ	C12-N1-C6	5.83	118.81	111.72
10	B	504	MES	C5-N4-C3	4.93	119.46	108.84
12	F	701	ACP	N3-C2-N1	-4.60	122.43	128.67
9	B	503	OBQ	C13-O4-C14	-4.51	108.37	111.00
9	D	503	OBQ	C12-N1-C7	4.40	117.87	110.61
5	C	501	GTP	C8-N7-C5	3.72	108.89	102.55
5	A	501	GTP	C8-N7-C5	3.53	108.56	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	503	OBQ	C12-N1-C7	3.12	115.75	110.61
9	B	503	OBQ	O2-C2-C3	3.01	112.67	109.62
11	B	505	GOL	C3-C2-C1	-2.98	100.86	111.80
5	A	501	GTP	C5-C6-N1	2.91	119.63	114.07
8	D	501	GDP	C8-N7-C5	2.88	107.46	102.55
5	C	501	GTP	C5-C6-N1	2.81	119.44	114.07
9	D	503	OBQ	O2-C2-C3	2.80	112.46	109.62
5	C	501	GTP	C2-N1-C6	-2.75	120.07	125.11
8	B	501	GDP	C8-N7-C5	2.74	107.21	102.55
5	A	501	GTP	C2-N1-C6	-2.67	120.22	125.11
12	F	701	ACP	PA-O5'-C5'	-2.64	106.23	121.35
9	B	503	OBQ	C7-C8-C9	2.58	115.80	111.34
9	D	503	OBQ	C1-O2-C2	-2.55	101.90	105.32
10	B	504	MES	C6-C5-N4	-2.52	106.30	110.12
10	B	504	MES	C7-N4-C5	2.39	117.60	111.24
9	D	503	OBQ	C7-C8-C9	2.36	115.42	111.34
9	B	503	OBQ	C1-O2-C2	-2.32	102.21	105.32
10	B	504	MES	C7-N4-C3	2.25	117.23	111.24
8	B	501	GDP	C5-C6-N1	2.23	118.32	114.07
5	A	501	GTP	O6-C6-C5	-2.22	119.91	124.32
10	B	504	MES	C8-C7-N4	-2.18	104.12	112.36
5	C	501	GTP	O2A-PA-O3A	2.17	113.13	107.27
9	B	503	OBQ	O4-C14-C15	-2.14	106.61	108.35
9	B	503	OBQ	O4-C13-C6	2.13	111.33	108.62
9	D	503	OBQ	O4-C13-C6	2.06	111.25	108.62
8	B	501	GDP	O2A-PA-O3A	2.02	112.74	107.27
5	C	501	GTP	O2B-PB-O3A	2.01	112.72	107.27

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
8	D	501	GDP	C5'-O5'-PA-O2A
10	B	504	MES	C8-C7-N4-C3
10	B	504	MES	C7-C8-S-O2S
12	F	701	ACP	C5'-O5'-PA-O2A
10	B	504	MES	C7-C8-S-O3S
12	F	701	ACP	O4'-C4'-C5'-O5'
9	D	503	OBQ	C3-C4-O3-C11
10	B	504	MES	C7-C8-S-O1S
9	D	503	OBQ	C5-C4-O3-C11
5	A	501	GTP	C5'-O5'-PA-O2A
12	F	701	ACP	C5'-O5'-PA-O1A
12	F	701	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
8	B	501	GDP	PB-O3A-PA-O2A
9	B	503	OBQ	C16-C17-O7-C21
5	C	501	GTP	PB-O3B-PG-O1G
12	F	701	ACP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
9	B	503	OBQ	C3-C4-O3-C11
9	B	503	OBQ	C18-C17-O7-C21
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3B-PG-O1G
12	F	701	ACP	C3'-C4'-C5'-O5'
5	C	501	GTP	C4'-C5'-O5'-PA
8	D	501	GDP	PB-O3A-PA-O2A

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	OBQ	3	0
8	D	501	GDP	1	0
5	A	501	GTP	1	0
11	B	505	GOL	1	0
9	D	503	OBQ	3	0
10	B	504	MES	1	0

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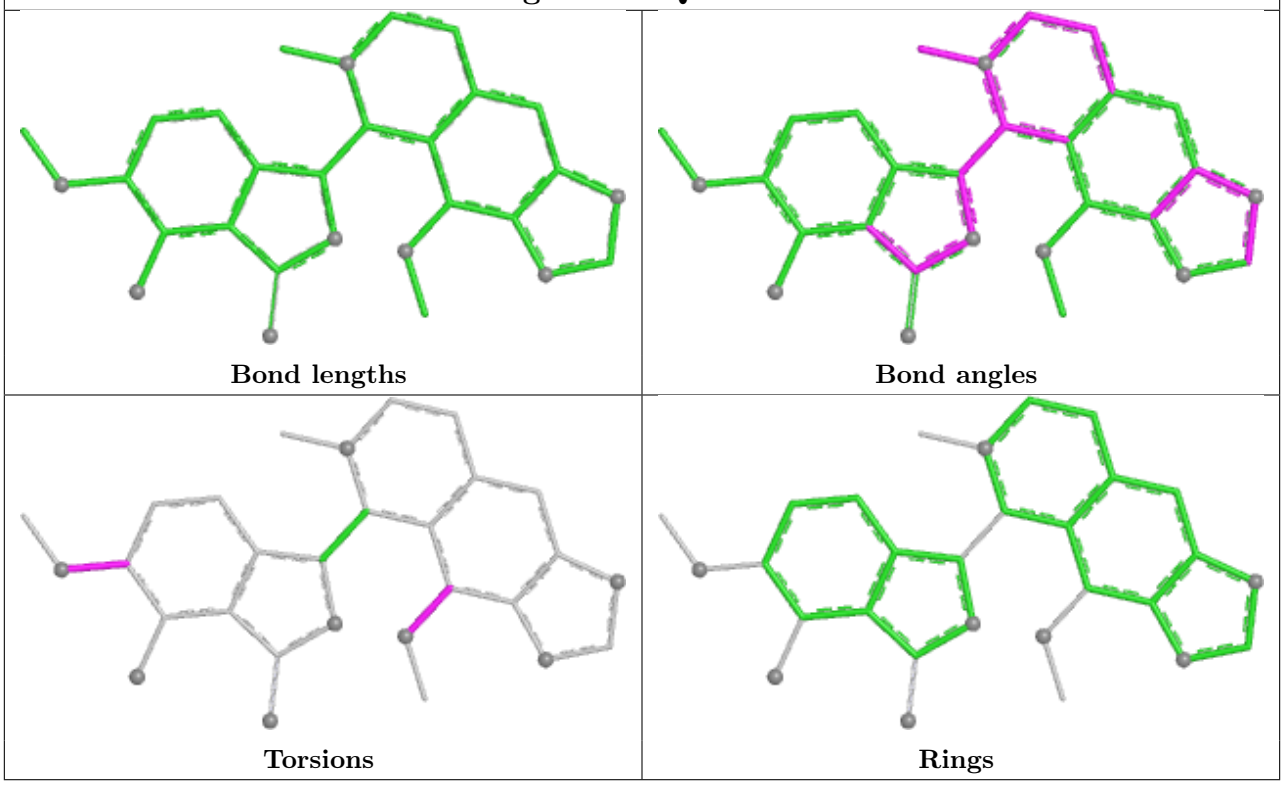
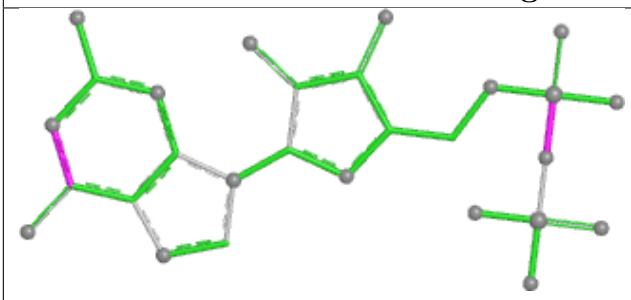
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	701	ACP	2	0

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 then 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.

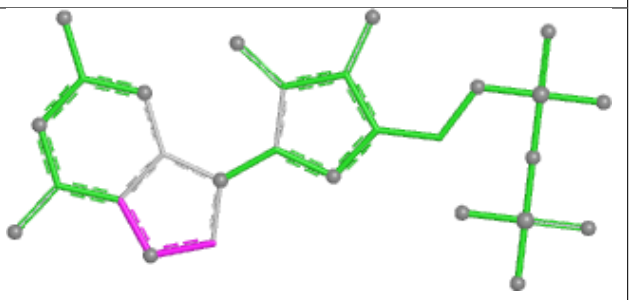
Ligand OBQ B 503



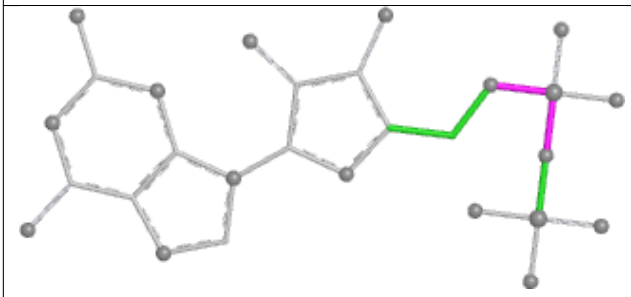
Ligand GDP D 501



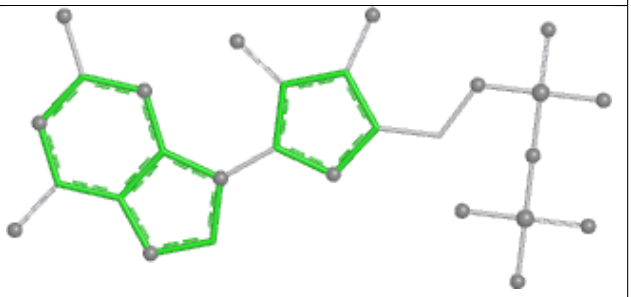
Bond lengths



Bond angles

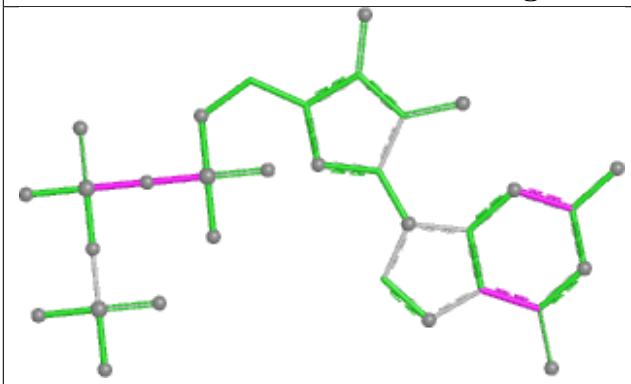


Torsions

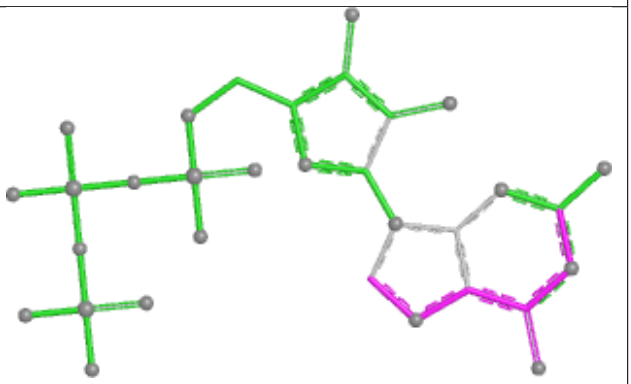


Rings

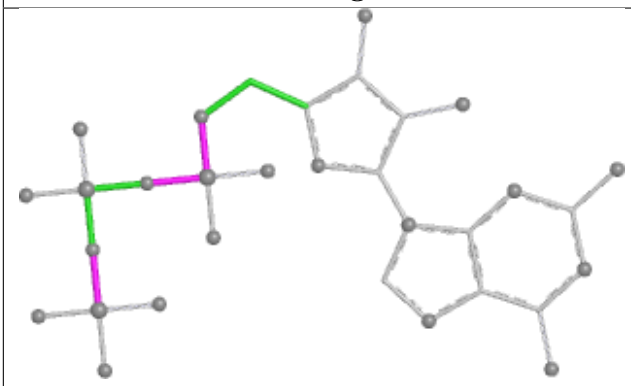
Ligand GTP A 501



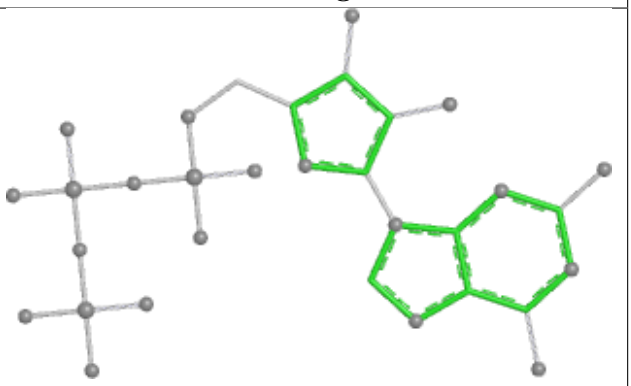
Bond lengths



Bond angles

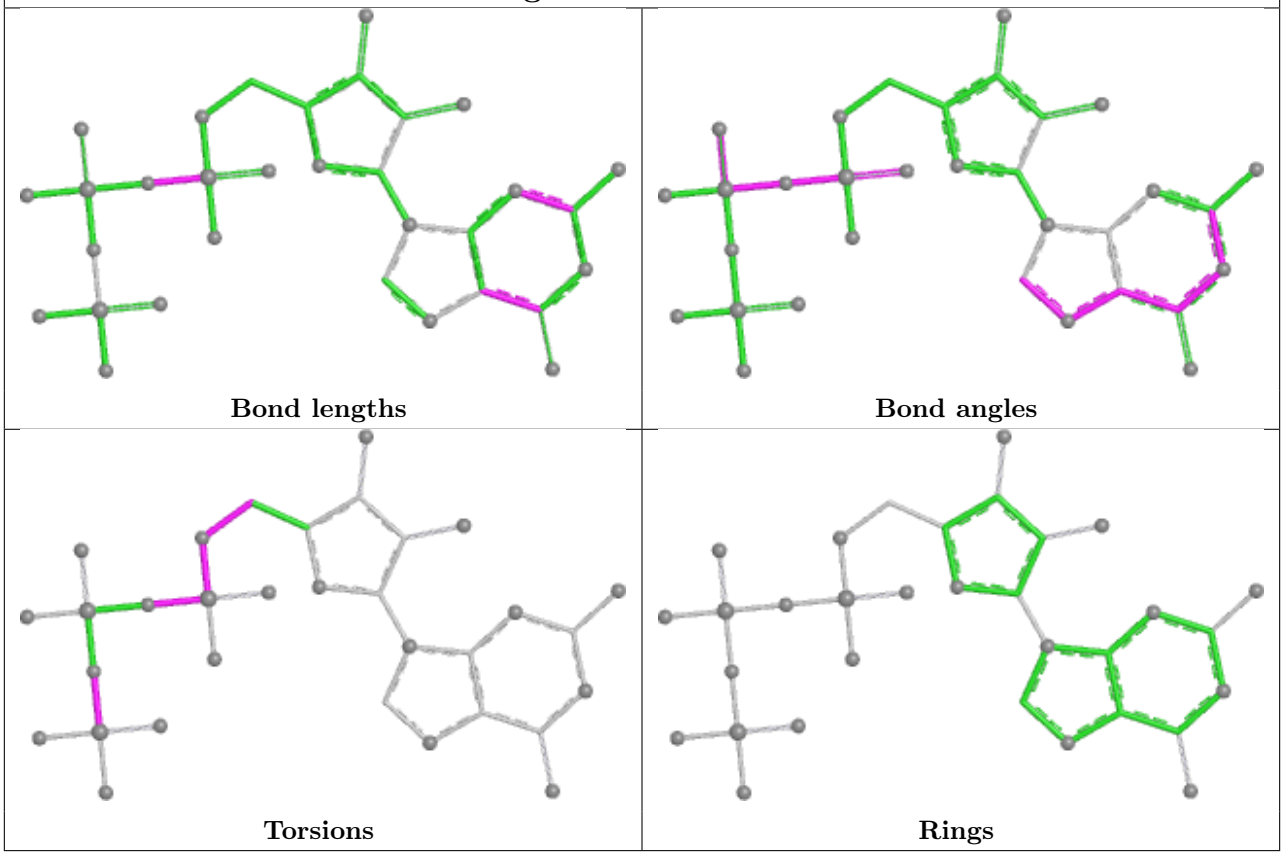


Torsions

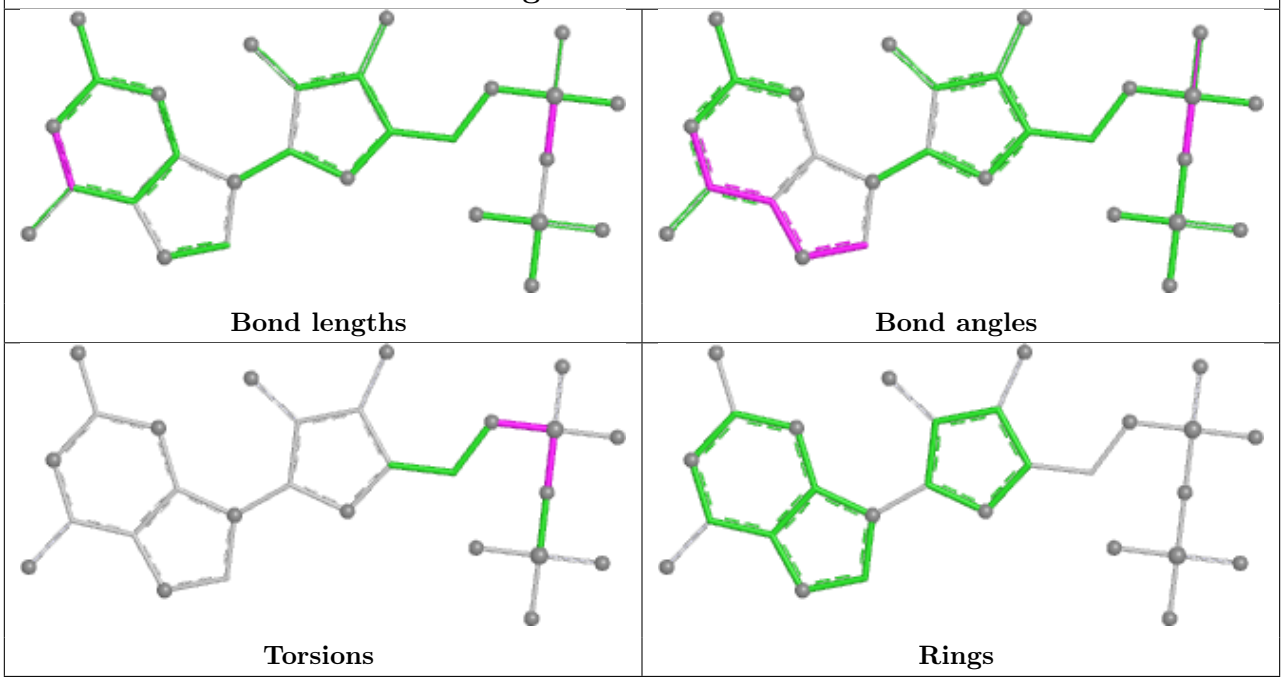


Rings

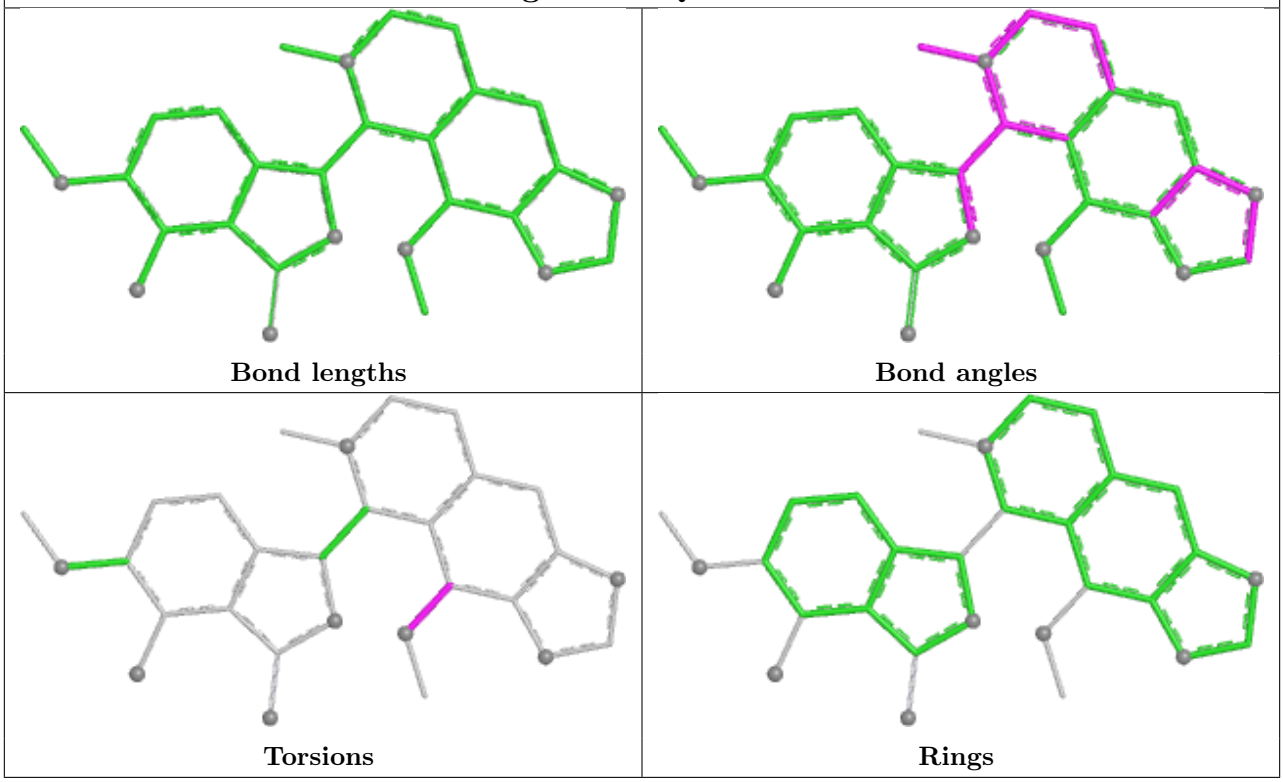
Ligand GTP C 501



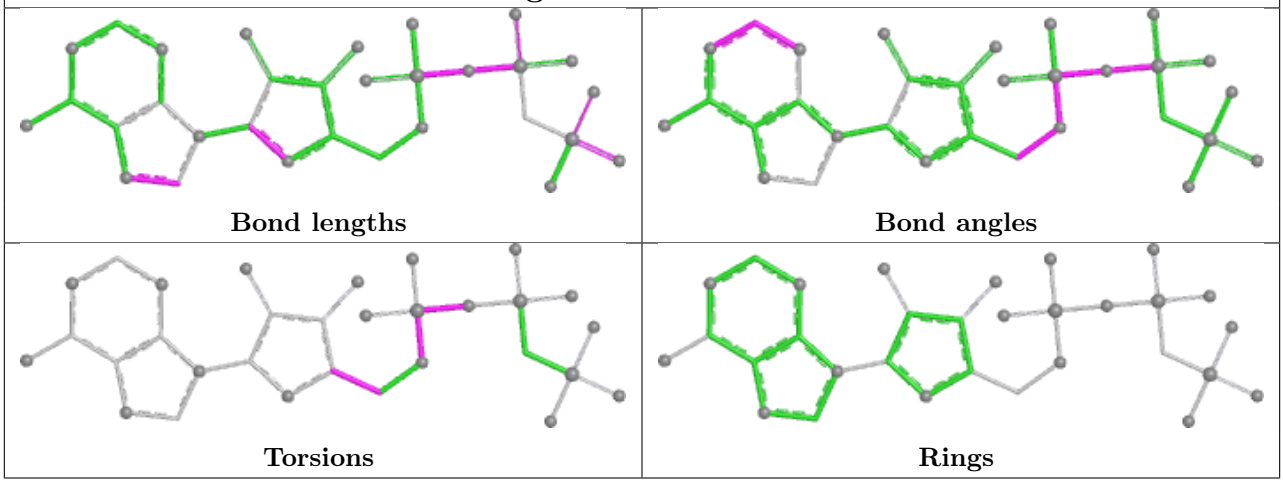
Ligand GDP B 501



Ligand OBQ D 503



Ligand ACP F 701



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	439/451 (97%)	0.25	18 (4%)	37	35	41, 63, 100, 148	0
1	C	440/451 (97%)	-0.08	5 (1%)	80	79	36, 49, 83, 111	0
2	B	422/445 (94%)	0.12	17 (4%)	38	36	38, 59, 99, 153	0
2	D	421/445 (94%)	0.34	32 (7%)	13	12	44, 68, 106, 188	0
3	E	122/143 (85%)	0.34	12 (9%)	7	6	49, 77, 117, 145	0
4	F	333/384 (86%)	1.32	101 (30%)	0	0	51, 90, 154, 183	0
All	All	2177/2319 (93%)	0.34	185 (8%)	10	9	36, 64, 119, 188	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	130	VAL	10.2
2	D	249	ASN	8.7
4	F	251	LYS	7.9
4	F	249	TYR	7.8
2	B	59	ASN	7.3
4	F	173	ILE	7.0
4	F	233	PHE	6.9
4	F	20	LEU	6.5
4	F	131	PHE	6.3
4	F	100	ILE	6.2
2	B	247	GLN	6.1
2	B	57	THR	6.0
4	F	166	ALA	5.9
4	F	132	LEU	5.9
4	F	253	TYR	5.7
4	F	24	THR	5.6
2	B	248	LEU	5.3
4	F	199	PHE	5.2
4	F	21	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
4	F	27	TRP	5.1
4	F	169	LEU	5.1
2	D	57	THR	5.1
4	F	361	LEU	5.0
4	F	133	ALA	4.9
4	F	182	ILE	4.8
2	D	179	ASP	4.8
4	F	252	ASN	4.8
4	F	362	ALA	4.8
4	F	101	TYR	4.8
4	F	17	VAL	4.7
3	E	26	PRO	4.7
4	F	25	GLY	4.7
4	F	250	SER	4.6
4	F	137	ARG	4.6
4	F	259	GLY	4.5
4	F	170	LEU	4.5
4	F	231	ALA	4.5
4	F	248	GLU	4.5
4	F	225	SER	4.4
4	F	129	GLU	4.3
4	F	256	TYR	4.3
4	F	167	SER	4.3
4	F	136	ASN	4.2
2	D	400	ARG	4.2
2	D	405	LEU	4.2
4	F	134	ALA	4.2
3	E	24	LEU	4.2
4	F	99	VAL	4.1
2	B	438	ALA	4.1
4	F	26	GLN	4.1
3	E	27	PRO	4.0
1	A	282	TYR	4.0
2	B	58	GLY	3.8
4	F	22	LEU	3.8
4	F	194	PRO	3.8
4	F	192	LEU	3.7
2	B	33	THR	3.7
4	F	255	ARG	3.7
4	F	247	LYS	3.6
1	A	37	PRO	3.6
2	B	337	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	28	LYS	3.6
2	B	249	ASN	3.6
4	F	224	SER	3.6
4	F	254	GLY	3.6
3	E	143	ALA	3.6
4	F	13	VAL	3.6
2	B	60	LYS	3.6
2	D	82	PRO	3.6
3	E	25	LYS	3.5
4	F	232	ASN	3.5
4	F	23	ALA	3.5
2	B	37	HIS	3.5
4	F	143	GLU	3.5
4	F	234	GLN	3.5
4	F	238	CYS	3.4
4	F	127	GLU	3.3
4	F	125	THR	3.3
1	A	281	ALA	3.2
4	F	226	GLU	3.2
2	D	220	THR	3.2
4	F	135	TYR	3.2
4	F	262	MET	3.2
2	D	252	LEU	3.1
2	B	36	TYR	3.1
4	F	31	ARG	3.1
1	A	42	ILE	3.1
4	F	9	GLU	3.1
4	F	245	ILE	3.1
4	F	197	ARG	3.1
4	F	140	GLU	3.1
2	D	399	PHE	3.1
2	D	202	TYR	3.0
4	F	161	LEU	3.0
1	A	57	GLY	3.0
4	F	168	GLU	3.0
2	D	94	PHE	3.0
2	D	58	GLY	3.0
4	F	228	TYR	3.0
2	D	401	ARG	3.0
4	F	4	PHE	3.0
3	E	142	GLU	2.9
2	D	250	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	147	TRP	2.9
3	E	141	GLU	2.9
4	F	126	ASP	2.9
4	F	240	LEU	2.9
1	A	171	ILE	2.9
4	F	223	THR	2.9
3	E	140	LYS	2.9
4	F	257	GLU	2.9
1	A	346	TRP	2.8
2	D	247	GLN	2.8
4	F	260	ASN	2.8
2	D	83	PHE	2.8
2	D	248	LEU	2.8
2	B	34	GLY	2.8
2	D	415	GLU	2.8
2	B	250	ALA	2.7
1	A	201	ALA	2.7
2	B	56	ALA	2.7
4	F	165	GLU	2.7
2	B	61	TYR	2.6
4	F	19	ARG	2.6
4	F	191	LEU	2.6
4	F	258	GLU	2.6
2	D	2[A]	ARG	2.6
2	D	56	ALA	2.6
4	F	244	CYS	2.6
4	F	343	TYR	2.6
4	F	243	HIS	2.6
4	F	246	GLN	2.6
4	F	172	PHE	2.5
4	F	227	PRO	2.5
2	D	260	VAL	2.4
4	F	267	PHE	2.4
4	F	229	ASN	2.4
1	A	41	THR	2.4
1	A	364	PRO	2.4
3	E	45	PRO	2.4
1	A	262	TYR	2.4
4	F	32	LYS	2.4
4	F	1	MET	2.4
2	D	79	ARG	2.3
4	F	128	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	138	ARG	2.3
4	F	171	ASP	2.3
2	B	38	GLY	2.3
1	C	1	MET	2.3
1	A	141	PHE	2.3
4	F	359	PHE	2.3
1	A	169	PHE	2.3
1	A	35	GLN	2.3
3	E	103	GLN	2.3
4	F	190	LEU	2.2
3	E	139	LEU	2.2
2	D	77	SER	2.2
4	F	341	LYS	2.2
1	A	38	SER	2.2
1	C	201	ALA	2.2
2	D	259	MET	2.2
2	D	407	TRP	2.2
2	D	255	LEU	2.2
1	A	283	HIS	2.1
1	C	179	THR	2.1
4	F	174	ASP	2.1
4	F	98	TYR	2.1
2	D	78	VAL	2.1
4	F	342	LEU	2.1
2	D	37	HIS	2.1
2	D	256	ALA	2.1
4	F	339	ALA	2.1
2	D	378	ILE	2.1
2	D	221	THR	2.1
1	A	43	GLY	2.1
4	F	163	SER	2.1
4	F	239	HIS	2.1
1	A	1	MET	2.1
1	C	340	SER	2.1
4	F	11	SER	2.1
4	F	181	VAL	2.1
4	F	142	ARG	2.0
2	D	219	LEU	2.0
3	E	48	GLU	2.0
1	C	200	CYS	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 monosaccharides in this entry.

6.4 Ligands (i)

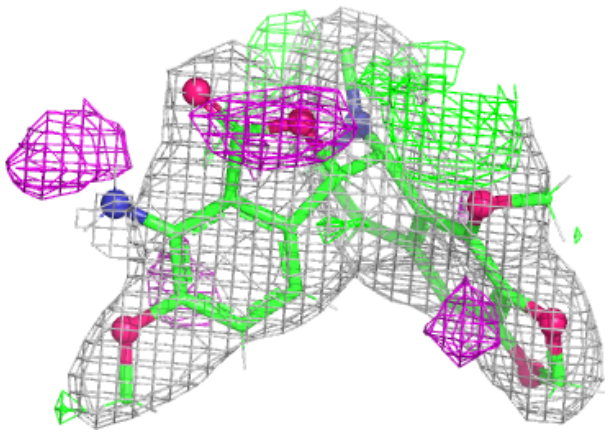
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

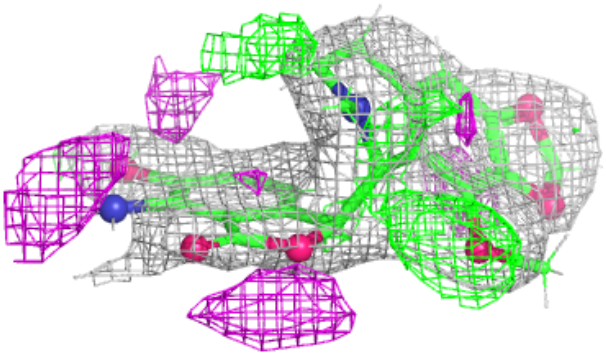
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	F	702	1/1	0.27	0.19	92,92,92,92	0
11	GOL	B	505	6/6	0.72	0.22	91,110,118,118	0
9	OBQ	D	503	29/29	0.78	0.32	53,75,98,100	51
7	CA	A	503	1/1	0.87	0.06	86,86,86,86	0
6	MG	D	502	1/1	0.90	0.13	79,79,79,79	0
9	OBQ	B	503	29/29	0.90	0.17	50,74,94,100	0
12	ACP	F	701	31/31	0.91	0.12	80,90,132,139	0
6	MG	A	502	1/1	0.95	0.16	47,47,47,47	0
10	MES	B	504	12/12	0.95	0.14	70,83,92,103	0
8	GDP	D	501	28/28	0.96	0.12	53,62,71,84	0
5	GTP	A	501	32/32	0.98	0.20	35,46,55,58	0
6	MG	B	502	1/1	0.98	0.13	40,40,40,40	0
6	MG	C	502	1/1	0.98	0.14	38,38,38,38	0
5	GTP	C	501	32/32	0.99	0.17	31,40,45,49	0
7	CA	C	503	1/1	0.99	0.03	69,69,69,69	0
8	GDP	B	501	28/28	0.99	0.17	35,43,46,48	0

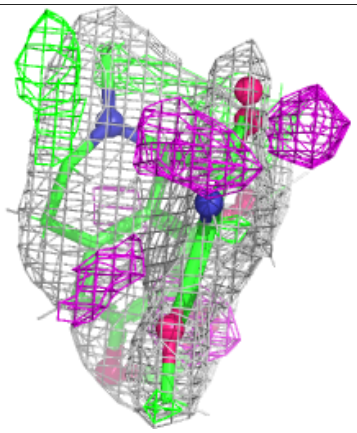
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OBQ 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)

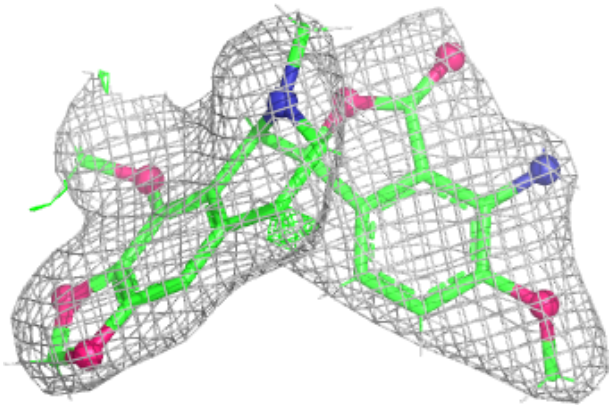


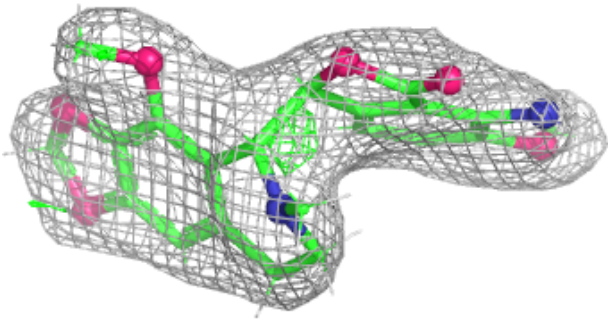


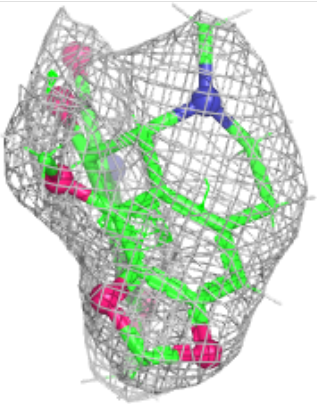


Electron density around OBQ B 503:

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

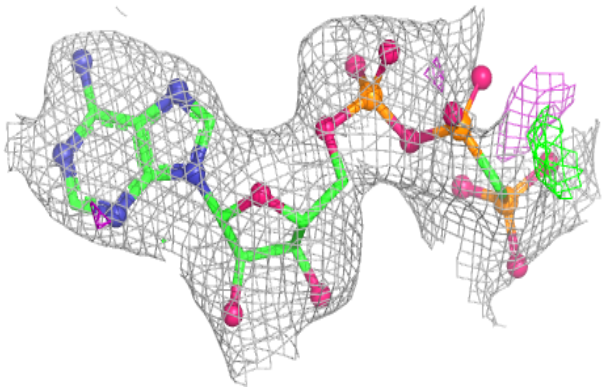


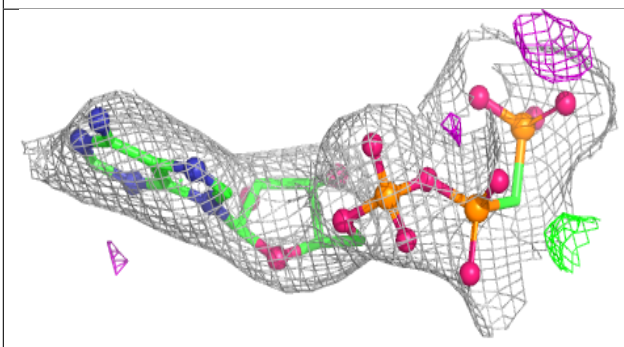


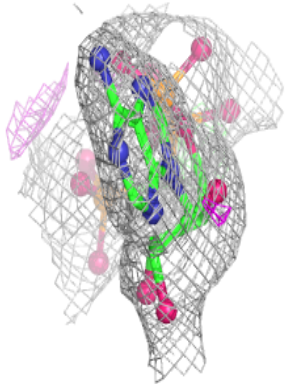


Electron density around ACP F 701:

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

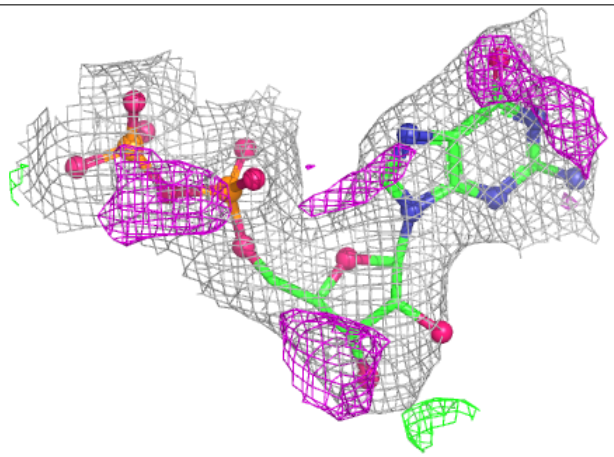


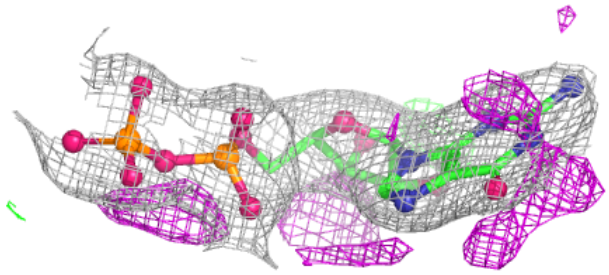


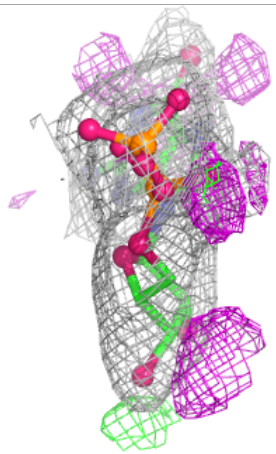


Electron density around GDP D 501:

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

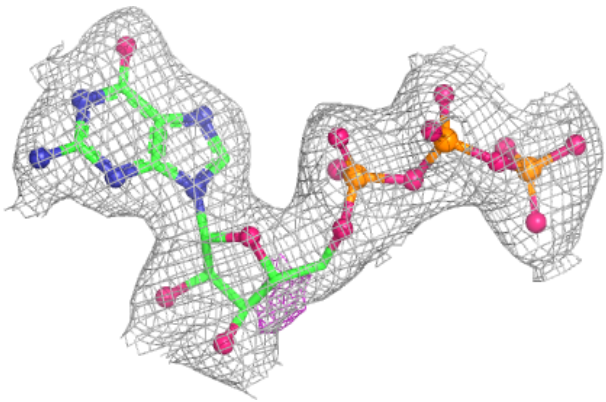


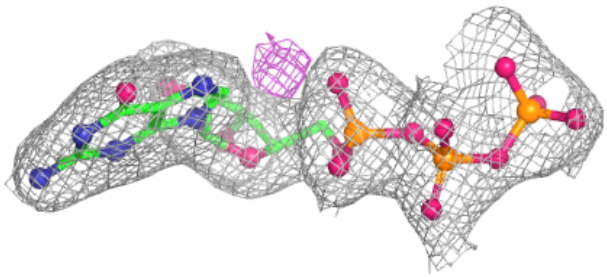


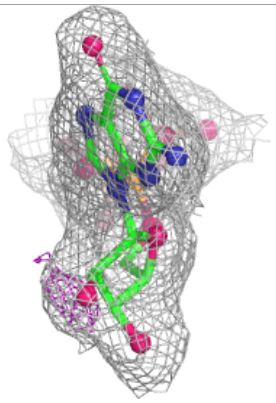


Electron density around GTP A 501:

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

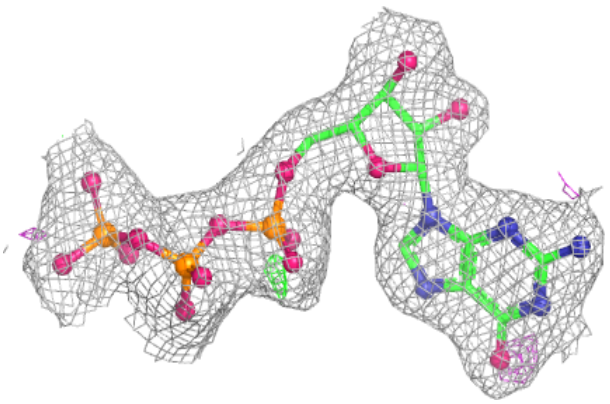


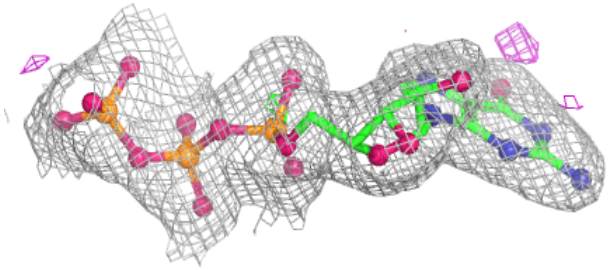


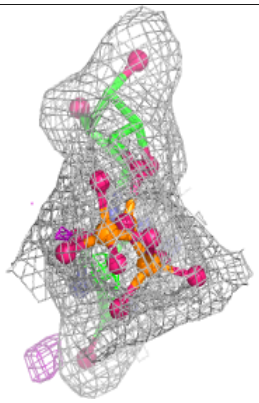


Electron density around GTP C 501:

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

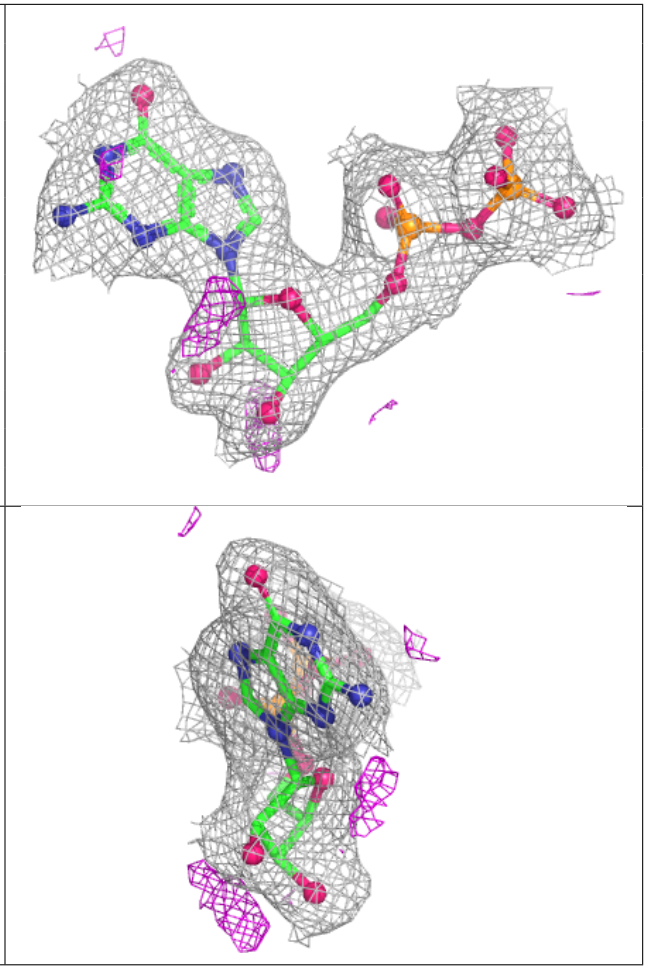






Electron density around GDP B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.