



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 7, 2016 – 02:13 PM EDT

PDB ID : 5FNV
Title : a new complex structure of tubulin with an alpha-beta unsaturated lactone
Authors : Wang, Y.; Naismith, J.; Zhu, X.
Deposited on : 2015-11-16
Resolution : 2.61 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-20027790
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-20027790

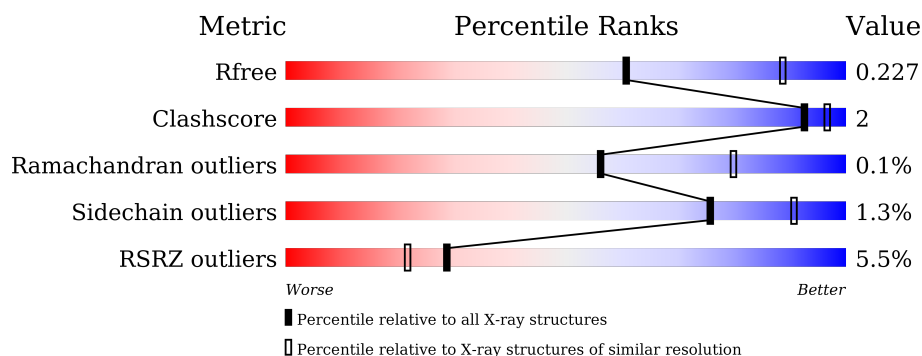
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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>4%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>5%</div> </div> </div>
1	C	451	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> </div>
2	B	445	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>6%</div> </div> </div>
2	D	445	<div> <div>8%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>6%</div> </div> </div>
3	E	143	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div></div> <div>17%</div> </div> </div>
4	F	384	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>6%</div> <div>20%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MES	B	1433	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17276 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	429	Total	C	N	O	S	0	3	0
			3373	2133	577	640	23			
1	C	439	Total	C	N	O	S	0	5	0
			3454	2184	585	662	23			

- Molecule 2 is a protein called TUBULIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	1	0
			3315	2086	567	637	25			
2	D	419	Total	C	N	O	S	0	1	0
			3288	2069	560	634	25			

- Molecule 3 is a protein called STATHMIN-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	119	Total	C	N	O	S	0	4	0
			1018	628	186	199	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	EXPRESSION TAG	UNP P63043
E	4	ALA	-	EXPRESSION TAG	UNP P63043

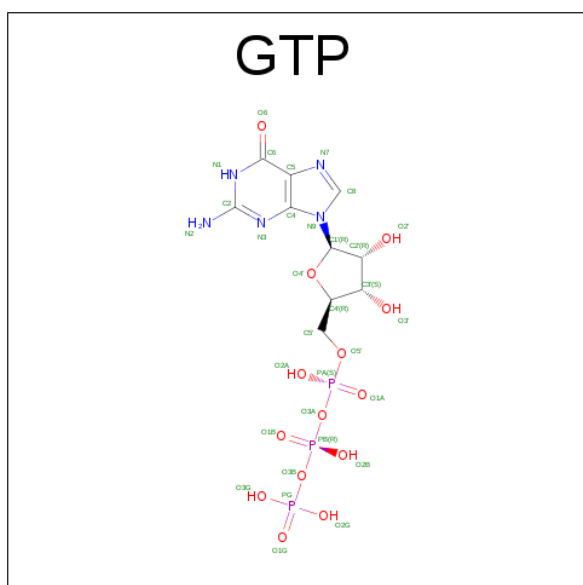
- Molecule 4 is a protein called TUBULIN TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	308	Total	C	N	O	S	0	2	0
			2551	1644	442	451	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		
5	D	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		

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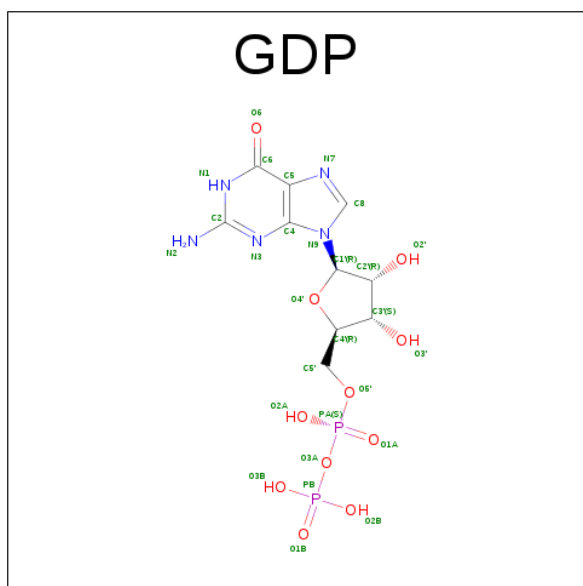
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		

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

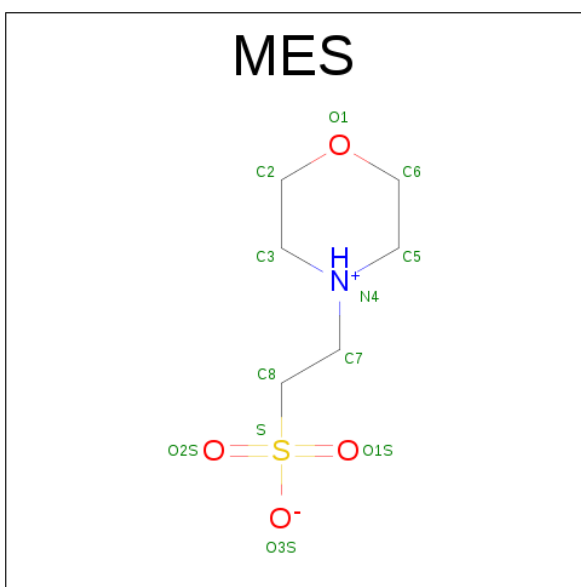
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



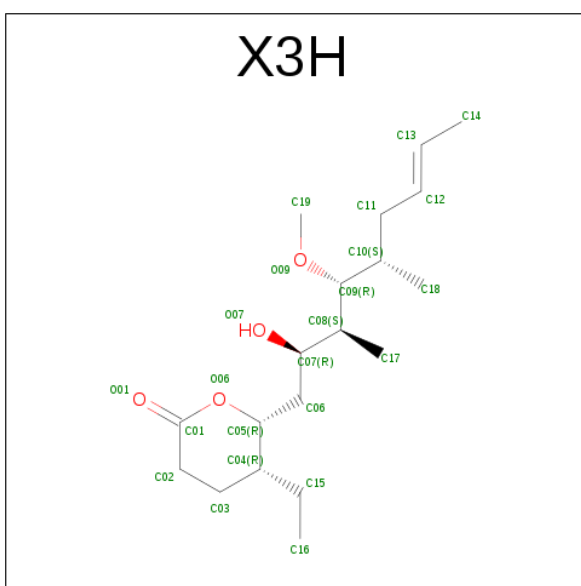
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0
			28	10	5	11	2	0

- 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		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

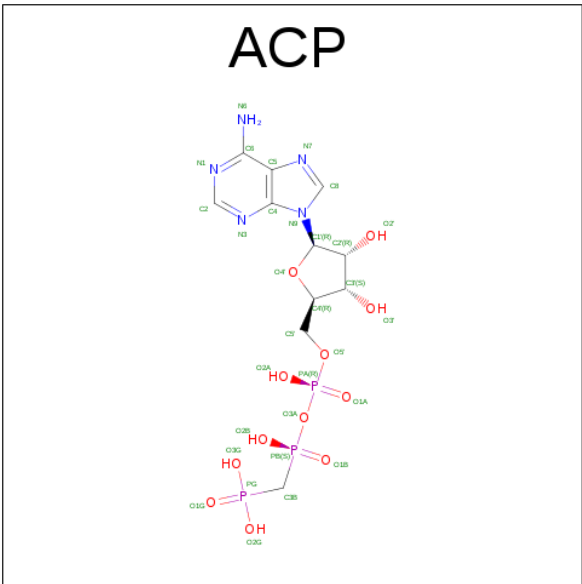
- Molecule 10 is PIRONETIN (three-letter code: X3H) (formula: $C_{19}H_{34}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			23	19	4		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-

letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

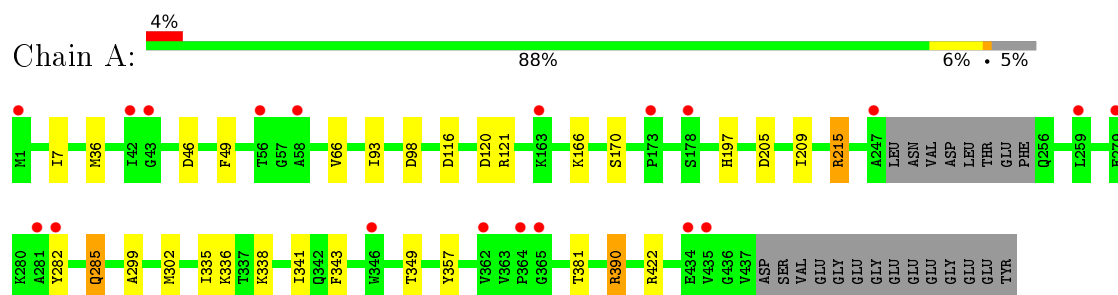
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	16	Total	O	0	0
			16	16		
12	B	16	Total	O	0	0
			16	16		
12	C	31	Total	O	0	0
			31	31		
12	D	3	Total	O	0	0
			3	3		
12	F	2	Total	O	0	0
			2	2		

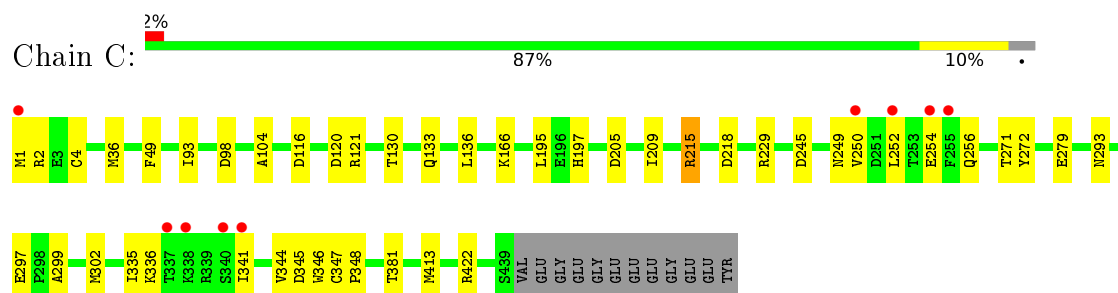
3 Residue-property plots

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.

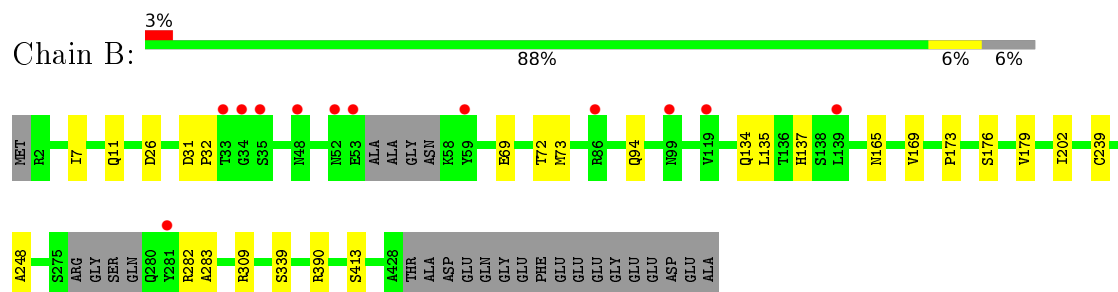
• Molecule 1: TUBULIN ALPHA-1B CHAIN



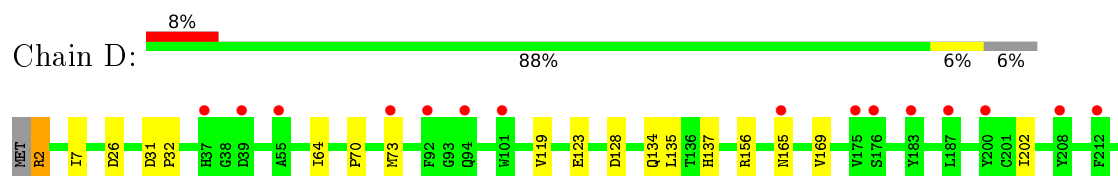
• Molecule 1: TUBULIN ALPHA-1B CHAIN

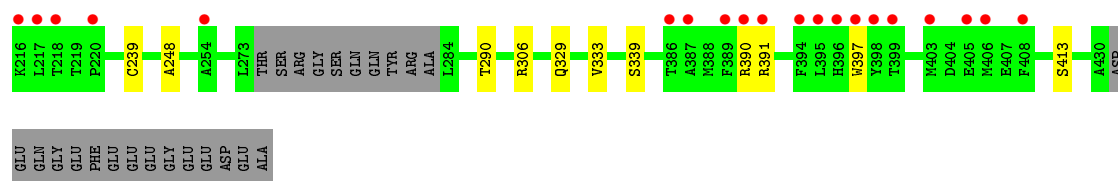


• Molecule 2: TUBULIN BETA CHAIN

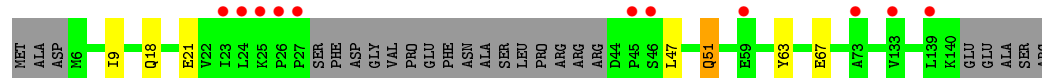
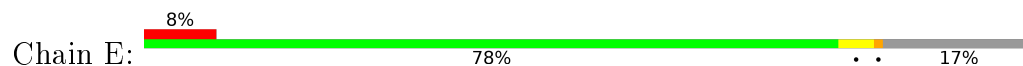


• Molecule 2: TUBULIN BETA CHAIN

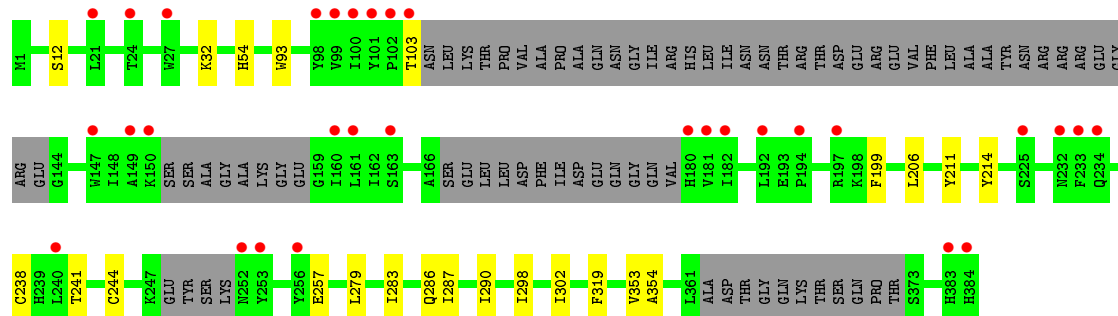
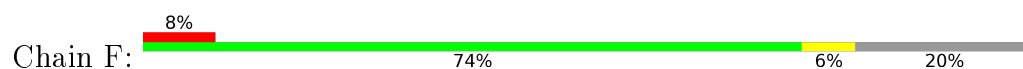




• Molecule 3: STATHMIN-4



• 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	106.16Å 157.20Å 181.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.88 – 2.61 45.49 – 2.61	Depositor EDS
% Data completeness (in resolution range)	94.6 (118.88-2.61) 94.7 (45.49-2.61)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.186 , 0.226 0.193 , 0.227	Depositor DCC
R_{free} test set	4397 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.6	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	0.95	EDS
Total number of atoms	17276	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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, MG, CA, GTP, ACP, MES, X3H

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	0.65	0/3452	0.84	7/4682 (0.1%)
1	C	0.72	0/3538	0.90	12/4803 (0.2%)
2	B	0.63	0/3388	0.79	1/4588 (0.0%)
2	D	0.59	0/3361	0.79	5/4555 (0.1%)
3	E	0.74	0/1030	0.82	0/1367
4	F	0.59	1/2614 (0.0%)	0.76	0/3531
All	All	0.65	1/17383 (0.0%)	0.82	25/23526 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	103	THR	C-O	6.44	1.35	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	C	245	ASP	CB-CG-OD2	-7.58	111.47	118.30
1	C	116	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	98	ASP	CB-CG-OD1	6.88	124.50	118.30
1	C	98	ASP	CB-CG-OD1	6.87	124.48	118.30
2	D	2	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	C	218	ASP	CB-CG-OD1	-6.50	112.45	118.30
1	A	116	ASP	CB-CG-OD1	6.15	123.83	118.30
1	C	205	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	C	422	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	205	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	345	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	215	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	C	120[A]	ASP	CB-CG-OD1	5.67	123.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	120[B]	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	215	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	422	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	205	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	390	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	B	73	MET	CA-CB-CG	-5.25	104.38	113.30
2	D	306	ARG	CB-CG-CD	5.20	125.12	111.60
2	D	156	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	170	SER	CB-CA-C	5.14	119.87	110.10
2	D	2	ARG	NE-CZ-NH2	-5.13	117.74	120.30
2	D	397	TRP	CA-CB-CG	5.03	123.25	113.70

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	3373	0	3288	12	0
1	C	3454	0	3357	23	0
2	B	3315	0	3196	13	0
2	D	3288	0	3169	14	0
3	E	1018	0	1031	4	0
4	F	2551	0	2524	9	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	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
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
9	B	24	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	23	0	0	0	0
11	F	31	0	14	0	0
12	A	16	0	0	0	0
12	B	16	0	0	0	0
12	C	31	0	0	0	0
12	D	3	0	0	0	0
12	F	2	0	0	0	0
All	All	17276	0	16653	69	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 2.

All (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:ILE:HD12	2:D:119:VAL:HG12	1.63	0.80
2:B:309:ARG:NH1	2:B:339:SER:O	2.24	0.70
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.38	0.64
2:B:69:GLU:OE2	1:C:250:VAL:N	2.37	0.57
2:D:64:ILE:HD11	2:D:123:GLU:HG3	1.86	0.57
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.40	0.57
1:C:133:GLN:CB	1:C:252:LEU:HD12	2.35	0.57
3:E:47:LEU:HD11	3:E:51:GLN:NE2	2.22	0.55
1:C:104:ALA:HB2	1:C:413:MET:SD	2.48	0.54
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.88	0.53
1:C:346:TRP:CZ3	1:C:347:CYS:SG	3.02	0.53
2:D:329:GLN:O	2:D:333:VAL:HG23	2.09	0.52
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.91	0.52
4:F:199:PHE:HA	4:F:241:THR:HG21	1.91	0.51
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.92	0.51
1:C:293:ASN:OD1	1:C:335:ILE:HD11	2.11	0.51
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.42	0.50
1:A:336:LYS:NZ	1:A:341:ILE:O	2.44	0.50
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.47	0.50
1:A:209:ILE:HD11	1:A:302:MET:SD	2.52	0.49
2:D:70:PRO:O	2:D:73:MET:HB3	2.12	0.49
1:C:209:ILE:HD11	1:C:302:MET:SD	2.52	0.49
1:A:390:ARG:HD3	4:F:54:HIS:CD2	2.48	0.48
1:A:36:MET:HE3	1:A:49:PHE:CE1	2.48	0.48
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.94	0.48
1:C:133:GLN:HB3	1:C:252:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:63:TYR:CZ	3:E:67:GLU:OE1	2.67	0.48
1:C:336:LYS:HA	1:C:341:ILE:HD11	1.95	0.47
1:C:36:MET:HE3	1:C:49:PHE:CE1	2.50	0.47
4:F:286:GLN:O	4:F:290:ILE:HG12	2.15	0.46
2:D:2:ARG:CZ	2:D:2:ARG:HB3	2.45	0.46
4:F:287:ILE:HD12	4:F:319:PHE:CD2	2.51	0.46
2:B:173:PRO:HA	2:B:176:SER:HB2	1.98	0.46
2:D:390:ARG:O	2:D:391:ARG:HG2	2.16	0.46
1:A:7:ILE:HG23	1:A:66:VAL:HG23	1.98	0.45
1:A:285:GLN:HE21	1:A:285:GLN:HA	1.81	0.45
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.99	0.45
1:C:2:ARG:HA	1:C:133:GLN:HG2	1.99	0.44
2:D:64:ILE:HD12	2:D:119:VAL:CG1	2.42	0.44
2:B:282:ARG:NH1	2:B:283:ALA:O	2.51	0.44
2:D:2:ARG:HE	2:D:128:ASP:HB3	1.83	0.44
1:A:215:ARG:NH2	1:A:299:ALA:O	2.51	0.44
1:C:133:GLN:HB2	1:C:252:LEU:HD12	1.99	0.43
2:B:94:GLN:O	1:C:250:VAL:HG11	2.17	0.43
1:C:271[B]:THR:OG1	1:C:272:TYR:N	2.51	0.43
1:C:215:ARG:NH2	1:C:299:ALA:O	2.51	0.43
1:C:166:LYS:HE2	1:C:197:HIS:O	2.19	0.43
2:D:134:GLN:HA	2:D:165:ASN:O	2.18	0.43
2:B:134:GLN:HA	2:B:165:ASN:O	2.18	0.43
2:B:169:VAL:HA	2:B:202:ILE:O	2.18	0.43
2:D:169:VAL:HA	2:D:202:ILE:O	2.19	0.43
1:A:166:LYS:HE2	1:A:197:HIS:O	2.19	0.42
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.49	0.42
2:B:11:GLN:HA	2:B:72:THR:HG21	2.01	0.42
2:B:69:GLU:OE2	1:C:249:ASN:HA	2.18	0.42
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.50	0.42
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.02	0.42
2:B:239:CYS:O	2:B:248:ALA:HA	2.21	0.41
1:C:1:MET:HB3	1:C:130:THR:OG1	2.20	0.41
1:C:279:GLU:N	1:C:279:GLU:OE1	2.48	0.41
4:F:93:TRP:CG	4:F:290:ILE:HD12	2.55	0.41
2:D:239:CYS:O	2:D:248:ALA:HA	2.20	0.41
3:E:9:ILE:HD11	3:E:21:GLU:OE1	2.20	0.41
4:F:214:TYR:CE2	4:F:353:VAL:CG1	3.04	0.41
2:B:7:ILE:O	2:B:135:LEU:HA	2.19	0.41
2:D:7:ILE:O	2:D:135:LEU:HA	2.21	0.41
1:A:335:ILE:HD13	1:A:335:ILE:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:LYS:HA	1:C:341:ILE:CD1	2.52	0.40
2:B:179:VAL:HG12	1:C:348:PRO:HG2	2.04	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	428/451 (95%)	416 (97%)	11 (3%)	1 (0%)	52	76
1	C	441/451 (98%)	425 (96%)	15 (3%)	1 (0%)	52	76
2	B	414/445 (93%)	403 (97%)	11 (3%)	0	100	100
2	D	415/445 (93%)	403 (97%)	12 (3%)	0	100	100
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	298/384 (78%)	280 (94%)	18 (6%)	0	100	100
All	All	2115/2319 (91%)	2044 (97%)	69 (3%)	2 (0%)	56	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	LYS
1	C	254	GLU

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	363/379 (96%)	358 (99%)	5 (1%)	74	90
1	C	374/379 (99%)	370 (99%)	4 (1%)	80	92
2	B	364/381 (96%)	360 (99%)	4 (1%)	80	92
2	D	360/381 (94%)	356 (99%)	4 (1%)	80	92
3	E	111/127 (87%)	110 (99%)	1 (1%)	84	94
4	F	281/342 (82%)	275 (98%)	6 (2%)	61	84
All	All	1853/1989 (93%)	1829 (99%)	24 (1%)	76	91

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	A	120	ASP
1	A	282	TYR
1	A	285	GLN
1	A	381	THR
2	B	26	ASP
2	B	137	HIS
2	B	390	ARG
2	B	413	SER
1	C	195	LEU
1	C	256	GLN
1	C	297	GLU
1	C	381	THR
2	D	26	ASP
2	D	137	HIS
2	D	339	SER
2	D	413	SER
3	E	51	GLN
4	F	12	SER
4	F	32	LYS
4	F	211	TYR
4	F	238	CYS
4	F	244	CYS
4	F	257	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	165	ASN

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Mol	Chain	Res	Type
2	D	94	GLN
2	D	165	ASN
2	D	195	ASN
3	E	51	GLN
4	F	252	ASN

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 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	1438	6	26,34,34	1.09	3 (11%)	29,54,54	2.13	5 (17%)
8	GDP	B	1429	6	24,30,30	1.27	3 (12%)	26,47,47	2.18	8 (30%)
9	MES	B	1432	-	12,12,12	2.18	1 (8%)	15,16,16	1.92	2 (13%)
9	MES	B	1433	-	12,12,12	2.20	1 (8%)	15,16,16	1.52	3 (20%)
5	GTP	C	1440	6	26,34,34	0.99	2 (7%)	29,54,54	2.14	7 (24%)
10	X3H	C	1443	1	23,23,23	1.38	2 (8%)	25,30,30	2.04	6 (24%)
5	GTP	D	1431	6	26,34,34	1.15	3 (11%)	29,54,54	2.11	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	ACP	F	1385	-	29,33,33	1.69	7 (24%)	29,52,52	1.72	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	1438	6	-	0/18/38/38	0/3/3/3
8	GDP	B	1429	6	-	0/12/32/32	0/3/3/3
9	MES	B	1432	-	-	0/6/14/14	0/1/1/1
9	MES	B	1433	-	-	0/6/14/14	0/1/1/1
5	GTP	C	1440	6	-	0/18/38/38	0/3/3/3
10	X3H	C	1443	1	-	0/24/37/37	0/1/1/1
5	GTP	D	1431	6	-	0/18/38/38	0/3/3/3
11	ACP	F	1385	-	-	0/15/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1433	MES	C8-S	-7.34	1.66	1.77
9	B	1432	MES	C8-S	-7.19	1.66	1.77
10	C	1443	X3H	O06-C05	-3.56	1.41	1.46
5	D	1431	GTP	C2'-C1'	-2.41	1.49	1.53
11	F	1385	ACP	PG-O3G	-2.40	1.49	1.54
8	B	1429	GDP	C2'-C1'	-2.26	1.50	1.53
5	A	1438	GTP	C2'-C1'	-2.01	1.50	1.53
11	F	1385	ACP	C2-N3	2.08	1.35	1.32
11	F	1385	ACP	PB-O3A	2.09	1.60	1.58
5	C	1440	GTP	C6-C5	2.12	1.45	1.41
11	F	1385	ACP	PB-O2B	2.40	1.62	1.56
11	F	1385	ACP	PG-O2G	2.75	1.61	1.54
5	A	1438	GTP	C5-C4	2.87	1.47	1.40
5	C	1440	GTP	C5-C4	3.09	1.47	1.40
8	B	1429	GDP	C5-C4	3.12	1.47	1.40
5	D	1431	GTP	C5-C4	3.12	1.47	1.40
11	F	1385	ACP	C5-C4	3.13	1.47	1.40
5	D	1431	GTP	C6-C5	3.15	1.47	1.41
5	A	1438	GTP	C6-C5	3.22	1.47	1.41
8	B	1429	GDP	C6-C5	3.23	1.47	1.41
10	C	1443	X3H	O06-C01	4.79	1.42	1.34
11	F	1385	ACP	PG-O1G	5.24	1.61	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	1385	ACP	N3-C2-N1	-7.00	123.37	128.87
5	C	1440	GTP	C5-C6-N1	-5.06	116.91	123.52
10	C	1443	X3H	C03-C02-C01	-5.00	104.45	116.32
5	A	1438	GTP	C5-C6-N1	-4.80	117.25	123.52
5	D	1431	GTP	C5-C6-N1	-4.79	117.27	123.52
8	B	1429	GDP	C5-C6-N1	-4.44	117.72	123.52
8	B	1429	GDP	C1'-N9-C4	-4.29	122.02	126.81
5	C	1440	GTP	N3-C2-N1	-4.07	122.02	127.56
8	B	1429	GDP	C6-C5-C4	-3.99	116.30	120.86
5	A	1438	GTP	C1'-N9-C4	-3.93	122.42	126.81
5	A	1438	GTP	C6-C5-C4	-3.89	116.41	120.86
5	A	1438	GTP	N3-C2-N1	-3.83	122.35	127.56
5	D	1431	GTP	N3-C2-N1	-3.75	122.45	127.56
10	C	1443	X3H	C03-C04-C05	-3.63	102.19	109.23
8	B	1429	GDP	N3-C2-N1	-3.31	123.05	127.56
5	D	1431	GTP	C6-C5-C4	-3.09	117.33	120.86
5	C	1440	GTP	C6-C5-C4	-3.06	117.36	120.86
5	C	1440	GTP	C1'-N9-C4	-2.56	123.95	126.81
5	D	1431	GTP	O4'-C1'-N9	-2.29	103.78	108.11
10	C	1443	X3H	C11-C12-C13	-2.12	119.47	127.02
8	B	1429	GDP	O4'-C1'-N9	-2.12	104.11	108.11
5	C	1440	GTP	O3'-C3'-C4'	-2.04	104.92	111.01
9	B	1433	MES	O2S-S-O1S	-2.03	108.21	113.96
11	F	1385	ACP	C2-N1-C6	2.01	122.36	118.77
9	B	1432	MES	O3S-S-C8	2.04	109.22	104.99
8	B	1429	GDP	C2'-C1'-N9	2.04	118.94	113.47
10	C	1443	X3H	O06-C05-C06	2.06	110.43	106.55
11	F	1385	ACP	N6-C6-N1	2.11	122.05	118.52
5	D	1431	GTP	C4'-O4'-C1'	2.25	112.03	109.64
8	B	1429	GDP	O3B-PB-O2B	2.28	115.80	107.44
5	C	1440	GTP	O3G-PG-O2G	2.38	116.17	107.44
9	B	1433	MES	O3S-S-C8	2.81	110.83	104.99
5	D	1431	GTP	O3G-PG-O2G	3.20	119.19	107.44
9	B	1433	MES	O2S-S-C8	3.74	109.51	106.87
10	C	1443	X3H	C02-C03-C04	4.11	120.23	111.59
10	C	1443	X3H	O06-C01-C02	4.28	127.55	119.22
9	B	1432	MES	O1S-S-C8	5.78	110.95	106.87
8	B	1429	GDP	C6-N1-C2	6.19	123.14	115.88
5	A	1438	GTP	C6-N1-C2	6.51	123.51	115.88
5	D	1431	GTP	C6-N1-C2	6.55	123.56	115.88
5	C	1440	GTP	C6-N1-C2	7.06	124.15	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	429/451 (95%)	0.11	19 (4%) 38 31	48, 76, 119, 147	0
1	C	439/451 (97%)	-0.10	9 (2%) 67 61	44, 62, 101, 128	0
2	B	419/445 (94%)	0.08	12 (2%) 55 48	50, 69, 103, 127	1 (0%)
2	D	419/445 (94%)	0.38	35 (8%) 14 9	56, 88, 126, 149	4 (0%)
3	E	119/143 (83%)	0.45	11 (9%) 11 7	55, 87, 125, 132	0
4	F	308/384 (80%)	0.36	31 (10%) 9 5	54, 91, 132, 162	0
All	All	2133/2319 (91%)	0.17	117 (5%) 29 22	44, 77, 120, 162	5 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	182	ILE	6.0
1	A	282	TYR	5.7
3	E	26	PRO	5.7
1	A	247	ALA	5.7
4	F	233	PHE	5.5
4	F	161	LEU	5.4
3	E	25	LYS	5.1
4	F	234	GLN	4.7
2	D	395	LEU	4.5
2	D	405	GLU	3.9
4	F	102	PRO	3.9
2	D	396	HIS	3.8
1	C	341	ILE	3.8
2	D	216	LYS	3.8
2	D	398	TYR	3.7
1	C	255	PHE	3.7
4	F	232	ASN	3.7
2	D	387	ALA	3.7
4	F	100	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
4	F	99	VAL	3.6
2	B	48	ASN	3.6
1	C	340	SER	3.6
4	F	98	TYR	3.6
2	D	217	LEU	3.5
2	D	37	HIS	3.5
2	D	39	ASP	3.5
4	F	21	LEU	3.4
4	F	192	LEU	3.3
4	F	225	SER	3.3
4	F	101	TYR	3.3
1	C	337	THR	3.3
4	F	194	PRO	3.2
1	A	43	GLY	3.2
4	F	147	TRP	3.1
2	D	390	ARG	3.1
4	F	149	ALA	3.1
2	D	389	PHE	3.1
2	D	391	ARG	3.1
1	C	1	MET	3.0
1	A	1	MET	3.0
4	F	383	HIS	3.0
1	A	42	ILE	2.9
2	D	165	ASN	2.9
2	D	183	TYR	2.9
4	F	253	TYR	2.9
4	F	197	ARG	2.9
3	E	139	LEU	2.9
2	B	34	GLY	2.8
1	C	252	LEU	2.8
2	B	59	TYR	2.8
2	D	394	PHE	2.7
3	E	23	ILE	2.7
1	A	346	TRP	2.7
2	D	187	LEU	2.7
2	D	408	PHE	2.7
3	E	27	PRO	2.7
1	A	434	GLU	2.7
2	B	281	TYR	2.7
3	E	73	ALA	2.6
3	E	24	LEU	2.6
2	D	55	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	256	TYR	2.6
4	F	27	TRP	2.6
1	A	163	LYS	2.6
1	A	259	LEU	2.6
4	F	160	ILE	2.6
2	D	73	MET	2.6
2	D	403	MET	2.6
1	C	338	LYS	2.6
3	E	45	PRO	2.6
2	D	220	PRO	2.5
2	D	176	SER	2.5
2	B	86	ARG	2.5
4	F	240	LEU	2.5
4	F	24	THR	2.5
4	F	181	VAL	2.4
4	F	103	THR	2.4
4	F	163	SER	2.4
1	C	250	VAL	2.4
3	E	46	SER	2.3
3	E	59	GLU	2.3
1	C	254	GLU	2.3
2	D	92	PHE	2.3
3	E	133	VAL	2.3
2	D	200	TYR	2.3
1	A	365	GLY	2.3
2	B	99	ASN	2.3
4	F	180	HIS	2.2
2	D	208	TYR	2.2
1	A	362	VAL	2.2
2	D	175	VAL	2.2
1	A	281	ALA	2.2
4	F	150	LYS	2.2
2	D	101	TRP	2.2
2	B	33	THR	2.2
2	D	386	THR	2.2
2	D	399	THR	2.2
4	F	252	ASN	2.2
2	D	212	PHE	2.2
2	B	119	VAL	2.1
2	D	397	TRP	2.1
2	B	53	GLU	2.1
4	F	384	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	178	SER	2.1
2	D	94	GLN	2.1
1	A	173	PRO	2.1
1	A	364	PRO	2.1
2	B	52	ASN	2.1
2	B	35	SER	2.0
2	D	254	ALA	2.0
1	A	56	THR	2.0
2	B	139	LEU	2.0
1	A	435	VAL	2.0
1	A	58	ALA	2.0
2	D	218	THR	2.0
2	D	406	MET	2.0
1	A	279	GLU	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	MES	B	1433	12/12	0.96	0.29	2.50	93,103,107,111	0
9	MES	B	1432	12/12	0.95	0.17	0.07	60,67,74,82	0
5	GTP	C	1440	32/32	0.99	0.18	-0.02	41,48,51,53	0
10	X3H	C	1443	23/23	0.96	0.21	-0.05	58,63,72,72	0
8	GDP	B	1429	28/28	0.98	0.21	-0.07	47,55,58,66	0
5	GTP	A	1438	32/32	0.99	0.23	-0.27	44,52,55,57	0
6	MG	A	1439	1/1	0.97	0.18	-0.72	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	ACP	F	1385	31/31	0.92	0.15	-0.85	86,94,121,132	0
6	MG	C	1441	1/1	0.97	0.16	-1.00	50,50,50,50	0
5	GTP	D	1431	32/32	0.95	0.12	-1.15	69,79,97,108	0
7	CA	C	1442	1/1	0.95	0.09	-1.27	83,83,83,83	0
7	CA	A	1440	1/1	0.93	0.06	-2.03	97,97,97,97	0
6	MG	B	1430	1/1	0.90	0.61	-	75,75,75,75	0
6	MG	D	1432	1/1	0.88	0.26	-	85,85,85,85	0
7	CA	B	1431	1/1	0.92	0.15	-	97,97,97,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.