



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2014 – 11:46 PM EDT

PDB ID : 4O2A  
Title : Tubulin-BAL27862 complex  
Authors : Prota, A.E.; Franck, D.; Bachmann, F.; Bargsten, K.; Buey, R.M.; Pohlmann, J.; Reinelt, S.; Lane, H.; Steinmetz, M.O.  
Deposited on : 2013-12-17  
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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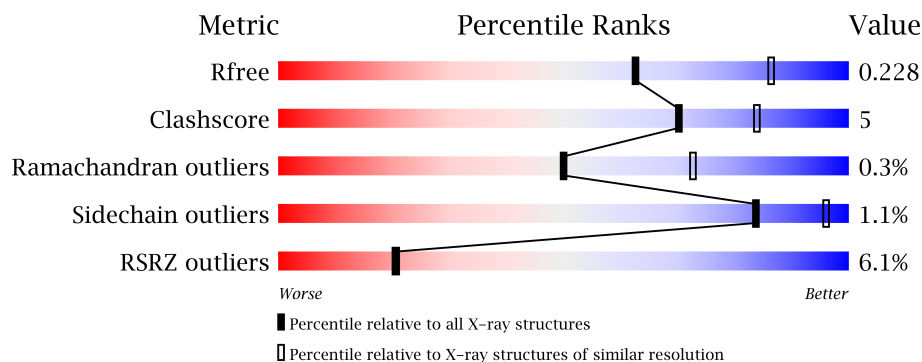
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : **FAILED**  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	IMD	A	506	-	X
12	2RR	D	604	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
14	ADP	F	401	-	X
6	MG	B	502	-	X
7	CA	B	503	-	X
9	GOL	A	505	-	X

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 18043 atoms, of which 0 are hydrogen and 0 are deuterium.

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	439	Total	C	N	O	S	0	12	0
			3487	2214	587	662	24			
1	C	440	Total	C	N	O	S	0	15	0
			3504	2224	587	667	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	418	Total	C	N	O	S	0	16	0
			3371	2127	566	650	28			
2	D	421	Total	C	N	O	S	0	4	0
			3324	2091	562	643	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	5	0
			1045	646	188	205	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	CLONING ARTIFACT	UNP P63043
E	4	ALA	-	CLONING ARTIFACT	UNP P63043

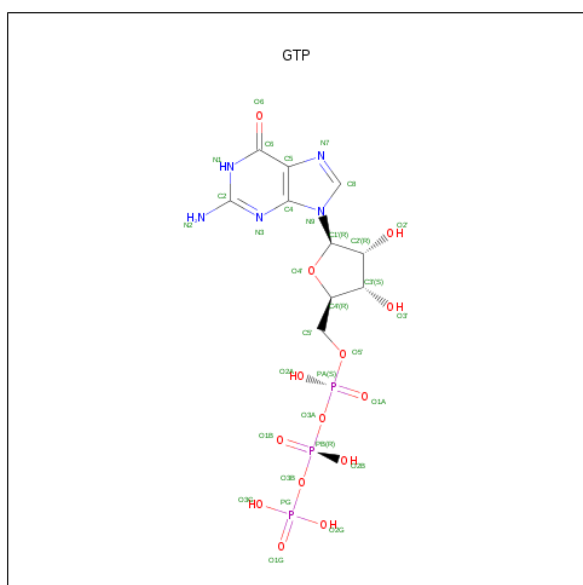
- Molecule 4 is a protein called TUBULIN-TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	0	4	0
			2740	1766	465	495	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	2	Total	Mg	0	0
			2	2		
6	A	1	Total	Mg	0	0
			1	1		
6	D	2	Total	Mg	0	0
			2	2		

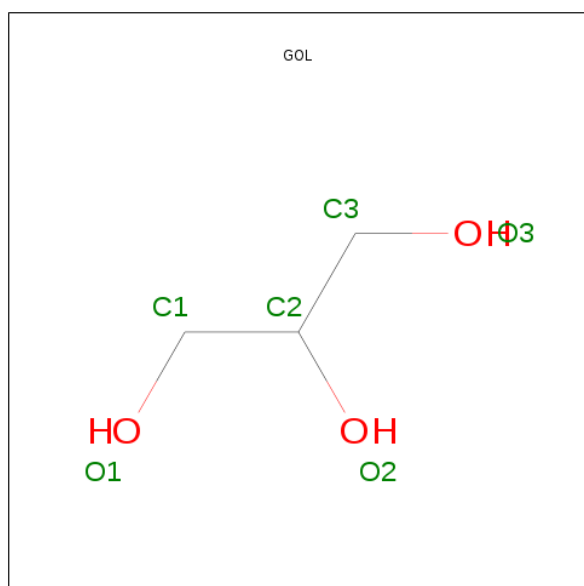
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

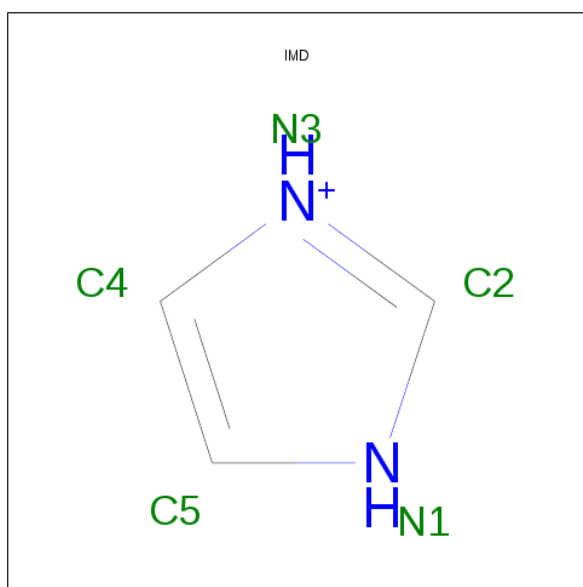
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



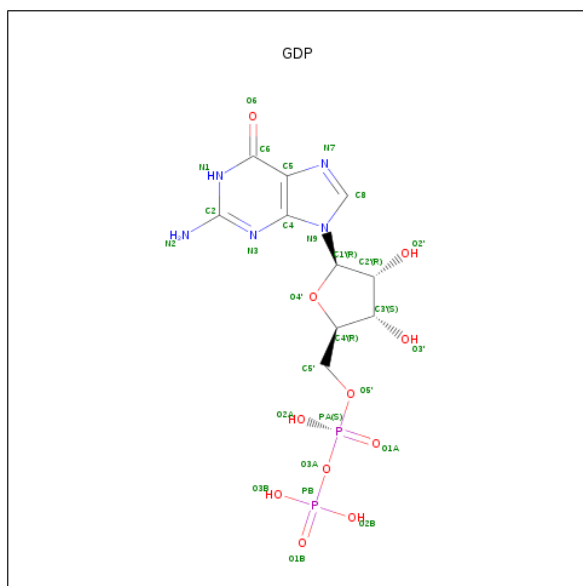
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0

- Molecule 10 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



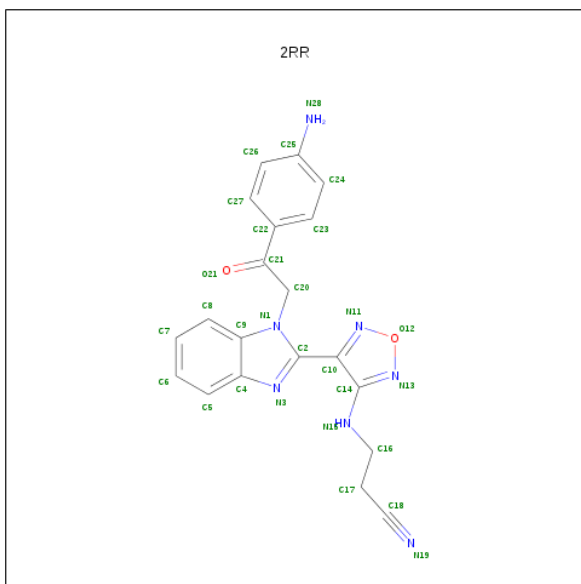
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	N	0	0
			5	3	2		

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



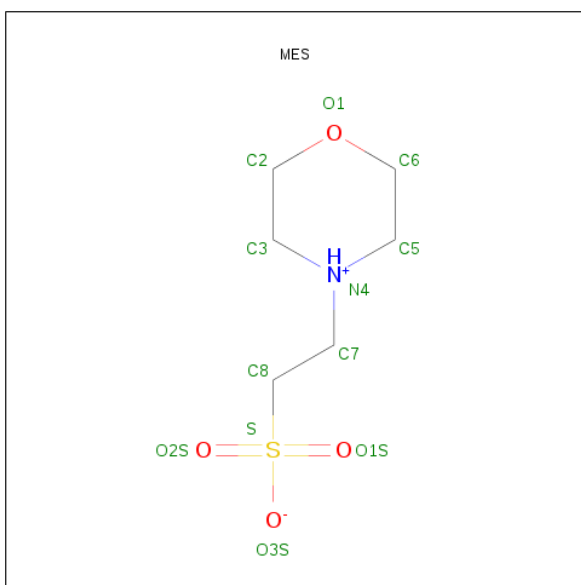
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
11	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 12 is 3-[(4-{1-[2-(4-AMINOPHENYL)-2-OXOETHYL]-1H-BENZIMIDAZOL-2-YL}-1,2,5-OXADIAZOL-3-YL)AMINO]PROPANENITRILE (three-letter code: 2RR) (formula:  $C_{20}H_{17}N_7O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			29	20	7	2		
12	D	1	Total	C	N	O	0	0
			29	20	7	2		

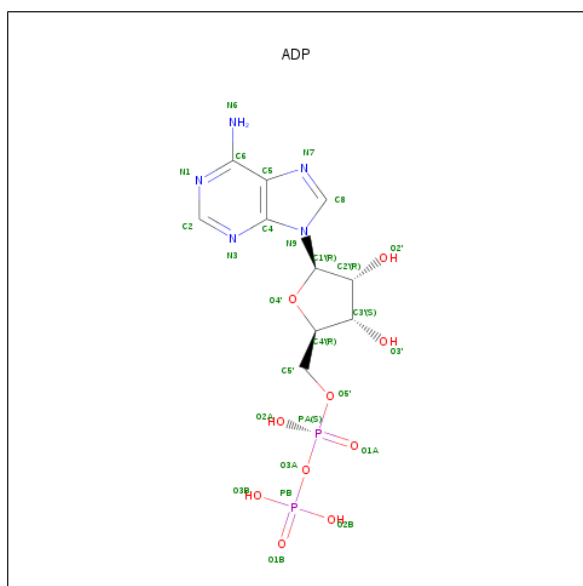
- Molecule 13 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).





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

- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 15 is water.

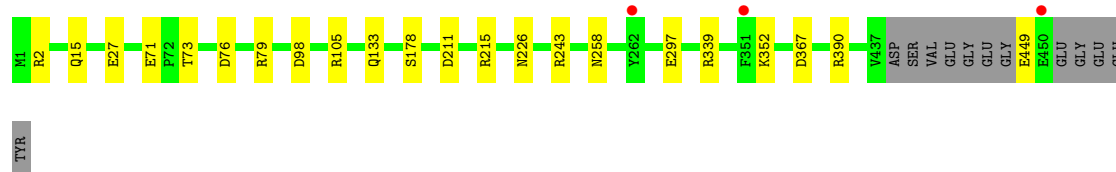
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	63	Total	O	0	0
			63	63		
15	B	70	Total	O	0	0
			70	70		
15	C	144	Total	O	0	0
			144	144		
15	D	26	Total	O	0	0
			26	26		
15	E	13	Total	O	0	0
			13	13		
15	F	18	Total	O	0	0
			18	18		

### 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.

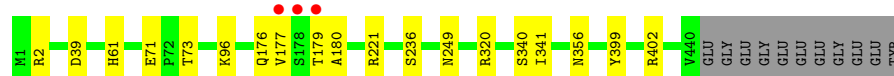
- Molecule 1: Tubulin alpha-1B chain

Chain A: 



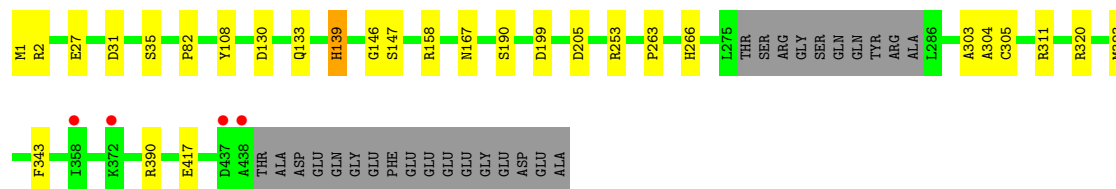
- Molecule 1: Tubulin alpha-1B chain

Chain C: 



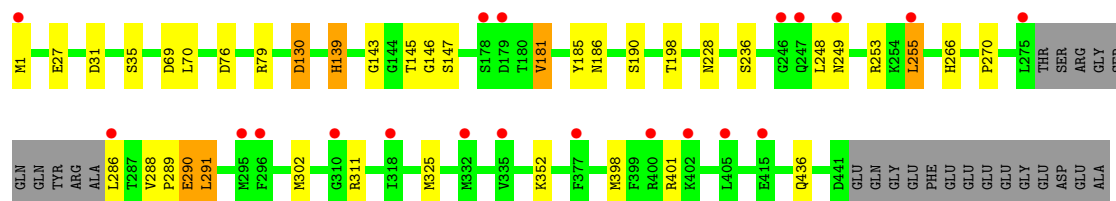
- Molecule 2: Tubulin beta-2B chain

Chain B: 



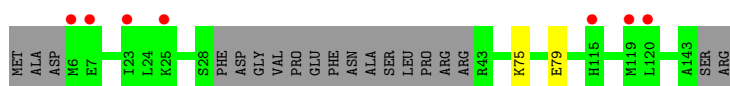
- Molecule 2: Tubulin beta-2B chain

Chain D: 



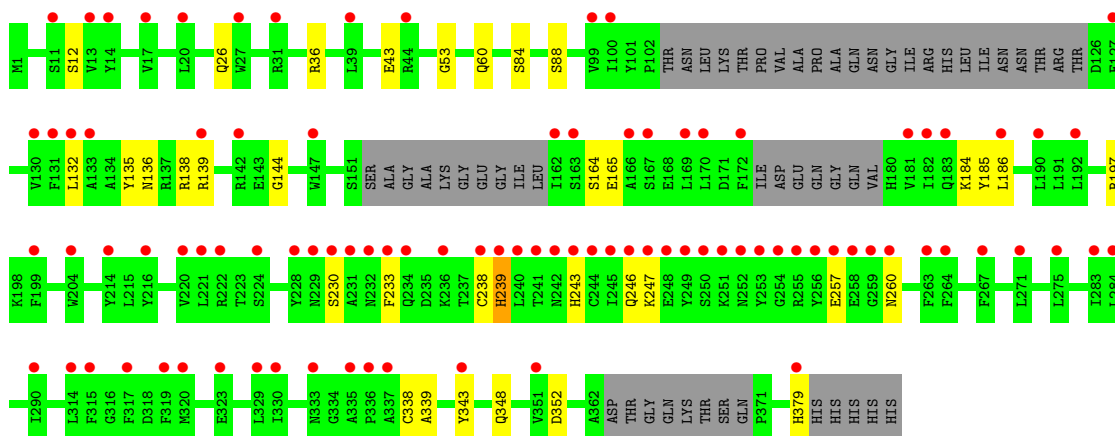
- Molecule 3: Stathmin-4

Chain E: 



• Molecule 4: TUBULIN-TYROSINE LIGASE

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.53Å 158.12Å 179.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.36 – 2.50 78.45 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (59.36-2.50) 99.7 (78.45-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, $R_{free}$	0.194 , 0.232 0.191 , 0.228	Depositor DCC
$R_{free}$ test set	5149 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 29.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 103225 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18043	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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, IMD, ADP, CL, CA, GTP, MES, 2RR

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	0.21	0/3600	0.38	0/4886
1	C	0.23	0/3628	0.40	0/4926
2	B	0.22	0/3489	0.38	0/4724
2	D	0.22	0/3409	0.42	2/4619 (0.0%)
3	E	0.20	0/1069	0.31	0/1419
4	F	0.22	0/2815	0.37	0/3801
All	All	0.22	0/18010	0.39	2/24375 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	289	PRO	C-N-CA	5.32	135.00	121.70
2	D	289	PRO	CA-C-N	5.01	128.22	117.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3487	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3504	0	0	10	0
2	B	3371	0	0	16	0
2	D	3324	0	0	20	0
3	E	1045	0	0	1	0
4	F	2740	0	2	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	2	0	0	0	0
6	D	2	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
7	E	1	0	0	0	0
8	A	1	0	0	0	0
9	A	6	0	8	0	0
10	A	5	0	5	0	0
11	B	28	0	12	1	0
11	D	28	0	12	3	0
12	B	29	0	0	1	0
12	D	29	0	0	5	0
13	B	12	0	12	3	0
14	F	27	0	12	2	0
15	A	63	0	0	0	0
15	B	70	0	0	1	0
15	C	144	0	0	0	0
15	D	26	0	0	2	0
15	E	13	0	0	0	0
15	F	18	0	0	2	0
All	All	18043	0	87	82	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (82) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:238:CYS:SG	4:F:239:HIS:CE1	2.03	1.50
4:F:238:CYS:SG	4:F:239:HIS:ND1	2.11	1.22
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.25	0.70
2:B:1:MET:SD	2:B:253[B]:ARG:NH1	2.66	0.69
4:F:184:LYS:O	14:F:401:ADP:N6	2.30	0.65
4:F:36:ARG:NH2	15:F:513:HOH:O	2.31	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:186:LEU:N	14:F:401:ADP:N1	2.47	0.63
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.32	0.61
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.17	0.61
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.19	0.60
2:D:147[B]:SER:OG	2:D:190:SER:OG	2.20	0.60
2:B:311:ARG:NH2	2:B:343:PHE:O	2.37	0.58
11:B:501:GDP:O1A	15:B:639:HOH:O	2.16	0.58
1:A:98:ASP:O	1:A:105[B]:ARG:NH2	2.37	0.57
1:A:211[B]:ASP:OD2	1:A:215:ARG:NH2	2.38	0.57
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.38	0.56
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.39	0.56
2:B:253[A]:ARG:NH1	13:B:505:MES:O3S	2.38	0.56
4:F:132:LEU:O	4:F:136:ASN:ND2	2.39	0.55
4:F:26:GLN:NE2	15:F:514:HOH:O	2.39	0.55
4:F:243:HIS:O	4:F:247:LYS:N	2.40	0.55
1:C:221:ARG:NH1	2:D:325:MET:SD	2.80	0.55
2:D:311:ARG:NH1	2:D:436:GLN:O	2.39	0.55
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.24	0.54
4:F:139:ARG:NH1	4:F:165:GLU:OE1	2.40	0.54
2:D:185:TYR:OH	2:D:398:MET:O	2.26	0.54
2:D:253:ARG:NE	15:D:717:HOH:O	2.40	0.53
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.42	0.53
4:F:43:GLU:N	4:F:43:GLU:OE2	2.42	0.53
1:C:96:LYS:NZ	2:D:130:ASP:OD2	2.42	0.53
2:B:27:GLU:OE2	2:B:320:ARG:NH2	2.42	0.53
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.42	0.52
2:D:228:ASN:OD1	11:D:602:GDP:N1	2.29	0.52
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.43	0.52
4:F:184:LYS:NZ	4:F:185:TYR:O	2.42	0.52
2:B:2:ARG:NH1	2:B:130:ASP:OD2	2.42	0.52
1:C:341:ILE:CD1	1:C:341:ILE:N	2.73	0.52
1:A:258:ASN:OD1	1:A:352:LYS:NZ	2.45	0.50
4:F:84:SER:O	4:F:88:SER:N	2.45	0.50
1:C:236:SER:OG	1:C:320:ARG:NH1	2.46	0.49
2:D:143:GLY:O	2:D:186:ASN:ND2	2.46	0.49
2:D:1:MET:SD	15:D:717:HOH:O	2.60	0.49
4:F:239:HIS:N	4:F:239:HIS:ND1	2.60	0.49
1:A:2:ARG:O	1:A:133:GLN:NE2	2.47	0.47
2:D:270:PRO:O	2:D:302:MET:N	2.48	0.47
2:B:31:ASP:OD1	2:B:35:SER:N	2.47	0.47
2:D:31:ASP:OD1	2:D:35:SER:N	2.48	0.46
4:F:138:ARG:NH1	4:F:144:GLY:O	2.47	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.33	0.46
2:D:288:VAL:O	2:D:291:LEU:N	2.49	0.46
2:D:255:LEU:CG	12:D:604:2RR:C26	2.94	0.46
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.49	0.46
2:D:27:GLU:OE1	2:D:236:SER:OG	2.34	0.45
12:D:604:2RR:N11	12:D:604:2RR:C21	2.80	0.45
2:B:199:ASP:OD2	13:B:505:MES:H52	2.17	0.45
4:F:135:TYR:OH	4:F:164:SER:O	2.33	0.45
2:D:145:THR:N	11:D:602:GDP:O3B	2.50	0.45
2:B:303:ALA:O	2:B:305:CYS:N	2.50	0.45
2:D:69:ASP:OD1	2:D:70:LEU:N	2.50	0.45
4:F:230:SER:O	4:F:233:PHE:CZ	2.70	0.45
2:B:139:HIS:ND1	2:B:146:GLY:O	2.49	0.45
1:C:39:ASP:OD2	1:C:61:HIS:NE2	2.50	0.45
4:F:246:GLN:NE2	4:F:260:ASN:OD1	2.50	0.45
12:D:604:2RR:C16	12:D:604:2RR:N3	2.81	0.44
1:C:180:ALA:CA	12:D:604:2RR:C17	2.96	0.44
2:D:198:THR:OG1	2:D:266:HIS:NE2	2.51	0.44
1:C:180:ALA:N	12:D:604:2RR:C17	2.81	0.44
12:B:504:2RR:N11	12:B:504:2RR:C20	2.81	0.44
2:B:263:PRO:O	2:B:266:HIS:ND1	2.51	0.44
2:B:2:ARG:O	2:B:133:GLN:NE2	2.51	0.44
1:C:399:TYR:O	1:C:402:ARG:NH2	2.52	0.43
4:F:338:CYS:SG	4:F:339:ALA:N	2.92	0.43
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.52	0.43
2:B:253[A]:ARG:NH2	13:B:505:MES:O2S	2.52	0.43
2:D:228:ASN:ND2	11:D:602:GDP:O6	2.51	0.42
1:A:449:GLU:OE1	4:F:12:SER:N	2.52	0.42
4:F:12:SER:OG	4:F:343:TYR:OH	2.39	0.41
2:B:205:ASP:OD2	2:B:390:ARG:NH1	2.54	0.41
2:D:139:HIS:ND1	2:D:146:GLY:O	2.54	0.41
4:F:53:GLY:N	4:F:60:GLN:OE1	2.54	0.41
2:D:76:ASP:OD1	2:D:79:ARG:NH1	2.53	0.41

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	447/451 (99%)	431 (96%)	15 (3%)	1 (0%)	56	79
1	C	453/451 (100%)	443 (98%)	9 (2%)	1 (0%)	56	79
2	B	430/445 (97%)	417 (97%)	11 (3%)	2 (0%)	38	60
2	D	421/445 (95%)	402 (96%)	17 (4%)	2 (0%)	38	60
3	E	125/143 (87%)	124 (99%)	1 (1%)	0	100	100
4	F	325/384 (85%)	313 (96%)	12 (4%)	0	100	100
All	All	2201/2319 (95%)	2130 (97%)	65 (3%)	6 (0%)	50	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	290	GLU
2	D	181	VAL
1	C	177	VAL
1	A	178	SER
2	B	304	ALA
2	B	82	PRO

### 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	382/379 (101%)	381 (100%)	1 (0%)	96	99
1	C	386/379 (102%)	382 (99%)	4 (1%)	85	97
2	B	378/383 (99%)	374 (99%)	4 (1%)	84	96
2	D	368/383 (96%)	357 (97%)	11 (3%)	53	80
3	E	115/127 (91%)	115 (100%)	0	100	100
4	F	303/342 (89%)	301 (99%)	2 (1%)	91	98
All	All	1932/1993 (97%)	1910 (99%)	22 (1%)	84	96

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	390	ARG
2	B	139	HIS
2	B	167[A]	ASN
2	B	167[B]	ASN
2	B	323	MET
1	C	2	ARG
1	C	176	GLN
1	C	179	THR
1	C	340	SER
2	D	130	ASP
2	D	139	HIS
2	D	181	VAL
2	D	248	LEU
2	D	249	ASN
2	D	255	LEU
2	D	286	LEU
2	D	290	GLU
2	D	291	LEU
2	D	352	LYS
2	D	401	ARG
4	F	239	HIS
4	F	379	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	439/451 (97%)	0.20	3 (0%)	84 86	25, 44, 77, 114	0
1	C	440/451 (97%)	0.18	3 (0%)	84 86	15, 31, 65, 98	0
2	B	418/445 (93%)	0.27	4 (0%)	79 81	19, 41, 78, 112	2 (0%)
2	D	421/445 (94%)	0.42	20 (4%)	29 30	24, 58, 93, 116	6 (1%)
3	E	124/143 (86%)	0.42	7 (5%)	24 24	32, 58, 102, 130	0
4	F	331/384 (86%)	1.41	94 (28%)	1 1	32, 65, 143, 162	0
All	All	2173/2319 (93%)	0.45	131 (6%)	21 21	15, 47, 99, 162	8 (0%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	9.5
4	F	249	TYR	9.2
4	F	240	LEU	8.2
4	F	251	LYS	7.5
4	F	233	PHE	6.6
4	F	253	TYR	6.6
4	F	241	THR	6.3
4	F	252	ASN	6.1
4	F	250	SER	6.0
4	F	170	LEU	5.9
4	F	243	HIS	5.5
1	C	177	VAL	5.4
4	F	132	LEU	5.0
4	F	245	ILE	5.0
4	F	169	LEU	4.8
4	F	234	GLN	4.7
4	F	242	ASN	4.6
4	F	166	ALA	4.6
4	F	229	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	438	ALA	4.3
2	D	335	VAL	4.3
4	F	231	ALA	4.3
4	F	232	ASN	4.2
2	D	402	LYS	4.1
2	D	275	LEU	4.1
4	F	256	TYR	4.0
4	F	248	GLU	3.9
4	F	131	PHE	3.9
4	F	330	ILE	3.8
4	F	379	HIS	3.7
2	D	295	MET	3.6
4	F	283	ILE	3.6
4	F	181	VAL	3.5
4	F	257	GLU	3.4
2	B	437	ASP	3.4
4	F	259	GLY	3.3
4	F	236	LYS	3.3
4	F	264	PHE	3.2
3	E	7	GLU	3.2
4	F	100	ILE	3.2
4	F	263	PHE	3.2
3	E	25	LYS	3.2
4	F	335	ALA	3.2
4	F	99	VAL	3.2
4	F	182	ILE	3.1
1	A	450	GLU	3.1
3	E	119	MET	3.1
4	F	199	PHE	3.1
2	D	296	PHE	3.0
4	F	329	LEU	3.0
4	F	246	GLN	3.0
4	F	133	ALA	2.9
4	F	315	PHE	2.9
2	D	179	ASP	2.9
4	F	247	LYS	2.9
4	F	162	ILE	2.9
2	D	400	ARG	2.9
4	F	167	SER	2.9
2	D	332	MET	2.9
4	F	14	TYR	2.9
2	D	255	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
4	F	319	PHE	2.8
1	A	351	PHE	2.8
1	C	178	SER	2.8
4	F	258	GLU	2.8
4	F	17	VAL	2.8
2	D	1	MET	2.8
4	F	221	LEU	2.8
4	F	238	CYS	2.7
4	F	239	HIS	2.7
4	F	39	LEU	2.7
2	D	377	PHE	2.7
4	F	44	ARG	2.7
4	F	284[A]	LEU	2.6
4	F	271[A]	LEU	2.6
4	F	204	TRP	2.6
2	D	286	LEU	2.6
4	F	147	TRP	2.6
4	F	320	MET	2.6
4	F	351	VAL	2.5
1	A	262	TYR	2.5
4	F	20	LEU	2.5
2	D	415	GLU	2.5
4	F	220	VAL	2.5
2	D	247	GLN	2.5
4	F	267	PHE	2.5
3	E	120	LEU	2.5
4	F	224	SER	2.4
4	F	255	ARG	2.4
4	F	260	ASN	2.4
3	E	23	ILE	2.4
4	F	190	LEU	2.4
4	F	228	TYR	2.4
4	F	333	ASN	2.4
4	F	290	ILE	2.4
2	B	372	LYS	2.4
2	D	246	GLY	2.4
4	F	130	VAL	2.3
4	F	216	TYR	2.3
4	F	254	GLY	2.3
2	D	318	ILE	2.3
4	F	337	ALA	2.3
2	D	405	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	323	GLU	2.3
4	F	31	ARG	2.3
4	F	127	GLU	2.3
3	E	6	MET	2.3
4	F	343	TYR	2.3
4	F	163	SER	2.2
4	F	186	LEU	2.2
4	F	317	PHE	2.2
4	F	183	GLN	2.2
2	D	178	SER	2.2
3	E	115[A]	HIS	2.1
4	F	172	PHE	2.1
4	F	192	LEU	2.1
4	F	214	TYR	2.1
2	B	358	ILE	2.1
4	F	27	TRP	2.1
4	F	275	LEU	2.1
4	F	336	PRO	2.1
2	D	310	GLY	2.1
4	F	222	ARG	2.1
4	F	11	SER	2.1
1	C	179	THR	2.1
4	F	13	VAL	2.1
4	F	139	ARG	2.1
2	D	249	ASN	2.1
4	F	314	LEU	2.1
4	F	142	ARG	2.0
4	F	230	SER	2.0

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
12	2RR	D	604	29/29	0.76	9.63	60,72,78,80	0
6	MG	B	502	1/1	0.34	7.78	47,47,47,47	0
10	IMD	A	506	5/5	0.23	5.73	92,92,94,95	0
7	CA	B	503	1/1	0.32	5.36	81,81,81,81	0
14	ADP	F	401	27/27	0.62	2.35	165,168,234,394	0
9	GOL	A	505	6/6	0.20	2.15	90,97,99,99	0
7	CA	E	700	1/1	0.21	0.88	84,84,84,84	0
7	CA	A	503	1/1	0.15	0.76	62,62,62,62	0
8	CL	A	504	1/1	0.15	0.64	78,78,78,78	0
11	GDP	B	501	28/28	0.18	0.57	18,27,36,43	0
12	2RR	B	504	29/29	0.19	0.37	34,47,54,55	0
11	GDP	D	602	28/28	0.17	0.29	35,44,62,69	0
6	MG	A	502	1/1	0.16	0.07	25,25,25,25	0
5	GTP	A	501	32/32	0.17	0.07	13,31,36,67	0
7	CA	C	502	1/1	0.15	0.06	58,58,58,58	0
5	GTP	C	501	32/32	0.15	-0.37	11,22,35,62	0
6	MG	D	601	1/1	0.15	-0.40	23,23,23,23	0
13	MES	B	505	12/12	0.16	-0.44	41,50,67,67	0
6	MG	B	506	1/1	0.13	-0.93	42,42,42,42	0
6	MG	D	603	1/1	0.10	-4.11	44,44,44,44	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.