Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 05:37 PM JST

PDB ID	:	6LSM
Title	:	Tubulin Polymerization Inhibitors
Authors	:	Gang, L.; Wang, Y.X.; Chen, J.J.
Deposited on	:	2020-01-17
Resolution	:	2.75 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:

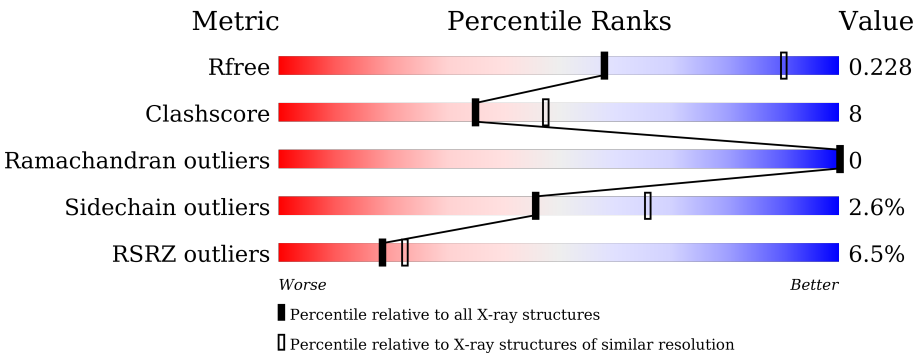
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	450	2%, 82%, 15%, • •
1	C	450	84%, 13%, • •
2	B	445	2%, 76%, 19%, 5%
2	D	445	8%, 71%, 23%, 5%
3	E	143	13%, 64%, 22%, •, 13%
4	F	384	17%, 68%, 22%, •, 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	GDP	D	600	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 17751 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
			Total	C	N	O	S			
1	A	440	3435	2175	581	657	22	0	1	0
1	C	440	3451	2184	585	660	22	0	4	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	424	3344	2104	569	645	26	0	2	0
2	D	421	3300	2074	562	639	25	0	2	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	124	1021	628	184	204	5	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

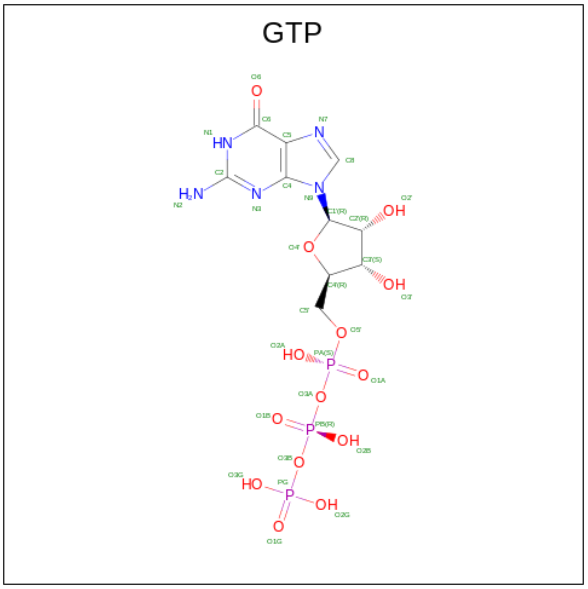
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	351	2891	1852	499	525	15	0	2	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	2	2	2	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

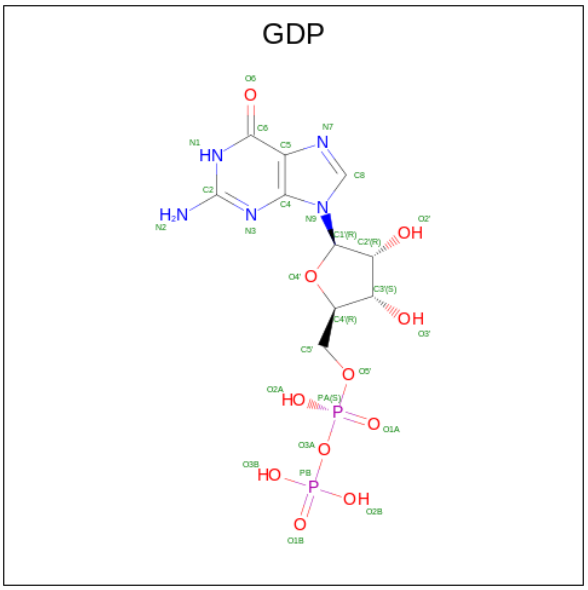
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
8	A	1	1	1	0	0

- Molecule 9 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		
9	B	1	28	10	5	11	2	0	0

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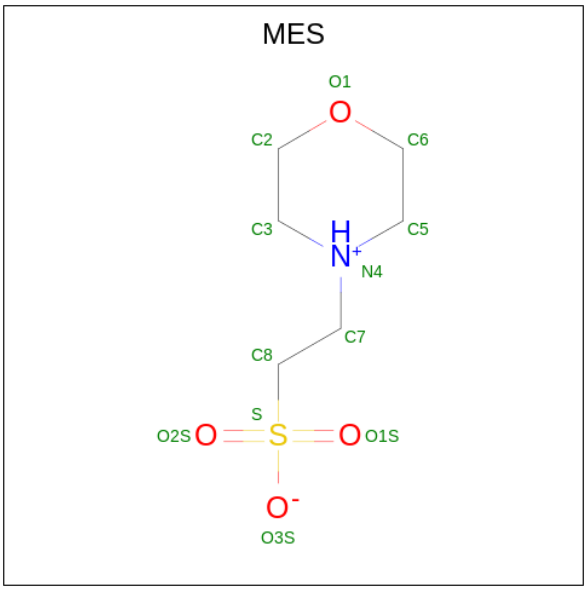
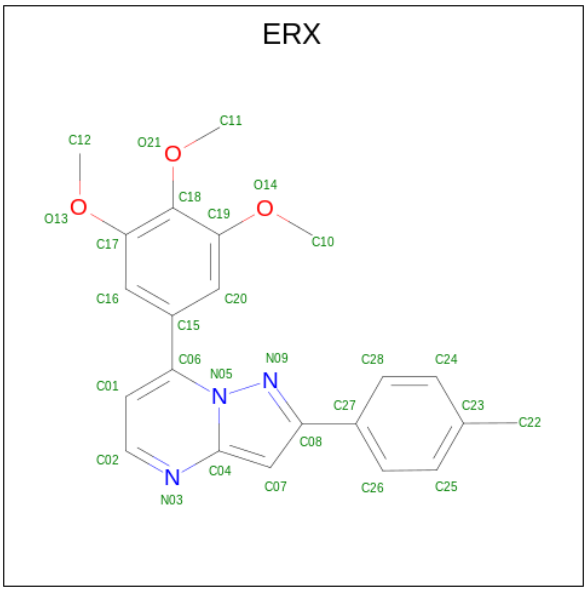
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	D	1	28	10	5	11	2	0	0

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



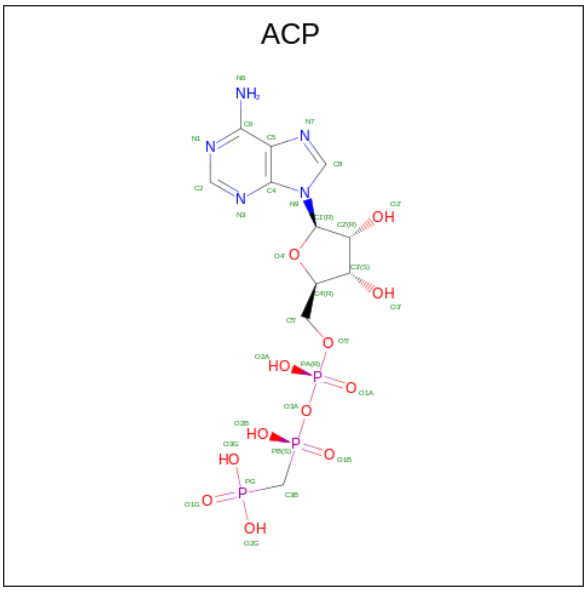
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
10	B	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
10	B	1	12	6	1	4	1	0	0

- Molecule 11 is 2-(4-methylphenyl)-7-(3,4,5-trimethoxyphenyl)pyrazolo[1,5-a]pyrimidine (three-letter code: ERX) (formula: $C_{22}H_{21}N_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	B	1	28	22	3	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.

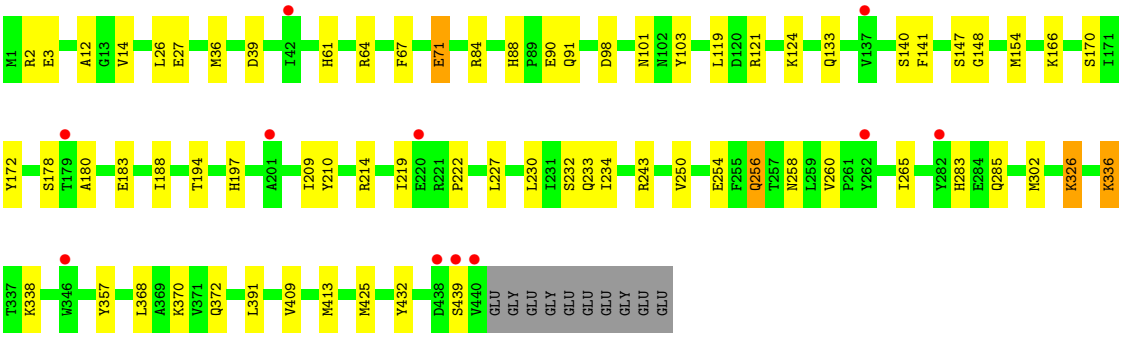
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	14	14	14	0	0
			Total	O		
13	B	27	27	27	0	0
			Total	O		
13	C	35	35	35	0	0
			Total	O		
13	D	3	3	3	0	0
			Total	O		
13	E	8	8	8	0	0
			Total	O		
13	F	8	8	8	0	0

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.

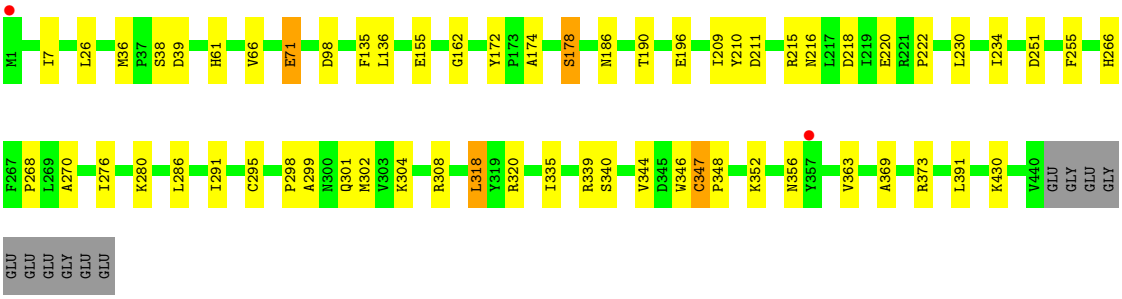
• Molecule 1: Tubulin alpha-1B chain

Chain A:



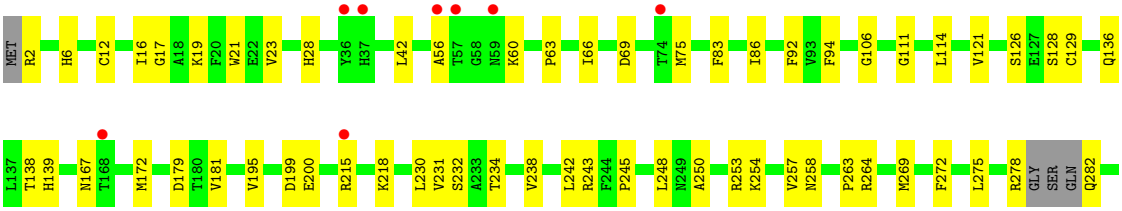
• Molecule 1: Tubulin alpha-1B chain

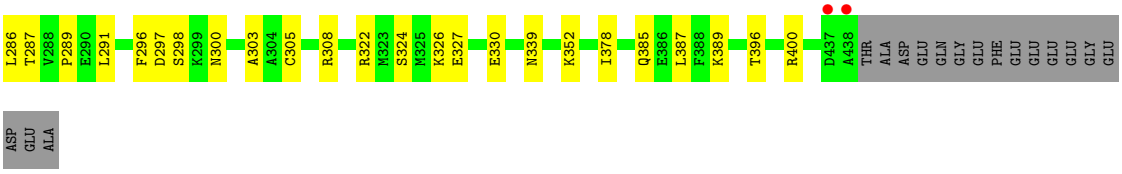
Chain C:



• Molecule 2: Tubulin beta chain

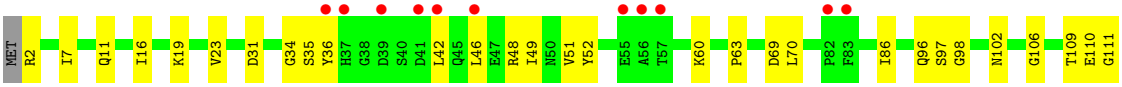
Chain B:

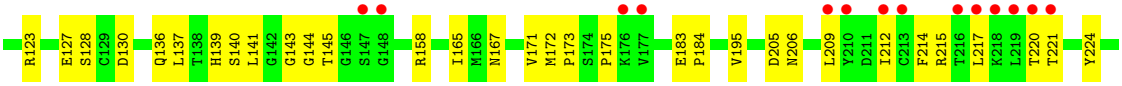


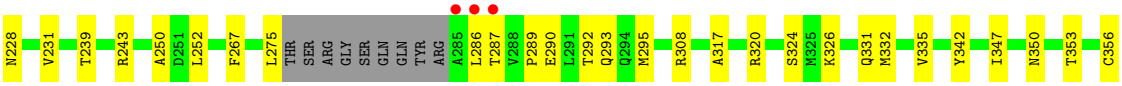


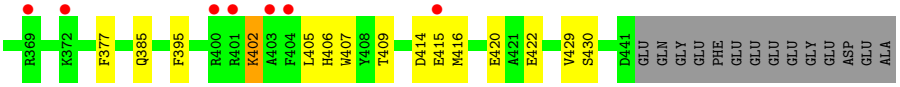
- Molecule 2: Tubulin beta chain

Chain D:



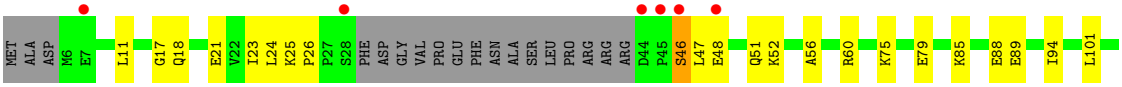


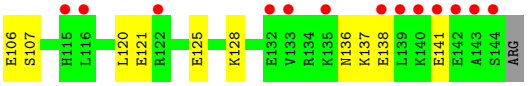




- Molecule 3: Stathmin-4

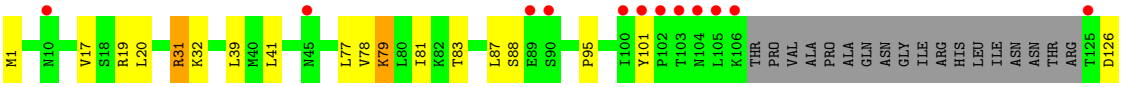
Chain E:

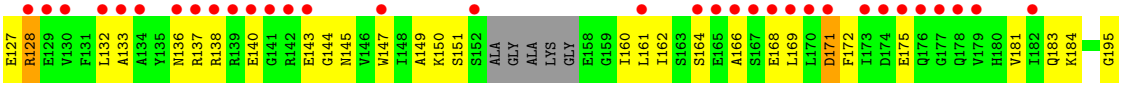


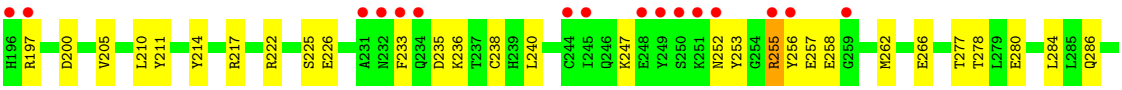


- Molecule 4: Tubulin tyrosine ligase

Chain F:







H289
I290
I291
R292
S293
K305
F315
A339
L342
G349
V353
L361
ALA
ASP
THR
GLY
GLN
LYS
THR
SER
GLN
PRO
T372
F375
L378
H379
H380
H381
H382
H383
H384

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.55Å 158.08Å 182.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.75 29.87 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.87-2.75) 99.8 (29.87-2.75)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.181 , 0.227 0.182 , 0.228	Depositor DCC
R_{free} test set	1999 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å^2)	55.3	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17751	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, CA, ACP, GDP, ERX, CL, MES, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.47	0/3516	0.63	0/4775
1	C	0.56	2/3538 (0.1%)	0.69	2/4803 (0.0%)
2	B	0.48	0/3424	0.63	0/4638
2	D	0.48	1/3376 (0.0%)	0.61	0/4576
3	E	0.50	0/1032	0.59	0/1371
4	F	0.43	0/2964	0.63	2/4003 (0.0%)
All	All	0.49	3/17850 (0.0%)	0.64	4/24166 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	175	PRO	N-CD	-7.11	1.37	1.47
1	C	347	CYS	CB-SG	-6.64	1.71	1.82
1	C	295	CYS	CB-SG	-6.60	1.71	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	280	LYS	CD-CE-NZ	9.25	132.97	111.70
1	C	318	LEU	CB-CG-CD2	6.14	121.45	111.00
4	F	171	ASP	CB-CG-OD2	-5.25	113.58	118.30
4	F	171	ASP	CB-CG-OD1	5.08	122.87	118.30

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	3435	0	3345	47	0
1	C	3451	0	3364	33	0
2	B	3344	0	3226	58	0
2	D	3300	0	3169	73	0
3	E	1021	0	1029	23	0
4	F	2891	0	2857	56	0
5	A	32	0	12	0	0
5	C	32	0	11	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	10	2	0
9	D	28	0	12	15	0
10	B	24	0	25	5	0
11	B	28	0	0	1	0
12	F	31	0	13	2	0
13	A	14	0	0	1	0
13	B	27	0	0	5	0
13	C	35	0	0	2	0
13	D	3	0	0	0	0
13	E	8	0	0	0	0
13	F	8	0	0	0	0
All	All	17751	0	17073	284	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 8.

All (284) 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:D:143:GLY:HA3	9:D:600:GDP:O2A	1.45	1.14
2:D:16:ILE:HG22	2:D:228:ASN:OD1	1.74	0.88
2:D:144:GLY:N	9:D:600:GDP:O2B	2.11	0.82
2:D:206:ASN:HA	2:D:209:LEU:HD23	1.61	0.79
2:D:205:ASP:O	2:D:209:LEU:HD22	1.83	0.78
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.17	0.77
2:D:143:GLY:CA	9:D:600:GDP:O2A	2.31	0.75
1:C:255:PHE:CZ	1:C:318:LEU:HD22	2.22	0.74
1:C:36:MET:SD	1:C:39:ASP:HB2	2.31	0.70
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.75	0.68
9:D:600:GDP:H5'	9:D:600:GDP:H8	1.58	0.68
2:B:339:ASN:HA	13:B:602:HOH:O	1.95	0.67
1:C:211[A]:ASP:OD2	1:C:304:LYS:NZ	2.28	0.67
2:B:298:SER:N	10:B:505:MES:O1S	2.22	0.66
9:D:600:GDP:H8	9:D:600:GDP:C5'	2.09	0.66
3:E:11:LEU:HD11	3:E:18:GLN:HE21	1.61	0.65
4:F:128:ARG:O	4:F:132:LEU:HD12	1.96	0.65
4:F:168:GLU:O	4:F:171:ASP:HB3	1.95	0.65
2:B:172:MET:HG2	2:B:387:LEU:HD21	1.80	0.64
2:D:228:ASN:ND2	9:D:600:GDP:HN1	1.96	0.64
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.79	0.63
2:D:317:ALA:HB3	2:D:353:THR:HG22	1.80	0.63
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.32	0.62
4:F:277:THR:HG22	4:F:278:THR:H	1.64	0.62
2:D:16:ILE:CG2	2:D:228:ASN:OD1	2.45	0.62
1:A:209:ILE:HD11	1:A:302:MET:SD	2.41	0.61
3:E:48:GLU:O	3:E:52:LYS:HG2	2.01	0.61
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.83	0.60
2:D:228:ASN:CG	9:D:600:GDP:HN1	2.05	0.60
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.20	0.60
2:D:145:THR:H	9:D:600:GDP:PB	2.25	0.60
2:D:136:GLN:HA	2:D:167:ASN:O	2.03	0.59
2:D:7:ILE:O	2:D:137:LEU:HD12	2.03	0.59
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.84	0.59
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.84	0.59
9:D:600:GDP:C5'	9:D:600:GDP:C8	2.85	0.59
1:C:196:GLU:HB2	13:C:616:HOH:O	2.03	0.58
4:F:349:GLY:O	4:F:353:VAL:HG12	2.03	0.57
2:D:214:PHE:HD2	2:D:215:ARG:HG2	1.70	0.57
2:D:402:LYS:HG3	2:D:405:LEU:HD13	1.86	0.57
4:F:247:LYS:HD2	4:F:253:TYR:CZ	2.39	0.57
2:B:136:GLN:HA	2:B:167:ASN:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:LEU:HD12	13:C:610:HOH:O	2.04	0.57
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.40	0.57
2:B:230:LEU:O	2:B:234:THR:HG23	2.03	0.57
2:B:167:ASN:OD1	2:B:200:GLU:HG3	2.03	0.57
2:B:263:PRO:HD2	13:B:610:HOH:O	2.04	0.57
2:D:332:MET:HG3	2:D:353:THR:HG21	1.86	0.57
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.40	0.57
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.87	0.56
2:D:70:LEU:HB3	2:D:98:GLY:HA2	1.87	0.56
2:D:220:THR:HG23	2:D:221:THR:HG22	1.86	0.56
2:D:239:THR:O	2:D:243:ARG:HG3	2.06	0.56
2:D:287:THR:HB	2:D:289:PRO:HD2	1.88	0.56
2:D:331:GLN:O	2:D:335:VAL:HG23	2.06	0.56
2:B:106:GLY:O	2:B:111:GLY:HA3	2.06	0.56
4:F:210:LEU:O	4:F:305:LYS:NZ	2.38	0.55
2:B:195:VAL:HG13	2:B:264:ARG:HB3	1.89	0.55
4:F:79:LYS:O	4:F:83:THR:OG1	2.21	0.55
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.88	0.55
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.88	0.54
2:D:63:PRO:HG2	2:D:86:ILE:HG23	1.89	0.54
2:D:145:THR:N	9:D:600:GDP:O2B	2.40	0.54
1:C:174:ALA:O	1:C:178:SER:HB2	2.07	0.54
2:D:48:ARG:HH12	2:D:250:ALA:HB1	1.73	0.53
3:E:11:LEU:HD11	3:E:18:GLN:NE2	2.23	0.53
2:B:322:ARG:HG2	2:B:322:ARG:HH21	1.74	0.53
4:F:150:LYS:HD3	4:F:160:ILE:HG12	1.91	0.53
1:A:101:ASN:HD22	2:B:258:ASN:HD21	1.56	0.53
1:A:230:LEU:O	1:A:234:ILE:HD12	2.09	0.53
2:D:205:ASP:O	2:D:209:LEU:CD2	2.54	0.53
2:B:396:THR:O	2:B:400:ARG:HG2	2.08	0.53
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.91	0.52
4:F:200:ASP:OD2	12:F:402:ACP:O3'	2.27	0.52
4:F:162:ILE:HB	4:F:233:PHE:HB3	1.91	0.52
4:F:286:GLN:O	4:F:290:ILE:HG13	2.08	0.52
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.90	0.52
1:A:180:ALA:O	1:A:183:GLU:HG3	2.10	0.52
2:B:248:LEU:HD11	2:B:352:LYS:HE2	1.92	0.52
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.44	0.52
2:D:414:ASP:OD1	2:D:415:GLU:N	2.43	0.52
4:F:101:TYR:HD2	4:F:126:ASP:HB2	1.75	0.52
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:HG2	1:A:64:ARG:NH2	2.25	0.51
4:F:160:ILE:HD13	4:F:240:LEU:HD21	1.92	0.51
2:D:69:ASP:OD1	2:D:70:LEU:N	2.44	0.51
4:F:292:ARG:HG3	4:F:378:LEU:HB3	1.93	0.51
1:C:7:ILE:HG23	1:C:66:VAL:HG13	1.93	0.51
2:D:295:MET:CG	2:D:377:PHE:HB2	2.40	0.51
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.41	0.51
2:B:308:ARG:HE	10:B:505:MES:H71	1.75	0.51
3:E:137:LYS:O	3:E:141:GLU:HG2	2.11	0.51
3:E:56:ALA:HB1	3:E:60:ARG:HH12	1.76	0.51
4:F:150:LYS:NZ	4:F:151:SER:O	2.29	0.51
2:B:253:ARG:O	2:B:257:VAL:HG23	2.10	0.50
1:A:250:VAL:HG22	1:A:254:GLU:OE2	2.12	0.50
2:B:296:PHE:O	10:B:505:MES:H81	2.12	0.50
2:D:123:ARG:O	2:D:127:GLU:HG2	2.12	0.50
2:B:234:THR:O	2:B:238:VAL:HG13	2.11	0.50
4:F:136:ASN:O	4:F:140:GLU:HG3	2.10	0.50
9:D:600:GDP:C8	9:D:600:GDP:H5"	2.46	0.50
4:F:184:LYS:O	12:F:402:ACP:N6	2.44	0.50
3:E:25:LYS:HG2	3:E:26:PRO:HD2	1.93	0.49
1:A:141:PHE:O	1:A:147:SER:HB3	2.12	0.49
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.47	0.49
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.42	0.49
2:B:238:VAL:HB	2:B:378:ILE:HD11	1.92	0.49
2:B:242:LEU:HA	2:B:250:ALA:HB1	1.95	0.49
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.94	0.49
1:A:326:LYS:HE2	1:A:326:LYS:H	1.78	0.49
4:F:138:ARG:NH1	4:F:144:GLY:O	2.46	0.49
3:E:125:GLU:HA	3:E:128:LYS:HG2	1.94	0.49
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.47	0.49
1:A:2:ARG:O	1:A:133:GLN:NE2	2.45	0.48
2:B:69:ASP:O	2:B:94:PHE:HA	2.14	0.48
2:B:326:LYS:HE3	2:B:330:GLU:OE2	2.13	0.48
4:F:31:ARG:HH21	4:F:32:LYS:HD3	1.78	0.48
4:F:161:LEU:HD23	4:F:172:PHE:CZ	2.49	0.48
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.96	0.48
2:D:416:MET:O	2:D:420:GLU:HG3	2.13	0.48
2:B:42:LEU:HD22	2:B:245:PRO:HG2	1.95	0.48
4:F:280:GLU:HA	4:F:284:LEU:CB	2.44	0.47
2:D:31:ASP:OD1	2:D:34:GLY:N	2.47	0.47
1:C:26:LEU:HD12	1:C:363:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:GLN:HB3	9:D:600:GDP:O1A	2.15	0.47
4:F:133:ALA:O	4:F:137:ARG:HG3	2.14	0.47
1:A:154:MET:HG3	1:A:194:THR:HG23	1.95	0.47
2:B:28:HIS:NE2	2:B:243:ARG:HB3	2.29	0.47
3:E:75:LYS:O	3:E:79:GLU:HG3	2.15	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.47
2:D:19:LYS:O	2:D:23:VAL:HG23	2.13	0.47
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.50	0.47
3:E:21:GLU:OE1	3:E:23:ILE:HD11	2.14	0.47
4:F:132:LEU:CD2	4:F:166:ALA:HB1	2.45	0.47
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.96	0.47
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.97	0.47
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.63	0.47
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.49	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.51	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.96	0.46
3:E:121:GLU:O	3:E:125:GLU:HG2	2.14	0.46
1:A:336:LYS:HD3	3:E:24:LEU:CD1	2.45	0.46
2:B:234:THR:HG22	2:B:272:PHE:HB2	1.97	0.46
2:D:140:SER:HA	2:D:171:VAL:HB	1.97	0.46
2:D:228:ASN:ND2	9:D:600:GDP:N1	2.63	0.46
4:F:17:VAL:HA	4:F:20:LEU:HD12	1.96	0.46
4:F:137:ARG:HA	4:F:140:GLU:OE2	2.16	0.46
4:F:161:LEU:HD13	4:F:161:LEU:HA	1.79	0.46
2:D:51:VAL:HG13	2:D:52:TYR:CD2	2.50	0.46
1:A:88:HIS:N	1:A:91:GLN:OE1	2.38	0.46
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.51	0.46
2:B:339:ASN:ND2	13:B:602:HOH:O	2.22	0.46
1:A:101:ASN:ND2	2:B:254:LYS:HG2	2.31	0.46
1:C:186:ASN:O	1:C:190:THR:HG22	2.16	0.46
2:D:286:LEU:HD12	2:D:286:LEU:HA	1.78	0.46
1:A:166:LYS:HE2	1:A:197:HIS:O	2.16	0.46
2:B:282:GLN:N	13:B:608:HOH:O	2.50	0.45
2:B:303:ALA:O	2:B:305:CYS:N	2.45	0.45
2:D:395:PHE:CE1	2:D:422:GLU:HG3	2.51	0.45
2:D:406:HIS:CD2	2:D:407:TRP:HD1	2.34	0.45
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.99	0.45
4:F:226:GLU:HB3	4:F:238:CYS:HB3	1.98	0.45
1:A:90:GLU:O	1:A:121:ARG:HD2	2.15	0.45
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.52	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:ARG:O	2:D:51:VAL:HG23	2.17	0.45
3:E:85:LYS:HE2	3:E:89:GLU:OE2	2.17	0.45
4:F:138:ARG:NH2	4:F:143:GLU:OE2	2.49	0.45
2:B:16[A]:ILE:HD11	2:B:138:THR:HB	2.00	0.44
1:C:215:ARG:HD2	1:C:216:ASN:OD1	2.18	0.44
4:F:145:ASN:OD1	4:F:147:TRP:NE1	2.49	0.44
1:A:326:LYS:HD3	1:A:326:LYS:N	2.32	0.44
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.99	0.44
2:B:16[A]:ILE:HG13	2:B:17:GLY:N	2.32	0.44
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.98	0.44
1:A:372:GLN:NE2	13:A:606:HOH:O	2.50	0.44
2:B:19:LYS:HG2	2:B:232:SER:OG	2.18	0.44
2:B:324:SER:OG	2:B:327:GLU:HB2	2.17	0.44
1:A:88:HIS:HB3	1:A:91:GLN:HG3	1.98	0.44
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.99	0.44
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.99	0.44
1:A:256:GLN:HG2	1:A:260:VAL:HB	1.99	0.44
1:A:233:GLN:HG3	1:A:368:LEU:HD12	2.00	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.43
4:F:339:ALA:HB3	4:F:342:LEU:HD12	2.00	0.43
2:D:48:ARG:O	2:D:51:VAL:HG12	2.19	0.43
2:D:96:GLN:NE2	2:D:97:SER:H	2.15	0.43
4:F:262:MET:SD	4:F:266:GLU:HG2	2.59	0.43
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.86	0.43
2:D:70:LEU:HD23	2:D:70:LEU:HA	1.84	0.43
2:D:292:THR:HG22	2:D:335:VAL:HG21	2.00	0.43
4:F:19:ARG:HG3	4:F:20:LEU:N	2.33	0.43
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.43
4:F:95:PRO:HB2	4:F:183:GLN:CG	2.49	0.43
2:B:83:PHE:O	2:B:86:ILE:HG22	2.18	0.43
1:A:256:GLN:O	1:A:256:GLN:OE1	2.36	0.43
3:E:47:LEU:HD12	3:E:47:LEU:O	2.19	0.43
3:E:88:GLU:OE1	3:E:88:GLU:HA	2.19	0.43
4:F:150:LYS:HD3	4:F:160:ILE:CG1	2.48	0.43
4:F:169:LEU:HD23	4:F:169:LEU:HA	1.43	0.43
1:A:39:ASP:OD2	1:A:61:HIS:NE2	2.44	0.43
2:B:352:LYS:HD2	11:B:507:ERX:C08	2.49	0.43
1:C:255:PHE:CE2	1:C:318:LEU:HD22	2.54	0.43
2:B:199:ASP:OD2	10:B:504:MES:H52	2.19	0.43
2:B:287:THR:HB	2:B:289:PRO:HD2	2.00	0.43
2:D:228:ASN:OD1	9:D:600:GDP:N1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:406:HIS:HA	2:D:409:THR:HG22	2.01	0.43
2:D:141:LEU:HD12	2:D:172:MET:SD	2.59	0.43
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.01	0.43
2:B:56:ALA:HB3	2:B:60:LYS:HB2	2.01	0.42
1:C:215:ARG:CZ	1:C:299:ALA:HB1	2.49	0.42
3:E:46:SER:OG	3:E:48:GLU:N	2.52	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.42
1:C:266:HIS:O	1:C:268:PRO:HD3	2.19	0.42
4:F:161:LEU:HD23	4:F:172:PHE:CE2	2.54	0.42
2:D:172:MET:HG3	2:D:173:PRO:HD2	2.01	0.42
3:E:46:SER:OG	3:E:47:LEU:N	2.52	0.42
4:F:289:HIS:O	4:F:293:SER:OG	2.29	0.42
2:D:46:LEU:HA	2:D:49:ILE:HB	2.02	0.42
2:D:275:LEU:HD23	2:D:275:LEU:HA	1.85	0.42
2:D:290:GLU:O	2:D:293:GLN:HB3	2.20	0.42
1:A:12:ALA:CB	1:A:140:SER:HB3	2.50	0.42
2:B:12:CYS:HB2	9:B:501:GDP:N7	2.35	0.42
2:B:297:ASP:HA	10:B:505:MES:O1S	2.20	0.42
1:C:155:GLU:HB3	3:E:101:LEU:HD22	2.02	0.42
1:C:230:LEU:O	1:C:234:ILE:HD12	2.20	0.42
2:D:34:GLY:O	2:D:60:LYS:HA	2.20	0.42
2:D:48:ARG:NH1	2:D:250:ALA:HB1	2.34	0.42
4:F:126:ASP:OD1	4:F:127:GLU:N	2.53	0.42
4:F:205:VAL:HG22	4:F:315:PHE:HB2	2.02	0.42
2:D:228:ASN:HA	2:D:231:VAL:HG22	2.01	0.41
4:F:149:ALA:O	4:F:160:ILE:HG23	2.19	0.41
2:B:128:SER:O	2:B:128:SER:OG	2.36	0.41
3:E:120:LEU:HD23	3:E:120:LEU:HA	1.93	0.41
2:B:179:ASP:O	1:C:352:LYS:NZ	2.37	0.41
2:D:212:ILE:HG22	2:D:217:LEU:HD12	2.02	0.41
2:D:228:ASN:O	2:D:231:VAL:HG22	2.20	0.41
1:C:209:ILE:HD11	1:C:302:MET:SD	2.60	0.41
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.35	0.41
2:D:385:GLN:HB2	2:D:429:VAL:HG13	2.02	0.41
4:F:205:VAL:HG11	4:F:291:ILE:HD13	2.01	0.41
2:B:28:HIS:HE1	2:B:243:ARG:O	2.03	0.41
2:B:215:ARG:O	2:B:218:LYS:NZ	2.52	0.41
1:C:135:PHE:O	1:C:136:LEU:HD23	2.20	0.41
1:C:220:GLU:OE2	2:D:326:LYS:HD3	2.20	0.41
3:E:47:LEU:HD11	3:E:51:GLN:NE2	2.35	0.41
2:D:102:ASN:ND2	2:D:407:TRP:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:109:THR:OG1	2:D:110:GLU:N	2.53	0.41
2:D:224:TYR:O	2:D:228:ASN:ND2	2.48	0.41
4:F:149:ALA:HB2	4:F:169:LEU:HD13	2.02	0.41
4:F:247:LYS:HD2	4:F:253:TYR:CE2	2.56	0.41
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.85	0.41
2:B:269:MET:HG3	2:B:303:ALA:HB3	2.02	0.41
9:D:600:GDP:H5'	9:D:600:GDP:C8	2.46	0.41
4:F:31:ARG:HA	4:F:31:ARG:HD2	1.73	0.41
4:F:87:LEU:O	4:F:88:SER:OG	2.33	0.41
2:D:195:VAL:HG22	2:D:267:PHE:CE2	2.56	0.41
1:A:26:LEU:HA	1:A:26:LEU:HD23	1.81	0.41
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.56	0.41
1:A:357:TYR:OH	3:E:18:GLN:HG3	2.20	0.41
2:B:126:SER:O	2:B:129:CYS:HB2	2.21	0.41
2:B:385:GLN:O	2:B:389:LYS:HG3	2.21	0.41
2:D:206:ASN:CA	2:D:209:LEU:HD23	2.42	0.41
1:A:188:ILE:HG13	1:A:425:MET:HG3	2.03	0.41
1:A:214:ARG:HG2	1:A:219:ILE:O	2.21	0.41
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.35	0.41
2:D:320:ARG:HA	2:D:356:CYS:O	2.21	0.41
1:C:270:ALA:O	1:C:302:MET:HB2	2.22	0.40
1:C:301:GLN:HE21	1:C:301:GLN:HB2	1.59	0.40
1:C:320:ARG:HA	1:C:356:ASN:O	2.22	0.40
2:D:290:GLU:H	2:D:290:GLU:HG2	1.71	0.40
4:F:252:ASN:O	4:F:255:ARG:HB2	2.21	0.40
2:B:66:ILE:HG12	2:B:121:VAL:HG12	2.03	0.40
2:B:114:LEU:O	2:B:114:LEU:HG	2.21	0.40
2:D:183:GLU:HB2	2:D:184:PRO:HD3	2.02	0.40
4:F:77:LEU:O	4:F:81:ILE:HG13	2.21	0.40
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.90	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.40
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.57	0.40
1:C:276:ILE:HG23	1:C:369:ALA:HB3	2.03	0.40
1:C:291:ILE:HD13	1:C:373:ARG:HG3	2.02	0.40
2:D:402:LYS:HE2	2:D:402:LYS:HB2	1.78	0.40
1:A:283:HIS:HD2	1:A:285:GLN:NE2	2.19	0.40
2:B:2:ARG:N	13:B:613:HOH:O	2.54	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	439/450 (98%)	422 (96%)	17 (4%)	0	100	100
1	C	441/450 (98%)	426 (97%)	15 (3%)	0	100	100
2	B	422/445 (95%)	408 (97%)	14 (3%)	0	100	100
2	D	418/445 (94%)	403 (96%)	15 (4%)	0	100	100
3	E	121/143 (85%)	119 (98%)	2 (2%)	0	100	100
4	F	345/384 (90%)	331 (96%)	14 (4%)	0	100	100
All	All	2186/2317 (94%)	2109 (96%)	77 (4%)	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	371/378 (98%)	360 (97%)	11 (3%)	41	61
1	C	374/378 (99%)	366 (98%)	8 (2%)	53	71
2	B	368/383 (96%)	366 (100%)	2 (0%)	88	92
2	D	361/383 (94%)	352 (98%)	9 (2%)	47	67
3	E	111/127 (87%)	106 (96%)	5 (4%)	27	46
4	F	319/342 (93%)	305 (96%)	14 (4%)	28	47
All	All	1904/1991 (96%)	1855 (97%)	49 (3%)	46	66

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	84	ARG
1	A	124	LYS
1	A	178	SER
1	A	232	SER
1	A	256	GLN
1	A	326	LYS
1	A	336	LYS
1	A	338	LYS
1	A	370	LYS
1	A	439	SER
2	B	139	HIS
2	B	278	ARG
1	C	38	SER
1	C	71	GLU
1	C	178	SER
1	C	218	ASP
1	C	251	ASP
1	C	340	SER
1	C	347	CYS
1	C	430	LYS
2	D	35	SER
2	D	42	LEU
2	D	128	SER
2	D	130	ASP
2	D	139	HIS
2	D	158	ARG
2	D	324	SER
2	D	402	LYS
2	D	430	SER
3	E	46	SER
3	E	106	GLU
3	E	107	SER
3	E	136	ASN
3	E	138	GLU
4	F	1	MET
4	F	31	ARG
4	F	79	LYS
4	F	128	ARG
4	F	164	SER
4	F	175	GLU
4	F	211	TYR

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Mol	Chain	Res	Type
4	F	217	ARG
4	F	222	ARG
4	F	225	SER
4	F	235	ASP
4	F	255	ARG
4	F	256	TYR
4	F	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	101	ASN
1	A	128	GLN
1	A	301	GLN
2	B	50	ASN
2	B	59	ASN
2	B	334	ASN
2	B	385	GLN
1	C	128	GLN
1	C	285	GLN
1	C	372	GLN
1	C	406	HIS
2	D	96	GLN
3	E	18	GLN
3	E	51	GLN
3	E	136	ASN
4	F	10	ASN
4	F	136	ASN
4	F	176	GLN
4	F	333	ASN
4	F	381	HIS

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 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	MES	B	504	-	12,12,12	1.65	2 (16%)	14,16,16	1.98	5 (35%)
12	ACP	F	402	6	27,33,33	4.81	9 (33%)	32,52,52	2.14	6 (18%)
5	GTP	A	501	6	26,34,34	4.91	12 (46%)	32,54,54	1.72	8 (25%)
11	ERX	B	507	-	28,31,31	1.32	5 (17%)	35,44,44	2.00	9 (25%)
5	GTP	C	501	6	26,34,34	5.04	14 (53%)	32,54,54	1.86	9 (28%)
9	GDP	D	600	-	24,30,30	1.48	4 (16%)	30,47,47	1.78	11 (36%)
9	GDP	B	501	6	24,30,30	3.73	13 (54%)	30,47,47	1.57	6 (20%)
10	MES	B	505	-	12,12,12	1.60	1 (8%)	14,16,16	2.30	6 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MES	B	504	-	-	2/6/14/14	0/1/1/1
12	ACP	F	402	6	-	6/15/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
11	ERX	B	507	-	-	4/14/14/14	0/4/4/4
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
9	GDP	D	600	-	-	5/12/32/32	0/3/3/3
9	GDP	B	501	6	-	4/12/32/32	0/3/3/3
10	MES	B	505	-	-	2/6/14/14	0/1/1/1

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	C2'-C1'	-16.44	1.28	1.53
5	A	501	GTP	C2'-C1'	-16.30	1.29	1.53
12	F	402	ACP	O4'-C1'	15.15	1.62	1.41
12	F	402	ACP	C2'-C1'	-14.87	1.31	1.53
5	C	501	GTP	O4'-C1'	13.72	1.60	1.41
5	A	501	GTP	O4'-C1'	13.23	1.59	1.41
9	B	501	GDP	C3'-C4'	-8.90	1.30	1.53
12	F	402	ACP	PB-O3A	8.87	1.68	1.58
9	B	501	GDP	O4'-C4'	7.02	1.60	1.45
5	A	501	GTP	O4'-C4'	-6.48	1.30	1.45
5	C	501	GTP	O4'-C4'	-6.31	1.30	1.45
12	F	402	ACP	O4'-C4'	-6.11	1.31	1.45
9	B	501	GDP	C2-N2	6.05	1.48	1.34
9	B	501	GDP	O4'-C1'	-5.68	1.33	1.41
5	C	501	GTP	C2-N3	5.55	1.46	1.33
5	A	501	GTP	C2-N3	5.45	1.46	1.33
9	B	501	GDP	C4-N3	4.97	1.49	1.37
5	C	501	GTP	C6-N1	4.82	1.45	1.37
9	B	501	GDP	C2-N3	4.71	1.44	1.33
9	B	501	GDP	C6-N1	4.61	1.44	1.37
5	C	501	GTP	C2-N2	4.52	1.44	1.34
5	C	501	GTP	C4-N3	4.46	1.48	1.37
5	A	501	GTP	C6-N1	4.41	1.44	1.37
5	A	501	GTP	C4-N3	4.34	1.47	1.37
5	C	501	GTP	C5-C6	3.95	1.55	1.47
5	A	501	GTP	C5-C6	3.89	1.55	1.47
5	A	501	GTP	C2-N2	3.88	1.43	1.34
10	B	505	MES	C8-S	3.88	1.83	1.77
9	D	600	GDP	C6-N1	-3.67	1.32	1.37
10	B	504	MES	C8-S	3.51	1.82	1.77
9	B	501	GDP	O2'-C2'	-3.39	1.35	1.43
11	B	507	ERX	C15-C06	3.36	1.52	1.48
12	F	402	ACP	C6-N6	3.32	1.46	1.34
9	B	501	GDP	C2'-C1'	-3.25	1.48	1.53
9	B	501	GDP	O6-C6	-3.03	1.17	1.23
12	F	402	ACP	O2'-C2'	2.89	1.49	1.43
9	D	600	GDP	C2'-C1'	-2.87	1.49	1.53
12	F	402	ACP	O3'-C3'	-2.75	1.36	1.43
5	A	501	GTP	O2'-C2'	2.73	1.49	1.43
9	B	501	GDP	C5-C4	-2.73	1.36	1.43
11	B	507	ERX	O13-C17	2.68	1.41	1.37
5	A	501	GTP	C2-N1	2.65	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	PG-O1G	2.65	1.59	1.50
5	C	501	GTP	C2-N1	2.63	1.44	1.37
5	C	501	GTP	O3'-C3'	-2.61	1.36	1.43
11	B	507	ERX	C27-C08	2.47	1.52	1.48
10	B	504	MES	O1S-S	2.44	1.52	1.45
5	C	501	GTP	O2'-C2'	2.44	1.48	1.43
9	B	501	GDP	C5-C6	2.44	1.52	1.47
12	F	402	ACP	C5-C4	-2.42	1.34	1.40
12	F	402	ACP	C2-N3	2.42	1.36	1.32
5	C	501	GTP	PB-O1B	2.40	1.59	1.50
11	B	507	ERX	O14-C19	2.40	1.41	1.37
9	B	501	GDP	PA-O5'	2.39	1.69	1.59
11	B	507	ERX	C06-N05	-2.36	1.37	1.41
5	C	501	GTP	O5'-C5'	-2.29	1.35	1.44
5	A	501	GTP	O3'-C3'	-2.20	1.37	1.43
5	A	501	GTP	O6-C6	-2.08	1.19	1.23
9	D	600	GDP	O4'-C4'	-2.04	1.40	1.45
9	D	600	GDP	PA-O2A	-2.02	1.45	1.55

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	402	ACP	C5-C6-N6	7.41	131.62	120.35
12	F	402	ACP	N3-C2-N1	-5.18	120.58	128.68
10	B	505	MES	O2S-S-C8	5.16	113.12	106.92
11	B	507	ERX	O13-C17-C18	5.13	124.18	115.16
11	B	507	ERX	O13-C17-C16	-4.69	116.06	124.12
12	F	402	ACP	N6-C6-N1	-4.67	108.87	118.57
5	C	501	GTP	PB-O3B-PG	-4.49	117.42	132.83
5	A	501	GTP	PB-O3B-PG	-4.28	118.15	132.83
11	B	507	ERX	C07-C08-C27	-4.07	123.78	129.44
9	B	501	GDP	C5-C6-N1	3.83	120.71	113.95
5	C	501	GTP	C5-C6-N1	3.74	120.56	113.95
10	B	504	MES	O3S-S-O2S	-3.73	102.16	111.27
5	C	501	GTP	C2-N1-C6	-3.65	118.38	125.10
5	A	501	GTP	PA-O3A-PB	-3.58	120.53	132.83
11	B	507	ERX	C27-C08-N09	3.38	126.29	120.92
5	A	501	GTP	C5-C6-N1	3.37	119.91	113.95
5	A	501	GTP	C2-N1-C6	-3.32	118.99	125.10
10	B	505	MES	O3S-S-O2S	-3.29	103.24	111.27
10	B	505	MES	O3S-S-C8	3.24	111.01	105.77
11	B	507	ERX	O14-C19-C18	3.20	120.78	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	402	ACP	C3'-C2'-C1'	3.19	105.78	100.98
11	B	507	ERX	C12-O13-C17	3.11	122.23	117.53
9	D	600	GDP	C3'-C2'-C1'	3.11	105.66	100.98
10	B	504	MES	O1S-S-C8	3.06	110.60	106.92
9	B	501	GDP	C2-N1-C6	-3.06	119.46	125.10
5	C	501	GTP	PA-O3A-PB	-3.03	122.42	132.83
11	B	507	ERX	C01-C02-N03	-2.98	119.96	124.58
5	C	501	GTP	O4'-C1'-C2'	-2.92	102.66	106.93
9	D	600	GDP	C5-C6-N1	2.88	119.04	113.95
9	D	600	GDP	O2A-PA-O1A	2.87	126.42	112.24
9	D	600	GDP	C2-N1-C6	-2.86	119.83	125.10
12	F	402	ACP	O3G-PG-C3B	2.83	113.28	106.40
11	B	507	ERX	C02-N03-C04	2.77	120.28	116.73
9	B	501	GDP	O6-C6-N1	-2.74	117.41	120.65
10	B	505	MES	C6-C5-N4	2.71	114.21	110.10
10	B	504	MES	O2S-S-C8	2.69	110.16	106.92
5	C	501	GTP	N2-C2-N1	2.65	122.36	116.71
9	D	600	GDP	O2A-PA-O5'	-2.64	95.49	107.75
9	D	600	GDP	O4'-C1'-C2'	-2.60	103.13	106.93
5	A	501	GTP	C8-N7-C5	2.55	107.85	102.99
9	B	501	GDP	PA-O3A-PB	-2.55	124.09	132.83
10	B	504	MES	O3S-S-C8	2.53	109.85	105.77
9	B	501	GDP	O3'-C3'-C2'	-2.43	103.95	111.82
10	B	504	MES	C5-N4-C3	2.43	114.30	108.83
12	F	402	ACP	PB-O3A-PA	-2.43	124.86	132.56
11	B	507	ERX	O14-C19-C20	-2.42	119.95	124.12
5	C	501	GTP	O5'-C5'-C4'	-2.42	100.67	108.99
9	D	600	GDP	C8-N7-C5	2.34	107.45	102.99
5	A	501	GTP	N2-C2-N1	2.32	121.66	116.71
10	B	505	MES	O1-C6-C5	2.28	116.81	111.80
9	D	600	GDP	O4'-C4'-C5'	-2.28	101.88	109.37
9	B	501	GDP	C8-N7-C5	2.28	107.33	102.99
5	C	501	GTP	C8-N7-C5	2.27	107.31	102.99
9	D	600	GDP	O6-C6-C5	-2.25	119.98	124.37
5	A	501	GTP	O6-C6-N1	-2.24	118.01	120.65
5	A	501	GTP	C3'-C2'-C1'	2.22	104.33	100.98
9	D	600	GDP	PA-O3A-PB	-2.19	125.30	132.83
9	D	600	GDP	O3B-PB-O2B	2.08	115.58	107.64
5	C	501	GTP	C3'-C2'-C1'	2.07	104.10	100.98
10	B	505	MES	C6-O1-C2	2.05	116.75	109.89

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	D	600	GDP	C5'-O5'-PA-O3A
9	D	600	GDP	C5'-O5'-PA-O2A
9	D	600	GDP	O4'-C4'-C5'-O5'
10	B	504	MES	C7-C8-S-O1S
10	B	504	MES	C7-C8-S-O2S
10	B	505	MES	C7-C8-S-O1S
12	F	402	ACP	C5'-O5'-PA-O1A
12	F	402	ACP	C5'-O5'-PA-O2A
12	F	402	ACP	C5'-O5'-PA-O3A
12	F	402	ACP	O4'-C4'-C5'-O5'
9	D	600	GDP	C3'-C4'-C5'-O5'
12	F	402	ACP	C3'-C4'-C5'-O5'
11	B	507	ERX	C16-C17-O13-C12
11	B	507	ERX	C18-C17-O13-C12
11	B	507	ERX	N05-C06-C15-C16
11	B	507	ERX	N05-C06-C15-C20
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
9	D	600	GDP	C4'-C5'-O5'-PA
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	505	MES	C7-C8-S-O2S
12	F	402	ACP	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
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3A-PA-O2A

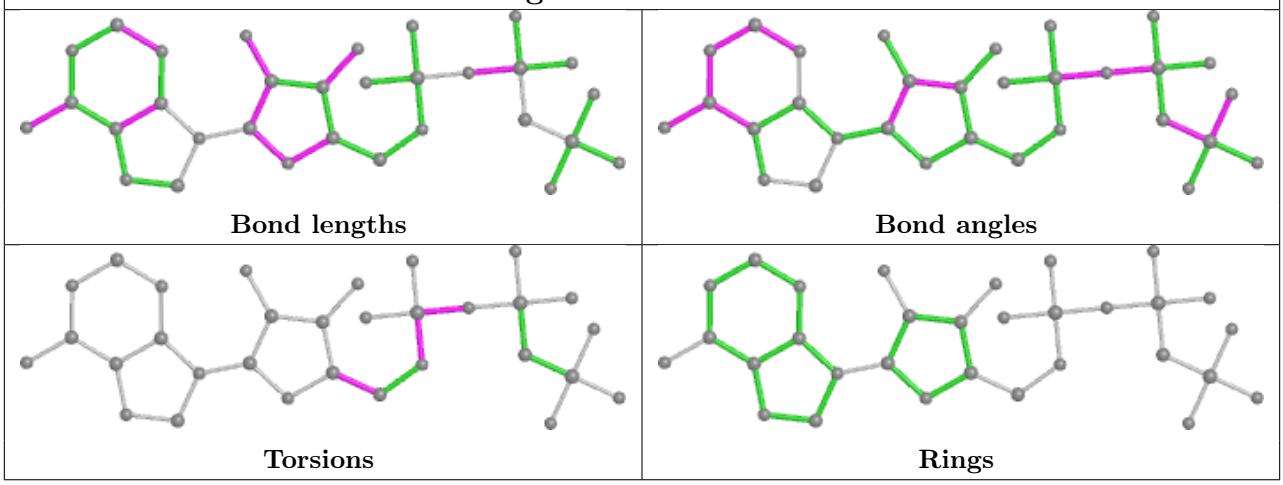
There are no ring outliers.

6 monomers are involved in 25 short contacts:

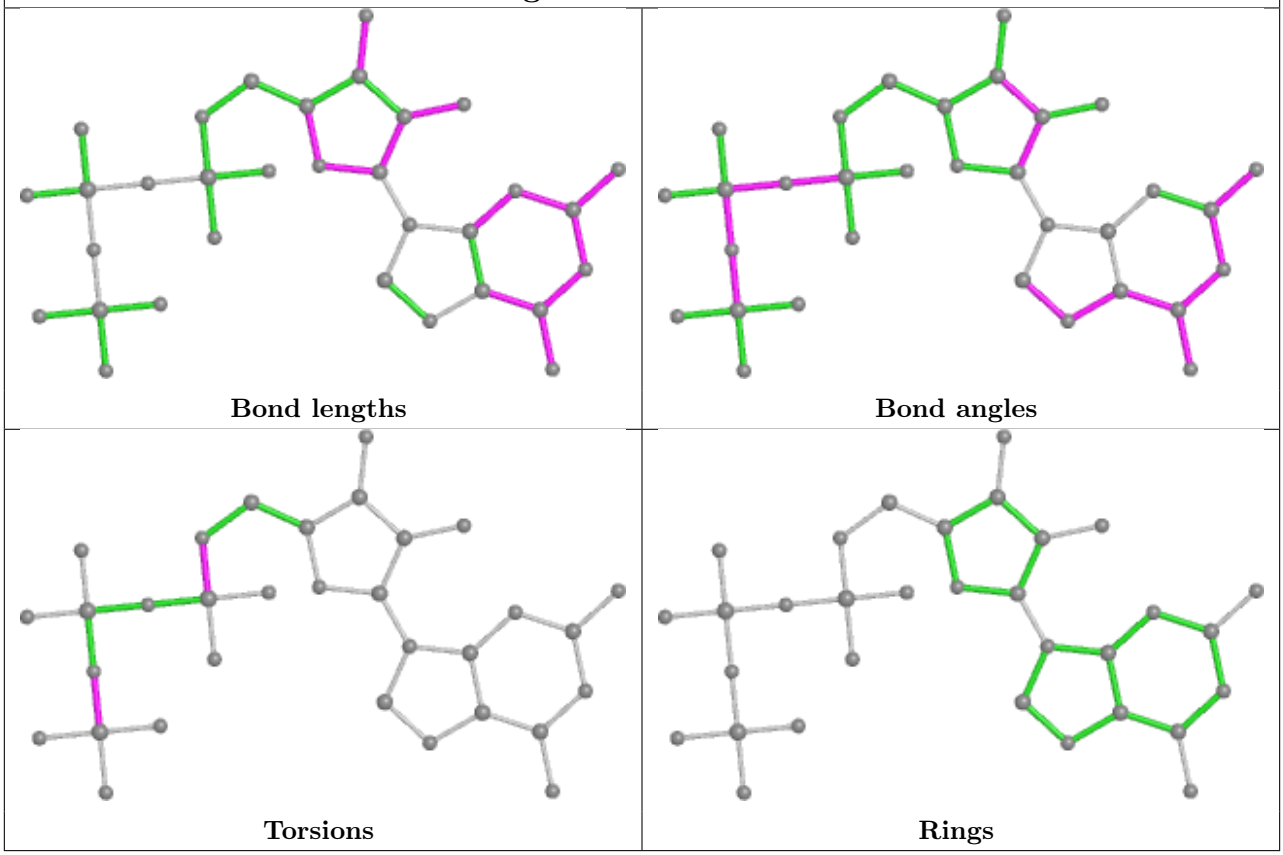
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	504	MES	1	0
12	F	402	ACP	2	0
11	B	507	ERX	1	0
9	D	600	GDP	15	0
9	B	501	GDP	2	0
10	B	505	MES	4	0

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.

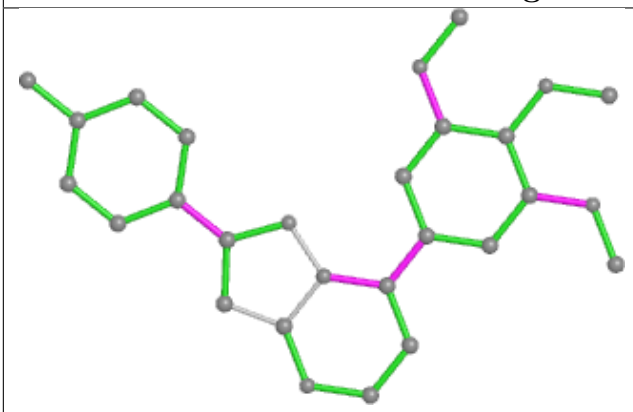
Ligand ACP F 402



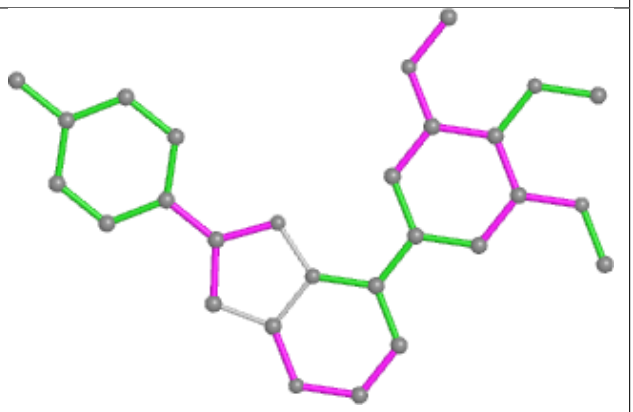
Ligand GTP A 501



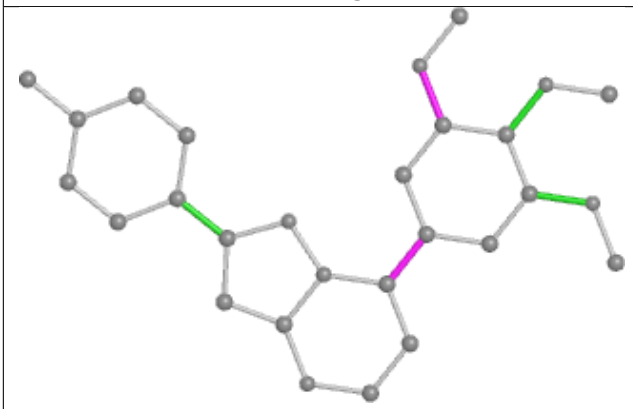
Ligand ERX B 507



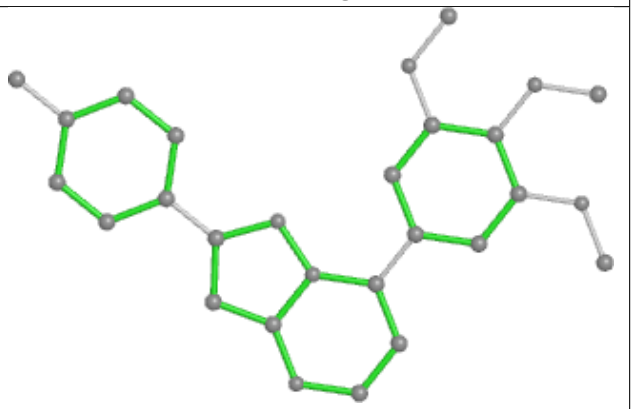
Bond lengths



Bond angles

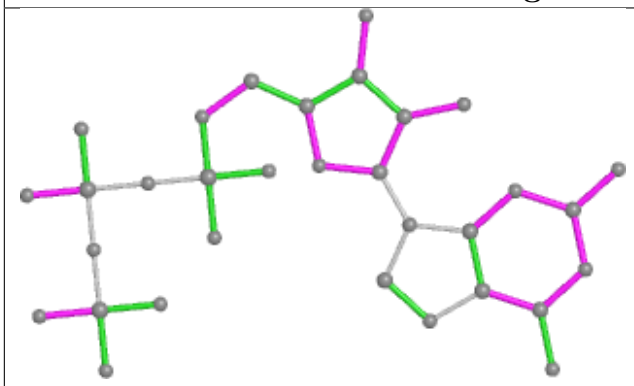


Torsions

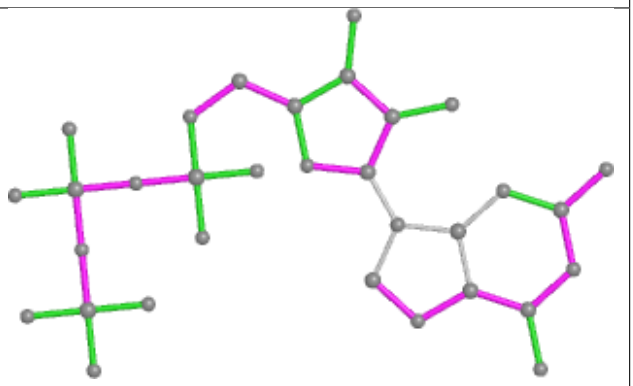


Rings

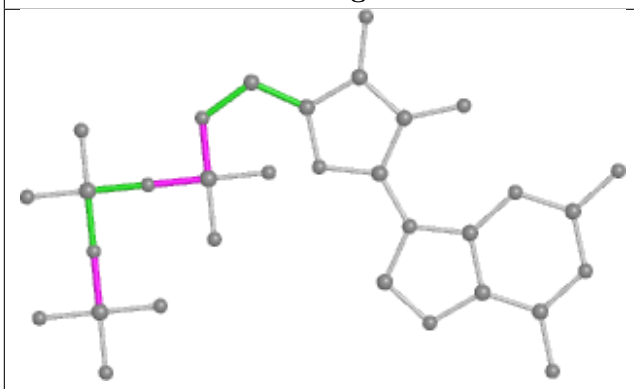
Ligand GTP C 501



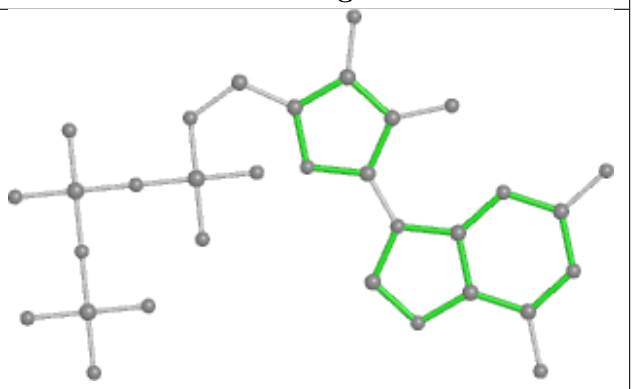
Bond lengths



Bond angles

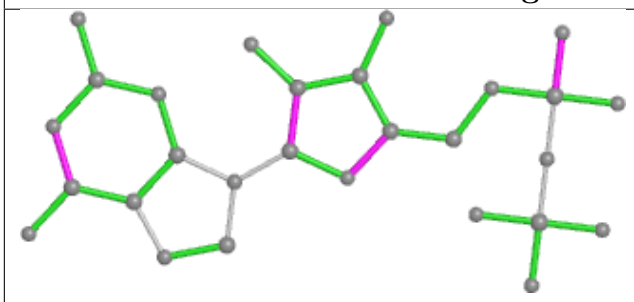


Torsions

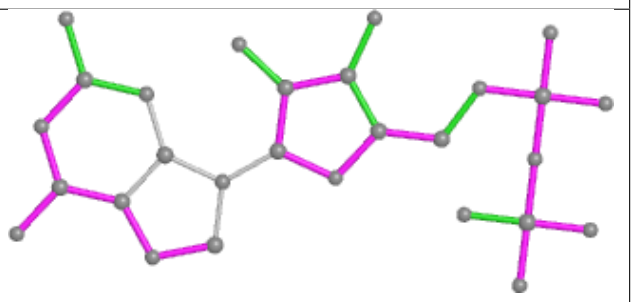


Rings

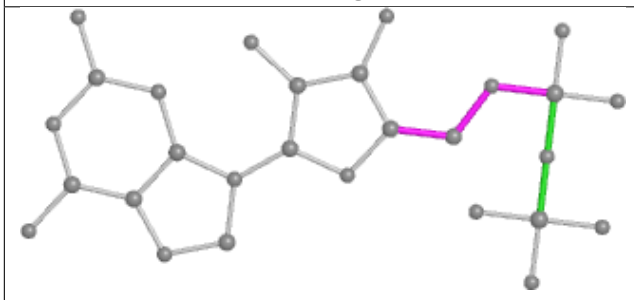
Ligand GDP D 600



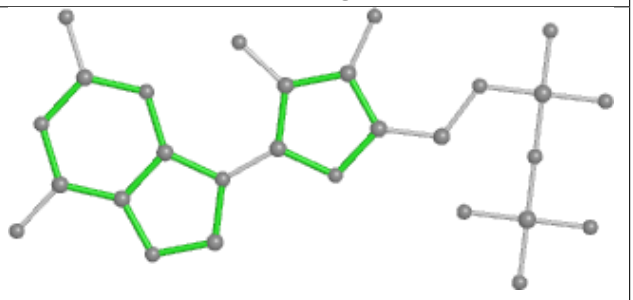
Bond lengths



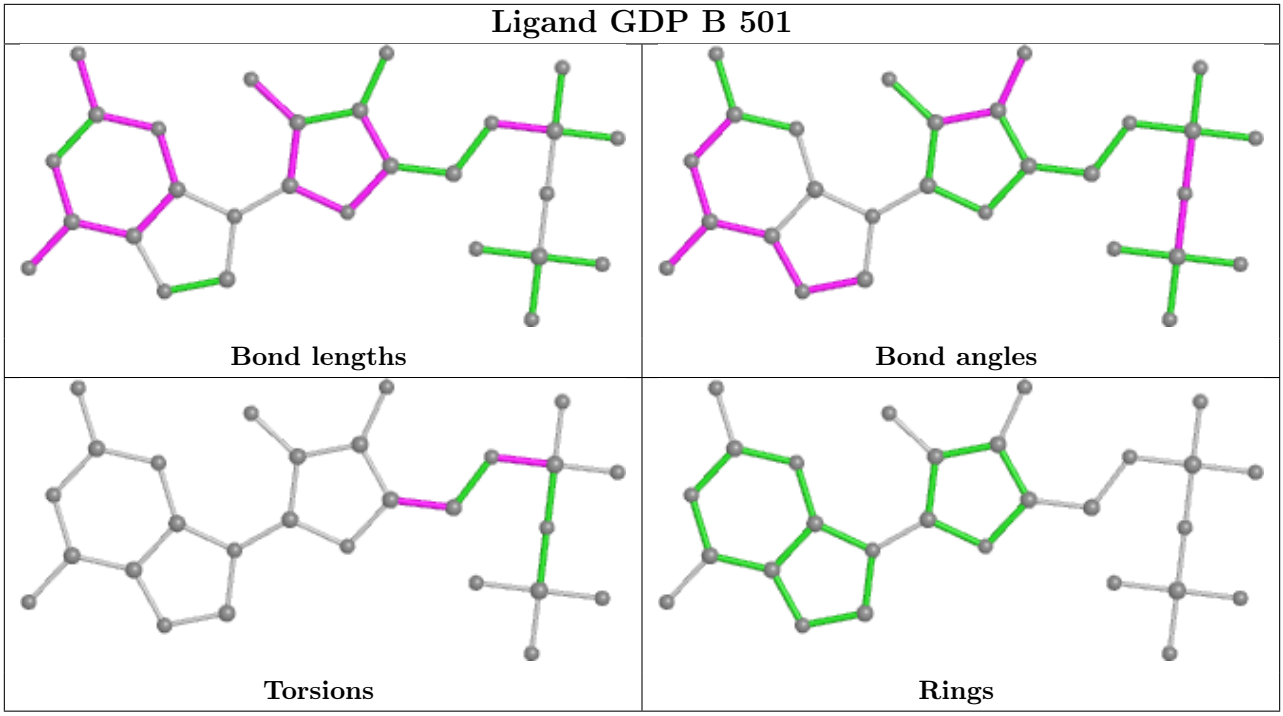
Bond angles



Torsions



Rings



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	440/450 (97%)	-0.04	11 (2%)	57	66	31, 51, 80, 127	0
1	C	440/450 (97%)	-0.39	2 (0%)	91	94	22, 39, 66, 85	0
2	B	424/445 (95%)	-0.07	10 (2%)	59	68	25, 48, 81, 130	0
2	D	421/445 (94%)	0.44	35 (8%)	11	13	35, 69, 107, 130	0
3	E	124/143 (86%)	0.71	19 (15%)	2	2	35, 68, 109, 136	0
4	F	351/384 (91%)	0.76	67 (19%)	1	1	39, 79, 147, 162	0
All	All	2200/2317 (94%)	0.15	144 (6%)	18	22	22, 57, 110, 162	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	167	SER	8.2
4	F	251	LYS	8.0
2	D	285	ALA	7.8
4	F	233	PHE	6.8
3	E	144	SER	6.7
4	F	105	LEU	6.3
3	E	143	ALA	6.2
4	F	381	HIS	6.2
2	B	57	THR	6.1
4	F	249	TYR	6.1
4	F	173	ILE	5.7
4	F	177	GLY	5.6
2	B	438	ALA	5.6
2	D	286	LEU	5.3
4	F	170	LEU	5.1
4	F	383	HIS	4.9
3	E	141	GLU	4.8
4	F	103	THR	4.8
2	D	177	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
4	F	232	ASN	4.7
2	D	213	CYS	4.7
4	F	161	LEU	4.5
4	F	231	ALA	4.5
1	A	439	SER	4.5
2	D	217	LEU	4.5
4	F	104	ASN	4.5
2	D	219	LEU	4.4
1	A	440	VAL	4.2
4	F	101	TYR	4.2
2	D	221	THR	4.2
4	F	134	ALA	4.2
2	D	176	LYS	4.1
4	F	136	ASN	4.1
2	D	216	THR	4.0
2	B	37	HIS	4.0
4	F	166	ALA	3.9
4	F	250	SER	3.9
4	F	382	HIS	3.9
4	F	384	HIS	3.9
3	E	140	LYS	3.9
4	F	178	GLN	3.8
4	F	137	ARG	3.8
4	F	139	ARG	3.8
3	E	45	PRO	3.8
4	F	175	GLU	3.7
4	F	140	GLU	3.7
4	F	152	SER	3.7
4	F	106	LYS	3.7
4	F	102	PRO	3.7
4	F	10	ASN	3.7
4	F	196	HIS	3.7
4	F	125	THR	3.6
4	F	130	VAL	3.6
1	A	282	TYR	3.6
4	F	255	ARG	3.5
3	E	46	SER	3.5
3	E	44	ASP	3.5
4	F	133	ALA	3.5
2	D	218	LYS	3.4
4	F	179	VAL	3.4
4	F	100	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	346	TRP	3.3
4	F	143	GLU	3.3
4	F	372	THR	3.3
2	D	220	THR	3.3
2	D	404	PHE	3.2
2	D	401	ARG	3.2
4	F	169	LEU	3.2
4	F	234	GLN	3.2
4	F	141	GLY	3.1
4	F	142	ARG	3.1
3	E	48	GLU	3.1
2	D	37	HIS	3.1
4	F	164	SER	3.1
2	D	82	PRO	3.0
2	D	56	ALA	3.0
2	D	369	ARG	3.0
3	E	28	SER	2.9
2	D	210	TYR	2.9
4	F	245	ILE	2.9
2	D	403	ALA	2.9
4	F	174	ASP	2.9
3	E	142	GLU	2.9
2	D	46	LEU	2.8
1	A	179	THR	2.8
2	D	400	ARG	2.8
4	F	252	ASN	2.8
2	D	212	ILE	2.8
4	F	132	LEU	2.8
4	F	256	TYR	2.7
2	B	74	THR	2.6
2	D	36	TYR	2.6
4	F	165	GLU	2.6
1	A	262	TYR	2.6
2	D	39	ASP	2.6
2	D	83	PHE	2.6
3	E	7	GLU	2.6
4	F	171	ASP	2.5
2	D	57	THR	2.5
2	D	415	GLU	2.5
2	D	41	ASP	2.5
2	D	209	LEU	2.5
3	E	139	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	56	ALA	2.5
1	A	220	GLU	2.5
4	F	176	GLN	2.4
4	F	45	ASN	2.4
2	D	55	GLU	2.4
2	B	59	ASN	2.4
4	F	182	ILE	2.4
2	D	148	GLY	2.4
2	D	287	THR	2.3
2	D	372	LYS	2.3
4	F	90	SER	2.3
4	F	129	GLU	2.3
2	D	42	LEU	2.3
4	F	128	ARG	2.3
4	F	197	ARG	2.3
4	F	89	GLU	2.3
3	E	116	LEU	2.3
4	F	168	GLU	2.2
1	C	357	TYR	2.2
1	A	42	ILE	2.2
4	F	380	HIS	2.2
3	E	135	LYS	2.2
4	F	259	GLY	2.1
2	B	215	ARG	2.1
2	B	36	TYR	2.1
2	B	437	ASP	2.1
4	F	244	CYS	2.1
1	A	137	VAL	2.1
4	F	248	GLU	2.1
2	B	168	THR	2.1
4	F	138	ARG	2.1
3	E	138	GLU	2.1
4	F	147	TRP	2.1
1	A	201	ALA	2.0
3	E	115	HIS	2.0
3	E	132	GLU	2.0
1	A	438	ASP	2.0
2	D	147[A]	SER	2.0
1	C	1	MET	2.0
3	E	122	ARG	2.0
3	E	133	VAL	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)

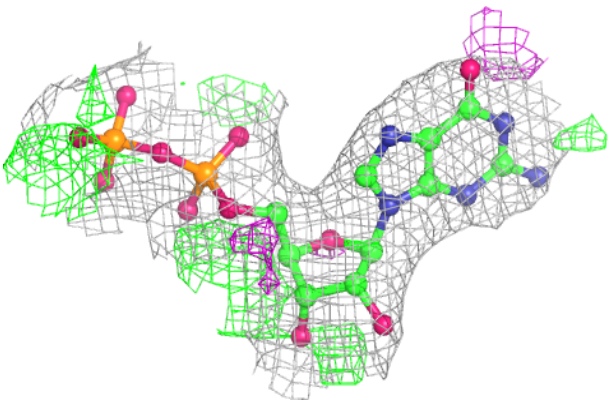
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

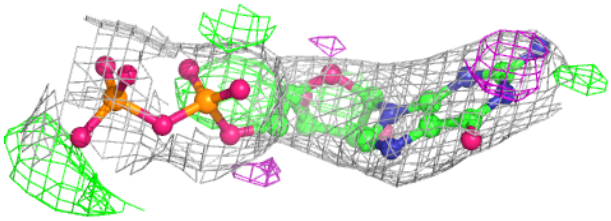
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	F	401	1/1	0.58	0.22	94,94,94,94	0
8	CL	A	504	1/1	0.77	0.19	73,73,73,73	0
7	CA	A	505	1/1	0.78	0.16	113,113,113,113	0
6	MG	D	601	1/1	0.80	0.13	64,64,64,64	0
6	MG	A	502	1/1	0.88	0.15	44,44,44,44	0
6	MG	B	506	1/1	0.90	0.05	87,87,87,87	0
9	GDP	D	600	28/28	0.91	0.18	52,64,92,98	0
7	CA	B	503	1/1	0.92	0.07	103,103,103,103	0
12	ACP	F	402	31/31	0.93	0.20	77,93,124,132	0
6	MG	C	502	1/1	0.94	0.15	46,46,46,46	0
10	MES	B	505	12/12	0.96	0.21	76,84,100,107	0
11	ERX	B	507	28/28	0.97	0.15	38,55,67,85	0
10	MES	B	504	12/12	0.97	0.11	40,56,79,97	0
5	GTP	C	501	32/32	0.98	0.15	26,34,42,43	0
5	GTP	A	501	32/32	0.98	0.14	35,41,50,54	0
6	MG	B	502	1/1	0.98	0.03	36,36,36,36	0
9	GDP	B	501	28/28	0.99	0.14	23,34,40,41	0
7	CA	C	503	1/1	0.99	0.05	57,57,57,57	0
7	CA	A	503	1/1	0.99	0.10	80,80,80,80	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 GDP D 600:

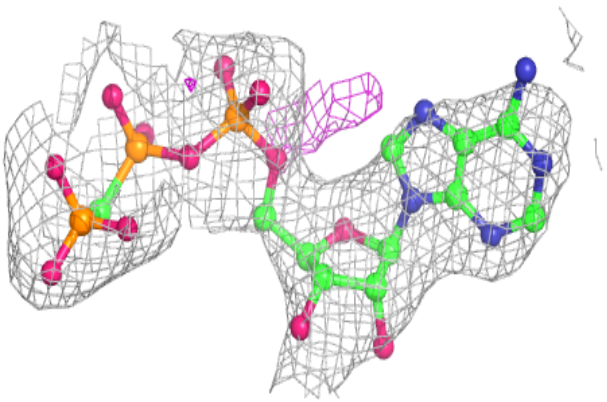
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

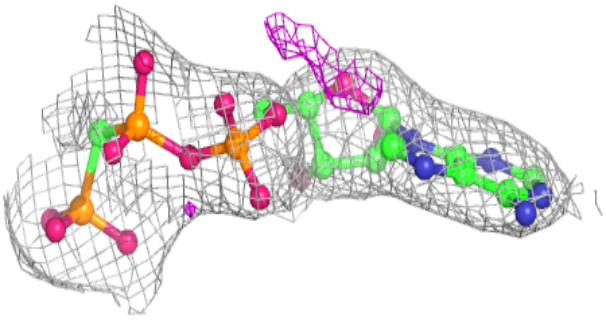


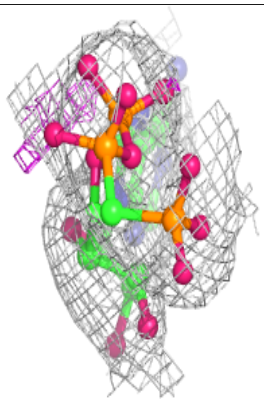


Electron density around ACP F 402:

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

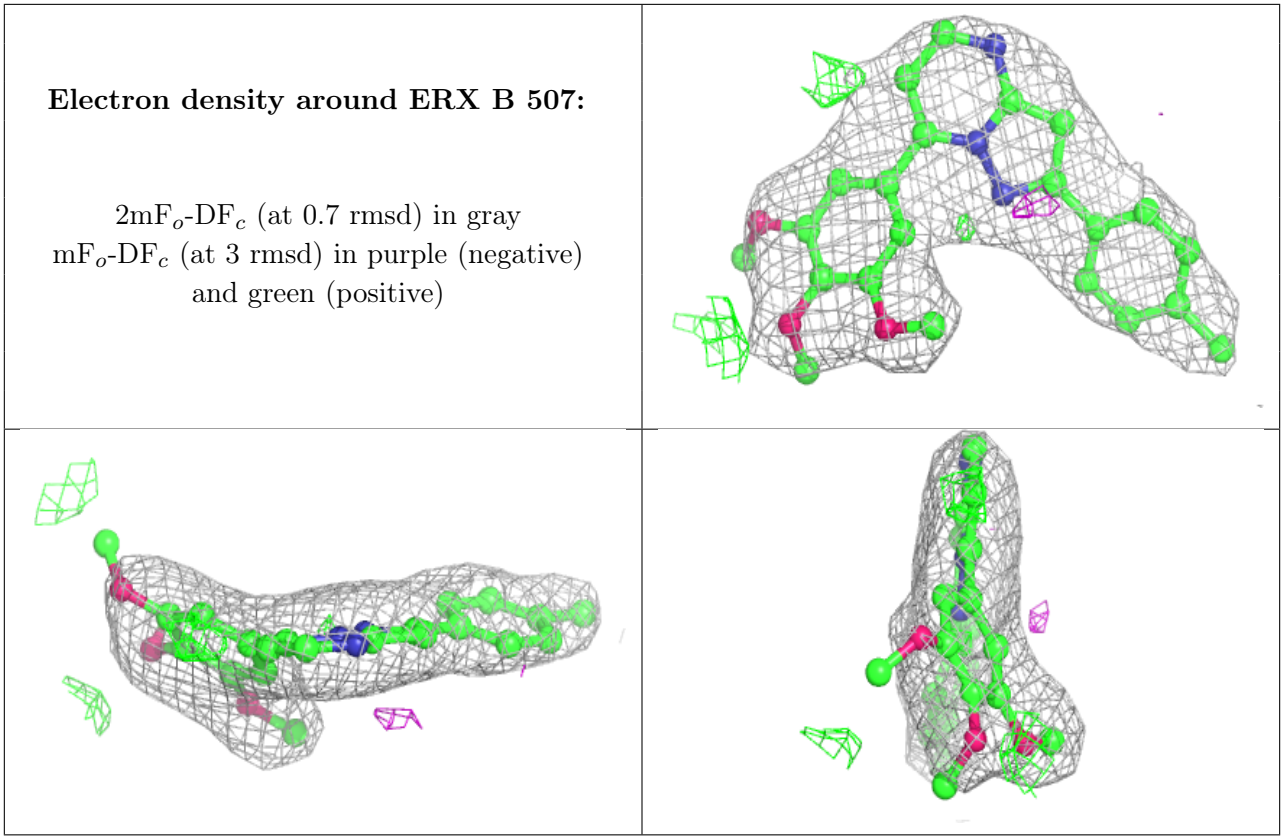






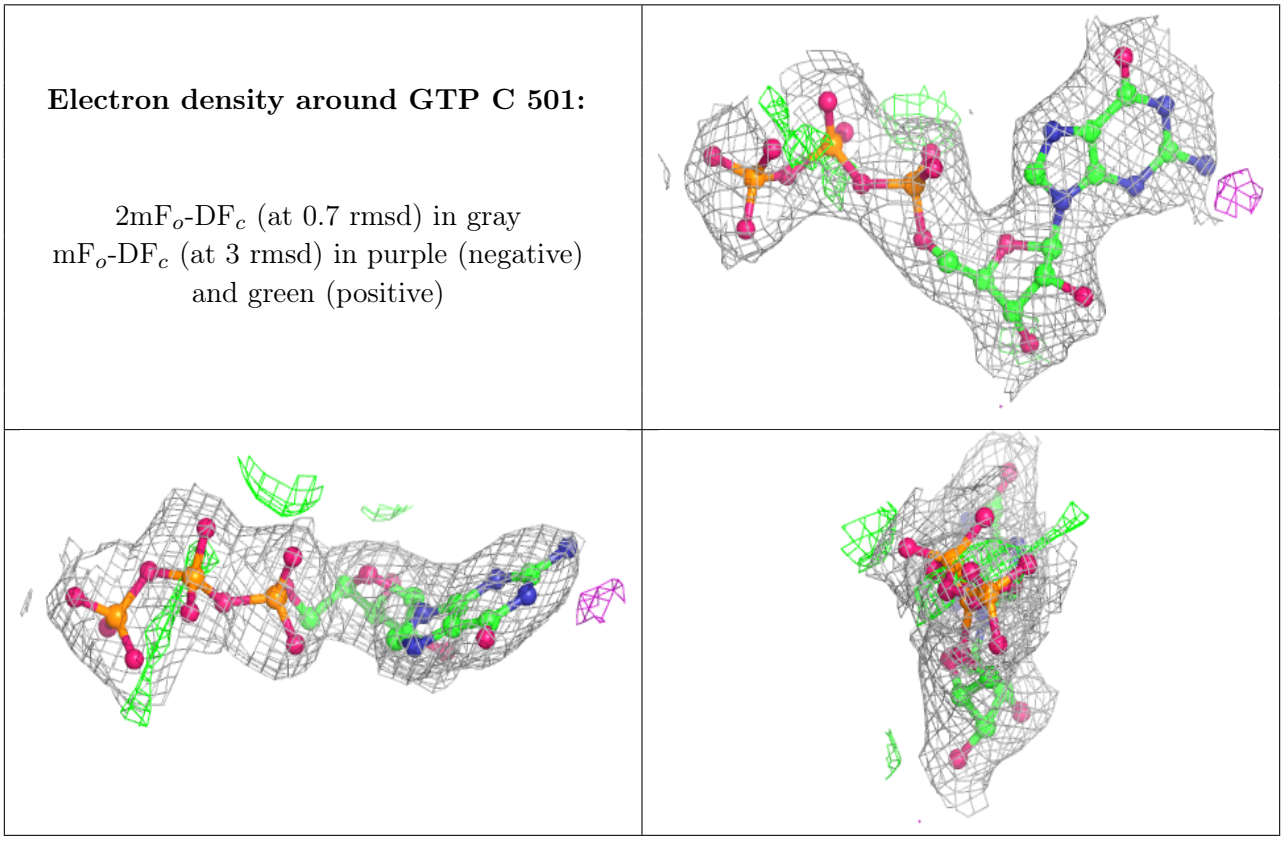
Electron density around ERX B 507:

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



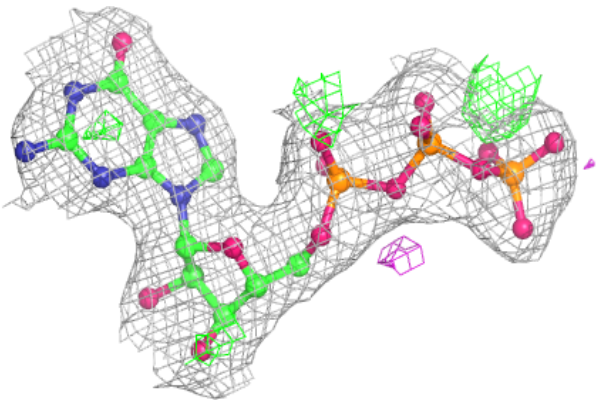
Electron density around GTP C 501:

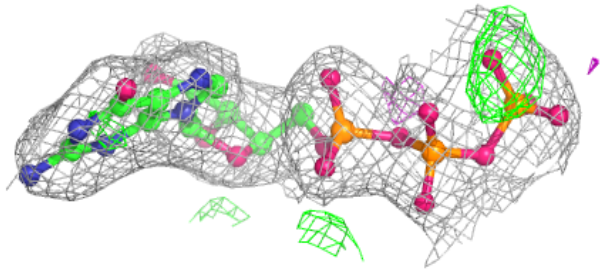
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

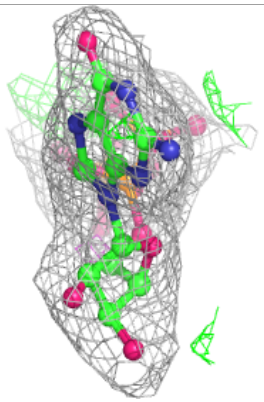


Electron density around GTP A 501:

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

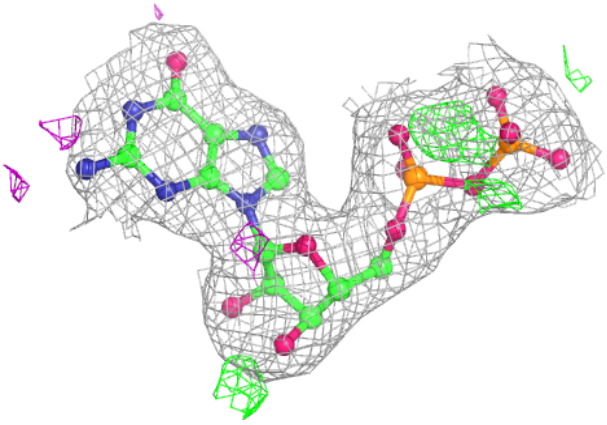


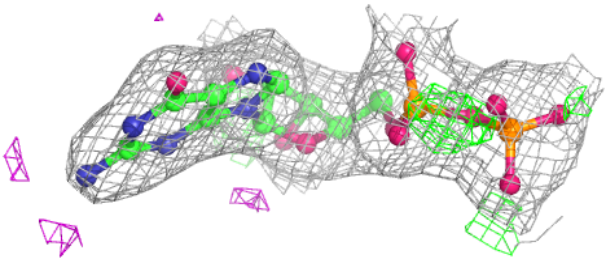


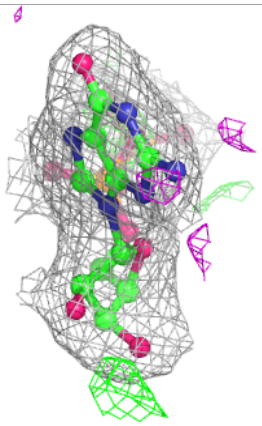


Electron density around GDP B 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.