



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2017 – 05:44 AM EST

PDB ID : 4IHJ
Title : Crystal structure of tubulin-stathmin-TTL-ADP complex
Authors : Prota, A.E.; Magiera, M.M.; Kuijpers, M.; Bargsten, K.; Frey, D.; Wieser, M.; Jaussi, R.; Hoogenraad, C.C.; Kammerer, R.A.; Janke, C.; Steinmetz, M.O.
Deposited on : unknown
Resolution : 2.00 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 : rb-20030345
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) : rb-20030345

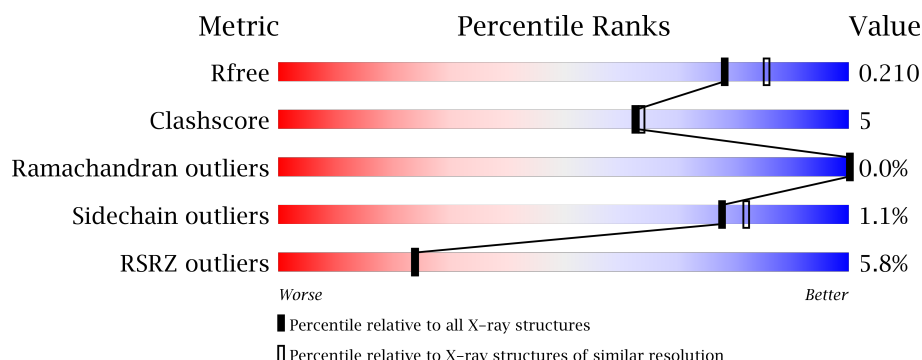
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	450	<div> <div>0.2%</div> <div>88%</div> <div>10%</div> <div>•</div> </div>
1	C	450	<div> <div>85%</div> <div>12%</div> <div>•</div> </div>
2	B	445	<div> <div>0.2%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
2	D	445	<div> <div>2%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>
3	E	143	<div> <div>80%</div> <div>5%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MG	A	502	-	-	-	X
6	MG	C	502	-	-	-	X
6	MG	D	602	-	-	-	X
7	CA	A	503	-	-	-	X
7	CA	A	505	-	-	-	X
7	CA	C	503	-	-	-	X

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 36041 atoms, of which 17304 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	442	Total	C	H	N	O	S	0	8	0
			6927	2210	3432	594	666	25			
1	C	440	Total	C	H	N	O	S	0	10	0
			6898	2203	3419	586	664	26			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	422	Total	C	H	N	O	S	0	5	0
			6591	2103	3250	567	644	27			
2	D	422	Total	C	H	N	O	S	0	5	0
			6555	2093	3224	563	648	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	3	0
			2062	629	1045	184	198	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, TTL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	344	Total	C	H	N	O	S	0	4	0
			5700	1837	2848	488	513	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	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	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	2	Total	Mg	0	0
			2	2		
6	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	2	Total	Mg	0	0
			2	2		

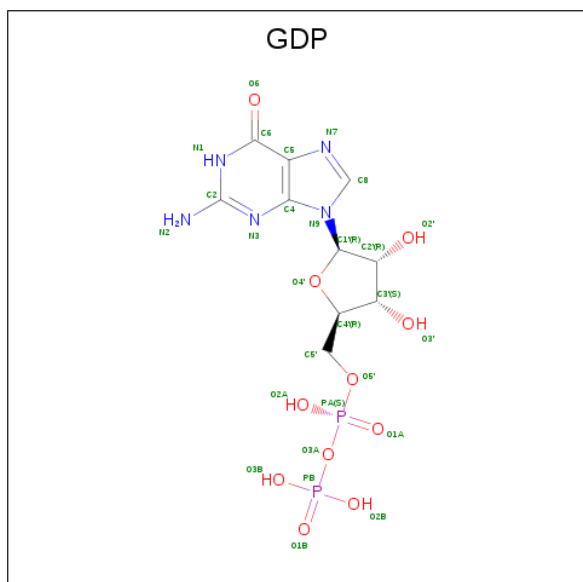
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



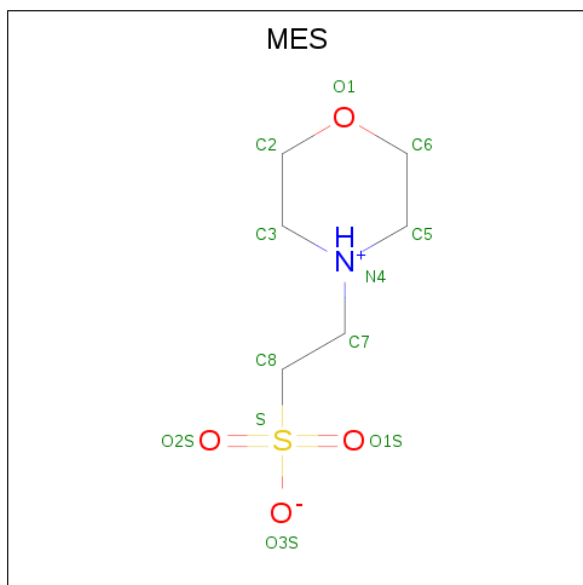
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	P	
			38	10	10	5	11	2	0

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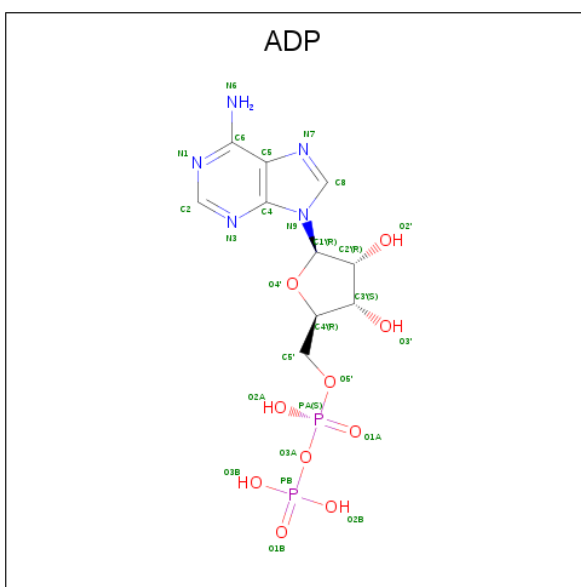
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	H	N	O	P	
			38	10	10	5	11	2	
								0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



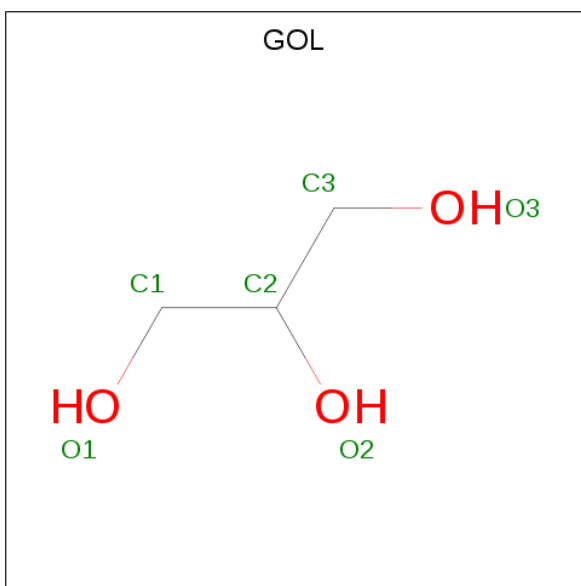
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	
10	B	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	
								0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	
			39	10	12	5	10	2	

- Molecule 12 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	F	1	Total	C	H	O		
			14	3	8	3	0	0

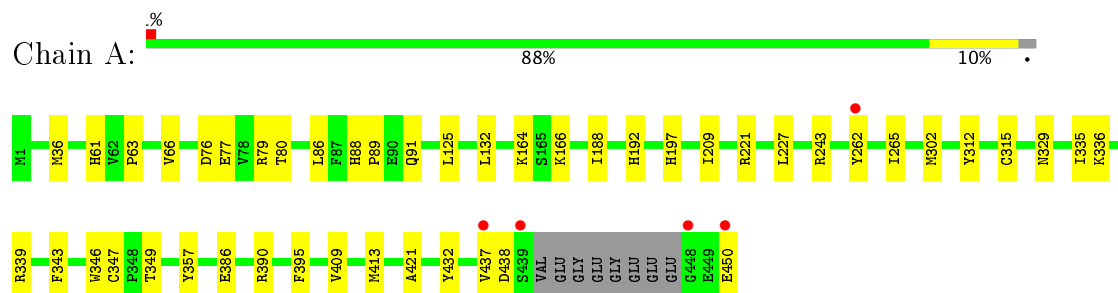
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	217	Total 217	O 217	0	0
13	B	189	Total 189	O 189	0	0
13	C	376	Total 376	O 376	0	0
13	D	117	Total 117	O 117	0	0
13	E	54	Total 54	O 54	0	0
13	F	80	Total 80	O 80	0	0

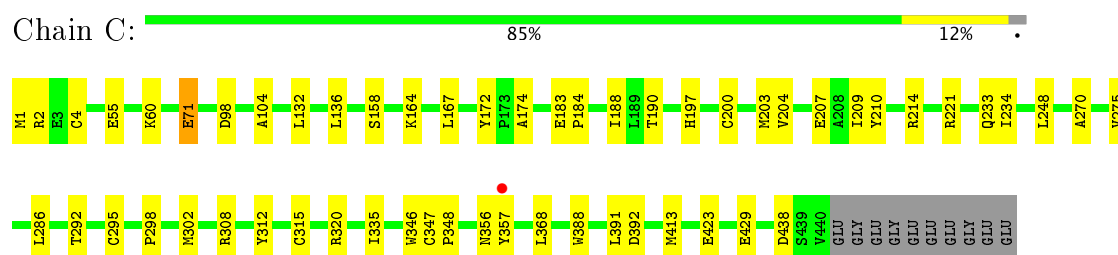
3 Residue-property plots [i](#)

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

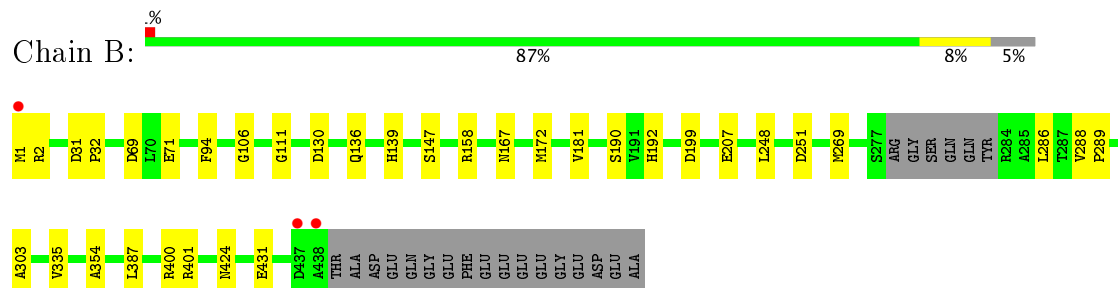
- Molecule 1: Tubulin alpha-1B chain



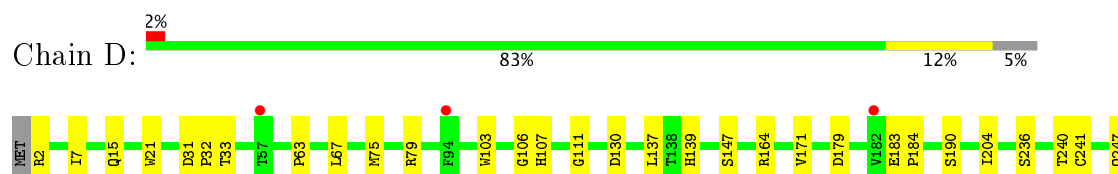
- Molecule 1: Tubulin alpha-1B chain

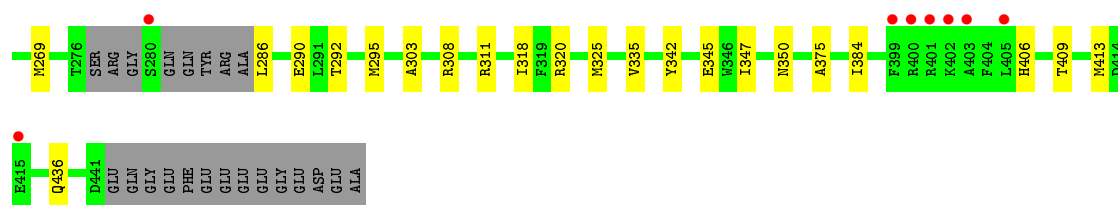


- Molecule 2: Tubulin beta-2B chain

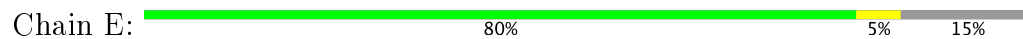


- Molecule 2: Tubulin beta-2B chain

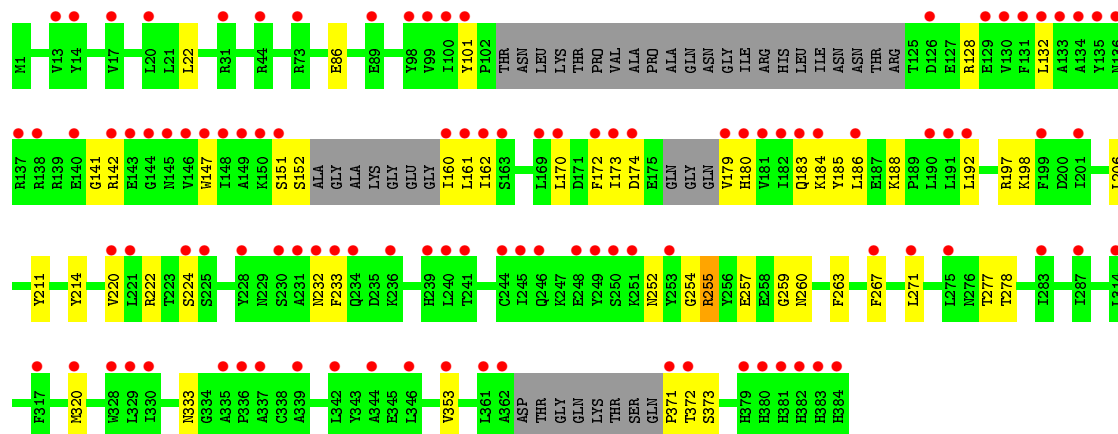
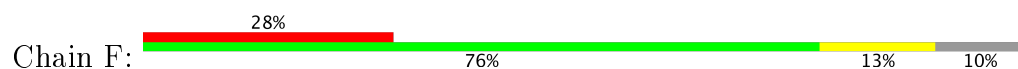




• Molecule 3: Stathmin-4



• Molecule 4: TUBULIN TYROSINE LIGASE, TTL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.52Å 157.31Å 180.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.10 – 2.00 78.45 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (72.10-2.00) 99.1 (78.45-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.168 , 0.217 0.161 , 0.210	Depositor DCC
R_{free} test set	10023 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36041	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, GOL, MG, ADP, CL, CA, GTP, 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	0.42	0/3596	0.61	2/4875 (0.0%)
1	C	0.53	1/3587 (0.0%)	0.63	0/4871
2	B	0.46	0/3429	0.57	0/4644
2	D	0.39	0/3420	0.53	0/4632
3	E	0.42	0/1035	0.51	0/1373
4	F	0.34	0/2932	0.51	0/3962
All	All	0.44	1/17999 (0.0%)	0.57	2/24357 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-5.25	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	243	ARG	NE-CZ-NH1	6.12	123.36	120.30

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	3495	3432	3419	31	0
1	C	3479	3419	3406	39	0
2	B	3341	3250	3240	35	0
2	D	3331	3224	3212	33	0
3	E	1017	1045	1040	5	0
4	F	2852	2848	2833	37	0
5	A	32	10	12	0	0
5	C	32	10	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	2	0	0	0	0
6	F	2	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	10	12	0	0
9	D	28	10	12	0	0
10	B	24	26	26	6	0
11	F	27	12	12	0	0
12	F	6	8	8	0	0
13	A	217	0	0	3	0
13	B	189	0	0	5	0
13	C	376	0	0	5	0
13	D	117	0	0	3	0
13	E	54	0	0	0	0
13	F	80	0	0	1	0
All	All	18737	17304	17244	173	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 5.

All (173) 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:B:192:HIS:ND1	13:B:770:HOH:O	1.98	0.96
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.07	0.94
2:B:199:ASP:OD2	10:B:504:MES:H32	1.75	0.87
1:C:270:ALA:HB3	1:C:302[B]:MET:SD	2.16	0.84
2:D:241[B]:CYS:SG	13:D:772:HOH:O	2.35	0.84
1:C:209:ILE:HD11	1:C:302[A]:MET:HG3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:801:HOH:O	2:B:1:MET:SD	2.44	0.75
2:D:147[B]:SER:HG	2:D:190:SER:HG	1.34	0.74
1:A:209:ILE:HD11	1:A:302[A]:MET:SD	2.27	0.73
1:C:190:THR:OG1	13:C:889:HOH:O	2.05	0.73
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.29	0.72
2:B:199:ASP:OD2	10:B:504:MES:C3	2.38	0.72
1:C:438:ASP:OD1	13:C:976:HOH:O	2.07	0.72
1:C:204:VAL:HG22	1:C:302[B]:MET:CE	2.22	0.68
2:B:192:HIS:CE1	2:B:424[B]:ASN:OD1	2.48	0.67
2:B:71:GLU:OE1	13:B:749:HOH:O	2.13	0.66
2:B:431:GLU:OE1	13:B:764:HOH:O	2.12	0.65
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.31	0.65
4:F:161:LEU:HD22	4:F:172:PHE:CG	2.33	0.64
2:B:192:HIS:CD2	2:B:424[A]:ASN:HD22	2.16	0.63
1:C:270:ALA:CB	1:C:302[B]:MET:SD	2.87	0.62
2:D:247:GLN:OE1	13:D:799:HOH:O	2.16	0.61
2:D:106:GLY:O	2:D:111:GLY:HA3	2.01	0.60
1:A:386:GLU:O	1:A:390[A]:ARG:HD3	2.01	0.60
1:C:207:GLU:OE2	13:C:892:HOH:O	2.16	0.60
2:B:1:MET:SD	13:B:721:HOH:O	2.57	0.59
1:C:234:ILE:HD13	1:C:302[A]:MET:SD	2.43	0.59
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.35	0.59
4:F:162:ILE:HB	4:F:233:PHE:HB3	1.86	0.58
2:D:240[B]:THR:HG21	2:D:320:ARG:HD2	1.85	0.58
2:D:236:SER:O	2:D:240[B]:THR:HG23	2.04	0.57
4:F:161:LEU:HD13	4:F:172:PHE:CZ	2.38	0.57
1:A:437:VAL:HG12	1:A:438:ASP:O	2.04	0.57
1:A:343:PHE:HB2	1:A:349:THR:HG22	1.86	0.57
2:B:192:HIS:ND1	2:B:424[B]:ASN:OD1	2.37	0.56
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.41	0.56
4:F:161:LEU:HD22	4:F:172:PHE:CB	2.36	0.56
2:B:199:ASP:CG	10:B:504:MES:H32	2.26	0.55
2:B:158:ARG:CZ	10:B:504:MES:H21	2.37	0.55
1:A:132:LEU:O	1:A:164:LYS:NZ	2.39	0.55
1:C:210:TYR:CD1	1:C:214:ARG:HD2	2.41	0.54
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.87	0.54
2:B:192:HIS:CD2	2:B:424[A]:ASN:ND2	2.74	0.54
2:D:292:THR:HG22	2:D:335:VAL:HG11	1.90	0.54
1:C:210:TYR:CE1	1:C:214:ARG:HD2	2.44	0.53
1:C:286:LEU:HB2	13:C:836:HOH:O	2.08	0.52
4:F:206:LEU:HD23	4:F:353[A]:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.91	0.52
1:A:349:THR:HG23	13:A:812:HOH:O	2.09	0.52
4:F:161:LEU:HD22	4:F:172:PHE:HB2	1.91	0.52
4:F:277:THR:HG22	4:F:278:THR:H	1.75	0.51
4:F:161:LEU:HD13	4:F:172:PHE:CE1	2.46	0.51
4:F:151:SER:OG	4:F:152:SER:N	2.44	0.51
2:B:251:ASP:OD2	13:B:708:HOH:O	2.19	0.51
1:A:262:TYR:CE2	1:A:346:TRP:CH2	2.98	0.50
2:D:2:ARG:NH1	2:D:130:ASP:CB	2.74	0.50
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.44	0.50
4:F:206:LEU:CD2	4:F:353[A]:VAL:CG2	2.89	0.50
4:F:101:TYR:CD1	4:F:179:VAL:HG22	2.47	0.49
4:F:371:PRO:N	4:F:372:THR:HB	2.27	0.49
4:F:371:PRO:CA	4:F:372:THR:HB	2.41	0.49
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.42	0.49
4:F:257:GLU:O	4:F:259:GLY:O	2.31	0.49
2:B:192:HIS:HD2	2:B:192:HIS:O	1.94	0.49
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.47	0.49
4:F:206:LEU:HD23	4:F:353[A]:VAL:HG21	1.93	0.49
4:F:373:SER:OG	13:F:856:HOH:O	2.20	0.49
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.42	0.49
1:A:209:ILE:CD1	1:A:302[A]:MET:SD	2.99	0.49
1:A:166:LYS:HE2	1:A:197:HIS:O	2.13	0.49
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.95	0.48
1:C:248:LEU:HD12	1:C:357:TYR:CE1	2.49	0.48
2:B:2:ARG:HB3	2:B:2:ARG:NH1	2.29	0.48
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.43	0.48
1:C:320:ARG:HA	1:C:356:ASN:O	2.13	0.48
1:A:357:TYR:CE1	3:E:17:GLY:HA2	2.49	0.48
4:F:371:PRO:HA	4:F:372:THR:C	2.33	0.48
1:A:450:GLU:HG3	4:F:333:ASN:HB3	1.95	0.48
2:B:192:HIS:CD2	2:B:192:HIS:O	2.67	0.48
4:F:252:ASN:O	4:F:255:ARG:HB2	2.14	0.48
1:A:66:VAL:HG23	1:A:125:LEU:HD12	1.96	0.47
1:C:346:TRP:CZ3	1:C:347[B]:CYS:SG	3.07	0.47
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.96	0.47
2:D:171:VAL:HA	2:D:204:ILE:O	2.14	0.47
2:B:69:ASP:O	2:B:94:PHE:HA	2.14	0.47
2:B:199:ASP:OD2	10:B:504:MES:H72	2.14	0.47
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.44	0.47
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ALA:HB2	1:C:413:MET:SD	2.55	0.47
2:D:311:ARG:NH1	2:D:436:GLN:O	2.46	0.47
1:A:88:HIS:CD2	1:A:89:PRO:HD2	2.49	0.47
1:C:234:ILE:CD1	1:C:302[A]:MET:SD	3.02	0.47
4:F:254:GLY:HA2	4:F:259:GLY:O	2.14	0.47
2:B:106:GLY:O	2:B:111:GLY:HA3	2.15	0.47
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.97	0.47
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.97	0.46
1:C:203:MET:SD	1:C:388:TRP:CH2	3.09	0.46
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.43	0.46
2:D:183:GLU:N	2:D:184:PRO:CD	2.79	0.46
2:D:75:MET:O	2:D:79:ARG:NH1	2.49	0.46
4:F:141:GLY:O	4:F:142:ARG:HB2	2.16	0.46
1:C:55:GLU:HA	1:C:60:LYS:O	2.16	0.45
2:D:31:ASP:OD1	2:D:33:THR:N	2.49	0.45
4:F:277:THR:HG22	4:F:278:THR:N	2.31	0.45
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.99	0.45
1:C:1:MET:O	1:C:2:ARG:HB2	2.16	0.45
1:C:392:ASP:OD1	1:C:429:GLU:OE1	2.34	0.45
2:B:2:ARG:HB3	2:B:2:ARG:HH11	1.82	0.45
2:B:147:SER:OG	2:B:190:SER:OG	2.35	0.44
2:D:164:ARG:NH2	13:D:768:HOH:O	2.51	0.44
4:F:186:LEU:HD23	4:F:320:MET:HE2	2.00	0.44
2:D:318:ILE:N	2:D:318:ILE:HD12	2.32	0.44
2:D:103:TRP:CH2	2:D:107:HIS:CD2	3.06	0.44
4:F:161:LEU:CD1	4:F:172:PHE:CE1	3.01	0.44
2:B:136:GLN:HA	2:B:167:ASN:O	2.18	0.44
2:B:2:ARG:NH1	2:B:130:ASP:HB3	2.32	0.44
2:B:181:VAL:HG12	1:C:348:PRO:HG2	2.00	0.43
2:D:7:ILE:O	2:D:137:LEU:HA	2.17	0.43
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.53	0.43
1:A:77:GLU:HA	1:A:80:THR:HG22	2.00	0.43
2:D:286:LEU:HD12	2:D:290:GLU:OE1	2.18	0.43
4:F:161:LEU:HD13	4:F:172:PHE:CE2	2.53	0.43
1:A:63:PRO:CD	1:A:86:LEU:HG	2.48	0.43
1:A:409:VAL:HA	1:A:413:MET:O	2.19	0.43
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.99	0.43
1:C:183:GLU:N	1:C:184:PRO:CD	2.82	0.43
4:F:147:TRP:CE3	4:F:184:LYS:N	2.87	0.43
2:B:248:LEU:HD23	2:B:354:ALA:HB2	1.99	0.43
3:E:72:LEU:O	3:E:76:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE1	2.53	0.42
1:A:349:THR:HG21	13:A:813:HOH:O	2.19	0.42
2:D:384:ILE:HG13	2:D:384:ILE:O	2.19	0.42
4:F:132:LEU:HD21	4:F:170:LEU:HD11	2.02	0.42
2:D:67:LEU:HD12	2:D:67:LEU:N	2.34	0.42
1:A:312:TYR:CD2	1:A:315[B]:CYS:SG	3.13	0.42
2:D:295:MET:CE	2:D:375:ALA:HB1	2.50	0.42
2:B:288:VAL:HB	2:B:289:PRO:HD3	2.01	0.42
4:F:151:SER:HB2	4:F:180:HIS:CE1	2.54	0.42
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.50	0.42
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.55	0.42
4:F:173:ILE:O	4:F:174:ASP:C	2.58	0.42
4:F:183:GLN:O	4:F:184:LYS:C	2.57	0.42
1:A:262:TYR:CE2	1:A:346:TRP:CZ2	3.08	0.42
1:C:158:SER:OG	1:C:197:HIS:HD2	2.02	0.42
1:C:2:ARG:NE	1:C:2:ARG:HA	2.35	0.42
1:C:132:LEU:O	1:C:164:LYS:CE	2.67	0.41
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.55	0.41
4:F:197:ARG:HD2	4:F:224:SER:O	2.19	0.41
2:D:409:THR:O	3:E:140:LYS:HE3	2.20	0.41
4:F:267:PHE:CE1	4:F:271[A]:LEU:CD1	3.03	0.41
1:A:329:ASN:HB3	3:E:6:MET:CE	2.51	0.41
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.03	0.41
2:D:31:ASP:C	2:D:31:ASP:OD1	2.59	0.41
1:C:423:GLU:HG2	13:C:688:HOH:O	2.20	0.41
1:A:192:HIS:CG	1:A:421:ALA:HA	2.56	0.41
4:F:371:PRO:HA	4:F:372:THR:HB	2.01	0.41
1:A:346:TRP:CZ3	1:A:347:CYS:SG	3.14	0.41
2:B:400:ARG:HG3	2:B:401:ARG:HG2	2.02	0.41
1:C:312:TYR:CD2	1:C:315[B]:CYS:SG	3.14	0.41
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.03	0.41
2:B:172:MET:HG3	2:B:387[B]:LEU:HD11	2.03	0.41
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.21	0.41
2:D:406:HIS:HA	2:D:409:THR:OG1	2.21	0.41
2:B:335:VAL:HG13	10:B:505:MES:H22	2.03	0.40
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.37	0.40
1:A:346:TRP:CE3	1:A:347:CYS:SG	3.13	0.40
1:A:88:HIS:N	1:A:91:GLN:OE1	2.45	0.40
2:B:288:VAL:N	2:B:289:PRO:CD	2.84	0.40
4:F:214:TYR:CE2	4:F:353[B]:VAL:HG11	2.55	0.40
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.04	0.40
2:D:409:THR:HA	2:D:413:MET:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/450 (99%)	435 (98%)	11 (2%)	0	100	100
1	C	448/450 (100%)	432 (96%)	16 (4%)	0	100	100
2	B	423/445 (95%)	412 (97%)	11 (3%)	0	100	100
2	D	422/445 (95%)	414 (98%)	8 (2%)	0	100	100
3	E	120/143 (84%)	118 (98%)	2 (2%)	0	100	100
4	F	338/384 (88%)	318 (94%)	19 (6%)	1 (0%)	44	40
All	All	2197/2317 (95%)	2129 (97%)	67 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	232	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/378 (100%)	379 (100%)	1 (0%)	94	96
1	C	381/378 (101%)	379 (100%)	2 (0%)	91	93
2	B	370/383 (97%)	367 (99%)	3 (1%)	85	88
2	D	370/383 (97%)	366 (99%)	4 (1%)	78	82
3	E	112/127 (88%)	111 (99%)	1 (1%)	82	87
4	F	316/342 (92%)	307 (97%)	9 (3%)	49	49
All	All	1929/1991 (97%)	1909 (99%)	20 (1%)	78	84

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
2	B	139	HIS
2	B	207	GLU
2	B	286	LEU
1	C	71	GLU
1	C	188	ILE
2	D	15	GLN
2	D	139	HIS
2	D	179	ASP
2	D	345	GLU
3	E	135	LYS
4	F	22	LEU
4	F	86	GLU
4	F	160	ILE
4	F	188	LYS
4	F	192	LEU
4	F	211	TYR
4	F	222	ARG
4	F	255	ARG
4	F	260	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	A	309	HIS
2	B	192	HIS
2	B	229	HIS
1	C	197	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 20 ligands modelled in this entry, 12 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	27,34,34	0.78	1 (3%)	24,54,54	0.99	2 (8%)
9	GDP	B	501	6	25,30,30	1.39	5 (20%)	23,47,47	1.35	3 (13%)
10	MES	B	504	-	12,12,12	1.93	1 (8%)	16,16,16	2.55	4 (25%)
10	MES	B	505	-	12,12,12	2.26	1 (8%)	16,16,16	1.98	5 (31%)
5	GTP	C	501	6	27,34,34	1.03	1 (3%)	24,54,54	0.88	1 (4%)
9	GDP	D	600	6	25,30,30	1.44	5 (20%)	23,47,47	1.29	2 (8%)
11	ADP	F	703	6	25,29,29	1.04	1 (4%)	24,45,45	1.75	3 (12%)
12	GOL	F	704	-	5,5,5	0.34	0	5,5,5	0.55	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
10	MES	B	504	-	-	0/6/14/14	0/1/1/1
10	MES	B	505	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
9	GDP	D	600	6	-	0/12/32/32	0/3/3/3
11	ADP	F	703	6	-	0/12/32/32	0/3/3/3
12	GOL	F	704	-	-	0/4/4/4	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	MES	C8-S	-6.93	1.67	1.77
10	B	504	MES	C8-S	-5.79	1.68	1.77
9	B	501	GDP	C6-N1	-2.27	1.33	1.36
9	D	600	GDP	C6-N1	-2.18	1.33	1.36
9	B	501	GDP	C2-N2	2.07	1.35	1.32
9	D	600	GDP	O4'-C1'	2.07	1.44	1.41
9	D	600	GDP	C2-N2	2.08	1.35	1.32
5	A	501	GTP	C2-N3	2.15	1.36	1.33
9	B	501	GDP	O4'-C1'	2.39	1.44	1.41
9	B	501	GDP	C5-C4	2.93	1.47	1.40
9	D	600	GDP	C5-C4	3.03	1.47	1.40
11	F	703	ADP	C5-C4	3.22	1.47	1.40
5	C	501	GTP	C2-N3	3.64	1.37	1.33
9	D	600	GDP	C6-C5	3.81	1.48	1.41
9	B	501	GDP	C6-C5	3.82	1.48	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	703	ADP	N3-C2-N1	-6.60	123.11	128.86
11	F	703	ADP	C4-C5-N7	-3.18	106.34	109.41
10	B	505	MES	C2-C3-N4	-3.05	105.60	110.06
9	D	600	GDP	C4-C5-N7	-2.66	106.84	109.41
10	B	505	MES	C8-C7-N4	-2.55	107.82	112.45
9	B	501	GDP	C4-C5-N7	-2.36	107.13	109.41
9	B	501	GDP	N2-C2-N3	-2.25	117.50	120.26
5	A	501	GTP	C4-C5-N7	-2.11	107.37	109.41
10	B	504	MES	C8-C7-N4	-2.10	108.64	112.45
11	F	703	ADP	C2-N1-C6	2.01	122.29	118.77
10	B	504	MES	C6-O1-C2	2.20	117.34	109.89
10	B	505	MES	O3S-S-C8	2.30	108.89	106.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C2-N3-C4	2.60	118.20	115.16
10	B	505	MES	C5-N4-C3	2.77	115.48	109.76
10	B	504	MES	O1-C6-C5	2.89	115.17	111.32
5	A	501	GTP	C2-N3-C4	2.93	118.58	115.16
9	B	501	GDP	C2-N3-C4	3.91	119.73	115.16
9	D	600	GDP	C2-N3-C4	4.27	120.15	115.16
10	B	505	MES	O1S-S-C8	4.31	110.49	106.79
10	B	504	MES	O1S-S-C8	8.31	113.93	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	504	MES	5	0
10	B	505	MES	1	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	442/450 (98%)	0.11	5 (1%)	80 80	24, 40, 78, 126	0
1	C	440/450 (97%)	0.20	1 (0%)	94 94	18, 31, 63, 95	0
2	B	422/445 (94%)	0.21	3 (0%)	87 87	21, 39, 80, 124	2 (0%)
2	D	422/445 (94%)	0.23	11 (2%)	56 56	25, 50, 89, 124	5 (1%)
3	E	121/143 (84%)	0.15	0	100 100	27, 56, 92, 108	0
4	F	344/384 (89%)	1.46	106 (30%)	0 1	33, 65, 125, 160	0
All	All	2191/2317 (94%)	0.38	126 (5%)	24 24	18, 44, 94, 160	7 (0%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	280	SER	9.3
4	F	182	ILE	8.9
2	D	401	ARG	8.5
4	F	173	ILE	7.8
4	F	186	LEU	7.7
4	F	161	LEU	7.7
4	F	99	VAL	6.8
4	F	231	ALA	6.6
4	F	134	ALA	6.5
4	F	169	LEU	6.5
4	F	170	LEU	5.9
4	F	179	VAL	5.6
2	B	1	MET	5.4
4	F	233	PHE	5.3
4	F	137	ARG	5.1
4	F	100	ILE	5.1
4	F	138	ARG	5.1
4	F	372	THR	5.1
4	F	132	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
4	F	181	VAL	4.8
4	F	135	TYR	4.8
2	B	438	ALA	4.8
4	F	381	HIS	4.6
4	F	101	TYR	4.6
4	F	131	PHE	4.6
4	F	249	TYR	4.6
4	F	240	LEU	4.3
4	F	151	SER	4.2
2	D	405	LEU	4.2
4	F	130	VAL	4.2
4	F	232	ASN	4.1
4	F	160	ILE	4.1
4	F	220[A]	VAL	3.9
4	F	184	LYS	3.8
4	F	330	ILE	3.8
4	F	320	MET	3.7
4	F	162	ILE	3.6
4	F	17	VAL	3.5
4	F	361	LEU	3.4
4	F	20	LEU	3.4
4	F	150	LYS	3.3
4	F	148	ILE	3.3
4	F	147	TRP	3.3
4	F	380	HIS	3.2
4	F	44	ARG	3.2
2	D	400	ARG	3.2
4	F	253	TYR	3.2
2	D	57	THR	3.1
4	F	191	LEU	3.1
4	F	371	PRO	3.1
4	F	73	ARG	3.1
4	F	163	SER	3.0
4	F	149	ALA	3.0
4	F	344	ALA	3.0
4	F	172	PHE	3.0
4	F	199	PHE	3.0
4	F	346	LEU	3.0
4	F	241	THR	3.0
4	F	353[A]	VAL	2.9
2	D	399	PHE	2.9
4	F	248	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	144	GLY	2.9
4	F	180	HIS	2.9
4	F	192	LEU	2.9
4	F	314	LEU	2.9
4	F	245	ILE	2.8
1	A	448	GLY	2.8
4	F	221	LEU	2.8
4	F	317	PHE	2.7
4	F	133	ALA	2.7
4	F	337	ALA	2.7
4	F	143	GLU	2.7
4	F	13	VAL	2.7
1	A	450	GLU	2.6
2	D	415	GLU	2.6
4	F	335	ALA	2.6
4	F	383	HIS	2.5
4	F	129	GLU	2.5
4	F	271[A]	LEU	2.5
4	F	382	HIS	2.5
4	F	362	ALA	2.5
4	F	142	ARG	2.5
4	F	234	GLN	2.4
4	F	239	HIS	2.4
4	F	379	HIS	2.4
1	A	262	TYR	2.4
4	F	225	SER	2.4
4	F	244	CYS	2.4
4	F	342	LEU	2.4
2	D	402	LYS	2.3
2	D	403	ALA	2.3
2	D	94	PHE	2.3
4	F	339	ALA	2.3
4	F	201	ILE	2.3
4	F	174	ASP	2.3
4	F	251	LYS	2.3
4	F	336	PRO	2.3
4	F	250	SER	2.3
4	F	329	LEU	2.2
1	C	357	TYR	2.2
4	F	31	ARG	2.2
4	F	89	GLU	2.2
4	F	14	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	98	TYR	2.2
4	F	140	GLU	2.2
4	F	190	LEU	2.2
4	F	283	ILE	2.2
1	A	437	VAL	2.2
4	F	267	PHE	2.2
4	F	384	HIS	2.2
4	F	146	VAL	2.1
2	D	182	VAL	2.1
4	F	136	ASN	2.1
4	F	145	ASN	2.1
4	F	287	ILE	2.1
4	F	230	SER	2.1
4	F	126	ASP	2.1
4	F	328	TRP	2.1
2	B	437	ASP	2.1
4	F	183	GLN	2.1
4	F	228	TYR	2.1
4	F	236	LYS	2.1
1	A	439	SER	2.0
4	F	246	GLN	2.0
4	F	275[A]	LEU	2.0
4	F	224	SER	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(\AA^2)	Q<0.9
7	CA	A	505	1/1	0.96	0.32	25.93	103,103,103,103	0
6	MG	C	502	1/1	0.99	0.19	6.48	27,27,27,27	0
7	CA	C	503	1/1	0.99	0.18	5.30	44,44,44,44	0
6	MG	A	502	1/1	0.99	0.21	4.60	28,28,28,28	0
6	MG	D	602	1/1	0.86	0.17	2.44	100,100,100,100	0
7	CA	A	503	1/1	0.97	0.15	2.42	59,59,59,59	0
5	GTP	A	501	32/32	0.99	0.16	1.90	23,26,31,32	0
5	GTP	C	501	32/32	1.00	0.15	1.52	19,23,26,28	0
9	GDP	B	501	28/28	0.99	0.16	0.64	22,27,34,35	0
10	MES	B	505	12/12	0.96	0.12	0.18	73,77,89,90	0
12	GOL	F	704	6/6	0.76	0.21	0.14	72,87,92,93	0
7	CA	B	503	1/1	0.97	0.14	-0.08	95,95,95,95	0
9	GDP	D	600	28/28	0.98	0.13	-0.21	50,54,67,69	0
10	MES	B	504	12/12	0.98	0.12	-0.56	50,57,62,64	0
11	ADP	F	703	27/27	0.98	0.14	-1.58	70,75,87,88	0
6	MG	F	701	1/1	0.98	0.12	-3.15	55,55,55,55	0
6	MG	F	702	1/1	0.98	0.07	-	66,66,66,66	0
6	MG	D	601	1/1	0.92	0.20	-	99,99,99,99	0
6	MG	B	502	1/1	0.99	0.20	-	27,27,27,27	0
8	CL	A	504	1/1	0.94	0.21	-	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.