Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2024 – 10:16 PM EST

PDB ID	:	5S66
Title	:	Tubulin-Z2856434929-complex
Authors	:	Muehlethaler, T.; Gioia, D.; Prota, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on	:	2020-11-08
Resolution	:	2.10 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:

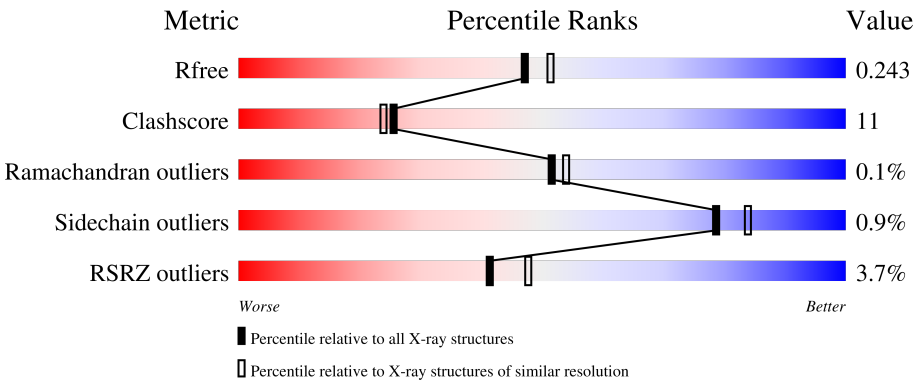
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	3%, 81%, 17%, •
1	C	451	%, 79%, 19%, •
2	B	445	4%, 69%, 24%, • 6%
2	D	445	2%, 73%, 21%, 5%
3	E	143	6%, 66%, 18%, • 14%

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Mol	Chain	Length	Quality of chain
4	F	384	9% 64% 24% 12%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 17859 atoms, of which 17 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	441	3446	2179	585	660	22	0	0	0
1	C	440	3440	2177	584	657	22	0	1	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	419	3294	2072	560	635	27	0	0	0
2	D	421	3309	2080	562	640	27	1	0	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	1014	625	183	201	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

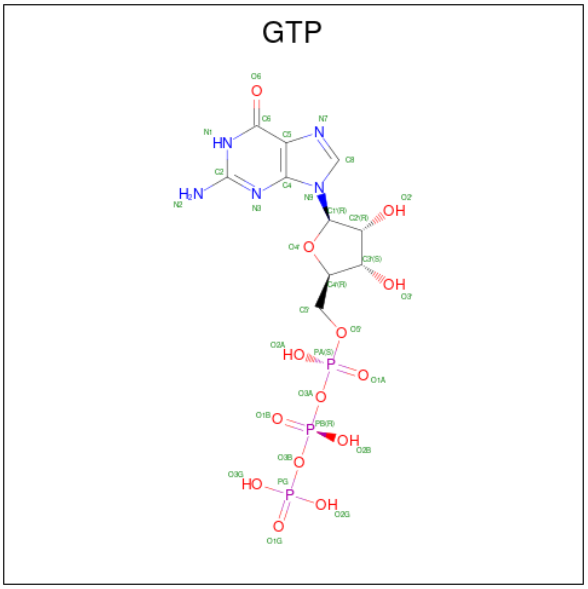
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	339	2781	1787	472	508	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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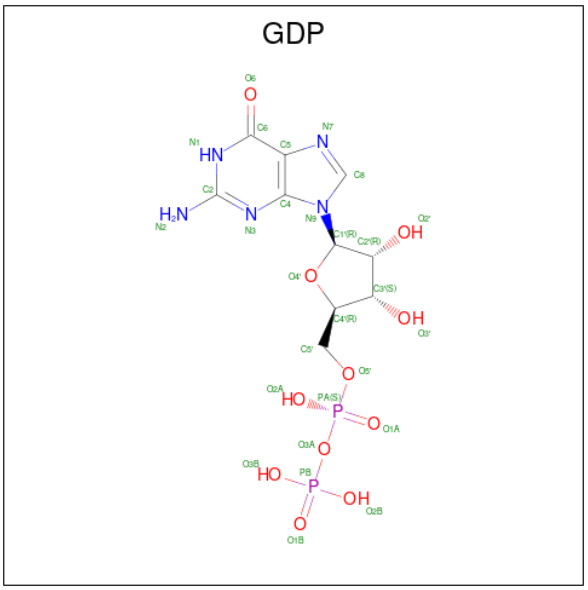
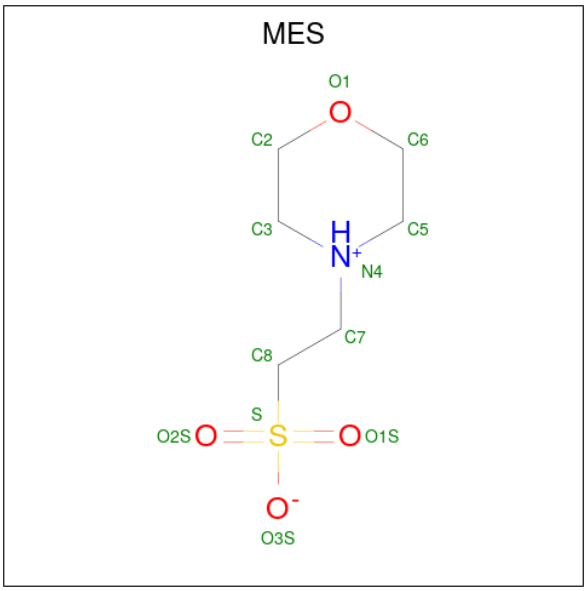
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	F	1	1	1	0	0

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



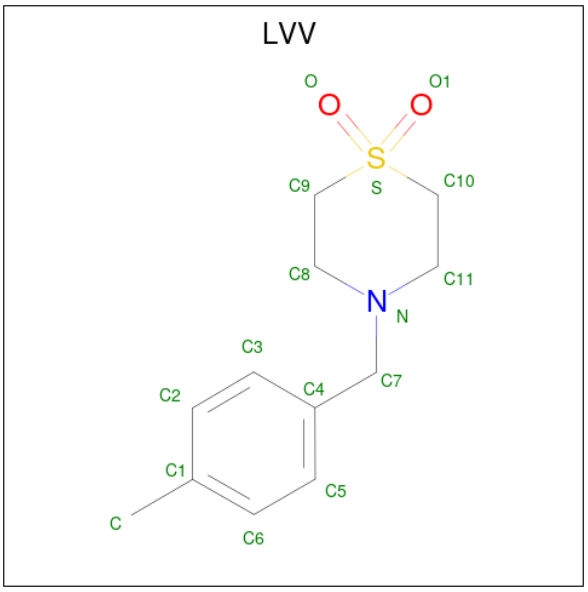
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	B	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
7	D	1	28	10	5	11	2	0	0

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



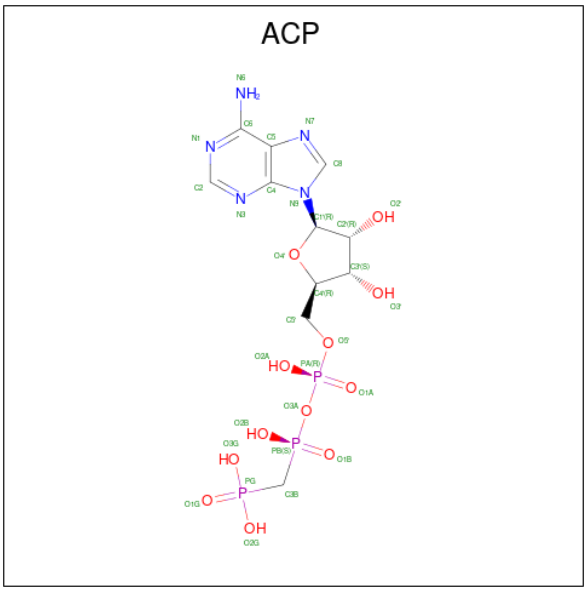
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
8	B	1	12	6	1	4	1	0	0

- Molecule 9 is 4-[(4-methylphenyl)methyl]-1,4-thiazinane 1,1-dioxide (three-letter code: LVV) (formula: $C_{12}H_{17}NO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
9	C	1	33	12	17	1	2	1	0	0

- Molecule 10 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		
10	F	1	31	11	5	12	3	0	0

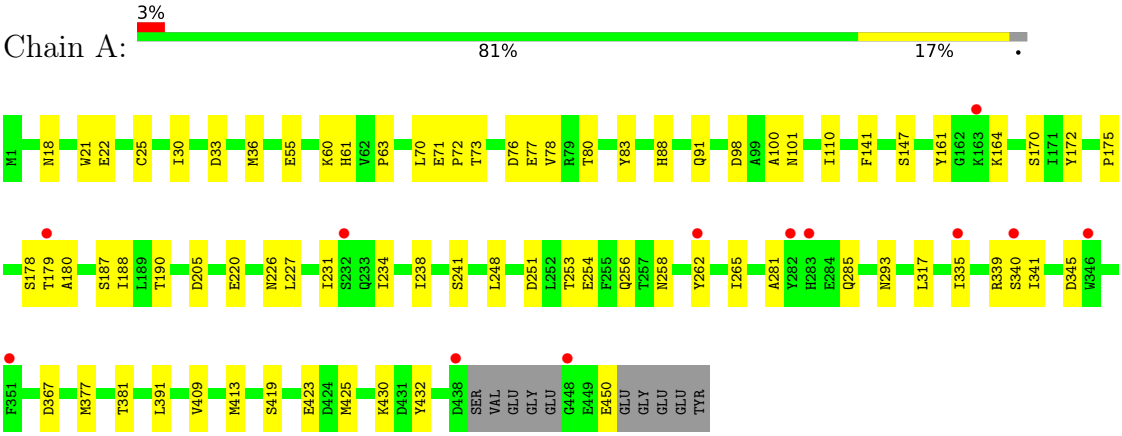
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	68	68	68	0	0
11	B	52	52	52	0	0
11	C	153	153	153	0	0
11	D	53	53	53	0	0
11	E	22	22	22	0	0
11	F	26	26	26	0	0

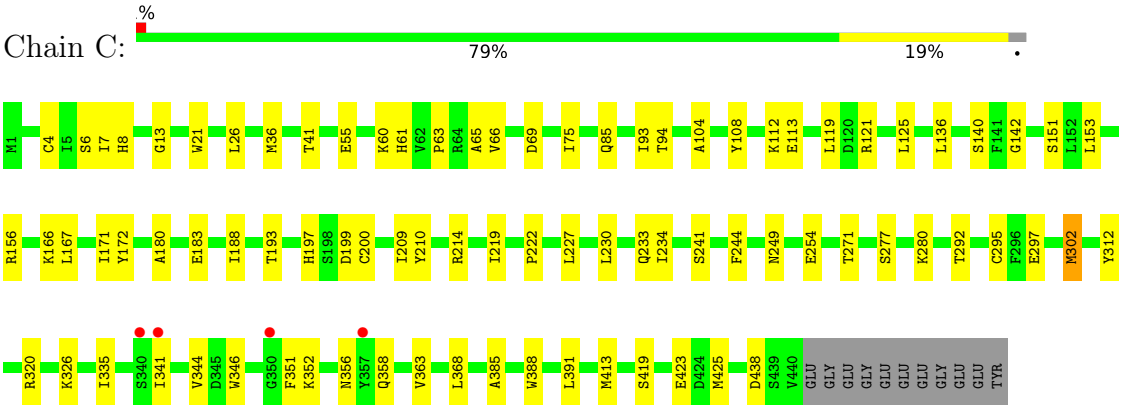
3 Residue-property plots (i)

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.

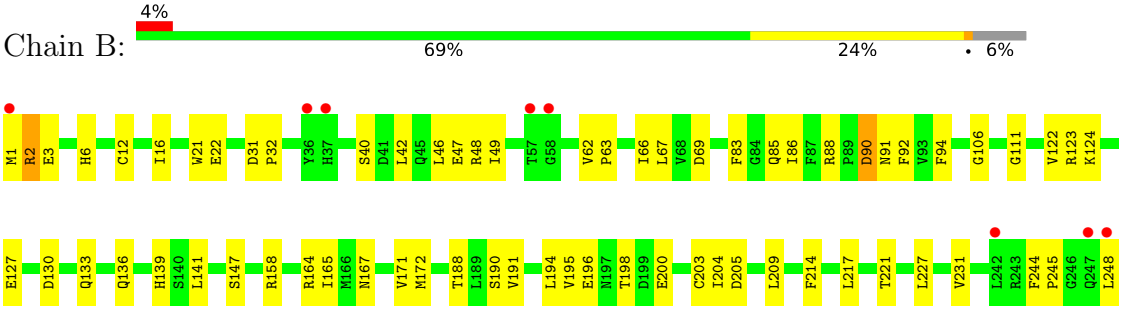
• Molecule 1: Tubulin alpha-1B chain

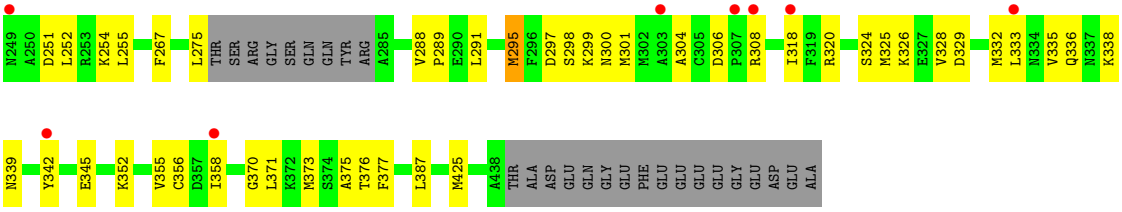


• Molecule 1: Tubulin alpha-1B chain



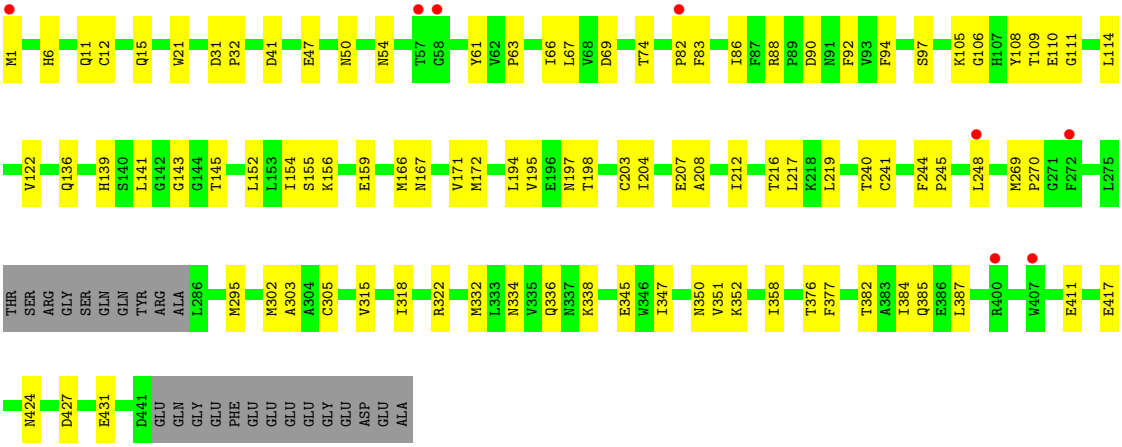
• Molecule 2: Tubulin beta-2B chain





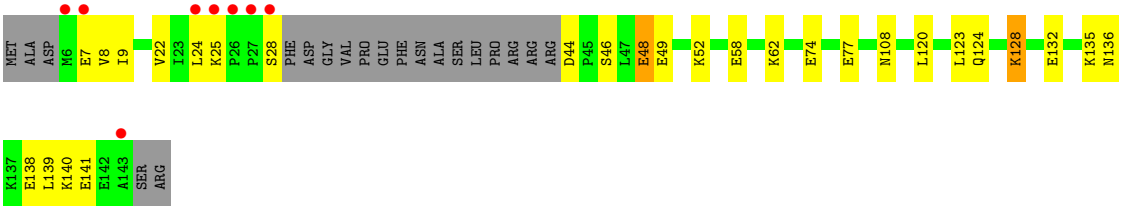
- Molecule 2: Tubulin beta-2B chain

Chain D:



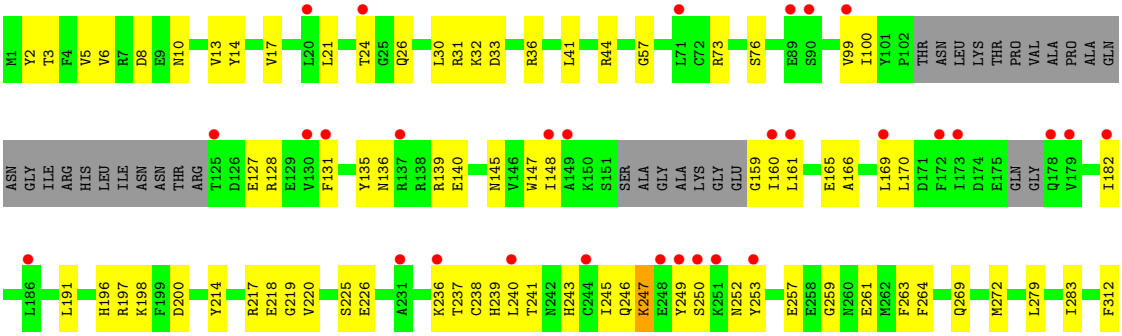
- Molecule 3: Stathmin-4

Chain E:



- Molecule 4: Tubulin-Tyrosine Ligase

Chain F:



D318
F319
M320
I330
E331
V332
N333
C338
A339
Q340
K341
L342
Y343
Q348
D352
I355
F359
A362
ASP
THR
GLY
GLN
LYS
THR
SER
GLN
P371
T372
F375
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	104.69Å 157.88Å 178.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.00 – 2.10 118.36 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (68.00-2.10) 99.8 (118.36-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.214 , 0.243 0.214 , 0.243	Depositor DCC
R_{free} test set	8621 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17859	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: GDP, LVV, MES, MG, ACP, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.25	0/3523	0.42	0/4780
1	C	0.26	0/3521	0.44	0/4780
2	B	0.25	0/3367	0.42	0/4560
2	D	0.25	0/3382	0.42	0/4581
3	E	0.24	0/1022	0.35	0/1356
4	F	0.24	0/2843	0.39	0/3839
All	All	0.25	0/17658	0.42	0/23896

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	3446	0	3349	55	0
1	C	3440	0	3354	55	0
2	B	3294	0	3178	103	0
2	D	3309	0	3189	63	0
3	E	1014	0	1029	15	0
4	F	2781	0	2757	83	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	B	28	0	12	1	0
7	D	28	0	12	3	0
8	B	12	0	12	3	0
9	C	16	17	0	0	0
10	F	31	0	14	3	0
11	A	68	0	0	1	0
11	B	52	0	0	2	0
11	C	153	0	0	3	0
11	D	53	0	0	1	0
11	E	22	0	0	1	0
11	F	26	0	0	2	0
All	All	17842	17	16930	366	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 11.

All (366) 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)
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.45	0.96
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.51	0.92
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.52	0.90
2:B:248:LEU:HD11	2:B:352:LYS:HB3	1.54	0.89
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.58	0.82
4:F:21:LEU:O	4:F:24:THR:HG22	1.82	0.80
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.65	0.79
1:C:60:LYS:NZ	1:C:85:GLN:O	2.16	0.77
2:B:123:ARG:O	2:B:127:GLU:HG3	1.83	0.77
2:B:188:THR:HA	2:B:425:MET:HE3	1.68	0.74
2:D:105:LYS:HA	2:D:109:THR:OG1	1.90	0.72
3:E:48:GLU:OE1	3:E:52:LYS:NZ	2.23	0.72
2:B:325:MET:HA	2:B:325:MET:CE	2.19	0.72
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.71	0.71
2:D:248:LEU:HD21	2:D:352:LYS:HB3	1.70	0.71
4:F:31:ARG:HD2	4:F:32:LYS:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:THR:HA	2:B:425:MET:CE	2.21	0.71
4:F:32:LYS:H	4:F:32:LYS:HD2	1.55	0.70
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.22	0.69
4:F:318:ASP:OD2	11:F:501:HOH:O	2.10	0.69
1:A:71:GLU:OE1	1:A:73:THR:HB	1.93	0.69
2:B:325:MET:SD	2:B:355:VAL:HG21	2.33	0.69
4:F:371:PRO:CA	4:F:372:THR:HB	2.22	0.69
4:F:135:TYR:OH	4:F:165:GLU:HA	1.94	0.68
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.76	0.67
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.77	0.67
4:F:139:ARG:HB3	4:F:145:ASN:HD22	1.59	0.67
2:B:3:GLU:OE1	2:B:130:ASP:N	2.27	0.66
2:B:69:ASP:O	2:B:94:PHE:HA	1.96	0.66
2:D:240:THR:HB	2:D:318:ILE:HD13	1.77	0.66
2:B:325:MET:CE	2:B:355:VAL:HG21	2.26	0.66
4:F:371:PRO:HA	4:F:372:THR:HB	1.77	0.66
4:F:32:LYS:N	4:F:32:LYS:HD2	2.11	0.65
3:E:46:SER:OG	3:E:49:GLU:HG3	1.96	0.65
2:D:109:THR:HG21	2:D:411:GLU:OE1	1.97	0.65
3:E:58:GLU:O	3:E:62:LYS:HG3	1.96	0.64
2:D:136:GLN:HA	2:D:167:ASN:O	1.96	0.64
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.79	0.64
1:A:175:PRO:HA	1:A:178:SER:HB3	1.80	0.64
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.12	0.64
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.25	0.63
3:E:8:VAL:HG22	3:E:22:VAL:HG12	1.80	0.63
4:F:246:GLN:HA	4:F:250:SER:HB3	1.79	0.62
1:A:98:ASP:OD2	11:B:601:HOH:O	2.16	0.62
1:A:450:GLU:OE2	4:F:333:ASN:HB3	1.99	0.62
2:B:62:VAL:HG11	2:B:88:ARG:HG3	1.82	0.62
2:B:325:MET:HE3	2:B:355:VAL:HG21	1.82	0.62
10:F:401:ACP:H3B2	11:F:501:HOH:O	2.00	0.62
1:C:320:ARG:HA	1:C:356:ASN:O	1.99	0.61
4:F:24:THR:HG23	4:F:26:GLN:H	1.65	0.61
2:D:1:MET:SD	2:D:50:ASN:HB2	2.40	0.61
4:F:100:ILE:HG23	4:F:128:ARG:HB2	1.82	0.61
2:B:141:LEU:HD12	2:B:172:MET:SD	2.41	0.61
2:B:251:ASP:OD2	11:B:601:HOH:O	2.15	0.60
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.83	0.60
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.35	0.60
2:D:11:GLN:O	2:D:15:GLN:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:371:PRO:HA	4:F:372:THR:O	2.01	0.60
1:A:251:ASP:OD2	1:A:253:THR:HB	2.02	0.60
2:D:41:ASP:OD1	11:D:601:HOH:O	2.16	0.60
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.20	0.60
2:B:47:GLU:HG2	2:B:245:PRO:HG3	1.84	0.60
1:A:22:GLU:HG3	1:A:83:TYR:CE2	2.37	0.60
2:B:62:VAL:HG11	2:B:88:ARG:CG	2.32	0.59
2:B:345:GLU:HG3	4:F:31:ARG:NH2	2.17	0.59
1:A:77:GLU:HA	1:A:80:THR:HG22	1.83	0.59
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.37	0.59
4:F:100:ILE:HD12	4:F:128:ARG:CA	2.30	0.59
4:F:259:GLY:O	4:F:261:GLU:HG3	2.02	0.59
4:F:8:ASP:OD1	4:F:44:ARG:HG3	2.03	0.59
2:D:83:PHE:O	2:D:86:ILE:HG22	2.03	0.59
2:D:240:THR:HB	2:D:318:ILE:CD1	2.32	0.59
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.38	0.58
2:B:191:VAL:O	2:B:195:VAL:HG23	2.03	0.58
1:C:419:SER:O	1:C:423:GLU:HG3	2.02	0.58
2:B:308:ARG:HD2	2:B:342:TYR:CE2	2.38	0.58
2:D:106:GLY:O	2:D:111:GLY:HA3	2.03	0.58
2:B:147:SER:HG	2:B:190:SER:HG	1.52	0.58
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.84	0.58
2:B:308:ARG:HD2	2:B:342:TYR:CZ	2.39	0.58
1:A:88:HIS:O	1:A:91:GLN:HG2	2.04	0.58
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.84	0.58
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.86	0.58
1:A:430:LYS:HE2	1:A:430:LYS:HA	1.85	0.57
2:D:208:ALA:O	2:D:212:ILE:HG13	2.03	0.57
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.39	0.57
4:F:31:ARG:CZ	4:F:33:ASP:HB2	2.34	0.57
2:B:370:GLY:O	2:B:371:LEU:HD23	2.05	0.57
4:F:5:VAL:CG2	4:F:32:LYS:HA	2.35	0.57
4:F:73:ARG:HB2	4:F:76:SER:OG	2.05	0.57
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.40	0.56
2:B:147:SER:OG	2:B:190:SER:OG	2.18	0.56
2:D:97:SER:OG	2:D:110:GLU:HG2	2.05	0.56
4:F:225:SER:HB3	4:F:252:ASN:HB2	1.87	0.56
1:C:297:GLU:HB2	11:C:639:HOH:O	2.04	0.56
4:F:241:THR:OG1	10:F:401:ACP:O3'	2.14	0.56
1:C:438:ASP:OD1	11:C:601:HOH:O	2.18	0.56
4:F:31:ARG:NH2	4:F:33:ASP:HB2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.87	0.56
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.35	0.56
4:F:10:ASN:HB2	4:F:44:ARG:HH12	1.70	0.56
2:D:241:CYS:SG	2:D:318:ILE:HD12	2.45	0.56
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.40	0.56
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.41	0.55
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.42	0.55
2:B:295:MET:CE	2:B:375:ALA:HB1	2.37	0.55
2:D:318:ILE:CG2	2:D:376:THR:HB	2.35	0.55
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.20	0.55
1:A:256:GLN:HB2	11:A:641:HOH:O	2.05	0.55
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.87	0.55
1:C:26:LEU:HD12	1:C:363:VAL:HG12	1.89	0.55
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.88	0.55
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.89	0.55
2:B:42:LEU:H	2:B:42:LEU:HD12	1.71	0.55
2:B:329:ASP:O	2:B:333:LEU:HD13	2.07	0.55
4:F:331:GLU:OE2	10:F:401:ACP:O3G	2.25	0.55
2:B:191:VAL:HB	2:B:425:MET:HE2	1.88	0.55
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.89	0.54
2:B:191:VAL:HB	2:B:425:MET:CE	2.37	0.54
2:B:338:LYS:HG3	2:B:339:ASN:OD1	2.07	0.54
1:C:151:SER:HB3	1:C:193:THR:HG21	1.90	0.54
2:D:141:LEU:HD12	2:D:172:MET:SD	2.48	0.54
3:E:74:GLU:O	3:E:77:GLU:HG2	2.08	0.54
1:A:22:GLU:HG3	1:A:83:TYR:HE2	1.73	0.54
4:F:371:PRO:N	4:F:372:THR:HB	2.23	0.54
2:B:338:LYS:HG3	2:B:339:ASN:H	1.73	0.53
1:A:187:SER:CB	1:A:391:LEU:HD21	2.39	0.53
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.90	0.53
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.89	0.53
4:F:245:ILE:HG23	4:F:249:TYR:HD2	1.74	0.53
2:B:324:SER:O	2:B:328:VAL:HG23	2.09	0.53
1:C:271:THR:HG21	1:C:295:CYS:O	2.09	0.53
4:F:136:ASN:O	4:F:140:GLU:HB3	2.08	0.53
2:B:106:GLY:O	2:B:111:GLY:HA3	2.08	0.53
2:B:297:ASP:OD2	2:B:299:LYS:HD3	2.08	0.53
4:F:31:ARG:NE	4:F:33:ASP:H	2.06	0.53
1:A:430:LYS:HE2	1:A:430:LYS:CA	2.39	0.53
1:A:340:SER:C	1:A:341:ILE:HD12	2.30	0.53
2:B:62:VAL:CG1	2:B:88:ARG:HG3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.43	0.53
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.35	0.53
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.91	0.52
2:D:145:THR:HB	7:D:501:GDP:O2B	2.09	0.52
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.91	0.52
1:A:98:ASP:HB2	5:A:501:GTP:O3G	2.09	0.52
2:D:217:LEU:CB	2:D:219:LEU:HD13	2.38	0.52
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.92	0.52
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.45	0.52
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.92	0.52
2:D:152:LEU:O	2:D:156:LYS:HG2	2.10	0.52
4:F:99:VAL:O	4:F:100:ILE:HD13	2.09	0.52
2:D:217:LEU:HB2	2:D:219:LEU:HD13	1.90	0.52
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.45	0.52
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.92	0.52
4:F:269:GLN:HA	4:F:272:MET:HE2	1.92	0.52
4:F:6:VAL:O	4:F:32:LYS:HG3	2.10	0.52
2:B:333:LEU:HD23	4:F:57:GLY:HA3	1.93	0.51
2:D:171:VAL:HA	2:D:204:ILE:O	2.11	0.51
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.92	0.51
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.46	0.51
3:E:120:LEU:O	3:E:124:GLN:NE2	2.43	0.51
4:F:31:ARG:HD2	4:F:32:LYS:H	1.74	0.51
4:F:3:THR:HB	4:F:30:LEU:HD11	1.93	0.50
1:A:101:ASN:ND2	1:A:180:ALA:HB2	2.27	0.50
4:F:31:ARG:HE	4:F:33:ASP:H	1.61	0.49
3:E:136:ASN:OD1	3:E:140:LYS:HE2	2.11	0.49
4:F:166:ALA:O	4:F:170:LEU:HD12	2.12	0.49
4:F:269:GLN:HA	4:F:272:MET:CE	2.43	0.49
1:A:76:ASP:O	1:A:80:THR:HG22	2.12	0.49
2:B:88:ARG:HH12	2:B:124:LYS:NZ	2.10	0.49
2:B:295:MET:HE1	2:B:375:ALA:HB1	1.95	0.49
2:B:306:ASP:OD2	2:B:308:ARG:HB2	2.13	0.49
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.48	0.49
4:F:371:PRO:CA	4:F:372:THR:CB	2.91	0.49
2:B:308:ARG:HD2	2:B:342:TYR:OH	2.12	0.49
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.48	0.49
2:B:88:ARG:NH1	2:B:91:ASN:OD1	2.46	0.48
2:D:69:ASP:O	2:D:94:PHE:HA	2.13	0.48
2:D:427:ASP:O	2:D:431:GLU:HG3	2.13	0.48
4:F:165:GLU:OE2	4:F:165:GLU:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.31	0.48
3:E:135:LYS:NZ	3:E:139:LEU:HD21	2.29	0.48
2:D:143:GLY:HA3	7:D:501:GDP:O3A	2.13	0.48
1:C:230:LEU:O	1:C:234:ILE:HD12	2.14	0.48
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.96	0.48
2:B:336:GLN:OE1	4:F:36:ARG:NH1	2.47	0.48
2:B:295:MET:HE2	2:B:376:THR:C	2.34	0.48
4:F:198:LYS:HD3	4:F:239:HIS:O	2.14	0.48
4:F:320:MET:CG	4:F:330:ILE:HD11	2.43	0.48
1:A:285:GLN:HA	1:A:285:GLN:NE2	2.28	0.47
3:E:44:ASP:N	11:E:202:HOH:O	2.47	0.47
4:F:17:VAL:O	4:F:21:LEU:HG	2.14	0.47
2:B:2:ARG:HB2	2:B:133:GLN:HE21	1.78	0.47
2:D:203:CYS:SG	2:D:384:ILE:HD11	2.54	0.47
2:B:2:ARG:HB2	2:B:133:GLN:NE2	2.29	0.47
2:B:335:VAL:HA	2:B:338:LYS:HD3	1.96	0.47
4:F:26:GLN:HE22	4:F:362:ALA:H	1.62	0.47
2:D:66:ILE:HD12	2:D:122:VAL:HG22	1.96	0.47
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.95	0.47
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.96	0.47
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.27	0.47
2:D:332:MET:O	2:D:336:GLN:HG3	2.15	0.47
2:D:67:LEU:N	2:D:67:LEU:HD12	2.30	0.47
2:B:221:THR:HG21	1:C:326:LYS:HA	1.95	0.47
1:C:341:ILE:HD13	1:C:351:PHE:HZ	1.78	0.47
2:D:159:GLU:HG3	3:E:123:LEU:HD13	1.96	0.47
2:D:387:LEU:HD23	2:D:387:LEU:C	2.35	0.47
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.50	0.47
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.47
4:F:243:HIS:NE2	4:F:247:LYS:HE3	2.30	0.47
2:B:66:ILE:CD1	2:B:122:VAL:HG22	2.46	0.46
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.50	0.46
1:C:104:ALA:HB2	1:C:413:MET:SD	2.55	0.46
1:A:293:ASN:ND2	1:A:339:ARG:HH21	2.13	0.46
2:B:194:LEU:HD22	2:B:198:THR:HG21	1.97	0.46
1:A:227:LEU:O	1:A:231:ILE:HG13	2.15	0.46
8:B:503:MES:H32	8:B:503:MES:H82	1.74	0.46
1:C:140:SER:HA	1:C:171:ILE:HB	1.98	0.46
2:D:334:ASN:OD1	2:D:338:LYS:HE3	2.15	0.46
2:B:200:GLU:OE2	2:B:255:LEU:HG	2.15	0.46
4:F:253:TYR:CZ	4:F:259:GLY:HA2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLU:OE2	2:B:326:LYS:HD3	2.15	0.46
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.51	0.46
2:B:335:VAL:O	2:B:338:LYS:HG2	2.16	0.46
4:F:161:LEU:HA	4:F:236:LYS:HE2	1.98	0.46
4:F:312:PHE:CZ	4:F:355:ILE:HD11	2.51	0.46
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.46	0.46
4:F:237:THR:O	4:F:246:GLN:NE2	2.48	0.46
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.52	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.97	0.45
1:C:199:ASP:HB2	11:C:617:HOH:O	2.16	0.45
2:D:12:CYS:HB2	7:D:501:GDP:C8	2.50	0.45
3:E:24:LEU:O	3:E:25:LYS:HE2	2.15	0.45
1:A:419:SER:O	1:A:423:GLU:HG3	2.16	0.45
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.46	0.45
1:A:254:GLU:HG2	1:A:258:ASN:HD21	1.81	0.45
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.99	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.51	0.45
2:B:325:MET:HA	2:B:325:MET:HE2	1.96	0.45
3:E:8:VAL:O	3:E:9:ILE:HD13	2.15	0.45
2:B:244:PHE:CE1	2:B:358:ILE:HD12	2.52	0.45
1:C:8:HIS:HB3	1:C:13:GLY:O	2.17	0.45
1:A:25:CYS:HB3	1:A:30:ILE:O	2.17	0.45
2:B:158:ARG:NH1	2:B:196:GLU:O	2.50	0.45
2:B:205:ASP:OD2	2:B:304:ALA:HB3	2.17	0.45
1:C:108:TYR:O	1:C:112:LYS:HG2	2.17	0.45
2:D:141:LEU:HD12	2:D:172:MET:HE3	1.99	0.45
2:B:1:MET:HG2	2:B:3:GLU:CD	2.37	0.45
1:C:4:CYS:HB3	1:C:136:LEU:CD1	2.47	0.45
2:D:54:ASN:O	2:D:61:TYR:HA	2.16	0.45
2:D:194:LEU:HD22	2:D:198:THR:HG21	1.99	0.45
1:A:71:GLU:OE1	1:A:73:THR:CB	2.64	0.44
2:B:85:GLN:HA	2:B:85:GLN:HE21	1.82	0.44
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.99	0.44
4:F:148:ILE:HG23	4:F:148:ILE:O	2.17	0.44
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.53	0.44
2:B:83:PHE:O	2:B:86:ILE:HG22	2.17	0.44
1:A:141:PHE:O	1:A:147:SER:HB3	2.18	0.44
1:A:234:ILE:O	1:A:238:ILE:HG13	2.17	0.44
1:A:241:SER:HB2	1:A:248:LEU:O	2.17	0.44
2:B:2:ARG:HE	2:B:48:ARG:NH2	2.15	0.44
2:B:40:SER:OG	2:B:42:LEU:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.83	0.44
1:C:351:PHE:CD1	1:C:351:PHE:N	2.86	0.44
2:D:141:LEU:HD12	2:D:172:MET:CE	2.48	0.44
1:A:341:ILE:HD12	1:A:341:ILE:N	2.33	0.44
2:B:325:MET:HA	2:B:325:MET:HE1	1.95	0.44
1:C:214:ARG:HG2	1:C:219:ILE:O	2.18	0.44
4:F:159:GLY:C	4:F:160:ILE:HD12	2.37	0.44
1:A:179:THR:HG23	2:B:248:LEU:HA	1.99	0.44
2:B:67:LEU:N	2:B:67:LEU:HD12	2.33	0.44
4:F:240:LEU:HD12	4:F:240:LEU:N	2.33	0.44
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.51	0.44
2:D:315:VAL:HB	2:D:351:VAL:HG22	2.00	0.44
4:F:99:VAL:O	4:F:127:GLU:HB2	2.18	0.44
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.99	0.44
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.00	0.43
2:B:88:ARG:NH1	2:B:90:ASP:OD1	2.51	0.43
2:B:335:VAL:HA	2:B:338:LYS:CD	2.48	0.43
1:C:75:ILE:HD12	1:C:94:THR:HG22	2.00	0.43
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.43
2:D:195:VAL:HG11	2:D:424:ASN:ND2	2.33	0.43
2:D:382:THR:O	2:D:385:GLN:HG2	2.17	0.43
4:F:5:VAL:HG23	4:F:32:LYS:HA	2.00	0.43
2:B:325:MET:HE1	2:B:328:VAL:HG21	2.01	0.43
2:D:212:ILE:O	2:D:216:THR:HB	2.19	0.43
2:D:240:THR:CG2	2:D:318:ILE:HD11	2.47	0.43
2:D:114:LEU:HG	2:D:114:LEU:O	2.19	0.43
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.54	0.43
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.00	0.43
2:B:171:VAL:HA	2:B:204:ILE:O	2.18	0.43
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.58	0.43
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.53	0.43
2:B:291:LEU:O	2:B:295:MET:HB3	2.18	0.43
2:B:318:ILE:N	2:B:318:ILE:HD12	2.34	0.43
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.01	0.43
2:B:387:LEU:C	2:B:387:LEU:HD23	2.39	0.43
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.54	0.43
1:C:69:ASP:O	1:C:94:THR:HA	2.19	0.43
4:F:13:VAL:O	4:F:17:VAL:HG23	2.19	0.43
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.54	0.43
1:C:75:ILE:HB	1:C:94:THR:HG21	2.01	0.43
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:HD11	1:C:302:MET:SD	2.58	0.42
1:C:277:SER:OG	1:C:280:LYS:HG2	2.19	0.42
2:B:42:LEU:HD12	2:B:42:LEU:N	2.33	0.42
1:C:41:THR:O	1:C:41:THR:OG1	2.38	0.42
1:A:293:ASN:HA	1:A:335:ILE:HD11	2.02	0.42
1:C:55:GLU:HA	1:C:60:LYS:O	2.20	0.42
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.01	0.42
1:C:142:GLY:CA	1:C:183:GLU:HG2	2.50	0.42
1:A:55:GLU:HA	1:A:60:LYS:O	2.20	0.42
2:B:288:VAL:N	2:B:289:PRO:HD2	2.34	0.42
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.01	0.42
2:B:136:GLN:HA	2:B:167:ASN:O	2.19	0.42
1:C:241:SER:HA	1:C:249:ASN:OD1	2.20	0.42
2:B:46:LEU:HA	2:B:49:ILE:HB	2.01	0.42
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.42	0.42
2:B:320:ARG:HA	2:B:356:CYS:O	2.19	0.41
1:A:234:ILE:HD12	1:A:234:ILE:N	2.35	0.41
1:A:317:LEU:HD23	1:A:377:MET:HG3	2.03	0.41
1:A:430:LYS:HE2	1:A:430:LYS:N	2.36	0.41
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.55	0.41
2:D:322:ARG:HD3	2:D:322:ARG:HA	1.75	0.41
1:A:293:ASN:HA	1:A:335:ILE:CD1	2.50	0.41
2:B:124:LYS:HE2	2:B:124:LYS:HB3	1.80	0.41
2:B:338:LYS:CG	2:B:339:ASN:H	2.33	0.41
3:E:128:LYS:O	3:E:132:GLU:HG2	2.20	0.41
4:F:226:GLU:HB2	4:F:238:CYS:HB3	2.02	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.03	0.41
2:B:301:MET:HE1	2:B:377:PHE:CE2	2.56	0.41
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.50	0.41
1:C:75:ILE:HB	1:C:94:THR:CG2	2.49	0.41
2:D:155:SER:OG	2:D:197:ASN:ND2	2.53	0.41
2:B:164:ARG:O	8:B:503:MES:H51	2.19	0.41
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.48	0.41
4:F:245:ILE:HG23	4:F:249:TYR:CD2	2.54	0.41
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.50	0.41
1:C:166:LYS:HE2	1:C:197:HIS:O	2.20	0.41
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.56	0.41
2:B:188:THR:HA	2:B:425:MET:HE1	1.98	0.41
2:B:12:CYS:HB2	7:B:501:GDP:C8	2.56	0.41
1:C:351:PHE:N	1:C:351:PHE:HD1	2.19	0.41
2:D:303:ALA:O	2:D:305:CYS:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:GLU:HG3	2:B:83:PHE:CE1	2.56	0.41
2:B:158:ARG:NE	8:B:503:MES:H62	2.36	0.41
4:F:198:LYS:HG3	4:F:241:THR:CG2	2.50	0.41
4:F:246:GLN:O	4:F:247:LYS:HG3	2.21	0.41
2:B:345:GLU:OE1	2:B:345:GLU:N	2.45	0.41
2:D:11:GLN:HA	2:D:74:THR:HG21	2.02	0.41
2:B:209:LEU:HB3	2:B:227:LEU:HG	2.03	0.40
2:B:320:ARG:O	2:B:373:MET:HA	2.21	0.40
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.01	0.40
3:E:138:GLU:O	3:E:141:GLU:HG2	2.21	0.40
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.84	0.40
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.54	0.40
2:B:248:LEU:CD1	2:B:352:LYS:HB3	2.38	0.40
4:F:14:TYR:HA	4:F:17:VAL:HB	2.02	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.22	0.40
1:C:6:SER:O	1:C:65:ALA:HA	2.22	0.40
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.02	0.40
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.51	0.40
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.03	0.40
1:A:265:ILE:O	1:A:265:ILE:HG22	2.22	0.40
2:B:297:ASP:OD1	2:B:298:SER:N	2.55	0.40
2:B:332:MET:O	2:B:335:VAL:HG12	2.21	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	437/451 (97%)	423 (97%)	13 (3%)	1 (0%)	47 49
1	C	439/451 (97%)	432 (98%)	7 (2%)	0	100 100
2	B	415/445 (93%)	403 (97%)	12 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	417/445 (94%)	405 (97%)	11 (3%)	1 (0%)	47	49
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	329/384 (86%)	314 (95%)	14 (4%)	1 (0%)	41	41
All	All	2156/2319 (93%)	2095 (97%)	58 (3%)	3 (0%)	51	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	247	LYS
1	A	281	ALA
2	D	82	PRO

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	371/379 (98%)	368 (99%)	3 (1%)	81	86
1	C	372/379 (98%)	371 (100%)	1 (0%)	92	95
2	B	362/383 (94%)	356 (98%)	6 (2%)	60	67
2	D	364/383 (95%)	361 (99%)	3 (1%)	81	86
3	E	110/127 (87%)	106 (96%)	4 (4%)	35	36
4	F	306/342 (90%)	306 (100%)	0	100	100
All	All	1885/1993 (95%)	1868 (99%)	17 (1%)	78	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	262	TYR
1	A	381	THR
2	B	2	ARG
2	B	90	ASP

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Mol	Chain	Res	Type
2	B	139	HIS
2	B	214	PHE
2	B	217	LEU
2	B	295	MET
1	C	302	MET
2	D	139	HIS
2	D	207	GLU
2	D	345	GLU
3	E	7	GLU
3	E	48	GLU
3	E	108	ASN
3	E	128	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
2	B	85	GLN
1	C	356	ASN
2	D	197	ASN
4	F	26	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 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GTP	A	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.38	6 (18%)
7	GDP	D	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.10	3 (10%)
9	LVV	C	503	-	17,17,17	0.96	0	21,24,24	0.84	0
8	MES	B	503	-	12,12,12	2.27	1 (8%)	14,16,16	2.28	6 (42%)
7	GDP	B	501	6	24,30,30	0.95	1 (4%)	30,47,47	1.08	4 (13%)
5	GTP	C	501	6	26,34,34	1.11	2 (7%)	32,54,54	1.42	6 (18%)
10	ACP	F	401	6	27,33,33	1.39	5 (18%)	32,52,52	1.45	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
7	GDP	D	501	6	-	5/12/32/32	0/3/3/3
9	LVV	C	503	-	-	0/4/16/16	0/2/2/2
8	MES	B	503	-	-	5/6/14/14	0/1/1/1
7	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
10	ACP	F	401	6	-	3/15/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	503	MES	C8-S	-7.56	1.66	1.77
5	A	501	GTP	C5-C6	-3.97	1.39	1.47
5	C	501	GTP	C5-C6	-3.85	1.39	1.47
10	F	401	ACP	PG-O2G	2.99	1.61	1.54
10	F	401	ACP	PG-O3G	2.96	1.61	1.54
10	F	401	ACP	PB-O3A	2.79	1.61	1.58
10	F	401	ACP	C5-C4	2.50	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	GDP	C6-N1	-2.44	1.34	1.37
7	D	501	GDP	C6-N1	-2.27	1.34	1.37
10	F	401	ACP	PB-O2B	2.21	1.61	1.56
5	C	501	GTP	C2-N3	2.13	1.38	1.33
5	A	501	GTP	C2-N3	2.12	1.38	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	503	MES	C5-N4-C3	4.18	118.25	108.83
10	F	401	ACP	PB-O3A-PA	-3.76	120.63	132.56
10	F	401	ACP	C3'-C2'-C1'	3.36	106.03	100.98
5	C	501	GTP	PB-O3B-PG	-3.19	121.89	132.83
8	B	503	MES	C2-C3-N4	-3.17	105.30	110.10
10	F	401	ACP	N3-C2-N1	-3.16	123.74	128.68
8	B	503	MES	O2S-S-C8	3.14	110.70	106.92
5	C	501	GTP	C5-C6-N1	3.12	119.46	113.95
8	B	503	MES	C6-C5-N4	-3.08	105.43	110.10
5	C	501	GTP	C8-N7-C5	3.04	108.78	102.99
5	A	501	GTP	C5-C6-N1	2.98	119.22	113.95
5	A	501	GTP	C8-N7-C5	2.97	108.66	102.99
8	B	503	MES	C7-N4-C5	2.75	118.26	111.23
5	C	501	GTP	C2-N1-C6	-2.75	120.04	125.10
5	A	501	GTP	PB-O3B-PG	-2.74	123.41	132.83
7	D	501	GDP	PA-O3A-PB	-2.70	123.57	132.83
10	F	401	ACP	C4-C5-N7	-2.68	106.61	109.40
5	A	501	GTP	C2-N1-C6	-2.68	120.17	125.10
8	B	503	MES	C7-N4-C3	2.63	117.95	111.23
5	C	501	GTP	PA-O3A-PB	-2.50	124.25	132.83
5	A	501	GTP	PA-O3A-PB	-2.47	124.36	132.83
7	B	501	GDP	C5-C6-N1	2.46	118.29	113.95
7	B	501	GDP	C8-N7-C5	2.41	107.58	102.99
7	B	501	GDP	PA-O3A-PB	-2.36	124.72	132.83
7	D	501	GDP	C8-N7-C5	2.36	107.48	102.99
7	D	501	GDP	C5-C6-N1	2.29	118.00	113.95
5	A	501	GTP	O6-C6-C5	-2.07	120.33	124.37
5	C	501	GTP	O6-C6-C5	-2.05	120.37	124.37
7	B	501	GDP	O6-C6-C5	-2.01	120.44	124.37

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
7	B	501	GDP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O2A
7	D	501	GDP	C5'-O5'-PA-O3A
7	D	501	GDP	C5'-O5'-PA-O1A
7	D	501	GDP	C5'-O5'-PA-O2A
8	B	503	MES	C8-C7-N4-C3
8	B	503	MES	C8-C7-N4-C5
10	F	401	ACP	O4'-C4'-C5'-O5'
10	F	401	ACP	C3'-C4'-C5'-O5'
8	B	503	MES	C7-C8-S-O3S
7	D	501	GDP	PA-O3A-PB-O3B
8	B	503	MES	C7-C8-S-O1S
8	B	503	MES	C7-C8-S-O2S
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
7	D	501	GDP	PA-O3A-PB-O1B
10	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
7	B	501	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

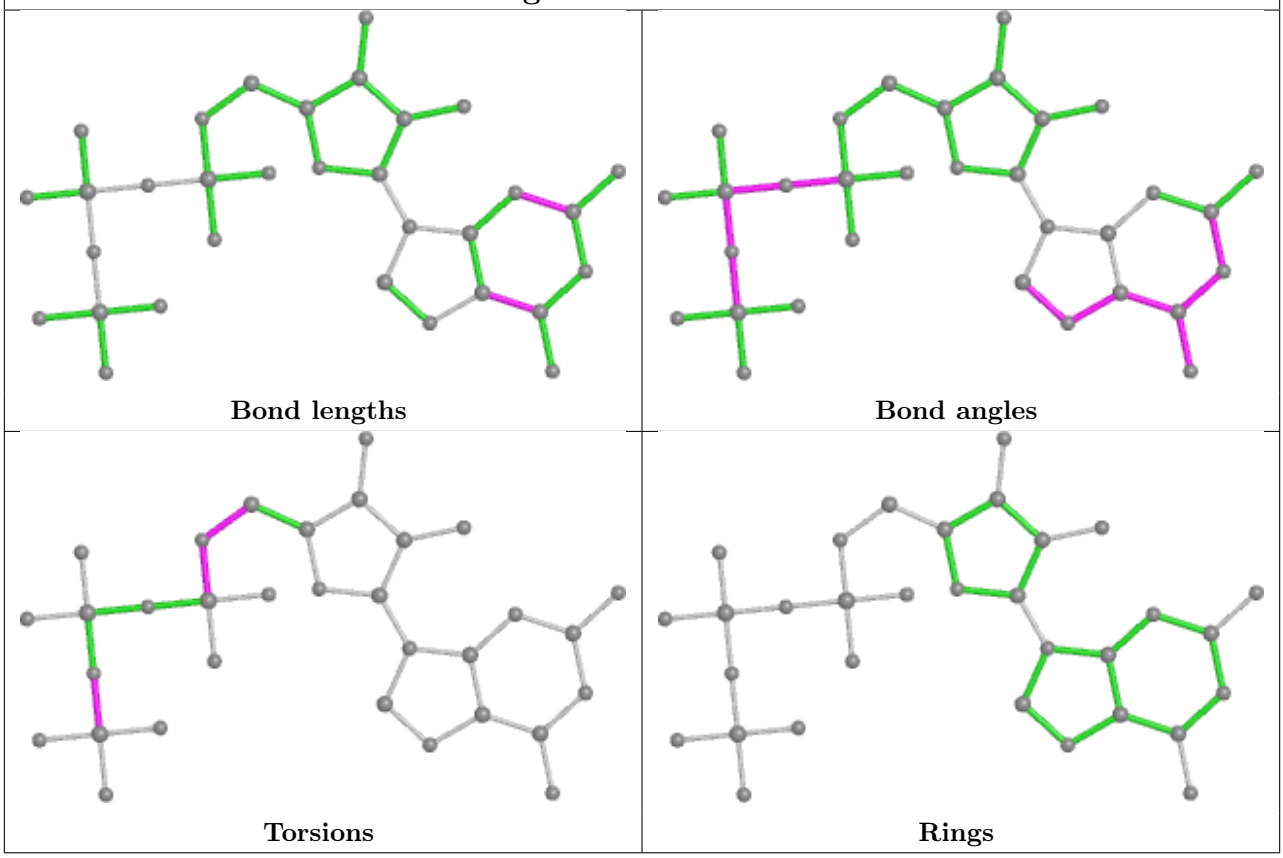
5 monomers are involved in 11 short contacts:

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

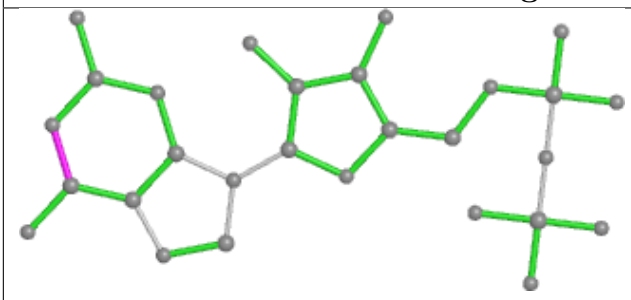
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

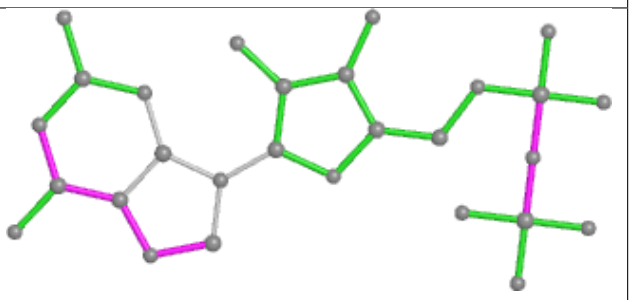
Ligand GTP A 501



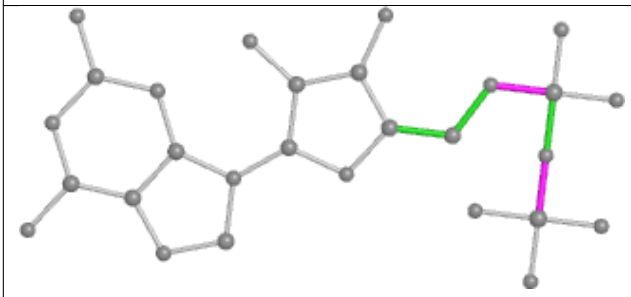
Ligand GDP D 501



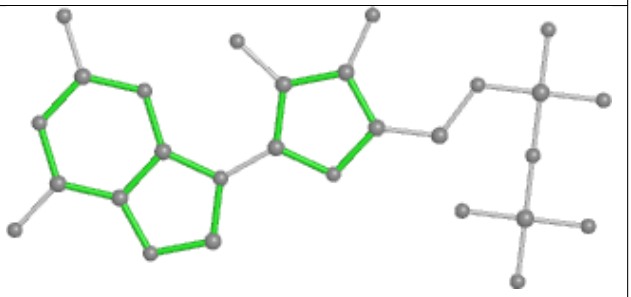
Bond lengths



Bond angles

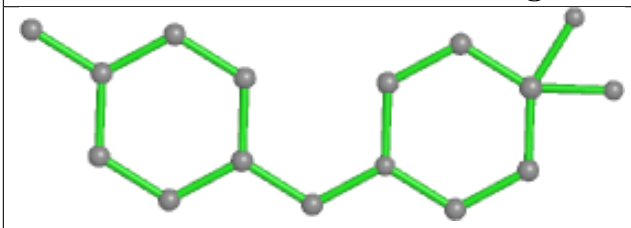


Torsions

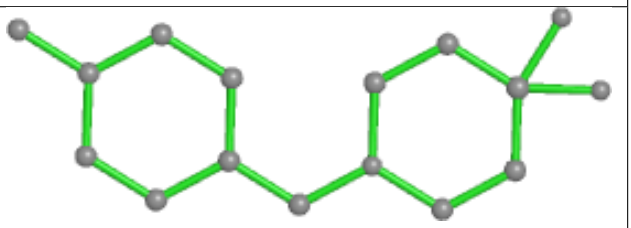


Rings

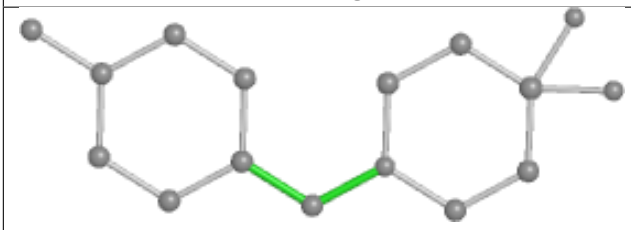
Ligand LVV C 503



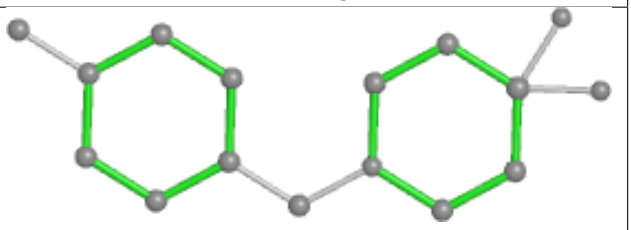
Bond lengths



Bond angles

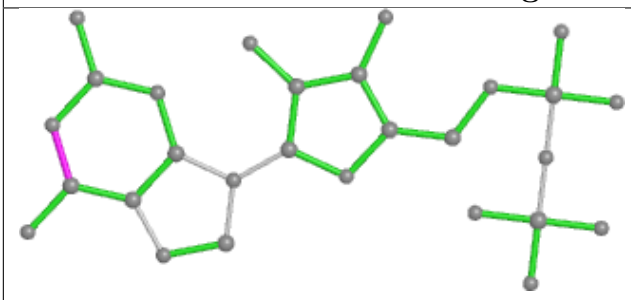


Torsions

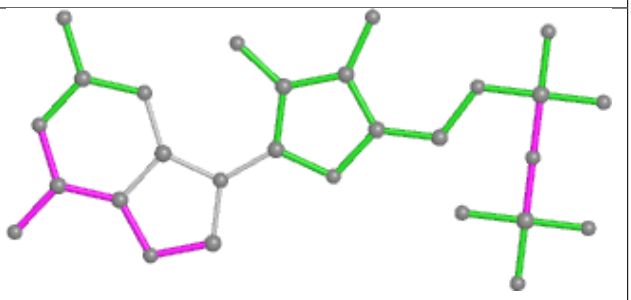


Rings

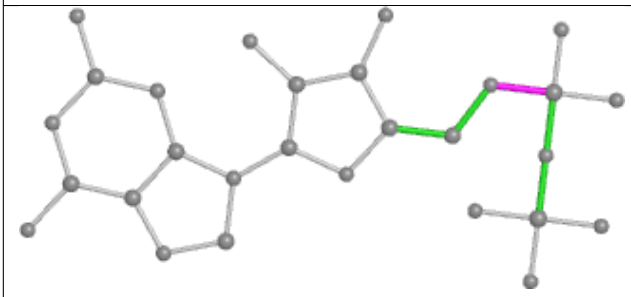
Ligand GDP B 501



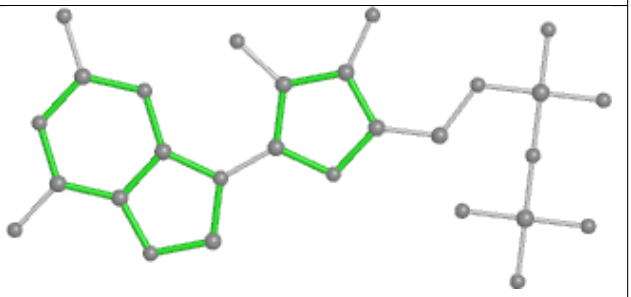
Bond lengths



Bond angles

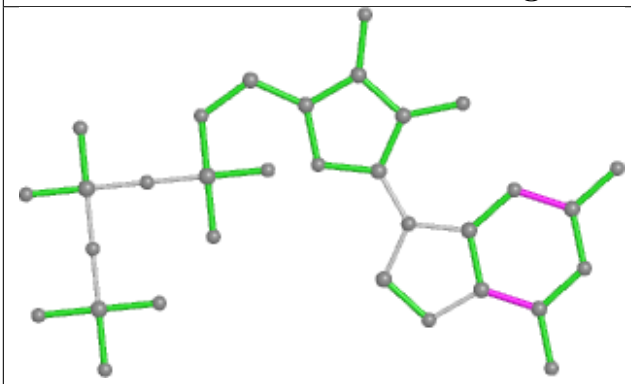


Torsions

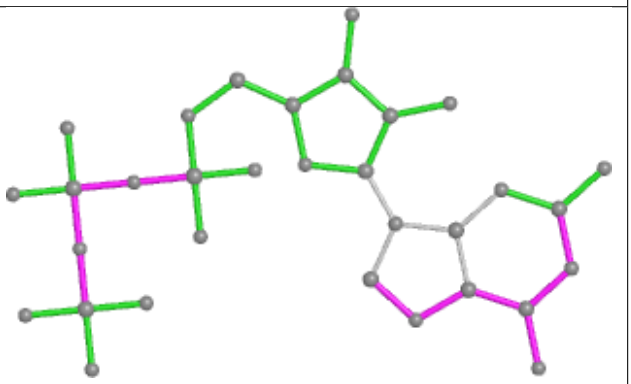


Rings

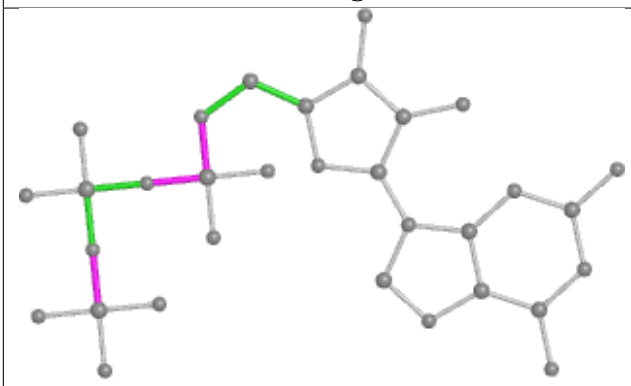
Ligand GTP C 501



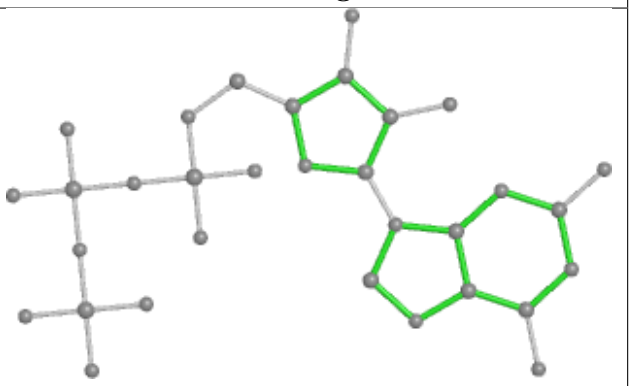
Bond lengths



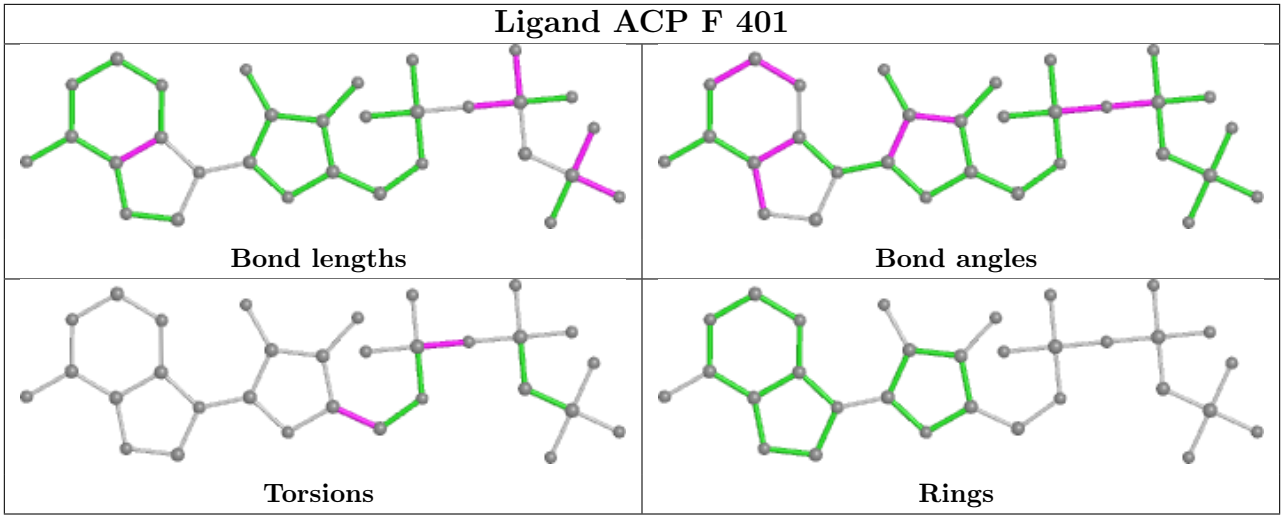
Bond angles



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	441/451 (97%)	0.33	12 (2%)	54	60	43, 62, 99, 159	0
1	C	440/451 (97%)	0.26	4 (0%)	84	86	38, 49, 69, 126	0
2	B	419/445 (94%)	0.50	16 (3%)	40	46	40, 61, 100, 131	1 (0%)
2	D	421/445 (94%)	0.22	8 (1%)	66	71	45, 66, 94, 132	4 (0%)
3	E	123/143 (86%)	0.57	8 (6%)	18	23	48, 70, 119, 150	0
4	F	339/384 (88%)	0.64	33 (9%)	7	10	54, 84, 142, 162	0
All	All	2183/2319 (94%)	0.39	81 (3%)	41	48	38, 63, 112, 162	5 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	248	LEU	8.8
4	F	173	ILE	7.1
4	F	372	THR	6.5
2	B	1	MET	6.2
4	F	99	VAL	6.1
1	A	179	THR	6.0
2	B	58	GLY	5.9
4	F	244	CYS	5.0
3	E	26	PRO	4.8
4	F	161	LEU	4.7
4	F	90	SER	4.6
1	A	448	GLY	4.4
2	B	249	ASN	4.0
1	A	438	ASP	3.8
3	E	7	GLU	3.7
4	F	249	TYR	3.7
3	E	25	LYS	3.5
4	F	125	THR	3.5
1	A	262	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	163	LYS	3.4
1	A	282	TYR	3.3
1	C	340	SER	3.3
2	B	303	ALA	3.3
2	B	57	THR	3.1
3	E	28	SER	3.1
4	F	148	ILE	3.1
2	D	407	TRP	3.0
4	F	182	ILE	3.0
4	F	169	LEU	3.0
4	F	253	TYR	3.0
4	F	149	ALA	3.0
4	F	89	GLU	2.9
4	F	371	PRO	2.9
4	F	240	LEU	2.9
2	B	333	LEU	2.8
4	F	179	VAL	2.8
2	D	82	PRO	2.8
4	F	130	VAL	2.7
2	B	358	ILE	2.7
1	A	335	ILE	2.7
1	A	346	TRP	2.6
4	F	160	ILE	2.6
1	C	357	TYR	2.6
4	F	131	PHE	2.6
1	A	351	PHE	2.5
3	E	24	LEU	2.5
4	F	236	LYS	2.4
1	C	341	ILE	2.4
1	A	340	SER	2.4
4	F	20	LEU	2.4
4	F	248	GLU	2.4
4	F	186	LEU	2.3
2	D	57	THR	2.3
2	B	247	GLN	2.3
2	B	307	PRO	2.3
2	B	36	TYR	2.3
2	D	248	LEU	2.3
4	F	250	SER	2.3
4	F	251	LYS	2.2
3	E	27	PRO	2.2
2	D	1	MET	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	37	HIS	2.2
4	F	178	GLN	2.2
4	F	231	ALA	2.2
2	B	342	TYR	2.2
2	B	308	ARG	2.2
1	A	232	SER	2.2
2	D	400	ARG	2.2
1	A	283	HIS	2.2
4	F	24	THR	2.2
4	F	137	ARG	2.2
2	B	318	ILE	2.1
4	F	71	LEU	2.1
4	F	320	MET	2.1
2	D	58	GLY	2.1
3	E	6	MET	2.1
4	F	172	PHE	2.1
3	E	143	ALA	2.1
2	B	242	LEU	2.0
1	C	350	GLY	2.0
2	D	272	PHE	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
10	ACP	F	401	31/31	0.83	0.16	82,93,102,104	0
6	MG	A	502	1/1	0.84	0.08	45,45,45,45	0
8	MES	B	503	12/12	0.85	0.17	59,63,79,82	0

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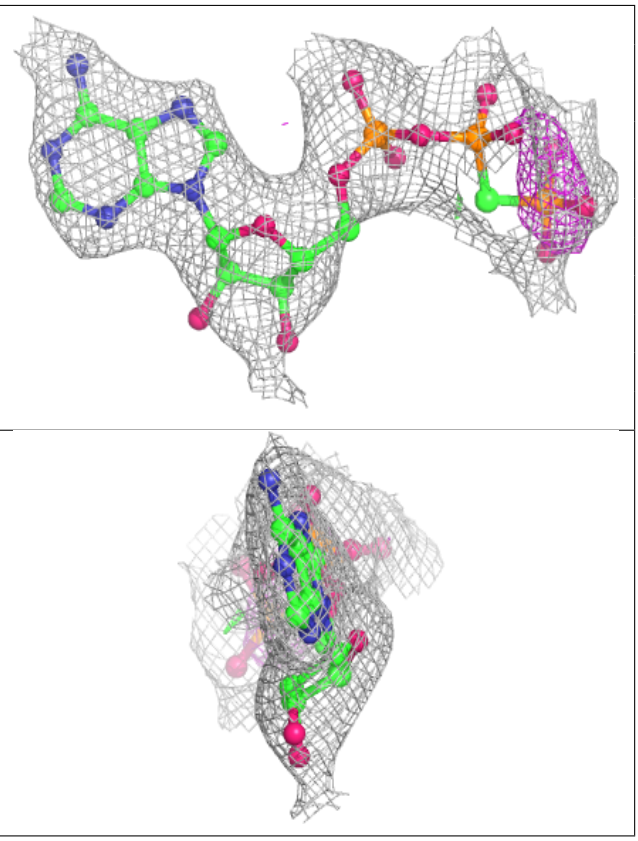
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	C	502	1/1	0.90	0.10	37,37,37,37	0
6	MG	D	502	1/1	0.93	0.12	64,64,64,64	0
9	LVV	C	503	16/16	0.94	0.17	44,55,63,63	33
6	MG	F	402	1/1	0.94	0.10	89,89,89,89	0
7	GDP	D	501	28/28	0.95	0.14	60,64,70,74	0
5	GTP	A	501	32/32	0.97	0.14	40,46,48,50	0
7	GDP	B	501	28/28	0.97	0.15	38,46,50,51	0
6	MG	B	502	1/1	0.97	0.17	38,38,38,38	0
5	GTP	C	501	32/32	0.98	0.15	38,42,43,45	0

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

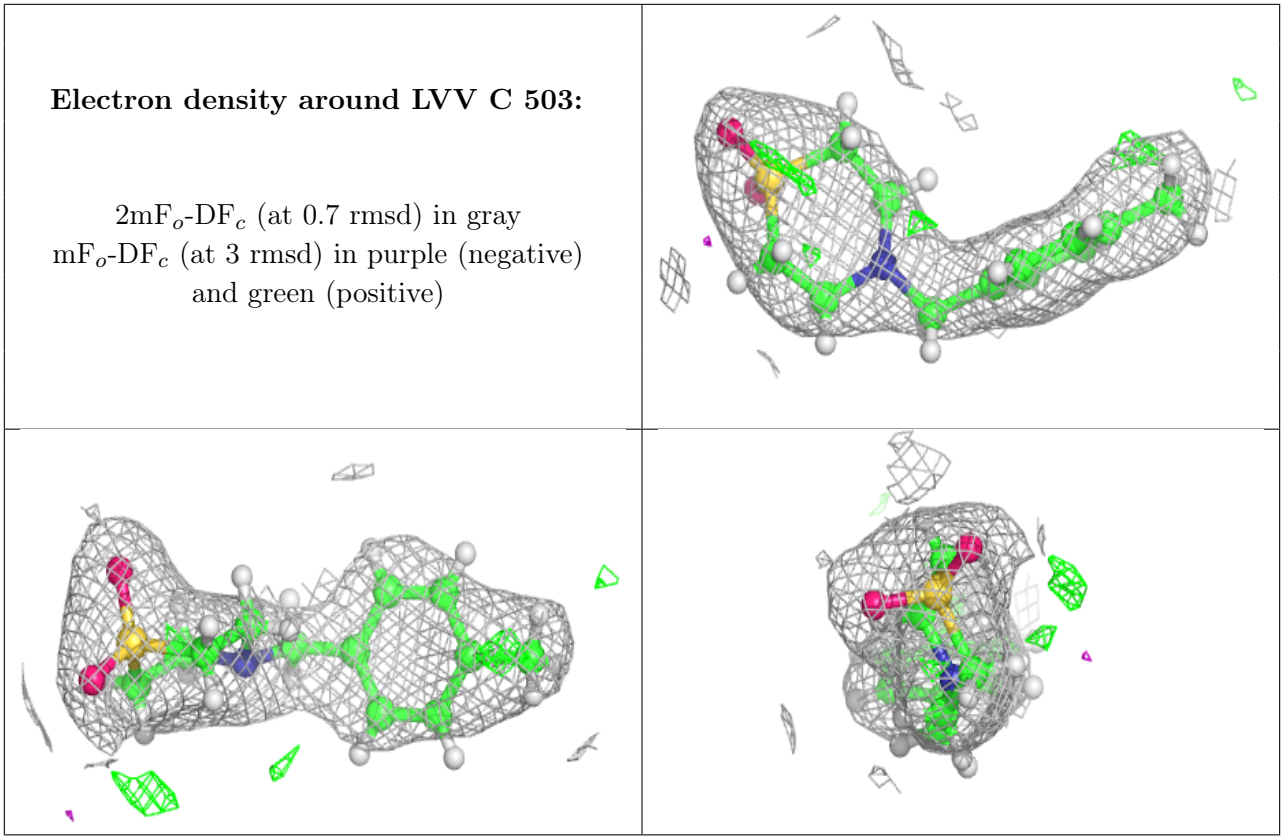
Electron density around ACP F 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



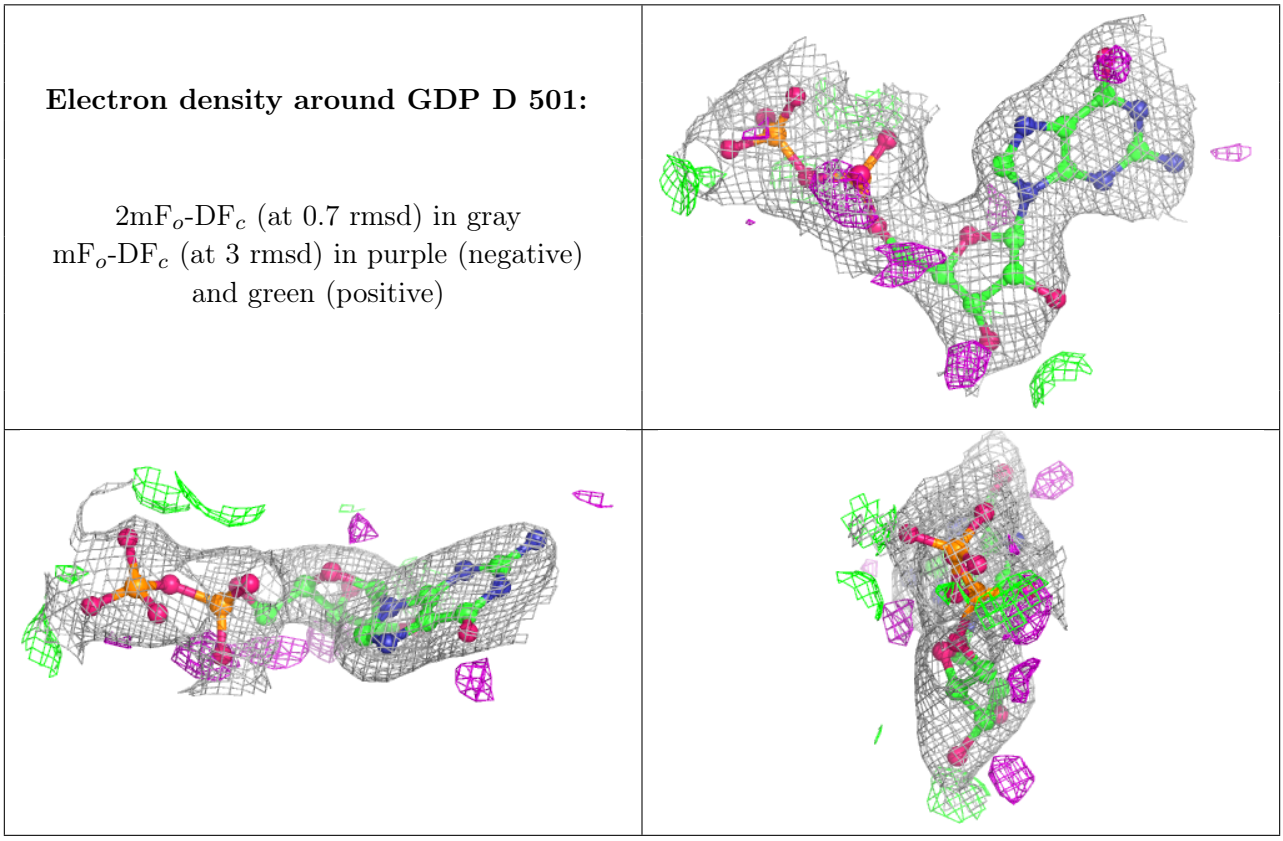
Electron density around LVV C 503:

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



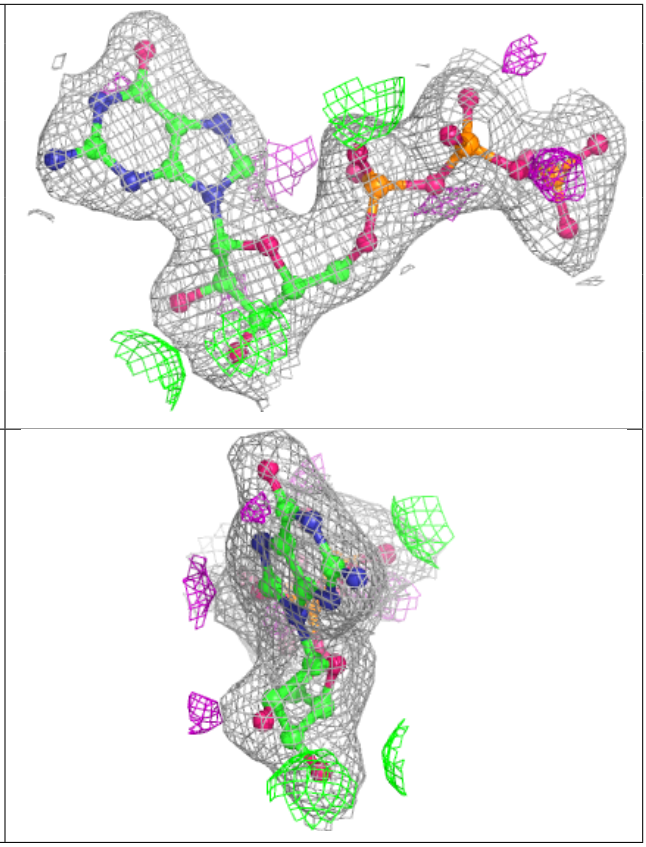
Electron density around GDP D 501:

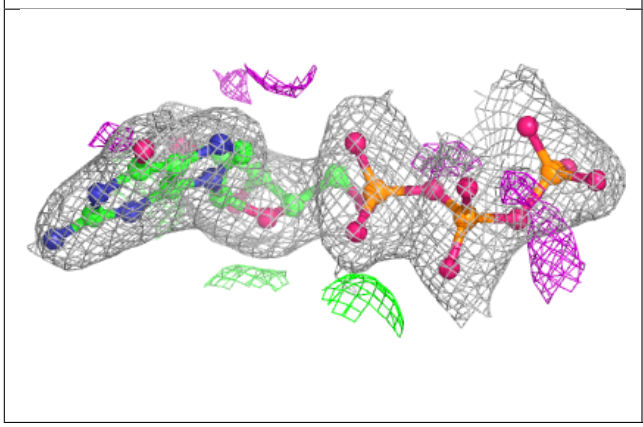
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GTP A 501:

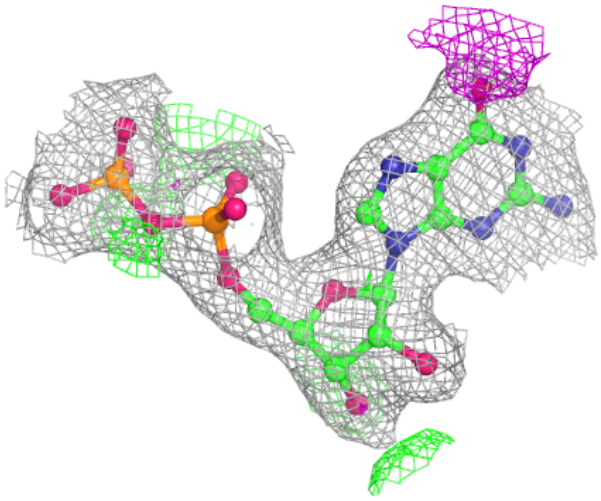
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

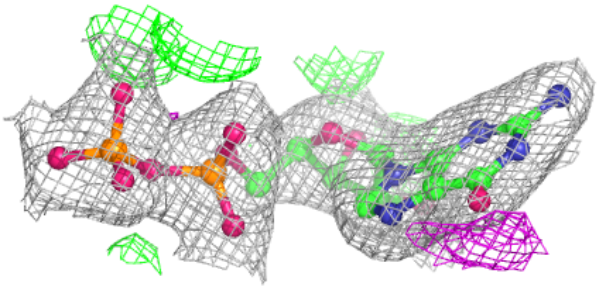


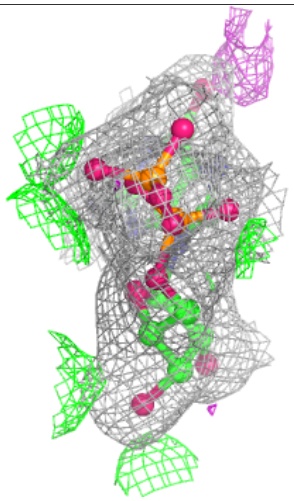


Electron density around GDP B 501:

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

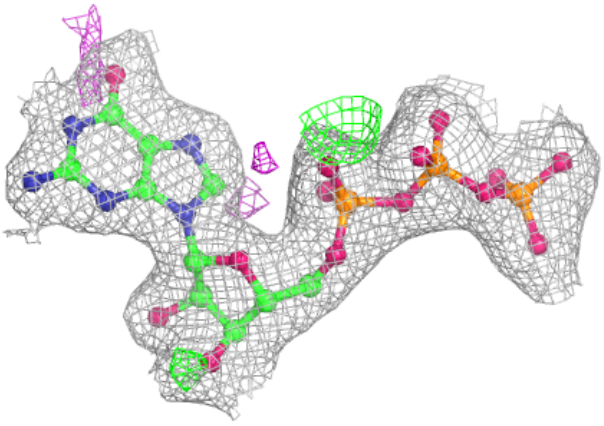


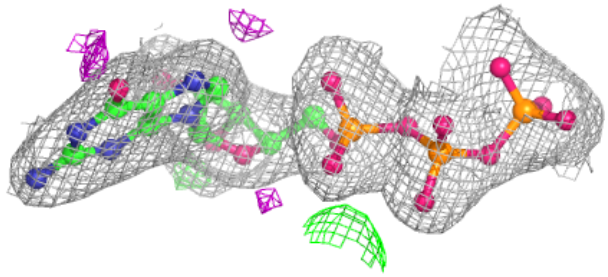


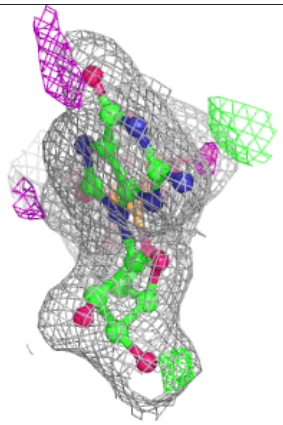


Electron density around GTP C 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.