



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:57 pm GMT

PDB ID : 4F6R
Title : Tubulin:Stathmin-like domain complex
Authors : Gigant, B.; Mignot, I.; Knossow, M.
Deposited on : 2012-05-15
Resolution : 2.64 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 : trunk28620
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) : recalc28949

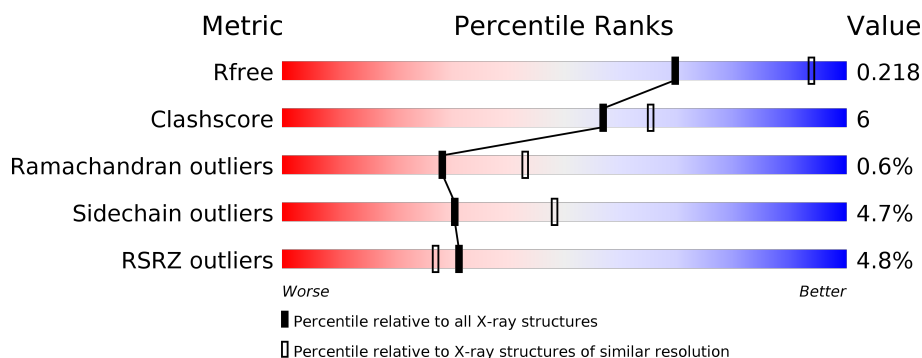
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	1044 (2.66-2.62)
Clashscore	112137	1092 (2.66-2.62)
Ramachandran outliers	110173	1077 (2.66-2.62)
Sidechain outliers	110143	1077 (2.66-2.62)
RSRZ outliers	101464	1047 (2.66-2.62)

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	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>••</div> </div> </div>
2	B	445	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>
3	C	87	<div> <div>9%</div> <div> <div></div> <div>62%</div> <div>11%</div> <div>26%</div> </div> </div>
4	D	169	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SO4	A	503	-	-	-	X
9	MES	B	502	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8626 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3396	2150	579	645	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
A	340	SER	THR	SEE REMARK 999	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	431	Total	C	N	O	S	0	0	0
			3378	2117	578	657	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
B	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	375	SER	ALA	SEE REMARK 999	UNP D0VWY9

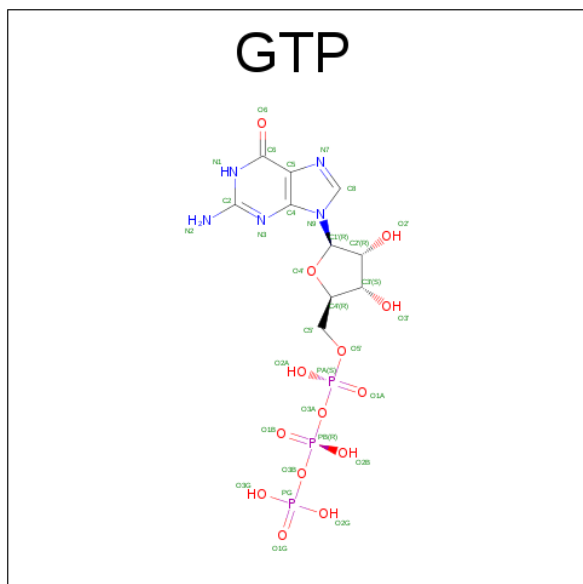
- Molecule 3 is a protein called Stathmin-like domain R1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	64	Total	C	N	O	S	0	0	0
			487	304	93	89	1			

- Molecule 4 is a protein called Designed ankyrin repeat protein (DARPIN) D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	159	Total	C	N	O	S	0	0	0
			1185	743	202	238	2			

- 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		

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

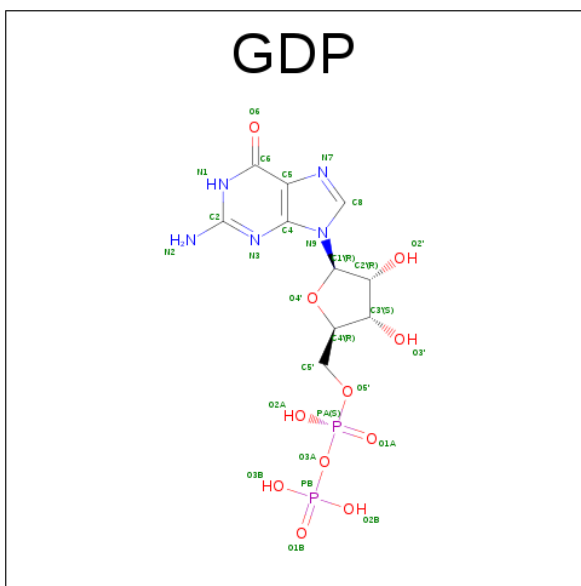
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg	0	0
			1 1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



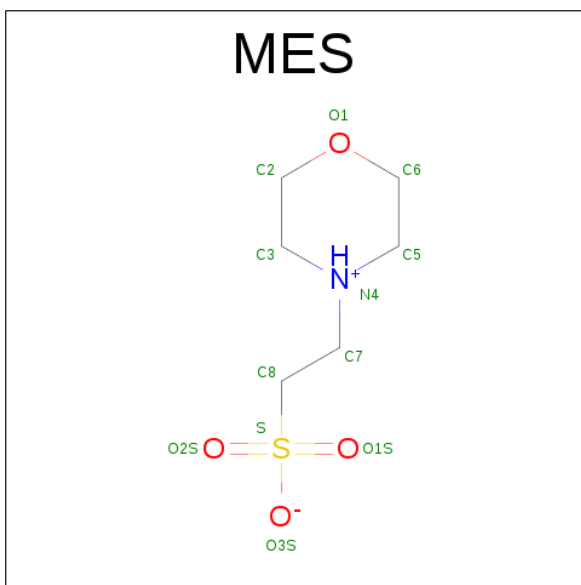
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	O	S		0	0
			5	4	1			

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



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

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

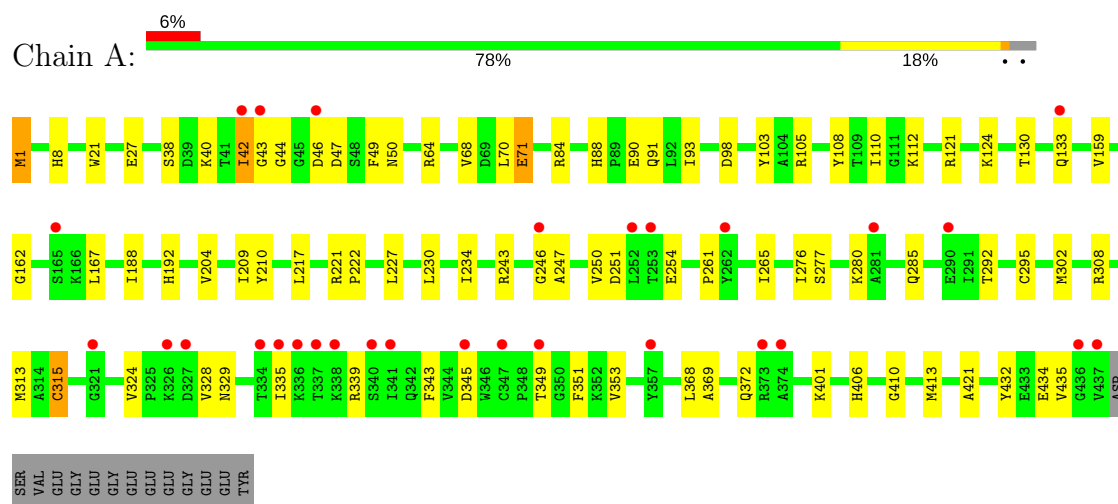
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	39	Total	O	0	0
			39	39		
10	B	43	Total	O	0	0
			43	43		
10	C	3	Total	O	0	0
			3	3		
10	D	17	Total	O	0	0
			17	17		

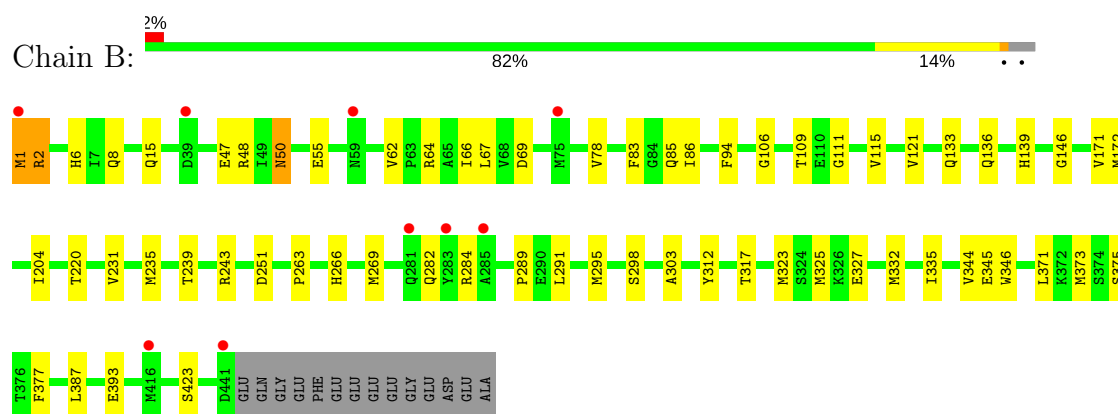
3 Residue-property plots [i](#)

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.

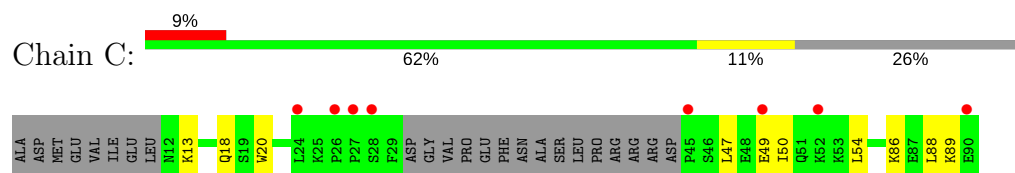
• Molecule 1: Tubulin alpha chain



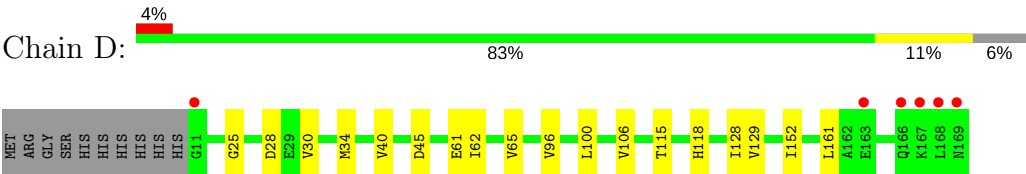
• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-like domain R1



• Molecule 4: Designed ankyrin repeat protein (DARPIN) D2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.06Å 75.57Å 155.68Å 90.00° 96.29° 90.00°	Depositor
Resolution (Å)	45.45 – 2.64 45.45 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.45-2.64) 98.3 (45.45-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.177 , 0.201 0.183 , 0.218	Depositor DCC
R_{free} test set	1614 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8626	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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, GTP, MG, SO4, 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	0.48	0/3472	0.73	0/4714
2	B	0.50	0/3452	0.72	0/4677
3	C	0.52	0/493	0.71	0/660
4	D	0.54	0/1200	0.74	0/1626
All	All	0.50	0/8617	0.72	0/11677

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	3396	0	3311	52	1
2	B	3378	0	3246	35	0
3	C	487	0	473	6	0
4	D	1185	0	1171	8	0
5	A	32	0	12	0	0
6	A	1	0	0	0	0
7	A	5	0	0	0	0
8	B	28	0	12	0	0
9	B	12	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	39	0	0	0	0
10	B	43	0	0	0	0
10	C	3	0	0	0	0
10	D	17	0	0	0	0
All	All	8626	0	8238	95	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (95) 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:329:ASN:HD21	3:C:20:TRP:HE1	1.33	0.75
1:A:47:ASP:HB2	1:A:49:PHE:CE2	2.24	0.73
2:B:1:MET:HG3	2:B:251:ASP:HB3	1.73	0.70
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.74	0.68
1:A:50:ASN:O	1:A:64:ARG:NH1	2.27	0.68
2:B:263:PRO:O	2:B:266:HIS:HD2	1.77	0.67
1:A:204:VAL:HG22	1:A:302:MET:CE	2.26	0.66
1:A:1:MET:N	1:A:130:THR:OG1	2.29	0.65
1:A:112:LYS:HE3	3:C:54:LEU:HB3	1.78	0.65
1:A:250:VAL:HG22	1:A:254:GLU:OE1	1.96	0.65
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.28	0.64
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.45	0.63
2:B:323:MET:HE2	2:B:373:MET:HG2	1.82	0.62
2:B:1:MET:HG3	2:B:251:ASP:CB	2.30	0.62
1:A:221:ARG:HG2	2:B:325:MET:HB3	1.81	0.61
1:A:410:GLY:HA3	9:B:502:MES:H32	1.80	0.61
1:A:88:HIS:HD2	1:A:90:GLU:H	1.48	0.61
2:B:323:MET:CE	2:B:373:MET:HG2	2.31	0.61
2:B:50:ASN:O	2:B:64:ARG:NH2	2.31	0.61
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.82	0.60
2:B:6:HIS:HE1	2:B:8:GLN:HG3	1.68	0.59
1:A:315:CYS:HG	1:A:351:PHE:HE2	1.51	0.58
1:A:88:HIS:HB3	1:A:91:GLN:HE21	1.67	0.58
1:A:204:VAL:HG22	1:A:302:MET:HE2	1.85	0.57
1:A:292:THR:HG22	1:A:335:ILE:HD12	1.87	0.57
1:A:108:TYR:CE1	1:A:413:MET:HE3	2.40	0.56
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.88	0.56
1:A:108:TYR:HE1	1:A:413:MET:HE3	1.71	0.56
1:A:276:ILE:HG13	1:A:369:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:CD2	1:A:90:GLU:H	2.22	0.56
4:D:115:THR:HG22	4:D:118:HIS:ND1	2.21	0.55
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.24	0.55
2:B:6:HIS:CE1	2:B:8:GLN:HG3	2.42	0.54
1:A:90:GLU:HB3	1:A:124:LYS:HE3	1.90	0.54
1:A:343:PHE:HB2	1:A:349:THR:HG22	1.90	0.53
1:A:47:ASP:HB2	1:A:49:PHE:HE2	1.71	0.53
2:B:106:GLY:O	2:B:111:GLY:HA3	2.08	0.53
2:B:317:THR:HG21	2:B:332:MET:CE	2.39	0.53
2:B:139:HIS:HD2	2:B:146:GLY:O	1.92	0.52
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.90	0.52
2:B:66:ILE:HG12	2:B:121:VAL:HG12	1.90	0.52
4:D:118:HIS:HD2	4:D:152:ILE:HD11	1.75	0.52
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.45	0.51
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.28	0.50
1:A:105:ARG:HG2	1:A:110:ILE:HD13	1.95	0.49
1:A:285:GLN:NE2	1:A:372:GLN:H	2.10	0.49
2:B:1:MET:HE3	2:B:48:ARG:HH21	1.77	0.49
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.12	0.49
2:B:1:MET:HE2	2:B:2:ARG:HA	1.94	0.49
2:B:332:MET:O	2:B:335:ILE:HG13	2.12	0.49
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.96	0.48
1:A:261:PRO:HG3	1:A:313:MET:HG3	1.95	0.48
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.95	0.48
2:B:317:THR:HG21	2:B:332:MET:HE2	1.96	0.48
1:A:406:HIS:HD2	9:B:502:MES:H61	1.78	0.48
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.96	0.48
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.61	0.48
1:A:234:ILE:HG21	1:A:302:MET:HE3	1.96	0.47
4:D:129:VAL:HG21	4:D:161:LEU:HD11	1.96	0.47
4:D:30:VAL:O	4:D:34:MET:HG2	2.15	0.47
1:A:70:LEU:HD22	1:A:110:ILE:HG22	1.95	0.47
1:A:103:TYR:HD2	1:A:413:MET:HE1	1.81	0.46
2:B:171:VAL:HA	2:B:204:ILE:O	2.15	0.46
1:A:108:TYR:HE1	1:A:413:MET:CE	2.28	0.46
4:D:25:GLY:HA2	4:D:62:ILE:HD12	1.96	0.46
1:A:234:ILE:CG2	1:A:302:MET:HE3	2.45	0.46
1:A:88:HIS:H	1:A:91:GLN:NE2	2.13	0.46
1:A:159:VAL:HG11	3:C:47:LEU:HB2	1.98	0.45
1:A:68:VAL:HG12	1:A:93:ILE:HB	1.98	0.45
2:B:295:MET:SD	2:B:375:SER:OG	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.37	0.44
4:D:25:GLY:HA2	4:D:62:ILE:CD1	2.48	0.44
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.53	0.43
1:A:292:THR:O	1:A:295:CYS:HB2	2.18	0.43
2:B:67:LEU:CD2	2:B:78:VAL:HG11	2.49	0.43
1:A:90:GLU:O	1:A:121:ARG:HG2	2.18	0.43
2:B:83:PHE:O	2:B:86:ILE:HG22	2.19	0.43
4:D:61:GLU:O	4:D:65:VAL:HG23	2.19	0.43
2:B:291:LEU:O	2:B:295:MET:HB2	2.19	0.42
1:A:285:GLN:HG3	1:A:372:GLN:HG3	2.00	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.55	0.42
2:B:295:MET:HE2	2:B:295:MET:HB3	1.92	0.42
2:B:69:ASP:O	2:B:94:PHE:HA	2.20	0.42
3:C:13:LYS:HG2	3:C:18:GLN:HG3	2.01	0.41
3:C:47:LEU:HA	3:C:50:ILE:HD12	2.02	0.41
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.56	0.41
4:D:96:VAL:HG11	4:D:128:ILE:HG23	2.01	0.41
1:A:88:HIS:CD2	1:A:90:GLU:HB2	2.55	0.41
1:A:43:GLY:HA3	1:A:44:GLY:HA3	1.71	0.41
2:B:289:PRO:HD3	2:B:327:GLU:OE1	2.21	0.41
2:B:109:THR:HG21	3:C:86:LYS:HD2	2.02	0.41
2:B:239:THR:O	2:B:243:ARG:HG2	2.21	0.41
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.38	0.41
2:B:231:VAL:HG12	2:B:235:MET:HE2	2.02	0.40
2:B:1:MET:HA	2:B:133:GLN:HG2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:OD2	1:A:251:ASP:OD2[2_656]	2.11	0.09

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	435/451 (96%)	415 (95%)	16 (4%)	4 (1%)	20	30
2	B	429/445 (96%)	418 (97%)	8 (2%)	3 (1%)	25	38
3	C	60/87 (69%)	59 (98%)	1 (2%)	0	100	100
4	D	157/169 (93%)	154 (98%)	3 (2%)	0	100	100
All	All	1081/1152 (94%)	1046 (97%)	28 (3%)	7 (1%)	28	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ILE
1	A	162	GLY
2	B	2	ARG
2	B	284	ARG
1	A	246	GLY
1	A	247	ALA
2	B	282	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	364/379 (96%)	346 (95%)	18 (5%)	29	46
2	B	371/385 (96%)	355 (96%)	16 (4%)	33	53
3	C	46/76 (60%)	43 (94%)	3 (6%)	20	32
4	D	121/131 (92%)	116 (96%)	5 (4%)	35	55
All	All	902/971 (93%)	860 (95%)	42 (5%)	30	48

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	38	SER
1	A	40	LYS
1	A	42	ILE
1	A	46	ASP
1	A	71	GLU
1	A	84	ARG
1	A	167	LEU
1	A	188	ILE
1	A	277	SER
1	A	280	LYS
1	A	308	ARG
1	A	315	CYS
1	A	324	VAL
1	A	339	ARG
1	A	345	ASP
1	A	434	GLU
1	A	435	VAL
2	B	1	MET
2	B	15	GLN
2	B	47	GLU
2	B	50	ASN
2	B	55	GLU
2	B	62	VAL
2	B	85	GLN
2	B	115	VAL
2	B	136	GLN
2	B	220	THR
2	B	298	SER
2	B	344	VAL
2	B	345	GLU
2	B	371	LEU
2	B	393	GLU
2	B	423	SER
3	C	49	GLU
3	C	88	LEU
3	C	89	LYS
4	D	28	ASP
4	D	40	VAL
4	D	45	ASP
4	D	100	LEU
4	D	106	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	15	GLN
1	A	61	HIS
1	A	88	HIS
1	A	91	GLN
1	A	139	HIS
1	A	197	HIS
1	A	249	ASN
1	A	258	ASN
1	A	285	GLN
1	A	301	GLN
1	A	329	ASN
1	A	356	ASN
1	A	406	HIS
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	37	HIS
2	B	101	ASN
2	B	136	GLN
2	B	139	HIS
2	B	247	GLN
2	B	266	HIS
2	B	300	ASN
2	B	385	GLN
3	C	78	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	1.08	2 (7%)	27,54,54	2.14	4 (14%)
7	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.10	0
8	GDP	B	501	-	25,30,30	1.03	2 (8%)	26,47,47	2.21	4 (15%)
9	MES	B	502	-	12,12,12	0.75	0	14,16,16	0.39	0

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
7	SO4	A	503	-	-	0/0/0/0	0/0/0/0
8	GDP	B	501	-	-	0/12/32/32	0/3/3/3
9	MES	B	502	-	-	0/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	C6-C5	2.79	1.46	1.41
8	B	501	GDP	C6-C5	2.79	1.46	1.41
8	B	501	GDP	C6-N1	3.02	1.38	1.33
5	A	501	GTP	C6-N1	3.24	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C5-C6-N1	-7.84	112.33	123.48
5	A	501	GTP	C5-C6-N1	-7.51	112.80	123.48
5	A	501	GTP	C6-C5-C4	-3.28	117.59	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C6-C5-C4	-2.97	117.89	120.84
5	A	501	GTP	N3-C2-N1	-2.80	123.37	127.46
8	B	501	GDP	N3-C2-N1	-2.68	123.54	127.46
5	A	501	GTP	C6-N1-C2	6.16	124.92	116.06
8	B	501	GDP	C6-N1-C2	6.32	125.15	116.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	502	MES	2	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	437/451 (96%)	0.38	29 (6%) 19 17	39, 60, 95, 124	6 (1%)
2	B	431/445 (96%)	0.05	9 (2%) 64 60	37, 53, 80, 126	4 (0%)
3	C	64/87 (73%)	0.55	8 (12%) 4 2	50, 70, 100, 133	0
4	D	159/169 (94%)	-0.08	6 (3%) 41 37	35, 51, 78, 130	0
All	All	1091/1152 (94%)	0.19	52 (4%) 31 27	35, 56, 90, 133	10 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	GLY	7.2
4	D	168	LEU	6.8
1	A	42	ILE	6.4
2	B	283	TYR	5.9
3	C	90	GLU	5.6
1	A	337	THR	5.5
2	B	281	GLN	4.7
4	D	169	ASN	4.6
2	B	1	MET	4.5
3	C	24	LEU	4.2
1	A	340	SER	4.1
1	A	321	GLY	3.8
1	A	338	LYS	3.8
4	D	166	GLN	3.8
3	C	27	PRO	3.7
1	A	281	ALA	3.7
1	A	341	ILE	3.6
1	A	345	ASP	3.5
1	A	46	ASP	3.5
1	A	165	SER	3.5
1	A	374	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	335	ILE	3.2
3	C	28	SER	3.2
1	A	349	THR	3.1
1	A	437	VAL	3.1
3	C	45	PRO	3.0
4	D	167	LYS	2.9
1	A	347	CYS	2.8
1	A	133	GLN	2.6
1	A	327	ASP	2.6
2	B	441	ASP	2.5
4	D	11	GLY	2.5
1	A	436	GLY	2.4
1	A	252	LEU	2.4
2	B	59	ASN	2.4
1	A	262	TYR	2.4
3	C	26	PRO	2.3
1	A	253	THR	2.3
1	A	246	GLY	2.3
1	A	336	LYS	2.3
1	A	290	GLU	2.2
1	A	334	THR	2.2
1	A	326	LYS	2.2
1	A	357	TYR	2.2
2	B	75	MET	2.2
3	C	52	LYS	2.1
2	B	285	ALA	2.1
2	B	39	ASP	2.1
1	A	373	ARG	2.1
4	D	163	GLU	2.1
2	B	416	MET	2.1
3	C	49	GLU	2.1

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	MES	B	502	12/12	0.90	0.28	3.78	129,135,136,136	0
7	SO4	A	503	5/5	0.79	0.34	2.39	126,126,127,128	0
8	GDP	B	501	28/28	0.98	0.17	-0.01	40,45,48,52	0
5	GTP	A	501	32/32	0.99	0.15	-0.70	39,46,51,57	0
6	MG	A	502	1/1	0.97	0.12	-2.44	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.