



Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 07:07 PM GMT

PDB ID : 4O4H
Title : Tubulin-Laulimalide complex
Authors : Prota, A.E.; Bargsten, K.; Northcote, P.T.; Marsh, M.; Altmann, K.H.; Miller, J.H.; Diaz, J.F.; Steinmetz, M.O.
Deposited on : 2013-12-18
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

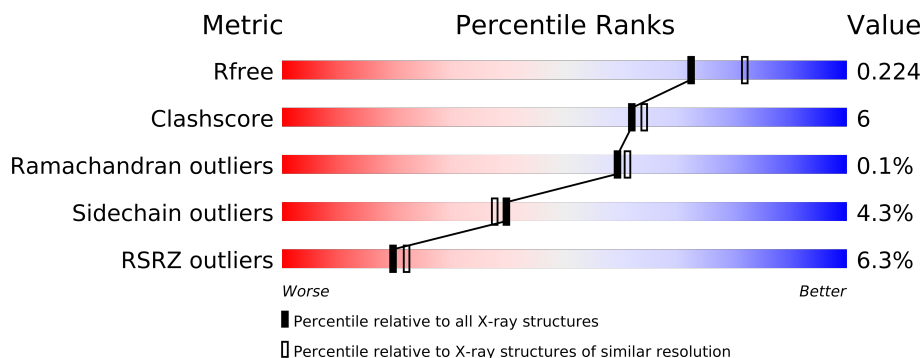
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22714
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) : trunk22714

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. 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	GOL	B	504	-	X
10	GOL	D	503	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	MG	A	502	-	X
6	MG	B	502	-	X
6	MG	C	502	-	X
6	MG	F	402	-	X
7	CA	A	503	-	X
9	LLM	B	503	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18548 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
			3481	2214	584	658	25			
1	C	440	Total	C	N	O	S	0	19	0
			3519	2235	586	672	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	10	0
			3397	2137	573	660	27			
2	D	427	Total	C	N	O	S	0	6	0
			3370	2117	571	653	29			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	5	0
			1039	642	187	205	5			

There are 2 discrepancies between the modelled and reference sequences:

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

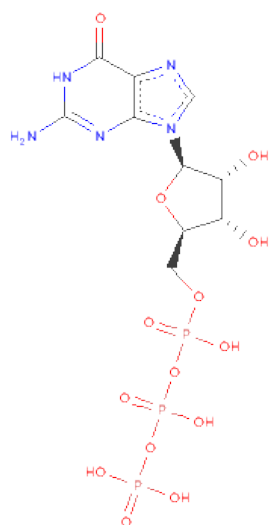
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	348	Total	C	N	O	S	0	6	0
			2878	1852	487	525	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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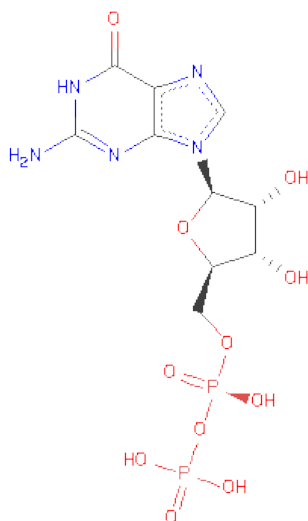
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

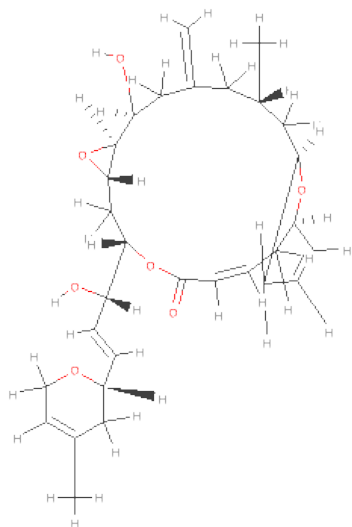
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	1	Total	Ca	0	0
			1	1		

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



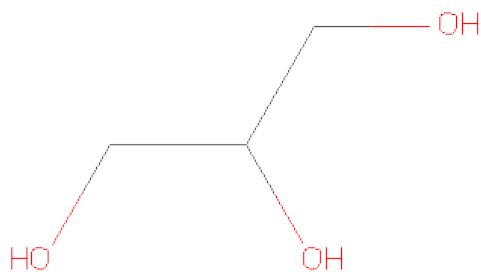
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is LAULIMALIDE (three-letter code: LLM) (formula: C₃₀H₄₂O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			37	30	7		

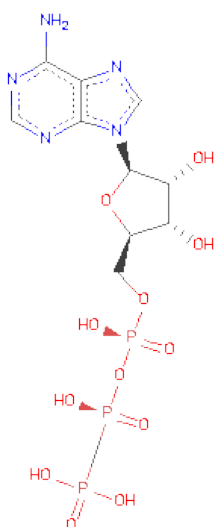
- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONICACID ADENYLATE ESTER (three-

letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

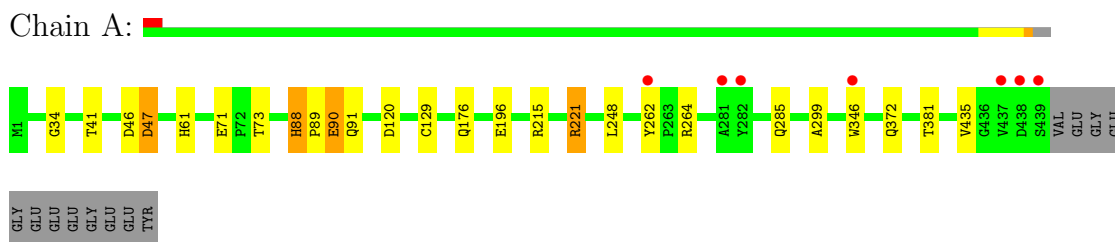
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	110	Total	O	0	0
			110	110		
12	B	142	Total	O	0	0
			142	142		
12	C	231	Total	O	0	0
			231	231		
12	D	102	Total	O	0	0
			102	102		
12	E	31	Total	O	0	0
			31	31		
12	F	40	Total	O	0	0
			40	40		

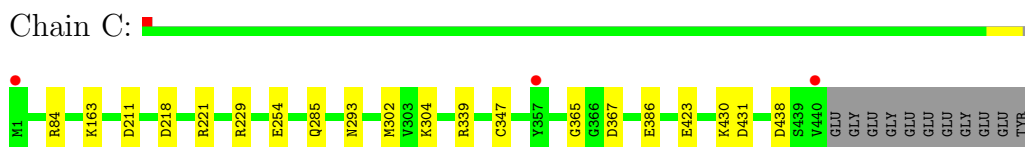
3 Residue-property plots

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.

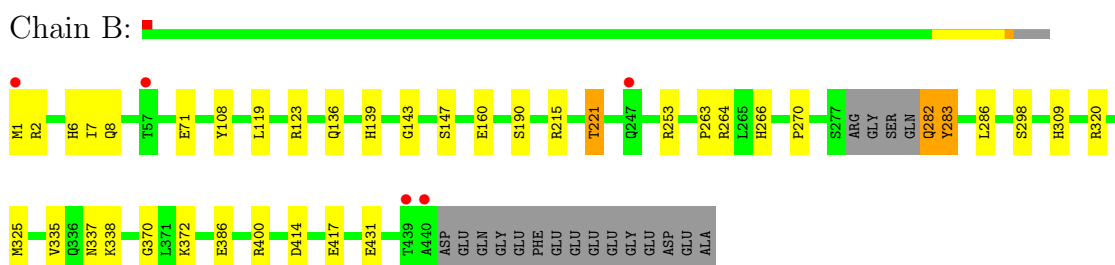
- Molecule 1: Tubulin alpha-1B chain



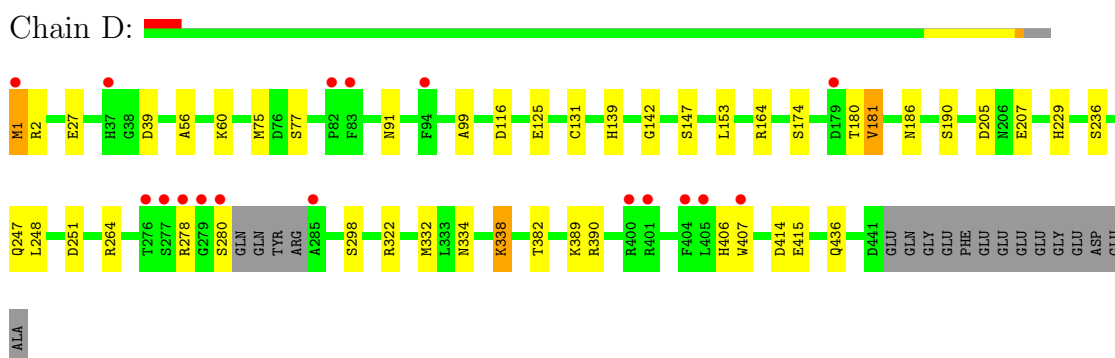
- Molecule 1: Tubulin alpha-1B chain



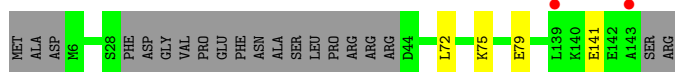
- Molecule 2: Tubulin beta-2B chain



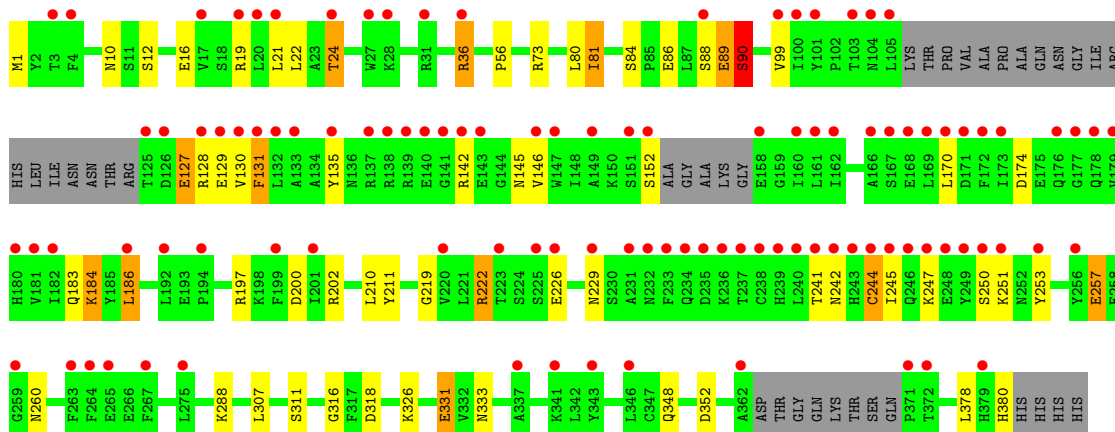
- Molecule 2: Tubulin beta-2B chain



- 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, α , β , γ	104.69Å 156.87Å 180.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.90 – 2.10 78.43 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.90-2.10) 99.8 (78.43-2.10)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.192 , 0.224 0.193 , 0.224	Depositor DCC
R_{free} test set	8656 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.1	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 172824 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18548	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, CA, GTP, ACP, LLM

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	0.31	1/3596 (0.0%)	0.51	1/4883 (0.0%)
1	C	0.33	0/3655	0.52	0/4965
2	B	0.31	0/3498	0.50	0/4738
2	D	0.31	0/3461	0.52	1/4689 (0.0%)
3	E	0.30	0/1063	0.42	0/1412
4	F	0.38	1/2961 (0.0%)	0.49	0/4002
All	All	0.33	2/18234 (0.0%)	0.50	2/24689 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	90	SER	CB-OG	-12.87	1.25	1.42
1	A	89	PRO	N-CD	5.28	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	338	LYS	CD-CE-NZ	-12.12	83.83	111.70
1	A	88	HIS	C-N-CD	5.62	140.19	128.40

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	3481	0	0	16	2
1	C	3519	0	0	11	0
2	B	3397	0	11	22	0
2	D	3370	0	0	21	1
3	E	1039	0	0	1	0
4	F	2878	0	0	29	3
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	B	37	0	0	1	0
10	B	6	0	8	1	0
10	D	6	0	8	0	0
11	F	31	0	14	5	0
12	A	110	0	0	8	0
12	B	142	0	0	11	0
12	C	231	0	0	8	0
12	D	102	0	0	9	0
12	E	31	0	0	0	0
12	F	40	0	0	3	0
All	All	18548	0	89	103	3

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 6.

All (103) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:163:LYS:NZ	12:C:770:HOH:O	2.09	0.85
2:B:320:ARG:NH1	10:B:504:GOL:O3	2.09	0.84
4:F:146:VAL:O	4:F:184:LYS:NZ	2.10	0.84
2:D:164:ARG:NH1	12:D:616:HOH:O	2.11	0.82
1:C:293[A]:ASN:OD1	1:C:339:ARG:NH1	2.13	0.82
2:B:71:GLU:O	12:B:724:HOH:O	1.99	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:21:LEU:O	4:F:24:THR:OG1	1.99	0.81
4:F:88:SER:OG	4:F:89:GLU:N	2.17	0.77
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.19	0.76
2:B:221:THR:N	12:B:685:HOH:O	2.18	0.76
11:F:401:ACP:C8	11:F:401:ACP:H3'	2.17	0.75
1:C:365:GLY:N	12:C:731:HOH:O	2.19	0.75
2:D:75:MET:N	12:D:702:HOH:O	2.19	0.74
2:B:370:GLY:N	12:B:693:HOH:O	2.18	0.74
2:D:180:THR:O	12:D:653:HOH:O	2.06	0.72
2:D:229:HIS:ND1	12:D:701:HOH:O	2.22	0.71
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.24	0.69
1:A:88:HIS:NE2	1:A:90:GLU:OE1	2.26	0.68
2:B:215:ARG:NH1	12:B:740:HOH:O	2.26	0.68
1:A:285:GLN:NE2	12:A:681:HOH:O	2.28	0.66
1:A:196:GLU:OE1	12:A:680:HOH:O	2.14	0.65
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.30	0.65
4:F:80:LEU:O	4:F:84:SER:OG	2.15	0.65
4:F:222:ARG:O	4:F:241:THR:OG1	2.14	0.65
2:B:338:LYS:NZ	12:B:671:HOH:O	2.30	0.64
4:F:56:PRO:O	12:F:521:HOH:O	2.15	0.64
4:F:288:LYS:NZ	12:F:527:HOH:O	2.32	0.63
2:B:337:ASN:ND2	12:B:687:HOH:O	2.32	0.61
1:C:438:ASP:OD1	12:C:725:HOH:O	2.16	0.61
1:A:264:ARG:NH1	12:A:680:HOH:O	2.34	0.60
4:F:242:ASN:ND2	11:F:401:ACP:O2B	2.33	0.60
1:A:88:HIS:N	1:A:91:GLN:OE1	2.34	0.60
4:F:90:SER:O	4:F:90:SER:OG	2.19	0.60
2:D:180:THR:OG1	2:D:181:VAL:N	2.35	0.60
11:F:401:ACP:H8	11:F:401:ACP:H5'1	1.84	0.60
2:D:174:SER:OG	2:D:207:GLU:OE1	2.19	0.60
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.36	0.59
4:F:81:ILE:O	4:F:88:SER:CA	2.52	0.57
1:A:88:HIS:CD2	1:A:90:GLU:N	2.73	0.56
4:F:226:GLU:OE2	4:F:250:SER:OG	2.22	0.56
2:D:56:ALA:N	2:D:60:LYS:O	2.39	0.56
2:B:400:ARG:NH1	12:B:702:HOH:O	2.39	0.55
1:C:430:LYS:NZ	1:C:431:ASP:OD1	2.40	0.55
9:B:503:LLM:C28	9:B:503:LLM:C29	2.86	0.54
1:A:88:HIS:CD2	1:A:90:GLU:CB	2.91	0.54
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.25	0.54
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.26	0.53
2:D:147[A]:SER:OG	2:D:190:SER:OG	2.27	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:282:GLN:CG	2:B:283:TYR:N	2.72	0.53
4:F:86:GLU:OE1	4:F:86:GLU:N	2.42	0.51
4:F:16:GLU:OE1	4:F:19:ARG:NH1	2.43	0.51
1:A:262:TYR:CE2	1:A:346:TRP:CH2	2.99	0.50
4:F:81:ILE:O	4:F:88:SER:N	2.44	0.50
1:A:248:LEU:N	12:A:625:HOH:O	2.45	0.50
1:C:254:GLU:OE2	12:C:831:HOH:O	2.20	0.49
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.29	0.49
2:B:2:ARG:NH1	12:B:677:HOH:O	2.45	0.49
1:A:372[B]:GLN:OE1	12:A:651:HOH:O	2.20	0.49
2:D:2:ARG:NH2	12:D:669:HOH:O	2.46	0.48
2:B:253:ARG:NH2	12:B:612:HOH:O	2.45	0.48
2:B:143:GLY:O	2:B:147[B]:SER:OG	2.32	0.48
2:D:99:ALA:N	12:D:675:HOH:O	2.47	0.48
2:D:382:THR:OG1	2:D:436:GLN:OE1	2.32	0.47
1:C:229:ARG:NH2	12:C:756:HOH:O	2.48	0.47
1:C:367:ASP:N	12:C:690:HOH:O	2.47	0.47
1:A:47:ASP:OD1	1:A:47:ASP:N	2.45	0.47
2:D:1:MET:N	2:D:131:CYS:SG	2.86	0.47
1:C:423:GLU:OE1	12:C:675:HOH:O	2.20	0.47
4:F:219:GLY:O	12:F:501:HOH:O	2.20	0.47
4:F:331:GLU:OE2	4:F:333:ASN:ND2	2.47	0.47
2:B:123:ARG:NE	2:B:160:GLU:OE2	2.48	0.46
2:B:309:HIS:ND1	2:B:386:GLU:OE1	2.48	0.46
2:D:334:ASN:ND2	12:D:659:HOH:O	2.48	0.46
4:F:202:ARG:NE	4:F:318:ASP:OD1	2.49	0.45
11:F:401:ACP:H8	11:F:401:ACP:H3'	1.94	0.45
2:D:27:GLU:OE1	2:D:236:SER:OG	2.35	0.45
4:F:99:VAL:N	4:F:127:GLU:OE1	2.50	0.44
2:B:337:ASN:OD1	4:F:36:ARG:NE	2.50	0.44
2:D:264:ARG:NH1	12:D:670:HOH:O	2.50	0.44
1:A:299:ALA:N	12:A:679:HOH:O	2.50	0.44
2:D:414:ASP:OD1	2:D:414:ASP:N	2.51	0.44
1:C:430:LYS:NZ	12:C:646:HOH:O	2.51	0.43
4:F:10:ASN:N	4:F:10:ASN:OD1	2.51	0.43
2:B:263:PRO:O	2:B:266:HIS:ND1	2.52	0.43
2:B:264:ARG:NE	2:B:431[B]:GLU:OE2	2.52	0.43
2:B:136:GLN:NE2	12:B:742:HOH:O	2.51	0.42
4:F:244:CYS:SG	4:F:245:ILE:N	2.92	0.42
2:D:406:HIS:NE2	2:D:407:TRP:CD1	2.88	0.42
2:D:142:GLY:O	2:D:186:ASN:ND2	2.52	0.41
4:F:253:TYR:CD1	4:F:253:TYR:C	2.93	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:221:ARG:N	12:A:688:HOH:O	2.53	0.41
4:F:128:ARG:O	4:F:130:VAL:N	2.53	0.41
4:F:135:TYR:O	4:F:145:ASN:ND2	2.54	0.41
1:A:129:CYS:O	12:A:684:HOH:O	2.22	0.41
2:B:253:ARG:NE	12:B:612:HOH:O	2.53	0.41
4:F:131:PHE:CD1	4:F:131:PHE:C	2.93	0.41
2:D:251:ASP:OD2	12:D:601:HOH:O	2.21	0.41
4:F:316:GLY:O	4:F:333:ASN:N	2.54	0.41
2:B:6:HIS:NE2	2:B:8:GLN:OE1	2.54	0.41
2:D:91:ASN:ND2	2:D:125:GLU:OE2	2.54	0.40
2:D:205:ASP:OD1	2:D:390:ARG:NH2	2.55	0.40
1:A:34:GLY:O	1:A:61:HIS:N	2.53	0.40
4:F:186:LEU:N	11:F:401:ACP:N1	2.70	0.40

All (3) 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	Distance(Å)	Clash(Å)
1:A:88:HIS:CE1	4:F:142:ARG:NH2[2_564]	1.14	1.06
1:A:88:HIS:ND1	4:F:142:ARG:NH2[2_564]	1.95	0.25
2:D:338:LYS:NZ	4:F:90:SER:OG[3_545]	2.05	0.15

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	449/451 (100%)	440 (98%)	9 (2%)	0	100	100
1	C	457/451 (101%)	447 (98%)	10 (2%)	0	100	100
2	B	432/445 (97%)	417 (96%)	14 (3%)	1 (0%)	56	57
2	D	429/445 (96%)	410 (96%)	18 (4%)	1 (0%)	56	57
3	E	124/143 (87%)	123 (99%)	1 (1%)	0	100	100
4	F	346/384 (90%)	327 (94%)	19 (6%)	0	100	100
All	All	2237/2319 (96%)	2164 (97%)	71 (3%)	2 (0%)	59	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	283	TYR
2	D	181	VAL

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%)	372 (97%)	10 (3%)	59	62
1	C	390/379 (103%)	380 (97%)	10 (3%)	59	62
2	B	378/383 (99%)	365 (97%)	13 (3%)	49	49
2	D	374/383 (98%)	359 (96%)	15 (4%)	42	41
3	E	115/127 (91%)	113 (98%)	2 (2%)	73	78
4	F	320/342 (94%)	286 (89%)	34 (11%)	10	5
All	All	1959/1993 (98%)	1875 (96%)	84 (4%)	40	37

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	46	ASP
1	A	47	ASP
1	A	90	GLU
1	A	120	ASP
1	A	176	GLN
1	A	215	ARG
1	A	221	ARG
1	A	381	THR
1	A	435	VAL
2	B	1	MET
2	B	7	ILE
2	B	119	LEU
2	B	139	HIS
2	B	221	THR
2	B	270	PRO
2	B	282	GLN

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Mol	Chain	Res	Type
2	B	286	LEU
2	B	298	SER
2	B	325	MET
2	B	335	VAL
2	B	372	LYS
2	B	414	ASP
1	C	84	ARG
1	C	218	ASP
1	C	221	ARG
1	C	285	GLN
1	C	302[A]	MET
1	C	302[B]	MET
1	C	347[A]	CYS
1	C	347[B]	CYS
1	C	386[A]	GLU
1	C	386[B]	GLU
2	D	1	MET
2	D	39	ASP
2	D	77	SER
2	D	116	ASP
2	D	139	HIS
2	D	153	LEU
2	D	247	GLN
2	D	248	LEU
2	D	278	ARG
2	D	280	SER
2	D	298	SER
2	D	322	ARG
2	D	332	MET
2	D	389	LYS
2	D	415	GLU
3	E	72	LEU
3	E	141	GLU
4	F	1	MET
4	F	12	SER
4	F	22	LEU
4	F	24	THR
4	F	36	ARG
4	F	73	ARG
4	F	81	ILE
4	F	89	GLU
4	F	90	SER

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Mol	Chain	Res	Type
4	F	127	GLU
4	F	129	GLU
4	F	131	PHE
4	F	152	SER
4	F	170	LEU
4	F	174	ASP
4	F	183	GLN
4	F	184	LYS
4	F	186	LEU
4	F	200	ASP
4	F	210	LEU
4	F	211	TYR
4	F	222	ARG
4	F	229	ASN
4	F	244	CYS
4	F	247	LYS
4	F	251	LYS
4	F	257	GLU
4	F	260	ASN
4	F	307	LEU
4	F	311	SER
4	F	326	LYS
4	F	331	GLU
4	F	378	LEU
4	F	380	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 ⓘ

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 16 ligands modelled in this entry, 8 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	34,34,34	0.95	1 (2%)	52,54,54	1.60	7 (13%)
8	GDP	B	501	6	30,30,30	1.28	5 (16%)	45,47,47	3.55	8 (17%)
9	LLM	B	503	-	40,40,40	3.30	14 (35%)	55,55,55	1.92	14 (25%)
10	GOL	B	504	-	5,5,5	0.39	0	5,5,5	0.41	0
5	GTP	C	501	6	34,34,34	1.07	1 (2%)	52,54,54	1.78	7 (13%)
8	GDP	D	501	6	30,30,30	1.26	4 (13%)	45,47,47	3.17	8 (17%)
10	GOL	D	503	-	5,5,5	0.40	0	5,5,5	0.38	0
11	ACP	F	401	-	33,33,33	2.38	12 (36%)	52,52,52	4.60	25 (48%)

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	-	0/22/38/38	0/3/3/3
8	GDP	B	501	6	-	0/16/32/32	0/3/3/3
9	LLM	B	503	-	-	0/39/64/64	0/1/4/4
10	GOL	B	504	-	-	0/4/4/4	0/0/0/0
5	GTP	C	501	6	-	0/22/38/38	0/3/3/3
8	GDP	D	501	6	-	0/16/32/32	0/3/3/3
10	GOL	D	503	-	-	0/4/4/4	0/0/0/0
11	ACP	F	401	-	-	0/20/38/38	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	LLM	C14-C13	-11.53	1.39	1.51
9	B	503	LLM	C12-C13	-10.67	1.40	1.51
9	B	503	LLM	C21-C22	6.21	1.52	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PG-O1G	5.13	1.61	1.50
9	B	503	LLM	C30-C25	-5.02	1.38	1.50
9	B	503	LLM	C5-C6	-4.96	1.40	1.50
11	F	401	ACP	C2-N3	4.40	1.39	1.32
11	F	401	ACP	PG-C3B	4.39	1.84	1.79
11	F	401	ACP	PB-O1B	4.04	1.62	1.51
9	B	503	LLM	C2-C1	-3.78	1.39	1.48
9	B	503	LLM	C8-C7	-3.62	1.41	1.49
5	A	501	GTP	C2-N3	3.57	1.37	1.33
5	C	501	GTP	C2-N3	3.48	1.37	1.33
11	F	401	ACP	C4-N9	-3.40	1.32	1.37
9	B	503	LLM	C4-C3	-3.32	1.39	1.50
11	F	401	ACP	C2-N1	3.28	1.40	1.33
9	B	503	LLM	C27-C26	-3.22	1.40	1.48
8	B	501	GDP	C4-N9	-3.12	1.33	1.37
11	F	401	ACP	PB-O2B	-3.11	1.48	1.56
11	F	401	ACP	C5-C4	-3.05	1.33	1.40
11	F	401	ACP	PG-O2G	-3.03	1.48	1.54
8	D	501	GDP	C5-C4	3.02	1.47	1.40
9	B	503	LLM	C16-C17	2.95	1.50	1.46
9	B	503	LLM	C6-C7	2.87	1.40	1.32
9	B	503	LLM	C29-C13	2.84	1.39	1.32
8	B	501	GDP	C5-C4	2.75	1.46	1.40
8	D	501	GDP	C4-N9	-2.71	1.33	1.37
11	F	401	ACP	C2'-C3'	-2.70	1.46	1.53
9	B	503	LLM	C2-C3	2.67	1.39	1.31
8	B	501	GDP	C2-N2	2.64	1.36	1.32
9	B	503	LLM	C24-C25	-2.58	1.41	1.50
11	F	401	ACP	C3'-C4'	2.57	1.60	1.53
8	D	501	GDP	C2-N2	2.48	1.36	1.32
8	D	501	GDP	C5-N7	-2.45	1.35	1.38
11	F	401	ACP	PA-O1A	2.41	1.60	1.51
8	B	501	GDP	O4'-C1'	2.05	1.43	1.41
8	B	501	GDP	C5-N7	-2.04	1.35	1.38

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C6-C5-N7	20.55	136.91	134.14
8	D	501	GDP	C6-C5-N7	17.24	136.46	134.14
11	F	401	ACP	O4'-C1'-C2'	-12.72	88.17	106.69
11	F	401	ACP	N3-C2-N1	-12.45	117.93	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	O4'-C4'-C5'	11.57	150.47	109.37
11	F	401	ACP	O4'-C4'-C3'	-10.17	84.48	105.16
11	F	401	ACP	C3'-C2'-C1'	-8.94	86.91	100.92
11	F	401	ACP	C1'-N9-C4	-8.85	111.34	126.64
11	F	401	ACP	C8-N9-C1'	8.19	141.56	126.15
5	C	501	GTP	C6-C5-N7	-7.99	133.06	134.14
11	F	401	ACP	C4'-O4'-C1'	7.91	118.41	109.72
5	A	501	GTP	C6-C5-N7	-6.88	133.21	134.14
8	D	501	GDP	C5-C4-N3	-6.15	118.99	126.07
11	F	401	ACP	C5'-C4'-C3'	-5.73	92.23	115.19
8	B	501	GDP	C5-C4-N3	-5.72	119.48	126.07
9	B	503	LLM	C20-C21-C22	-5.71	116.11	125.16
9	B	503	LLM	C23-C22-C21	-5.66	113.00	125.27
8	D	501	GDP	N3-C4-N9	5.33	134.72	126.91
8	B	501	GDP	N3-C4-N9	5.17	134.50	126.91
11	F	401	ACP	O4'-C1'-N9	4.97	118.91	108.10
8	B	501	GDP	C2-N3-C4	4.96	121.25	115.30
11	F	401	ACP	C5-C4-N3	-4.94	121.16	125.98
8	D	501	GDP	C2-N3-C4	4.89	121.16	115.30
9	B	503	LLM	C18-C17-C16	-4.74	114.42	124.53
11	F	401	ACP	PA-O3A-PB	-4.57	118.30	132.02
11	F	401	ACP	PB-C3B-PG	-4.50	110.36	118.95
11	F	401	ACP	O2G-PG-C3B	4.26	116.73	106.40
8	D	501	GDP	C6-N1-C2	4.12	122.53	120.20
11	F	401	ACP	O3'-C3'-C2'	-4.03	98.81	111.83
5	C	501	GTP	C2-N3-C4	3.94	120.03	115.30
8	B	501	GDP	C6-N1-C2	3.82	122.36	120.20
5	C	501	GTP	C5-C4-N3	-3.81	121.69	126.07
5	A	501	GTP	C5-C4-N3	-3.70	121.81	126.07
11	F	401	ACP	C2'-C3'-C4'	3.54	109.71	102.64
9	B	503	LLM	O27-C23-C24	-3.47	107.73	110.39
9	B	503	LLM	C16-O16-C17	3.43	62.67	60.60
5	A	501	GTP	C2-N3-C4	3.30	119.26	115.30
11	F	401	ACP	O3A-PB-O1B	-3.16	104.80	111.51
8	D	501	GDP	PA-O3A-PB	-3.09	123.38	131.93
5	C	501	GTP	N3-C4-N9	3.09	131.43	126.91
5	C	501	GTP	N2-C2-N1	3.01	121.05	117.82
11	F	401	ACP	N3-C4-N9	2.94	130.43	125.39
5	A	501	GTP	PA-O3A-PB	-2.91	123.86	131.93
11	F	401	ACP	C6-C5-C4	2.84	120.74	117.55
9	B	503	LLM	C11-C10-C9	-2.79	110.27	115.40
8	D	501	GDP	C4-C5-N7	-2.78	106.72	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C8-N9-C4	2.74	109.19	106.96
9	B	503	LLM	C15-C16-C17	-2.68	115.23	121.70
11	F	401	ACP	O3G-PG-O1G	-2.66	105.44	112.49
5	A	501	GTP	N3-C4-N9	2.65	130.79	126.91
5	A	501	GTP	PB-O3B-PG	-2.57	124.82	131.93
11	F	401	ACP	O5'-C5'-C4'	2.56	118.36	108.96
8	B	501	GDP	C4-C5-N7	-2.42	107.07	109.41
9	B	503	LLM	C15-C14-C13	-2.37	110.18	115.17
5	C	501	GTP	PA-O3A-PB	-2.34	125.45	131.93
9	B	503	LLM	C9-C8-C7	2.33	114.73	109.53
9	B	503	LLM	C18-C19-C20	-2.31	109.19	113.95
11	F	401	ACP	O3A-PA-O5'	2.27	108.93	102.91
11	F	401	ACP	O2'-C2'-C1'	-2.22	104.48	111.49
5	C	501	GTP	PB-O3B-PG	-2.16	125.95	131.93
11	F	401	ACP	C2-N3-C4	2.15	119.45	113.27
8	D	501	GDP	C8-N9-C4	2.11	108.68	106.96
11	F	401	ACP	C5-C6-N6	-2.11	115.94	120.72
9	B	503	LLM	C4-C5-C6	-2.11	109.16	113.10
9	B	503	LLM	C19-C20-C21	-2.09	108.63	111.09
9	B	503	LLM	O19-C1-C2	2.08	116.43	111.41
8	B	501	GDP	PA-O3A-PB	-2.05	126.26	131.93
9	B	503	LLM	C30-C25-C26	-2.03	118.19	122.55
5	A	501	GTP	N2-C2-N1	2.02	119.99	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	439/451 (97%)	0.17	7 (1%) 68 72	26, 44, 80, 131	0
1	C	440/451 (97%)	0.11	3 (0%) 84 88	22, 34, 58, 99	0
2	B	426/445 (95%)	0.20	5 (1%) 75 80	25, 41, 72, 126	2 (0%)
2	D	427/445 (95%)	0.33	17 (3%) 36 41	28, 47, 78, 123	6 (1%)
3	E	123/143 (86%)	0.49	2 (1%) 68 72	34, 56, 93, 139	0
4	F	348/384 (90%)	1.50	105 (30%) 1 1	34, 69, 131, 174	0
All	All	2203/2319 (94%)	0.42	139 (6%) 19 22	22, 45, 96, 174	8 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	105	LEU	10.5
4	F	249	TYR	8.1
4	F	104	ASN	7.0
4	F	173	ILE	6.4
4	F	182	ILE	6.0
2	D	285	ALA	6.0
2	D	277	SER	6.0
2	D	1	MET	5.6
4	F	161	LEU	5.6
4	F	142	ARG	5.5
4	F	178	GLN	5.4
2	D	276	THR	5.4
3	E	143	ALA	5.3
4	F	143	GLU	5.3
2	B	1	MET	5.2
4	F	131	PHE	5.0
4	F	244	CYS	4.9
4	F	179	VAL	4.7
2	D	405	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	4.7
4	F	170	LEU	4.6
4	F	251	LYS	4.5
4	F	17	VAL	4.4
4	F	166	ALA	4.3
4	F	234	GLN	4.3
4	F	245	ILE	4.2
4	F	233	PHE	4.1
4	F	181	VAL	4.1
4	F	177	GLY	4.1
4	F	176	GLN	4.0
2	D	279	GLY	4.0
4	F	24	THR	4.0
4	F	275[A]	LEU	3.9
1	A	282	TYR	3.9
4	F	172	PHE	3.9
2	D	278	ARG	3.9
4	F	372	THR	3.9
4	F	232	ASN	3.7
4	F	194	PRO	3.7
1	A	281	ALA	3.7
4	F	100	ILE	3.7
4	F	140	GLU	3.7
2	D	404	PHE	3.7
4	F	99	VAL	3.6
4	F	238	CYS	3.6
4	F	160	ILE	3.6
1	C	1	MET	3.5
4	F	31	ARG	3.5
4	F	259	GLY	3.5
4	F	225	SER	3.5
4	F	250	SER	3.4
4	F	231	ALA	3.4
4	F	20	LEU	3.4
2	D	400	ARG	3.4
4	F	237	THR	3.4
4	F	240	LEU	3.3
4	F	158	GLU	3.3
4	F	180	HIS	3.3
4	F	171	ASP	3.3
4	F	192	LEU	3.3
4	F	125	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	179	ASP	3.2
4	F	243	HIS	3.2
2	D	280	SER	3.2
4	F	129	GLU	3.2
4	F	371	PRO	3.2
4	F	162	ILE	3.2
4	F	242	ASN	3.2
4	F	229	ASN	3.1
4	F	132	LEU	3.1
4	F	247	LYS	3.1
4	F	199	PHE	3.0
4	F	267	PHE	3.0
4	F	362	ALA	3.0
4	F	138	ARG	2.9
4	F	21	LEU	2.9
2	B	439	THR	2.9
4	F	167	SER	2.9
4	F	152	SER	2.8
1	A	437	VAL	2.8
4	F	130	VAL	2.8
4	F	141	GLY	2.8
4	F	88	SER	2.7
4	F	137	ARG	2.7
2	D	82	PRO	2.7
4	F	263	PHE	2.7
2	D	83	PHE	2.7
4	F	135	TYR	2.7
4	F	379	HIS	2.7
1	C	440	VAL	2.6
4	F	201	ILE	2.6
4	F	147	TRP	2.6
4	F	226	GLU	2.6
4	F	27	TRP	2.6
4	F	220[A]	VAL	2.5
4	F	168	GLU	2.5
4	F	103	THR	2.5
4	F	149	ALA	2.5
4	F	101	TYR	2.5
4	F	236	LYS	2.4
4	F	128	ARG	2.4
4	F	256	TYR	2.4
4	F	235	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	2.4
4	F	253	TYR	2.4
4	F	133	ALA	2.4
1	A	438	ASP	2.4
4	F	28	LYS	2.3
1	A	439	SER	2.3
4	F	265	GLU	2.3
4	F	4	PHE	2.3
4	F	264	PHE	2.3
2	D	407	TRP	2.3
4	F	186	LEU	2.3
4	F	223	THR	2.3
4	F	248	GLU	2.2
4	F	239	HIS	2.2
4	F	343	TYR	2.2
4	F	36	ARG	2.2
4	F	126	ASP	2.2
2	B	440	ALA	2.2
2	D	94	PHE	2.2
4	F	151	SER	2.2
3	E	139	LEU	2.2
4	F	146	VAL	2.2
2	D	37	HIS	2.1
4	F	139	ARG	2.1
1	A	346	TRP	2.1
4	F	241	THR	2.1
4	F	341	LYS	2.1
2	D	401	ARG	2.1
4	F	346	LEU	2.1
2	B	57	THR	2.1
4	F	3	THR	2.1
2	B	247	GLN	2.1
4	F	19	ARG	2.1
1	C	357	TYR	2.1
4	F	246	GLN	2.0
4	F	337	ALA	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	MG	F	402	1/1	0.26	19.81	30,30,30,30	0
10	GOL	D	503	6/6	0.42	11.64	63,74,92,100	0
6	MG	C	502	1/1	0.22	10.82	34,34,34,34	0
6	MG	B	502	1/1	0.20	7.35	22,22,22,22	0
10	GOL	B	504	6/6	0.23	6.55	55,62,66,75	0
6	MG	A	502	1/1	0.23	6.35	38,38,38,38	0
9	LLM	B	503	37/37	0.23	2.70	91,93,102,104	0
7	CA	A	503	1/1	0.16	2.53	80,80,80,80	0
5	GTP	C	501	32/32	0.13	0.59	21,26,32,36	0
7	CA	B	505	1/1	0.17	0.52	109,109,109,109	0
5	GTP	A	501	32/32	0.14	0.33	25,30,34,43	0
8	GDP	D	501	28/28	0.13	-0.24	34,44,53,59	0
8	GDP	B	501	28/28	0.13	-0.29	21,27,33,37	0
11	ACP	F	401	31/31	0.16	-1.28	49,73,130,140	0
6	MG	D	502	1/1	0.07	-1.66	44,44,44,44	0
7	CA	B	506	1/1	0.09	-5.10	93,93,93,93	0

6.5 Other polymers ⓘ

There are no such residues in this entry.