



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2017 – 07:45 AM EDT

PDB ID : 5M8D
Title : Tubulin MTD265-R1 complex
Authors : Bohnacker, T.; Protá, A.E.; Steinmetz, M.O.; Wymann, M.P.
Deposited on : unknown
Resolution : 2.25 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

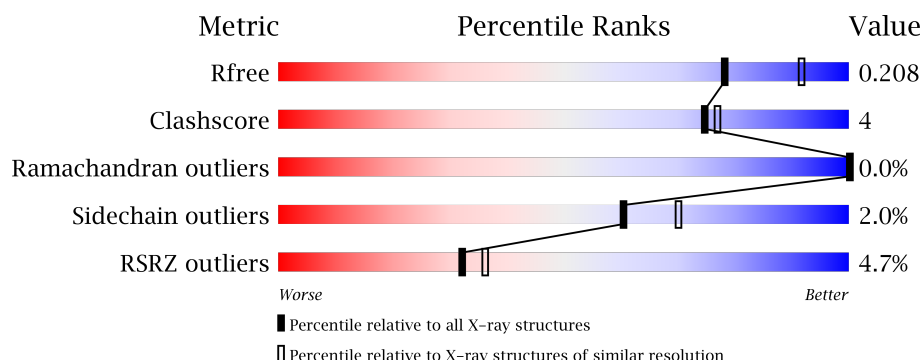
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
2	B	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div>21%</div><div></div><div>79%</div><div></div><div>9%</div><div></div><div>10%</div></div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18103 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3331	2094	568	643	26			
2	D	427	Total	C	N	O	S	0	0	0
			3349	2101	572	650	26			

- Molecule 3 is a protein called Stathmin-4.

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

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

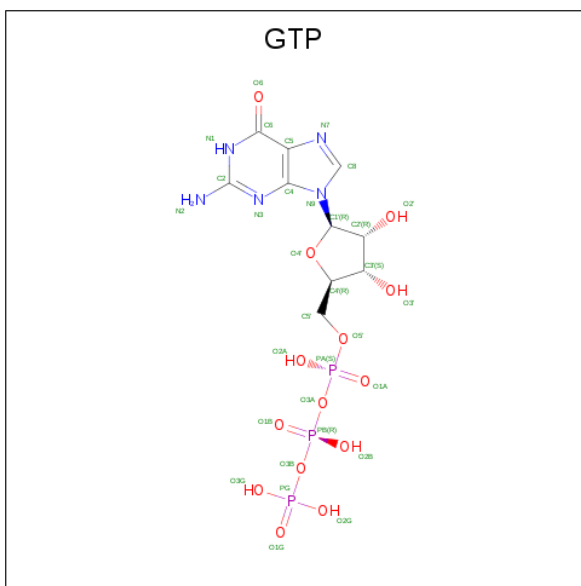
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	344	Total	C	N	O	S	0	0	0
			2808	1800	483	511	14			

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: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



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

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

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

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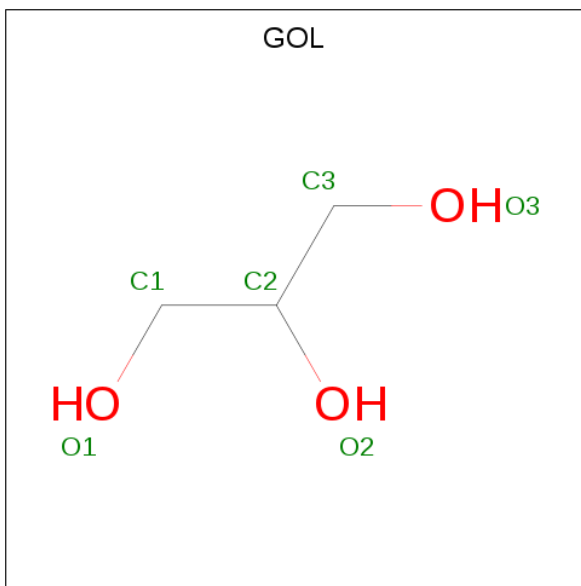
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

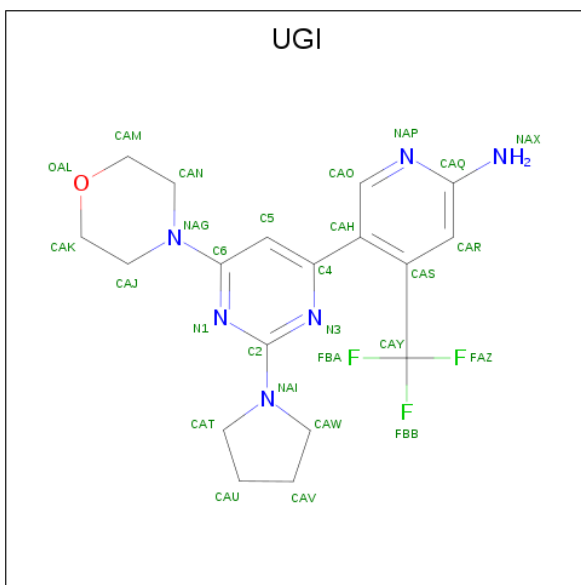
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



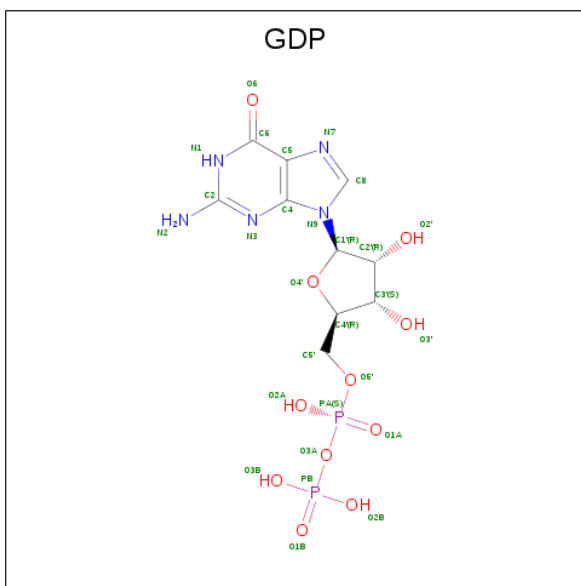
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 5-(6-morpholin-4-yl-2-pyrrolidin-1-yl-pyrimidin-4-yl)-4-(trifluoromethyl)pyridine-2-amine (three-letter code: UGI) (formula: C₁₈H₂₁F₃N₆O).



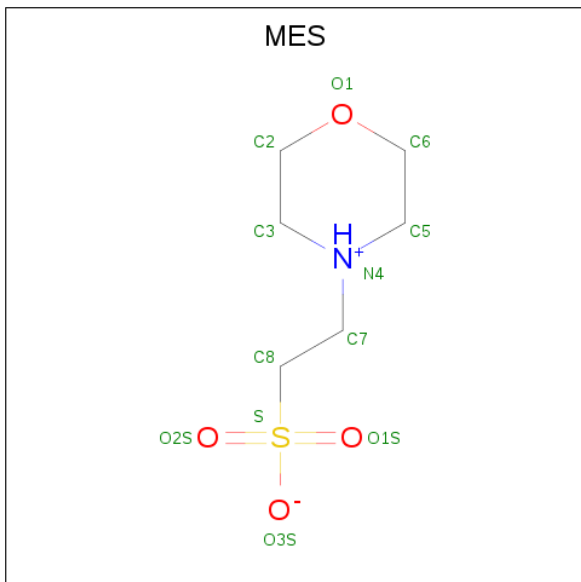
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	F	N	O	0	0
			28	18	3	6	1		

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



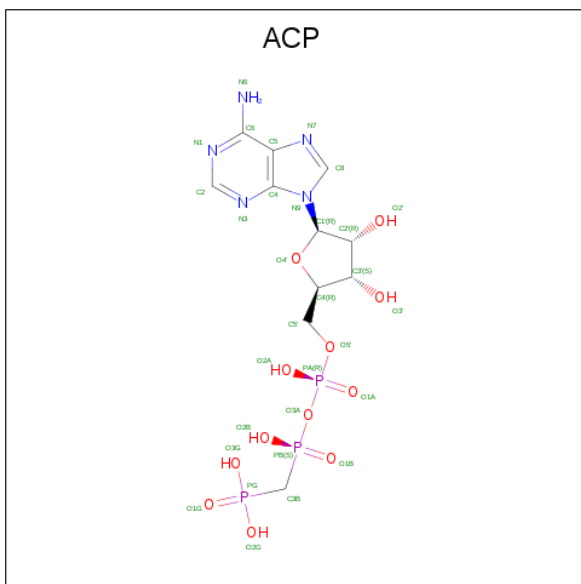
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
10	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

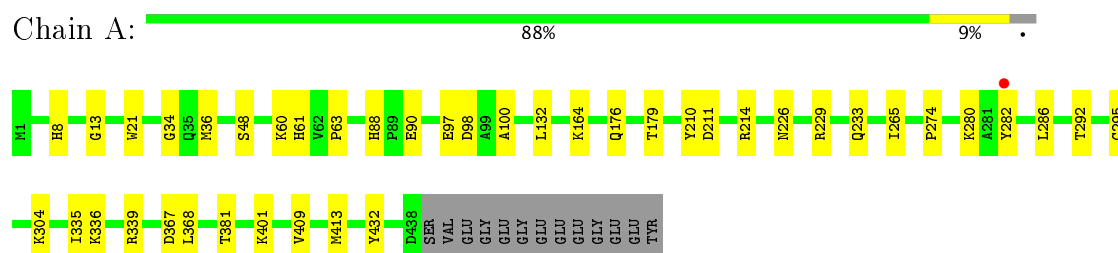
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	113	Total 113	O 113	0	0
13	B	95	Total 95	O 95	0	0
13	C	199	Total 199	O 199	0	0
13	D	69	Total 69	O 69	0	0
13	E	18	Total 18	O 18	0	0
13	F	39	Total 39	O 39	0	0

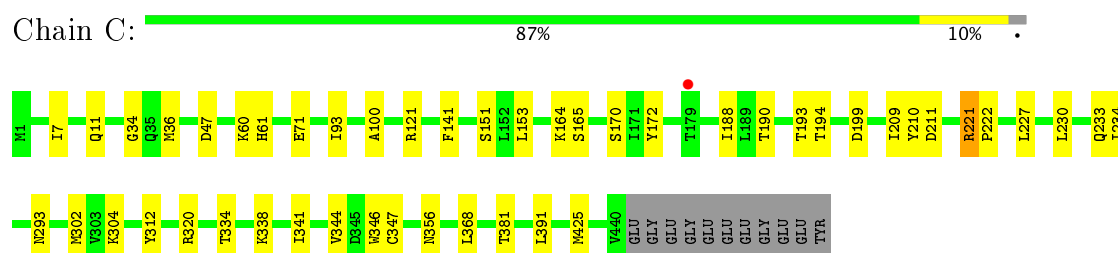
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

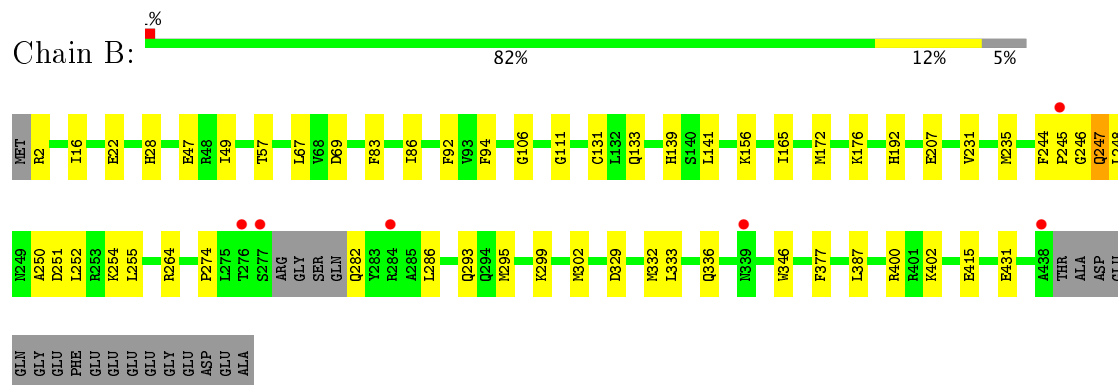
- Molecule 1: Tubulin alpha-1B chain



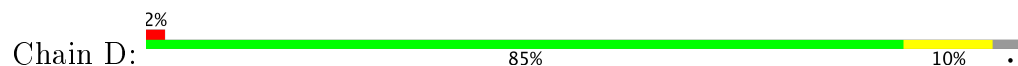
- Molecule 1: Tubulin alpha-1B chain

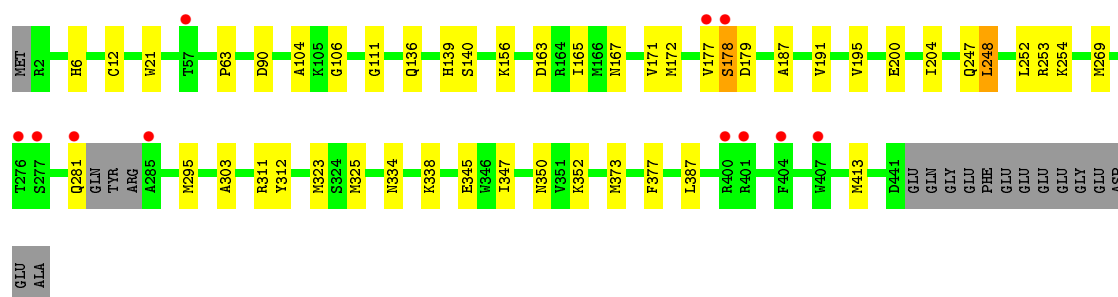


- Molecule 2: Tubulin beta-2B chain

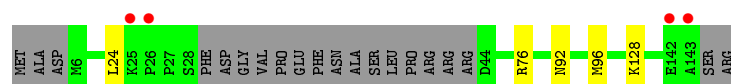
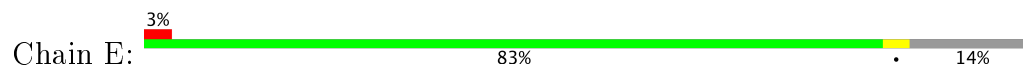


- Molecule 2: Tubulin beta-2B chain

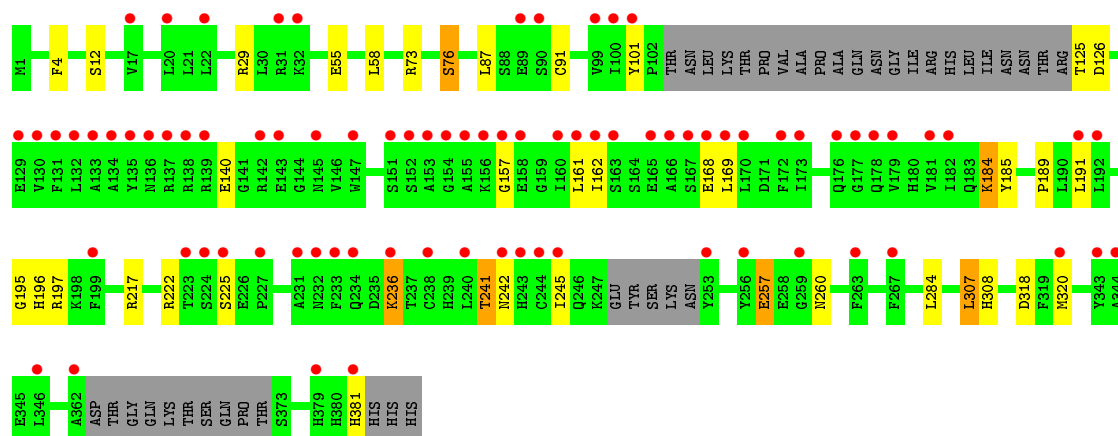
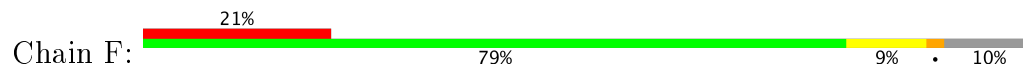




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.18Å 157.02Å 179.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.10 – 2.25 78.19 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (68.10-2.25) 99.5 (78.19-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.25Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.170 , 0.210 0.167 , 0.208	Depositor DCC
R_{free} test set	6888 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18103	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.38	0/3502	0.54	0/4754
1	C	0.48	1/3515 (0.0%)	0.58	0/4772
2	B	0.41	0/3405	0.56	0/4612
2	D	0.37	0/3422	0.53	0/4635
3	E	0.39	0/1022	0.48	0/1356
4	F	0.34	0/2872	0.50	0/3878
All	All	0.40	1/17738 (0.0%)	0.54	0/24007

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	347	CYS	CB-SG	-5.17	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3424	0	3335	22	0
1	C	3437	0	3348	25	0
2	B	3331	0	3208	35	0
2	D	3349	0	3223	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1014	0	1029	3	0
4	F	2808	0	2776	23	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	0	1	0
10	B	28	0	12	0	0
10	D	28	0	12	1	0
11	B	12	0	12	0	0
12	F	31	0	14	4	0
13	A	113	0	0	1	0
13	B	95	0	0	2	0
13	C	199	0	0	1	0
13	D	69	0	0	2	0
13	E	18	0	0	0	0
13	F	39	0	0	0	0
All	All	18103	0	17001	129	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 4.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLU:OE1	2:B:2:ARG:NH1	2.16	0.78
1:A:229:ARG:NH2	13:A:601:HOH:O	2.19	0.74
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.69	0.73
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.27	0.67
2:B:299:LYS:NZ	13:B:602:HOH:O	2.30	0.65
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.80	0.64
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.81	0.62
2:D:12:CYS:HB2	10:D:501:GDP:C8	2.34	0.62
2:D:281:GLN:NE2	13:D:602:HOH:O	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.35	0.61
2:D:311:ARG:NH2	2:D:345:GLU:OE1	2.33	0.61
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.82	0.60
2:B:2:ARG:HB3	2:B:133:GLN:HG3	1.82	0.60
4:F:241:THR:OG1	12:F:402:ACP:O2'	2.19	0.60
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.83	0.60
4:F:162:ILE:H	4:F:236:LYS:NZ	2.00	0.59
2:D:167:ASN:ND2	13:D:604:HOH:O	2.36	0.58
2:B:250:ALA:HB1	2:B:255:LEU:HD21	1.86	0.58
12:F:402:ACP:O1A	12:F:402:ACP:O3G	2.22	0.56
2:B:83:PHE:O	2:B:86:ILE:HG12	2.06	0.56
4:F:225:SER:OG	4:F:260:ASN:ND2	2.35	0.56
1:A:132:LEU:O	1:A:164:LYS:NZ	2.34	0.55
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.89	0.55
4:F:161:LEU:HD23	4:F:169:LEU:HD23	1.89	0.55
2:B:329:ASP:O	2:B:333:LEU:HG	2.07	0.55
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.43	0.54
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.89	0.53
2:B:69:ASP:O	2:B:94:PHE:HA	2.09	0.53
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.91	0.53
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.89	0.53
2:B:47:GLU:HB3	2:B:245:PRO:HG3	1.90	0.53
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.43	0.53
4:F:101:TYR:HD1	4:F:126:ASP:HB2	1.74	0.52
2:B:251:ASP:O	2:B:255:LEU:HG	2.10	0.52
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.40	0.51
4:F:241:THR:HG1	12:F:402:ACP:HO2'	1.58	0.51
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.92	0.51
1:C:47:ASP:OD2	13:C:601:HOH:O	2.19	0.51
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.93	0.51
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.46	0.51
1:C:320:ARG:HA	1:C:356:ASN:O	2.11	0.50
2:B:244:PHE:O	2:B:246:GLY:N	2.44	0.50
2:B:156:LYS:HD3	3:E:76:ARG:CZ	2.41	0.50
2:D:334:ASN:HD21	2:D:338:LYS:NZ	2.09	0.49
1:A:336:LYS:HG2	3:E:24:LEU:HD23	1.93	0.49
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.47	0.49
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.94	0.49
1:C:334:THR:HG23	1:C:338:LYS:HE2	1.94	0.49
4:F:189:PRO:HG2	4:F:191:LEU:HD21	1.95	0.49
2:B:106:GLY:O	2:B:111:GLY:HA3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.48	0.49
2:D:178:SER:CB	2:D:179:ASP:HA	2.43	0.49
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.48	0.48
1:C:151:SER:HB3	1:C:193:THR:HG21	1.93	0.48
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.94	0.48
2:B:176:LYS:HD3	2:B:207:GLU:HG3	1.97	0.47
1:C:230:LEU:O	1:C:234:ILE:HD12	2.15	0.47
2:B:332:MET:O	2:B:336:GLN:HG3	2.15	0.47
4:F:162:ILE:H	4:F:236:LYS:HZ2	1.61	0.47
1:C:11:GLN:HE22	2:D:247:GLN:HE22	1.63	0.47
4:F:318:ASP:OD2	12:F:402:ACP:O3G	2.32	0.47
2:B:264:ARG:NE	2:B:431:GLU:OE2	2.39	0.47
4:F:101:TYR:CD1	4:F:126:ASP:HB2	2.50	0.46
2:D:136:GLN:HA	2:D:167:ASN:O	2.16	0.46
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.96	0.46
1:C:190:THR:O	1:C:194:THR:HG23	2.15	0.46
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.34	0.46
2:D:248:LEU:HD11	2:D:352:LYS:HB3	1.97	0.46
2:D:163:ASP:O	2:D:253:ARG:NH2	2.49	0.46
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.51	0.46
1:C:221:ARG:HG3	2:D:325:MET:HB3	1.97	0.45
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.52	0.45
2:B:402:LYS:HD3	2:B:415:GLU:OE2	2.17	0.45
4:F:184:LYS:NZ	4:F:185:TYR:O	2.47	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.52	0.45
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.98	0.44
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.98	0.44
1:A:34:GLY:HA3	1:A:60:LYS:HG3	2.00	0.44
2:D:156:LYS:HA	2:D:156:LYS:HD2	1.85	0.44
2:B:286:LEU:HD12	2:B:286:LEU:HA	1.85	0.44
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.31	0.44
1:C:341:ILE:HD12	1:C:341:ILE:H	1.82	0.44
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.99	0.43
2:B:2:ARG:HA	2:B:131:CYS:O	2.18	0.43
2:B:141:LEU:HD12	2:B:172:MET:SD	2.57	0.43
2:B:293:GLN:NE2	13:B:601:HOH:O	2.28	0.43
3:E:92:ASN:O	3:E:96:MET:HG2	2.18	0.43
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.83	0.43
4:F:73:ARG:HB2	4:F:76:SER:OG	2.18	0.43
2:B:255:LEU:HD22	9:B:501:UGI:CAO	2.48	0.43
2:D:171:VAL:HA	2:D:204:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:101:TYR:N	4:F:126:ASP:OD2	2.31	0.43
2:D:187:ALA:O	2:D:191:VAL:HG23	2.18	0.43
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.54	0.43
1:A:280:LYS:HE2	1:A:282:TYR:O	2.18	0.42
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.01	0.42
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.53	0.42
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.54	0.42
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.42
1:A:292:THR:O	1:A:295:CYS:HB2	2.18	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.42
4:F:55:GLU:HB3	4:F:58:LEU:HD12	2.00	0.42
2:B:28:HIS:HB3	2:B:49:ILE:HD12	2.02	0.42
1:C:100:ALA:HA	2:D:254:LYS:HG3	2.02	0.42
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.55	0.42
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.55	0.42
1:C:165:SER:HA	1:C:199:ASP:OD2	2.19	0.42
2:B:244:PHE:C	2:B:246:GLY:H	2.23	0.41
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.37	0.41
2:D:104:ALA:HB2	2:D:413:MET:SD	2.60	0.41
2:D:12:CYS:HB3	2:D:140:SER:HB3	2.02	0.41
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.56	0.41
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.49	0.41
2:B:235:MET:HE2	2:B:235:MET:HB3	1.88	0.41
2:D:191:VAL:O	2:D:195:VAL:HG23	2.20	0.41
4:F:4:PHE:CZ	4:F:29:ARG:HB2	2.56	0.41
1:A:8:HIS:HB3	1:A:13:GLY:O	2.20	0.41
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.51	0.41
1:A:233:GLN:HG3	1:A:368:LEU:HD12	2.04	0.40
2:B:402:LYS:NZ	2:B:415:GLU:OE1	2.54	0.40
4:F:284:LEU:HA	4:F:284:LEU:HD12	1.97	0.40
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.56	0.40
2:D:323:MET:HB3	2:D:373:MET:HE2	2.03	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.40
1:C:34:GLY:HA3	1:C:60:LYS:HG3	2.02	0.40
4:F:87:LEU:O	4:F:91:CYS:HB2	2.21	0.40
1:C:164:LYS:HB2	1:C:164:LYS:HE2	1.83	0.40
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.22	0.40
4:F:157:GLY:HA2	4:F:245:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/451 (97%)	428 (98%)	8 (2%)	0	100	100
1	C	438/451 (97%)	427 (98%)	11 (2%)	0	100	100
2	B	419/445 (94%)	410 (98%)	8 (2%)	1 (0%)	51	60
2	D	423/445 (95%)	417 (99%)	6 (1%)	0	100	100
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	336/384 (88%)	325 (97%)	11 (3%)	0	100	100
All	All	2171/2319 (94%)	2126 (98%)	44 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	247	GLN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/379 (97%)	365 (99%)	4 (1%)	78	86
1	C	371/379 (98%)	366 (99%)	5 (1%)	73	83
2	B	366/383 (96%)	358 (98%)	8 (2%)	57	67
2	D	368/383 (96%)	362 (98%)	6 (2%)	68	78
3	E	110/127 (87%)	109 (99%)	1 (1%)	82	89
4	F	306/342 (90%)	292 (95%)	14 (5%)	31	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1890/1993 (95%)	1852 (98%)	38 (2%)	60	70

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	176	GLN
1	A	179	THR
1	A	381	THR
2	B	57	THR
2	B	139	HIS
2	B	192	HIS
2	B	247	GLN
2	B	248	LEU
2	B	282	GLN
2	B	302	MET
2	B	400	ARG
1	C	71	GLU
1	C	221	ARG
1	C	293	ASN
1	C	302	MET
1	C	381	THR
2	D	90	ASP
2	D	139	HIS
2	D	177	VAL
2	D	178	SER
2	D	200	GLU
2	D	248	LEU
3	E	128	LYS
4	F	12	SER
4	F	76	SER
4	F	125	THR
4	F	140	GLU
4	F	168	GLU
4	F	184	LYS
4	F	217	ARG
4	F	222	ARG
4	F	236	LYS
4	F	241	THR
4	F	257	GLU
4	F	307	LEU
4	F	320	MET

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Mol	Chain	Res	Type
4	F	381	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	176	GLN
2	D	15	GLN
2	D	247	GLN
2	D	334	ASN
4	F	260	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 10 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	$\# Z > 2$
5	GTP	A	501	6	27,34,34	0.87	1 (3%)	27,54,54	1.92	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	A	505	-	5,5,5	0.33	0	5,5,5	0.41	0
9	UGI	B	501	-	31,31,31	1.35	6 (19%)	38,45,45	1.72	9 (23%)
10	GDP	B	502	6	25,30,30	1.15	3 (12%)	26,47,47	2.01	8 (30%)
11	MES	B	506	-	12,12,12	1.84	1 (8%)	14,16,16	2.03	4 (28%)
5	GTP	C	501	6	27,34,34	1.05	2 (7%)	27,54,54	1.82	6 (22%)
10	GDP	D	501	6	25,30,30	1.08	2 (8%)	26,47,47	2.01	6 (23%)
12	ACP	F	402	6	27,33,33	1.68	6 (22%)	30,52,52	1.50	3 (10%)

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	-	0/18/38/38	0/3/3/3
8	GOL	A	505	-	-	0/4/4/4	0/0/0/0
9	UGI	B	501	-	-	0/18/33/33	0/4/4/4
10	GDP	B	502	6	-	0/12/32/32	0/3/3/3
11	MES	B	506	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
10	GDP	D	501	6	-	0/12/32/32	0/3/3/3
12	ACP	F	402	6	-	0/15/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	506	MES	C8-S	-6.01	1.68	1.77
9	B	501	UGI	CAY-CAS	-3.89	1.41	1.50
9	B	501	UGI	CAH-C4	-3.10	1.39	1.48
12	F	402	ACP	PB-O2B	-2.92	1.49	1.56
9	B	501	UGI	C2-NAI	-2.23	1.31	1.35
9	B	501	UGI	FBB-CAY	-2.22	1.24	1.32
9	B	501	UGI	FBA-CAY	-2.19	1.25	1.32
5	C	501	GTP	PG-O3B	2.03	1.63	1.60
10	B	502	GDP	O4'-C1'	2.08	1.44	1.41
5	A	501	GTP	C6-N1	2.25	1.37	1.33
9	B	501	UGI	CAO-NAP	2.26	1.39	1.34
10	B	502	GDP	C5-C4	2.40	1.45	1.40
10	D	501	GDP	C5-C4	2.71	1.46	1.40
12	F	402	ACP	PG-O3G	2.75	1.61	1.54
12	F	402	ACP	PG-O2G	2.82	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	402	ACP	C5-C4	3.05	1.47	1.40
5	C	501	GTP	C6-N1	3.21	1.38	1.33
10	D	501	GDP	C6-C5	3.34	1.47	1.41
10	B	502	GDP	C6-C5	3.69	1.48	1.41
12	F	402	ACP	PB-O1B	3.79	1.61	1.51
12	F	402	ACP	PB-O3A	3.85	1.62	1.58

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	402	ACP	N3-C2-N1	-5.95	123.67	128.86
5	A	501	GTP	N3-C2-N1	-5.21	119.86	127.46
5	C	501	GTP	N3-C2-N1	-5.03	120.11	127.46
10	B	502	GDP	C6-C5-C4	-4.58	116.28	120.84
10	D	501	GDP	C6-C5-C4	-4.17	116.70	120.84
9	B	501	UGI	CAO-CAH-C4	-3.96	113.98	120.86
5	A	501	GTP	C5-C6-N1	-3.75	118.14	123.48
10	D	501	GDP	C5-C6-N1	-3.64	118.31	123.48
10	D	501	GDP	N3-C2-N1	-3.31	122.62	127.46
10	B	502	GDP	C5-C6-N1	-3.30	118.79	123.48
5	C	501	GTP	C5-C6-N1	-3.23	118.88	123.48
10	B	502	GDP	N3-C2-N1	-3.13	122.88	127.46
9	B	501	UGI	C5-C4-N3	-2.89	118.91	122.38
10	D	501	GDP	C4-C5-N7	-2.74	106.76	109.41
9	B	501	UGI	N1-C2-N3	-2.73	121.76	126.32
10	B	502	GDP	C4-C5-N7	-2.72	106.78	109.41
5	A	501	GTP	C1'-N9-C4	-2.63	122.09	126.64
12	F	402	ACP	C4-C5-N7	-2.59	106.91	109.41
9	B	501	UGI	FBA-CAY-CAS	-2.50	108.19	112.69
10	B	502	GDP	C1'-N9-C4	-2.42	122.46	126.64
5	A	501	GTP	C6-C5-C4	-2.33	118.53	120.84
10	B	502	GDP	O3'-C3'-C4'	-2.23	104.58	111.09
12	F	402	ACP	PA-O3A-PB	-2.22	125.24	132.39
5	C	501	GTP	C4-C5-N7	-2.12	107.36	109.41
9	B	501	UGI	OAL-CAK-CAJ	-2.11	107.10	111.83
5	C	501	GTP	N2-C2-N1	2.18	120.72	117.24
11	B	506	MES	O1S-S-C8	2.21	108.69	106.79
9	B	501	UGI	CAM-CAN-NAG	2.28	114.08	109.98
11	B	506	MES	C7-N4-C3	2.40	117.42	111.26
9	B	501	UGI	C2-N1-C6	2.70	119.91	115.26
9	B	501	UGI	N3-C2-NAI	2.90	120.34	117.11
5	C	501	GTP	C6-N1-C2	3.04	120.43	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C2-N3-C4	3.23	118.93	115.16
11	B	506	MES	O3S-S-C8	3.86	110.80	106.06
5	C	501	GTP	C2-N3-C4	4.04	119.88	115.16
5	A	501	GTP	C6-N1-C2	4.08	121.93	116.06
10	B	502	GDP	C6-N1-C2	4.13	122.00	116.06
10	D	501	GDP	C6-N1-C2	4.25	122.17	116.06
10	B	502	GDP	C2-N3-C4	4.71	120.66	115.16
9	B	501	UGI	CAN-NAG-CAJ	4.84	121.83	111.57
10	D	501	GDP	C2-N3-C4	4.95	120.94	115.16
11	B	506	MES	C5-N4-C3	5.11	120.44	108.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
9	B	501	UGI	1	0
10	D	501	GDP	1	0
12	F	402	ACP	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	438/451 (97%)	-0.03	1 (0%) 94 96	36, 55, 89, 155	0
1	C	440/451 (97%)	-0.06	1 (0%) 94 96	30, 43, 73, 105	0
2	B	423/445 (95%)	0.06	6 (1%) 75 78	31, 53, 90, 125	2 (0%)
2	D	427/445 (95%)	-0.07	11 (2%) 56 60	37, 62, 98, 129	4 (0%)
3	E	123/143 (86%)	0.18	4 (3%) 47 51	41, 69, 112, 138	0
4	F	344/384 (89%)	1.10	81 (23%) 1 1	43, 81, 147, 165	0
All	All	2195/2319 (94%)	0.16	104 (4%) 32 36	30, 58, 110, 165	6 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	9.6
4	F	134	ALA	6.6
4	F	100	ILE	6.4
4	F	182	ILE	6.2
4	F	130	VAL	5.6
1	A	282	TYR	5.4
4	F	253	TYR	5.3
4	F	143	GLU	5.2
4	F	166	ALA	5.1
4	F	132	LEU	4.9
4	F	179	VAL	4.8
4	F	131	PHE	4.8
4	F	169	LEU	4.8
4	F	233	PHE	4.6
4	F	177	GLY	4.6
4	F	135	TYR	4.3
2	B	284	ARG	4.3
4	F	20	LEU	4.2
4	F	99	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
4	F	139	ARG	4.1
4	F	90	SER	4.1
2	D	401	ARG	4.1
2	B	276	THR	4.0
3	E	26	PRO	3.9
2	D	57	THR	3.9
4	F	225	SER	3.9
4	F	231	ALA	3.8
4	F	152	SER	3.8
4	F	178	GLN	3.8
4	F	170	LEU	3.6
4	F	32	LYS	3.6
4	F	137	ARG	3.6
4	F	172	PHE	3.6
4	F	161	LEU	3.6
4	F	259	GLY	3.4
4	F	234	GLN	3.4
2	D	400	ARG	3.4
4	F	240	LEU	3.4
4	F	162	ILE	3.3
4	F	17	VAL	3.3
4	F	181	VAL	3.3
4	F	244	CYS	3.2
4	F	101	TYR	3.2
4	F	199	PHE	3.2
4	F	31	ARG	3.2
4	F	256	TYR	3.2
4	F	379	HIS	3.1
4	F	136	ASN	3.0
2	B	277	SER	3.0
3	E	25	LYS	2.9
4	F	176	GLN	2.9
4	F	224	SER	2.9
3	E	143	ALA	2.9
4	F	165	GLU	2.9
4	F	381	HIS	2.9
2	D	177	VAL	2.8
4	F	263	PHE	2.8
4	F	133	ALA	2.8
4	F	236	LYS	2.8
4	F	156	LYS	2.7
4	F	227	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	142	GLU	2.7
2	D	285	ALA	2.7
2	D	276	THR	2.7
4	F	147	TRP	2.6
4	F	22	LEU	2.6
4	F	138	ARG	2.6
2	B	245	PRO	2.6
4	F	158	GLU	2.5
4	F	232	ASN	2.5
4	F	267	PHE	2.5
4	F	320	MET	2.5
4	F	191	LEU	2.5
4	F	153	ALA	2.5
2	D	277	SER	2.4
4	F	157	GLY	2.4
2	D	281	GLN	2.4
4	F	243	HIS	2.3
4	F	167	SER	2.3
4	F	344	ALA	2.3
4	F	151	SER	2.2
4	F	245	ILE	2.2
4	F	145	ASN	2.2
4	F	89	GLU	2.2
4	F	154	GLY	2.2
4	F	168	GLU	2.2
4	F	223	THR	2.2
2	B	438	ALA	2.2
4	F	362	ALA	2.2
2	B	339	ASN	2.1
4	F	346	LEU	2.1
4	F	238	CYS	2.1
1	C	179	THR	2.1
2	D	407	TRP	2.1
4	F	155	ALA	2.1
2	D	178	SER	2.1
2	D	404	PHE	2.1
4	F	192	LEU	2.0
4	F	142	ARG	2.0
4	F	343	TYR	2.0
4	F	242	ASN	2.0
4	F	129	GLU	2.0
4	F	160	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	163	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
9	UGI	B	501	28/28	0.91	0.17	0.64	41,56,73,85	28
7	CA	A	504	1/1	0.81	0.17	0.32	102,102,102,102	0
11	MES	B	506	12/12	0.97	0.14	0.18	48,53,69,71	0
5	GTP	A	501	32/32	0.98	0.14	0.05	29,38,43,55	0
10	GDP	B	502	28/28	0.99	0.15	0.01	27,37,41,44	0
5	GTP	C	501	32/32	0.99	0.14	-0.14	27,32,38,46	0
10	GDP	D	501	28/28	0.97	0.12	-0.24	45,55,64,65	0
7	CA	C	503	1/1	0.96	0.12	-0.27	63,63,63,63	0
6	MG	A	502	1/1	0.96	0.14	-0.40	37,37,37,37	0
12	ACP	F	402	31/31	0.92	0.15	-1.37	82,98,121,125	0
8	GOL	A	505	6/6	0.94	0.12	-1.87	73,77,90,92	0
7	CA	A	503	1/1	0.95	0.08	-2.33	71,71,71,71	0
6	MG	B	503	1/1	0.99	0.19	-	33,33,33,33	0
7	CA	B	505	1/1	0.92	0.25	-	92,92,92,92	0
7	CA	B	504	1/1	0.93	0.13	-	118,118,118,118	0
6	MG	F	401	1/1	0.86	0.05	-	78,78,78,78	0
6	MG	D	502	1/1	0.90	0.10	-	55,55,55,55	0
6	MG	C	502	1/1	0.98	0.15	-	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.