



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2016 – 06:22 AM EST

PDB ID : 5IYZ
Title : Tubulin-MMAE complex
Authors : Waight, A.B.; Bargsten, K.; Doronina, S.; Steinmetz, M.O.; Sussman, D.;
Prota, A.E.
Deposited on : 2016-03-24
Resolution : 1.80 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20028442

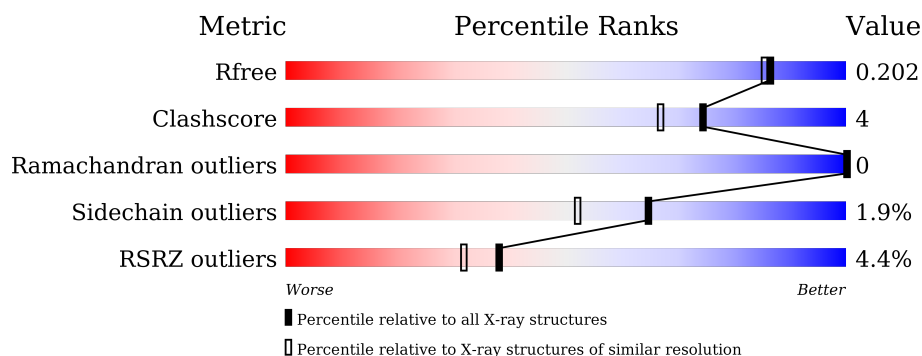
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	
4	F	384	

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
10	4Q5	D	503	-	-	-	X
7	CA	C	503	-	-	-	X
9	MES	B	503	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19140 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	437	Total	C	N	O	S	0	12	0
			3467	2206	582	654	25			
1	C	440	Total	C	N	O	S	0	11	0
			3482	2208	585	664	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	3	14	0
			3447	2169	586	663	29			
2	D	424	Total	C	N	O	S	0	3	0
			3347	2101	570	648	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	6	0
			1047	646	189	207	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

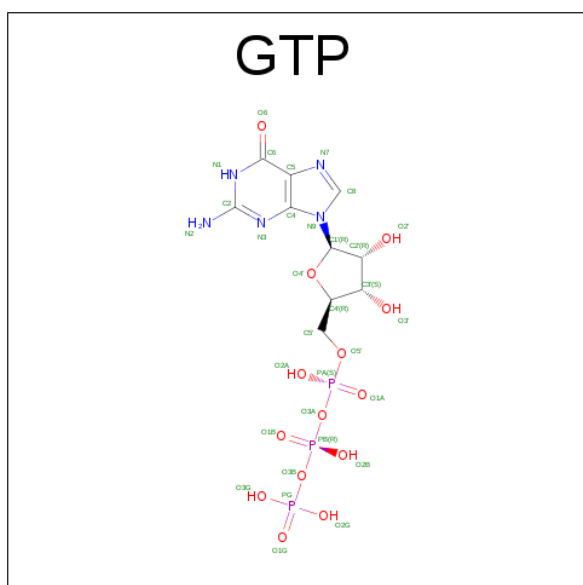
- Molecule 4 is a protein called TUBULIN-TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	0	3	0
			2725	1757	461	493	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: $C_{10}H_{16}N_5O_{14}P_3$).



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

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

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

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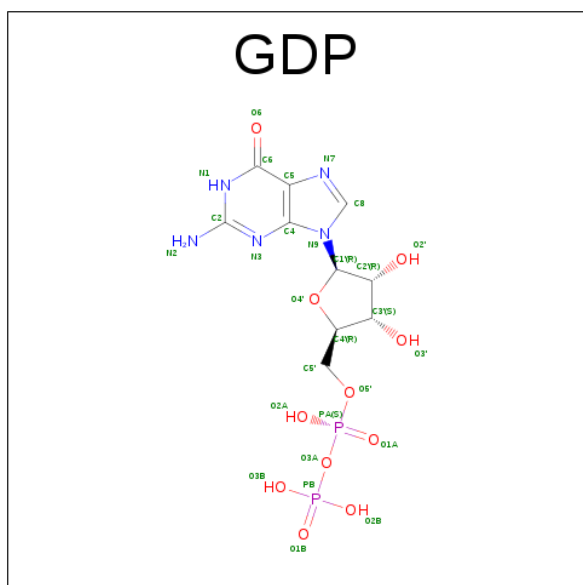
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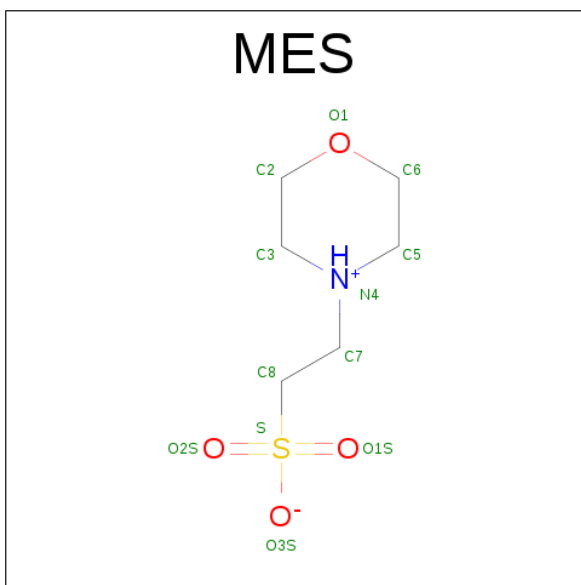
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

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

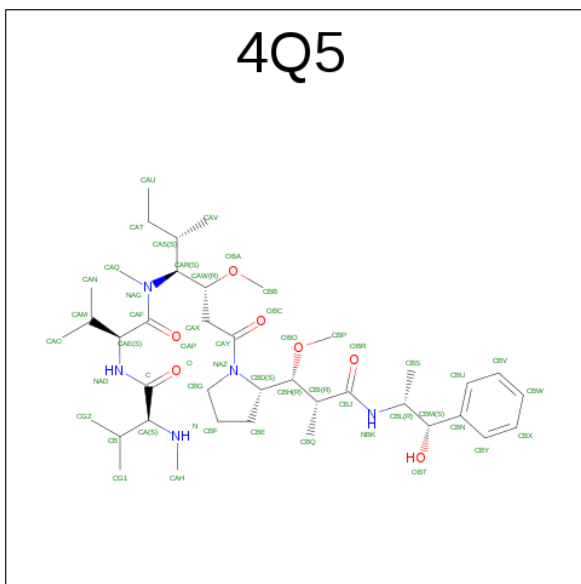
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





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

- Molecule 10 is N-methyl-L-valyl-N-[(3R,4S,5S)-1-{(2S)-2-[(1R,2R)-3-{[(1S,2R)-1-hydroxy-1-phenylpropan-2-yl]amino}-1-methoxy-2-methyl-3-oxopropyl]pyrrolidin-1-yl}-3-methoxy-5-methyl-1-oxoheptan-4-yl]-N-methyl-L-valinamide (three-letter code: 4Q5) (formula: C₃₉H₆₇N₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			51	39	5	7		

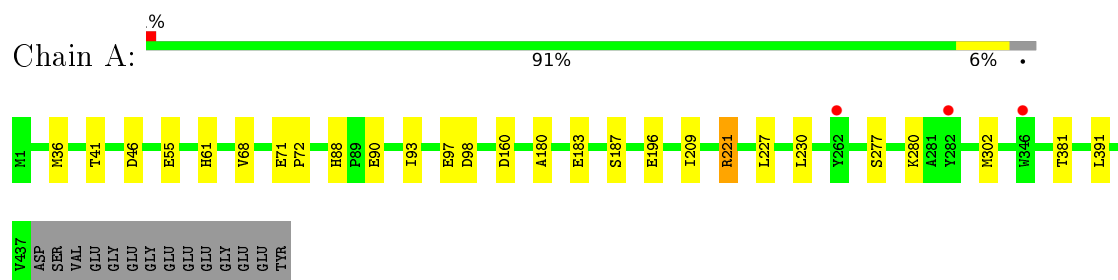
- # ACP
-
- The chemical structure of Adenosine 3'-phosphate (ACP) is shown. It consists of an adenosine moiety (adenine base and ribose sugar) linked to a triphosphate group. The structure is labeled with atom IDs in brackets.
- Atom IDs for the adenosine moiety:
- NH2: [N1], [N2]
 - N1: [N1]
 - N3: [N3]
 - N7: [N7]
 - C2: [C2]
 - C4: [C4]
 - C5: [C5]
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- Atom IDs for the triphosphate group:
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	259	Total O 259 259	0	0
12	B	314	Total O 314 314	0	0
12	C	434	Total O 434 434	0	0
12	D	178	Total O 178 178	0	0
12	E	67	Total O 67 67	0	0
12	F	101	Total O 101 101	0	0

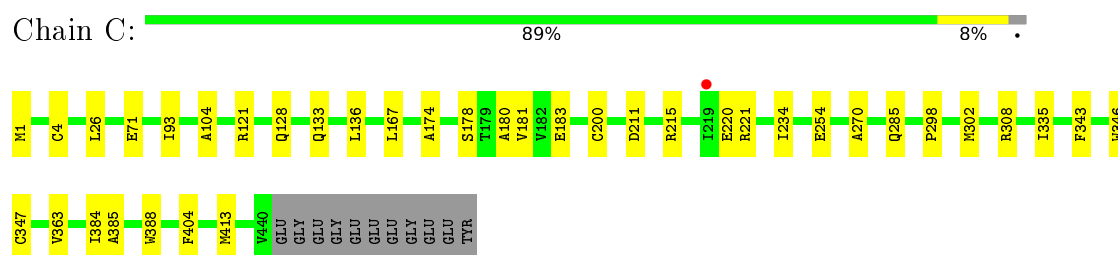
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

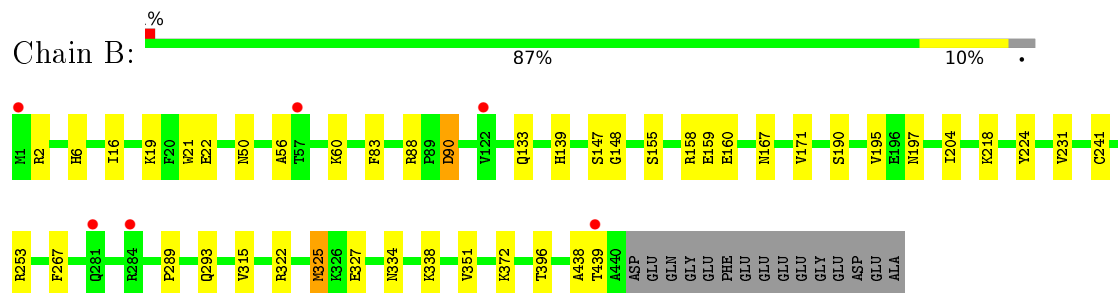
- Molecule 1: Tubulin alpha-1B chain



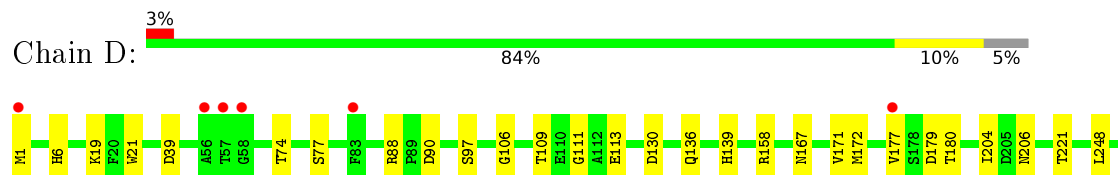
- Molecule 1: Tubulin alpha-1B chain

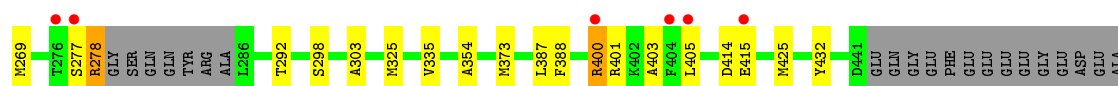


- Molecule 2: Tubulin beta-2B chain

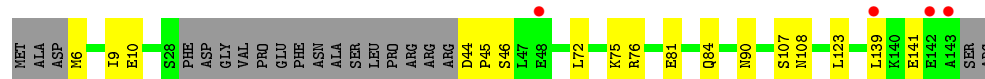
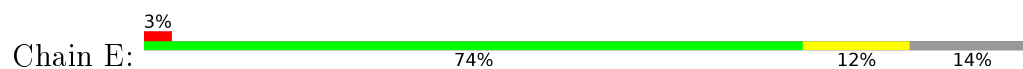


- Molecule 2: Tubulin beta-2B chain

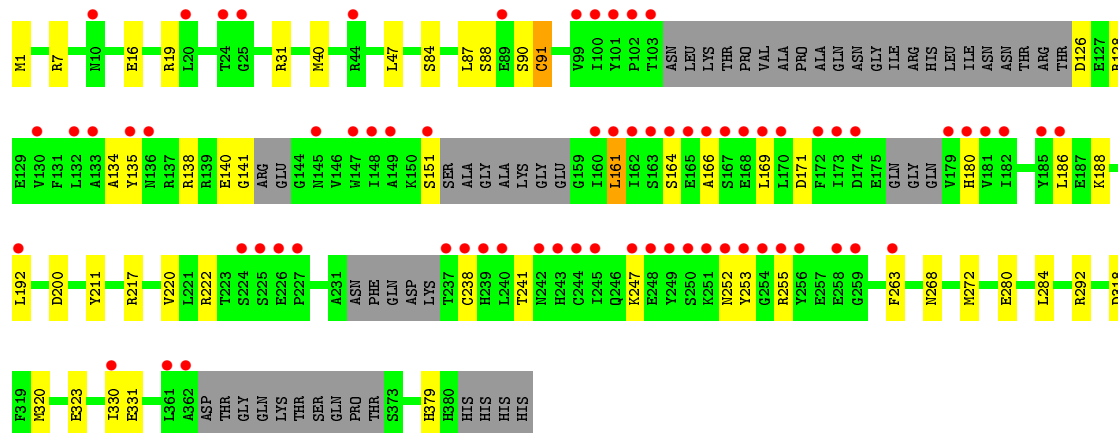
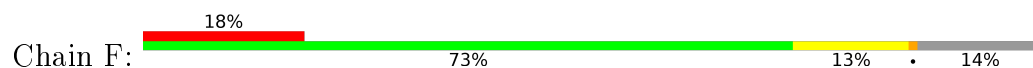




• Molecule 3: Stathmin-4



• 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	104.51Å 156.61Å 182.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.96 – 1.80 71.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (71.96-1.80) 99.9 (71.96-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.167 , 0.202 0.167 , 0.202	Depositor DCC
R_{free} test set	13776 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.5	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	0.97	EDS
Total number of atoms	19140	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, CA, GTP, 4Q5, 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	0.41	0/3582	0.54	0/4864
1	C	0.55	0/3590	0.60	0/4877
2	B	0.49	0/3559	0.55	0/4817
2	D	0.37	0/3426	0.50	0/4640
3	E	0.43	0/1071	0.46	0/1423
4	F	0.32	0/2794	0.49	0/3772
All	All	0.44	0/18022	0.54	0/24393

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	3467	0	3426	17	0
1	C	3482	0	3416	22	0
2	B	3447	0	3364	34	0
2	D	3347	0	3229	31	0
3	E	1047	0	1067	10	0
4	F	2725	0	2712	31	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	B	12	0	12	4	0
10	B	51	0	0	0	0
10	D	51	0	0	0	0
11	F	31	0	14	3	0
12	A	259	0	0	2	0
12	B	314	0	0	10	0
12	C	434	0	0	5	0
12	D	178	0	0	8	0
12	E	67	0	0	3	0
12	F	101	0	0	3	0
All	All	19140	0	17288	140	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 (140) 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:320:MET:HG2	4:F:330:ILE:HD11	1.60	0.83
1:C:128:GLN:NE2	12:C:601:HOH:O	2.11	0.83
4:F:40:MET:SD	12:F:595:HOH:O	2.40	0.78
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.05	0.74
3:E:6:MET:N	12:E:202:HOH:O	2.21	0.74
4:F:241:THR:OG1	11:F:402:ACP:O3'	2.07	0.71
4:F:217:ARG:NH1	12:F:501:HOH:O	2.22	0.70
4:F:272:MET:SD	12:F:542:HOH:O	2.48	0.70
4:F:252:ASN:HB3	4:F:255:ARG:HD3	1.74	0.69
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.75	0.68
2:B:438:ALA:O	12:B:601:HOH:O	2.11	0.67
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.78	0.65
1:A:88:HIS:CE1	1:A:90:GLU:HB2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.37	0.64
2:D:180:THR:OG1	12:D:601:HOH:O	2.14	0.64
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.80	0.64
2:B:88:ARG:NH1	12:B:609:HOH:O	2.30	0.64
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.38	0.63
3:E:108[B]:ASN:ND2	12:E:204:HOH:O	2.31	0.62
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.81	0.62
4:F:88:SER:OG	4:F:90:SER:O	2.19	0.61
1:A:97:GLU:OE2	2:B:2:ARG:NH1	2.33	0.60
2:D:432:TYR:OH	12:D:602:HOH:O	2.14	0.60
4:F:318:ASP:OD2	11:F:402:ACP:O3G	2.19	0.59
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.35	0.59
4:F:134:ALA:O	4:F:138:ARG:HG2	2.01	0.59
1:C:133:GLN:NE2	12:C:608:HOH:O	2.35	0.58
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.52	0.58
1:C:1:MET:O	12:C:602:HOH:O	2.18	0.57
2:B:241[B]:CYS:SG	12:B:779:HOH:O	2.57	0.57
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.87	0.55
3:E:90[B]:ASN:OD1	12:E:201:HOH:O	2.17	0.55
2:D:414:ASP:OD1	2:D:415:GLU:N	2.40	0.55
2:D:39:ASP:N	2:D:39:ASP:OD1	2.39	0.54
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.24	0.54
1:C:181[B]:VAL:HG12	12:D:615:HOH:O	2.07	0.54
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.43	0.53
2:D:278:ARG:HD2	2:D:278:ARG:H	1.72	0.53
1:A:68[B]:VAL:HG12	1:A:93:ILE:HB	1.90	0.53
1:C:180:ALA:O	1:C:183:GLU:HG3	2.09	0.53
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.90	0.52
4:F:126:ASP:OD1	4:F:128:ARG:HB2	2.09	0.52
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.90	0.52
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.92	0.51
2:B:327:GLU:OE2	12:B:604:HOH:O	2.19	0.51
2:D:278:ARG:CD	2:D:278:ARG:H	2.21	0.51
2:D:97:SER:OG	12:D:603:HOH:O	2.19	0.51
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.91	0.51
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.25	0.51
2:B:224:TYR:OH	12:B:602:HOH:O	2.18	0.51
2:D:167:ASN:ND2	12:D:613:HOH:O	2.42	0.51
2:B:159:GLU:OE1	12:B:603:HOH:O	2.19	0.51
1:A:88:HIS:ND1	1:A:90:GLU:OE1	2.44	0.51
4:F:40:MET:HE2	4:F:47:LEU:HG	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:ARG:HE	2:D:403:ALA:HB2	1.75	0.50
1:A:277:SER:HB3	1:A:280:LYS:HG3	1.92	0.50
2:B:197:ASN:HD21	3:E:75:LYS:NZ	2.09	0.50
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.30	0.49
2:B:155[B]:SER:OG	3:E:76:ARG:NH2	2.44	0.49
1:C:181[B]:VAL:HG11	1:C:404:PHE:CZ	2.48	0.49
1:C:211:ASP:O	1:C:215:ARG:HD2	2.11	0.49
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.94	0.49
2:D:373:MET:HE1	12:D:755:HOH:O	2.13	0.49
1:A:88:HIS:HE1	1:A:90:GLU:HB2	1.78	0.49
2:B:253[B]:ARG:NH1	9:B:503:MES:O3S	2.41	0.49
1:C:343:PHE:HD2	1:C:347[A]:CYS:SG	2.36	0.49
3:E:9:ILE:HG13	3:E:10:GLU:HG3	1.95	0.48
1:C:234:ILE:HG21	1:C:302:MET:SD	2.53	0.48
4:F:135:TYR:CZ	4:F:166:ALA:HB2	2.48	0.48
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.95	0.48
1:C:26:LEU:HD12	1:C:363[B]:VAL:HG12	1.96	0.48
4:F:151:SER:HG	4:F:180:HIS:CD2	2.32	0.47
2:B:50[B]:ASN:ND2	2:B:50[B]:ASN:H	2.13	0.47
4:F:161:LEU:HD23	4:F:169:LEU:HD23	1.96	0.47
4:F:247:LYS:HG3	4:F:253:TYR:CE2	2.49	0.47
4:F:140:GLU:HA	4:F:141:GLY:HA2	1.57	0.47
2:D:400:ARG:HG2	2:D:401:ARG:N	2.29	0.47
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.50	0.46
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.50	0.46
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.96	0.46
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.30	0.46
1:C:285:GLN:NE2	12:C:623:HOH:O	2.48	0.46
3:E:44:ASP:HB3	3:E:45:PRO:HD3	1.98	0.46
2:D:1:MET:HE2	12:D:776:HOH:O	2.15	0.45
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.34	0.45
2:D:106:GLY:O	2:D:111:GLY:HA3	2.17	0.45
2:B:2:ARG:HB3	2:B:133:GLN:HG2	1.98	0.45
2:B:289:PRO:O	2:B:293:GLN:HG2	2.17	0.45
1:A:180:ALA:O	1:A:183:GLU:HG3	2.17	0.45
2:D:171:VAL:HA	2:D:204:ILE:O	2.17	0.45
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE1	2.52	0.45
4:F:292:ARG:NH1	4:F:379:HIS:O	2.50	0.45
2:B:253[B]:ARG:NH2	9:B:503:MES:O2S	2.44	0.44
4:F:268:ASN:O	4:F:272:MET:HG3	2.17	0.44
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:503:MES:H51	9:B:503:MES:H82	1.59	0.44
1:C:174:ALA:O	1:C:178:SER:HB3	2.18	0.44
2:D:292:THR:HG22	2:D:335:VAL:HG21	2.00	0.44
2:B:218:LYS:NZ	12:B:624:HOH:O	2.51	0.43
2:D:109:THR:O	2:D:113:GLU:HG3	2.17	0.43
2:D:1:MET:HG3	2:D:130:ASP:OD2	2.18	0.43
2:D:388:PHE:HD1	2:D:425:MET:HE3	1.83	0.43
2:D:278:ARG:N	2:D:278:ARG:HD2	2.34	0.43
3:E:72:LEU:O	3:E:76:ARG:HG2	2.18	0.43
4:F:188:LYS:HD3	4:F:323:GLU:OE1	2.18	0.43
2:D:19:LYS:HA	2:D:19:LYS:HD3	1.86	0.43
4:F:151:SER:HG	4:F:180:HIS:CE1	2.31	0.43
1:A:196:GLU:OE1	12:A:601:HOH:O	2.21	0.43
4:F:186:LEU:HD13	4:F:320:MET:HE2	2.01	0.43
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.99	0.43
2:D:74:THR:O	2:D:77:SER:HB2	2.19	0.43
2:B:315:VAL:HB	2:B:351:VAL:HG22	2.00	0.43
1:C:254:GLU:OE1	12:C:603:HOH:O	2.22	0.43
4:F:84:SER:O	4:F:88:SER:N	2.51	0.43
4:F:87:LEU:O	4:F:91:CYS:HB2	2.19	0.42
4:F:200:ASP:OD1	4:F:222:ARG:NE	2.32	0.42
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.34	0.42
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.00	0.42
1:C:104:ALA:HB2	1:C:413:MET:SD	2.60	0.42
2:D:136:GLN:HA	2:D:167:ASN:O	2.19	0.42
2:B:158:ARG:CZ	9:B:503:MES:H21	2.49	0.42
2:B:167:ASN:ND2	12:B:628:HOH:O	2.52	0.41
2:B:334:ASN:HD21	2:B:338:LYS:NZ	2.17	0.41
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.55	0.41
1:A:209[A]:ILE:HG22	1:A:227:LEU:HD22	2.02	0.41
2:B:396:THR:HG23	12:B:631:HOH:O	2.20	0.41
2:B:438:ALA:C	2:B:439:THR:N	2.74	0.41
1:C:346:TRP:CZ3	1:C:347[B]:CYS:SG	3.14	0.41
1:C:270:ALA:HB3	1:C:302:MET:HE2	2.02	0.41
4:F:331:GLU:OE2	11:F:402:ACP:O2B	2.38	0.41
2:B:171:VAL:HA	2:B:204:ILE:O	2.21	0.41
2:B:160:GLU:HG3	12:B:758:HOH:O	2.20	0.41
2:B:195[B]:VAL:HG12	2:B:267:PHE:CE2	2.56	0.41
2:B:19:LYS:HA	2:B:19:LYS:HD3	1.94	0.41
2:D:74:THR:OG1	12:D:604:HOH:O	2.21	0.41
2:D:172:MET:HG3	2:D:387:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:HG3	2:B:325:MET:HB3	2.02	0.40
2:B:147[B]:SER:OG	2:B:148:GLY:N	2.55	0.40
3:E:81:GLU:HA	3:E:84[B]:GLN:HG2	2.03	0.40
1:A:160:ASP:OD2	12:A:602:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/451 (99%)	439 (98%)	8 (2%)	0	100	100
1	C	449/451 (100%)	437 (97%)	12 (3%)	0	100	100
2	B	440/445 (99%)	435 (99%)	5 (1%)	0	100	100
2	D	423/445 (95%)	417 (99%)	6 (1%)	0	100	100
3	E	125/143 (87%)	125 (100%)	0	0	100	100
4	F	320/384 (83%)	314 (98%)	6 (2%)	0	100	100
All	All	2204/2319 (95%)	2167 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/379 (100%)	375 (99%)	5 (1%)	76	68
1	C	382/379 (101%)	378 (99%)	4 (1%)	82	77
2	B	385/383 (100%)	380 (99%)	5 (1%)	76	68
2	D	370/383 (97%)	362 (98%)	8 (2%)	60	45
3	E	116/127 (91%)	112 (97%)	4 (3%)	44	26
4	F	301/342 (88%)	292 (97%)	9 (3%)	48	31
All	All	1934/1993 (97%)	1899 (98%)	35 (2%)	65	54

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	46	ASP
1	A	55	GLU
1	A	221	ARG
1	A	381	THR
2	B	90	ASP
2	B	139	HIS
2	B	322	ARG
2	B	325	MET
2	B	372	LYS
1	C	71	GLU
1	C	220	GLU
1	C	335	ILE
1	C	384	ILE
2	D	139	HIS
2	D	179	ASP
2	D	221	THR
2	D	277	SER
2	D	278	ARG
2	D	298	SER
2	D	400	ARG
2	D	405	LEU
3	E	46	SER
3	E	107	SER
3	E	139	LEU
3	E	141	GLU
4	F	1	MET
4	F	31	ARG
4	F	91	CYS
4	F	161	LEU

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Mol	Chain	Res	Type
4	F	164	SER
4	F	171	ASP
4	F	192	LEU
4	F	211	TYR
4	F	238	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	334	ASN

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 15 ligands modelled in this entry, 7 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	26,34,34	1.14	2 (7%)	29,54,54	2.06	6 (20%)
8	GDP	B	501	6	24,30,30	1.20	2 (8%)	26,47,47	2.13	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MES	B	503	-	12,12,12	2.19	1 (8%)	15,16,16	2.75	8 (53%)
10	4Q5	B	504	-	52,52,52	1.43	5 (9%)	54,72,72	1.64	9 (16%)
5	GTP	C	501	6	26,34,34	1.08	2 (7%)	29,54,54	1.85	7 (24%)
8	GDP	D	501	6	24,30,30	1.04	2 (8%)	26,47,47	2.06	6 (23%)
10	4Q5	D	503	-	52,52,52	1.25	2 (3%)	54,72,72	1.79	9 (16%)
11	ACP	F	402	6	29,33,33	1.47	5 (17%)	29,52,52	1.56	2 (6%)

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	GDP	B	501	6	-	0/12/32/32	0/3/3/3
9	MES	B	503	-	-	0/6/14/14	0/1/1/1
10	4Q5	B	504	-	-	0/76/86/86	0/2/2/2
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
8	GDP	D	501	6	-	0/12/32/32	0/3/3/3
10	4Q5	D	503	-	-	0/76/86/86	0/2/2/2
11	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)
10	D	503	4Q5	CBN-CBM	-7.73	1.40	1.51
9	B	503	MES	C8-S	-7.29	1.66	1.77
10	B	504	4Q5	CBN-CBM	-6.18	1.42	1.51
10	B	504	4Q5	OBA-CAW	2.04	1.49	1.43
10	B	504	4Q5	OBO-CBH	2.05	1.48	1.42
10	B	504	4Q5	CBF-CBG	2.07	1.59	1.51
5	C	501	GTP	C5-C4	2.11	1.45	1.40
11	F	402	ACP	PG-C3B	2.37	1.82	1.80
10	D	503	4Q5	CBE-CBD	2.39	1.58	1.53
8	D	501	GDP	C5-C4	2.66	1.46	1.40
5	A	501	GTP	C5-C4	2.71	1.46	1.40
11	F	402	ACP	PG-O2G	2.82	1.61	1.54
8	B	501	GDP	C6-C5	2.94	1.47	1.41
11	F	402	ACP	PB-O3A	2.94	1.61	1.58
8	D	501	GDP	C6-C5	3.01	1.47	1.41
11	F	402	ACP	PG-O3G	3.03	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	C5-C4	3.05	1.47	1.40
5	C	501	GTP	C6-C5	3.22	1.47	1.41
5	A	501	GTP	C6-C5	3.32	1.48	1.41
8	B	501	GDP	O4'-C1'	3.47	1.46	1.41
10	B	504	4Q5	CBH-CBD	4.10	1.58	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	402	ACP	N3-C2-N1	-6.53	123.74	128.87
10	D	503	4Q5	CBF-CBE-CBD	-6.01	94.09	104.28
10	D	503	4Q5	CBG-NAZ-CBD	-5.72	102.72	111.49
10	B	504	4Q5	CBE-CBF-CBG	-5.29	90.28	105.18
10	B	504	4Q5	CBG-NAZ-CBD	-5.23	103.48	111.49
10	D	503	4Q5	CBE-CBF-CBG	-4.85	91.52	105.18
5	A	501	GTP	C5-C6-N1	-4.70	117.37	123.52
8	D	501	GDP	C5-C6-N1	-4.50	117.64	123.52
8	B	501	GDP	N3-C2-N1	-4.13	121.93	127.56
5	C	501	GTP	N3-C2-N1	-4.07	122.02	127.56
8	B	501	GDP	C6-C5-C4	-4.01	116.27	120.86
5	A	501	GTP	N3-C2-N1	-3.81	122.38	127.56
5	C	501	GTP	C5-C6-N1	-3.78	118.58	123.52
8	B	501	GDP	C5-C6-N1	-3.75	118.62	123.52
8	D	501	GDP	N3-C2-N1	-3.71	122.51	127.56
8	B	501	GDP	C1'-N9-C4	-3.67	122.71	126.81
10	B	504	4Q5	CBF-CBE-CBD	-3.61	98.16	104.28
8	D	501	GDP	C6-C5-C4	-3.54	116.81	120.86
5	C	501	GTP	C6-C5-C4	-3.49	116.87	120.86
5	A	501	GTP	C6-C5-C4	-3.39	116.98	120.86
10	B	504	4Q5	CBE-CBD-CBH	-3.33	109.06	113.78
8	D	501	GDP	C1'-N9-C4	-2.48	124.04	126.81
10	D	503	4Q5	OBC-CAY-CAX	-2.43	117.41	122.12
5	A	501	GTP	C1'-N9-C4	-2.32	124.22	126.81
10	B	504	4Q5	CBQ-CBI-CBH	-2.24	108.08	113.03
10	D	503	4Q5	CBQ-CBI-CBJ	-2.10	105.14	108.47
10	B	504	4Q5	CAV-CAS-CAT	-2.08	106.50	111.81
5	C	501	GTP	O3'-C3'-C4'	-2.06	104.86	111.01
10	B	504	4Q5	CAF-CAE-NAD	-2.04	103.02	107.89
10	D	503	4Q5	CAV-CAS-CAT	-2.04	106.61	111.81
8	B	501	GDP	C4'-O4'-C1'	-2.01	107.51	109.64
5	C	501	GTP	C1'-N9-C4	-2.01	124.57	126.81
10	B	504	4Q5	CBF-CBG-NAZ	-2.00	100.10	103.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	O1-C2-C3	2.04	116.54	111.83
8	B	501	GDP	N2-C2-N1	2.06	120.61	117.20
11	F	402	ACP	O2G-PG-C3B	2.09	111.09	106.13
9	B	503	MES	O2S-S-C8	2.19	108.42	106.87
8	D	501	GDP	O3B-PB-O1B	2.20	117.80	110.63
5	C	501	GTP	O3G-PG-O2G	2.29	115.87	107.44
9	B	503	MES	O3S-S-C8	2.46	110.11	104.99
10	D	503	4Q5	OBC-CAY-NAZ	2.69	125.67	121.55
9	B	503	MES	C7-N4-C3	2.89	117.54	111.25
9	B	503	MES	C2-C3-N4	3.07	114.81	110.11
9	B	503	MES	C7-N4-C5	3.14	118.08	111.25
10	D	503	4Q5	OBO-CBH-CBI	3.14	113.83	106.07
5	A	501	GTP	O3G-PG-O2G	3.81	121.44	107.44
10	B	504	4Q5	CBG-NAZ-CAY	3.94	136.08	125.45
10	D	503	4Q5	CBG-NAZ-CAY	4.87	138.58	125.45
9	B	503	MES	O1S-S-C8	5.02	110.42	106.87
5	C	501	GTP	C6-N1-C2	5.05	121.80	115.88
8	B	501	GDP	C6-N1-C2	5.63	122.47	115.88
8	D	501	GDP	C6-N1-C2	6.00	122.91	115.88
9	B	503	MES	C5-N4-C3	6.15	122.64	108.87
5	A	501	GTP	C6-N1-C2	6.39	123.37	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	MES	4	0
11	F	402	ACP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	438:ALA	C	439:THR	N	2.74

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	437/451 (96%)	-0.19	3 (0%)	89 87	32, 49, 83, 104	0
1	C	440/451 (97%)	-0.10	1 (0%)	95 93	26, 37, 61, 103	0
2	B	430/445 (96%)	-0.05	6 (1%)	78 74	27, 41, 79, 132	2 (0%)
2	D	424/445 (95%)	0.02	12 (2%)	56 51	33, 54, 86, 121	3 (0%)
3	E	123/143 (86%)	0.09	4 (3%)	50 44	34, 61, 96, 132	0
4	F	331/384 (86%)	0.83	70 (21%)	1 1	39, 69, 125, 156	0
All	All	2185/2319 (94%)	0.06	96 (4%)	38 32	26, 49, 95, 156	5 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	7.8
4	F	173	ILE	7.4
4	F	169	LEU	7.1
4	F	249	TYR	6.2
2	D	57	THR	6.0
4	F	251	LYS	5.3
4	F	170	LEU	5.3
4	F	244	CYS	5.2
4	F	245	ILE	5.1
4	F	151	SER	4.9
4	F	186	LEU	4.9
4	F	172	PHE	4.8
4	F	100	ILE	4.6
4	F	166	ALA	4.5
4	F	248	GLU	4.4
4	F	182	ILE	4.3
4	F	250	SER	4.2
2	D	277	SER	4.1
1	A	262	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
4	F	20	LEU	4.0
4	F	133	ALA	3.9
4	F	148	ILE	3.8
2	B	281	GLN	3.7
2	D	177	VAL	3.7
2	D	276	THR	3.7
4	F	253	TYR	3.6
4	F	165	GLU	3.6
2	B	439	THR	3.5
4	F	240	LEU	3.5
4	F	252	ASN	3.4
4	F	239	HIS	3.4
4	F	160	ILE	3.4
4	F	162	ILE	3.4
4	F	247	LYS	3.3
4	F	225	SER	3.3
2	D	56	ALA	3.3
4	F	167	SER	3.2
4	F	180	HIS	3.2
2	D	1	MET	3.2
2	D	405	LEU	3.1
4	F	259	GLY	3.1
4	F	101	TYR	3.1
4	F	256	TYR	3.1
2	B	1	MET	3.0
4	F	181	VAL	3.0
4	F	255	ARG	3.0
3	E	142	GLU	3.0
4	F	238	CYS	3.0
4	F	132	LEU	2.9
4	F	145	ASN	2.9
1	A	282	TYR	2.8
2	B	57	THR	2.8
4	F	227	PRO	2.8
4	F	163	SER	2.8
4	F	361	LEU	2.8
4	F	136	ASN	2.8
3	E	48	GLU	2.7
4	F	10	ASN	2.7
2	D	415	GLU	2.6
4	F	258	GLU	2.6
4	F	243	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	58	GLY	2.6
4	F	192	LEU	2.6
2	D	83	PHE	2.5
4	F	149	ALA	2.5
4	F	168	GLU	2.5
4	F	99	VAL	2.5
4	F	254	GLY	2.5
4	F	102	PRO	2.4
4	F	263	PHE	2.4
4	F	179	VAL	2.4
1	A	346	TRP	2.4
4	F	174	ASP	2.3
4	F	44	ARG	2.3
4	F	224	SER	2.3
4	F	103	THR	2.3
4	F	89	GLU	2.3
4	F	164	SER	2.3
2	D	400	ARG	2.3
4	F	226	GLU	2.3
4	F	237	THR	2.2
3	E	143	ALA	2.2
4	F	185	TYR	2.2
2	D	404	PHE	2.2
2	B	122	VAL	2.2
4	F	25	GLY	2.2
4	F	147	TRP	2.2
4	F	135	TYR	2.2
4	F	130	VAL	2.1
1	C	219	ILE	2.1
4	F	330	ILE	2.1
4	F	24	THR	2.1
3	E	139	LEU	2.1
4	F	362	ALA	2.1
2	B	284	ARG	2.1
4	F	242	ASN	2.1

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

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
7	CA	C	503	1/1	0.93	0.31	18.08	86,86,86,86	0
10	4Q5	D	503	51/51	0.81	0.35	4.80	73,106,125,133	0
9	MES	B	503	12/12	0.88	0.18	2.32	55,86,118,124	0
5	GTP	C	501	32/32	0.99	0.12	0.58	25,30,32,33	0
8	GDP	B	501	28/28	0.99	0.12	0.31	25,28,30,31	0
5	GTP	A	501	32/32	0.98	0.09	0.11	30,33,38,39	0
8	GDP	D	501	28/28	0.97	0.09	-0.00	42,47,57,60	0
10	4Q5	B	504	51/51	0.97	0.09	-0.21	26,32,39,42	0
11	ACP	F	402	31/31	0.91	0.12	-1.09	61,70,108,130	0
7	CA	A	503	1/1	0.93	0.05	-2.48	67,67,67,67	0
6	MG	D	502	1/1	0.81	0.12	-	64,64,64,64	0
6	MG	C	502	1/1	0.97	0.14	-	32,32,32,32	0
6	MG	B	502	1/1	0.81	0.12	-	63,63,63,63	0
6	MG	F	401	1/1	0.86	0.11	-	78,78,78,78	0
6	MG	A	502	1/1	0.96	0.15	-	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.