



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:50 PM GMT

PDB ID : 4WBN
Title : Crystal structure of Tubulin-Stathmin-TTL complex solved by native-SAD phasing
Authors : Weinert, T.; Protá, A.E.; Wang, M.
Deposited on : 2014-09-03
Resolution : 2.30 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

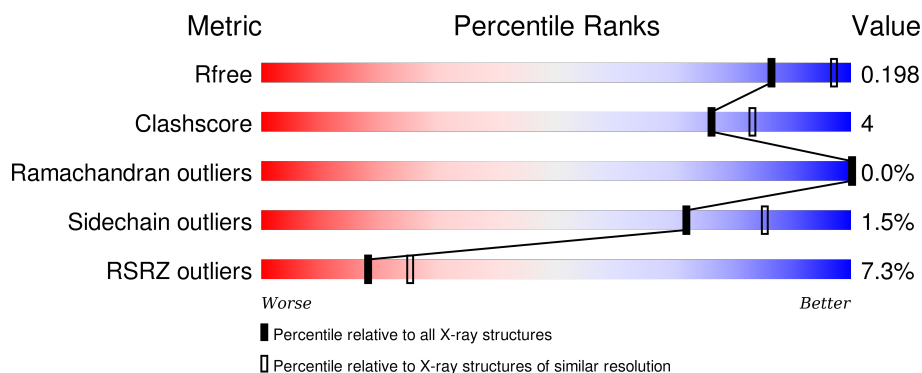
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>3%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	C	451	<div> <div>87%</div> <div>10%</div> <div>.</div> </div>
2	B	445	<div> <div>3%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
2	D	445	<div> <div>7%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>
3	E	143	<div> <div>6%</div> <div>76%</div> <div>8%</div> <div>16%</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
10	MES	B	504	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18021 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	9	0
			3480	2204	592	659	25			
1	C	440	Total	C	N	O	S	0	7	0
			3469	2197	586	662	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	2	0
			3326	2092	566	641	27			
2	D	421	Total	C	N	O	S	0	3	0
			3326	2090	566	644	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	3	0
			1011	626	183	196	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

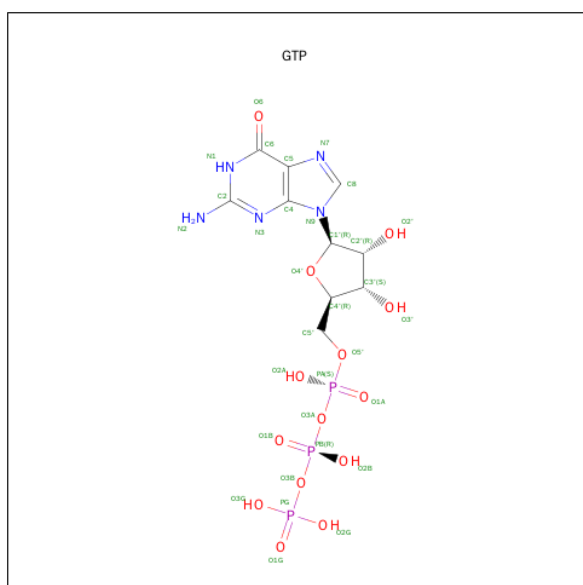
- Molecule 4 is a protein called TUBULIN-TYROSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	336	Total	C	N	O	S	0	0	0
			2760	1776	470	500	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	A	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

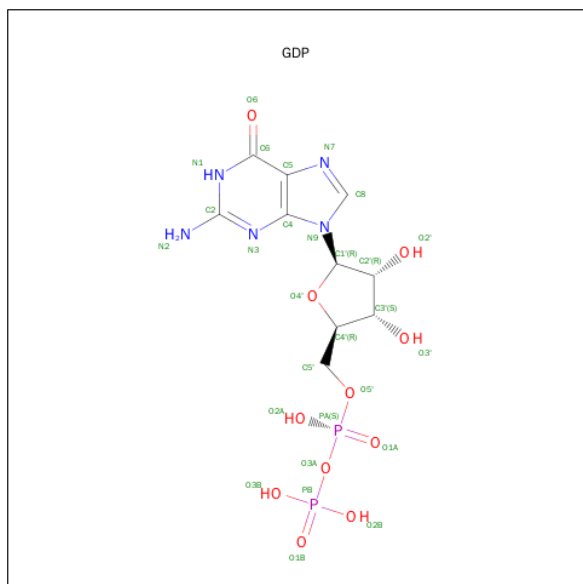
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

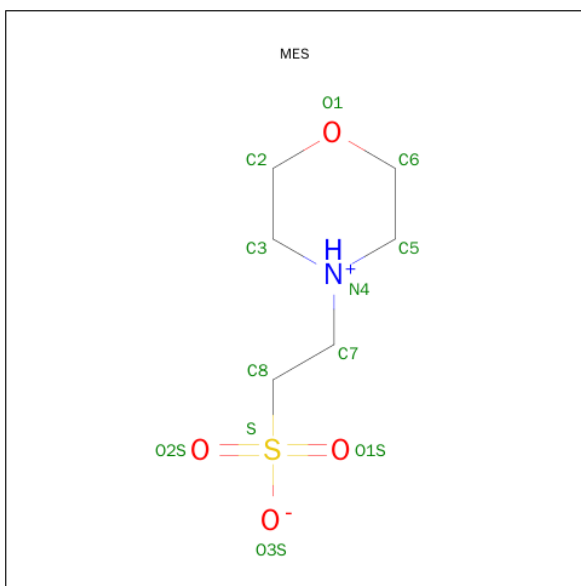
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

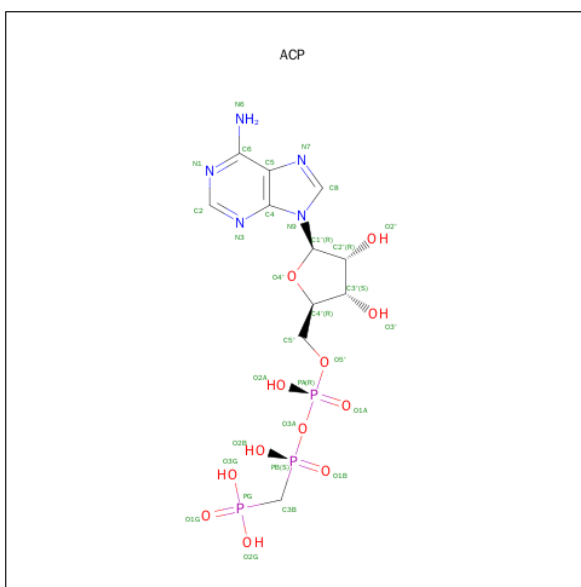
- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES)

(formula: $C_6H_{13}NO_4S$).



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

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID 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		

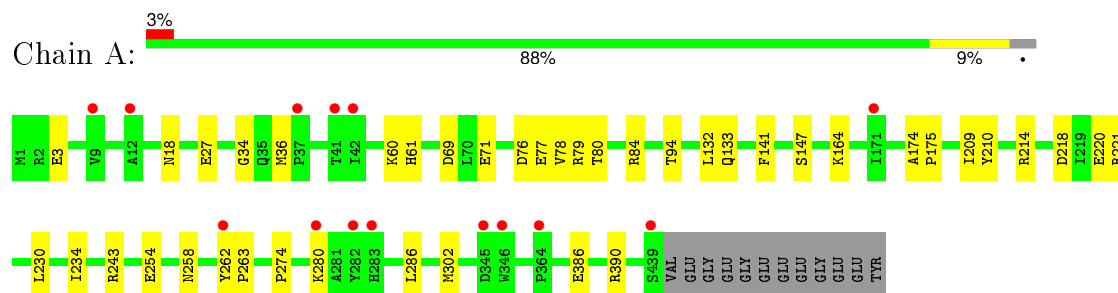
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	89	Total	O	0	0
			89	89		
12	B	97	Total	O	0	0
			97	97		
12	C	181	Total	O	0	0
			181	181		
12	D	43	Total	O	0	0
			43	43		
12	E	19	Total	O	0	0
			19	19		
12	F	35	Total	O	0	0
			35	35		

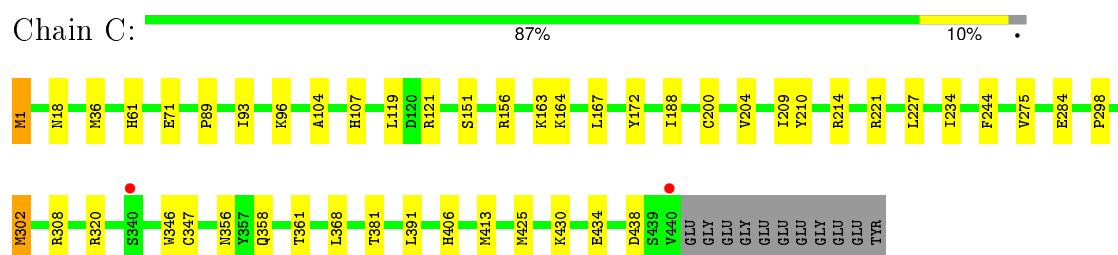
3 Residue-property plots [i](#)

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

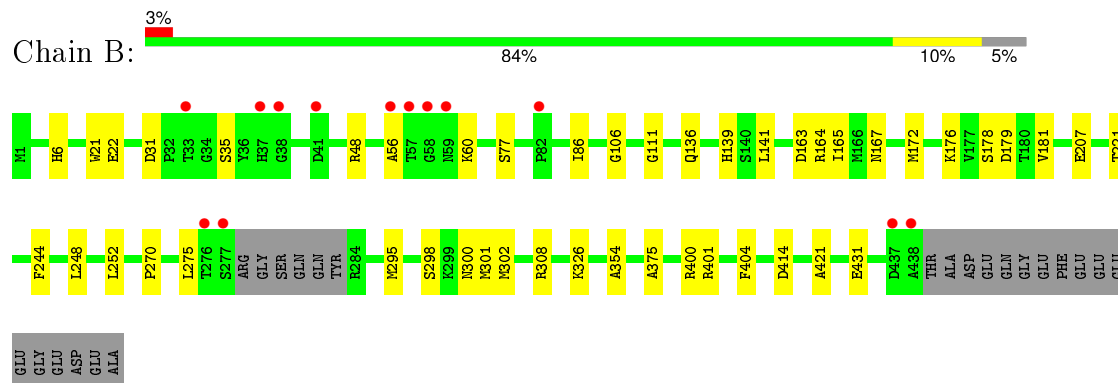
- Molecule 1: Tubulin alpha-1B chain



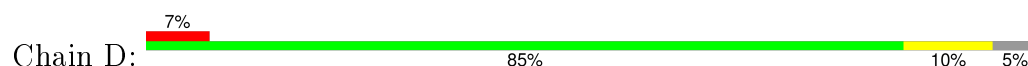
- Molecule 1: Tubulin alpha-1B chain

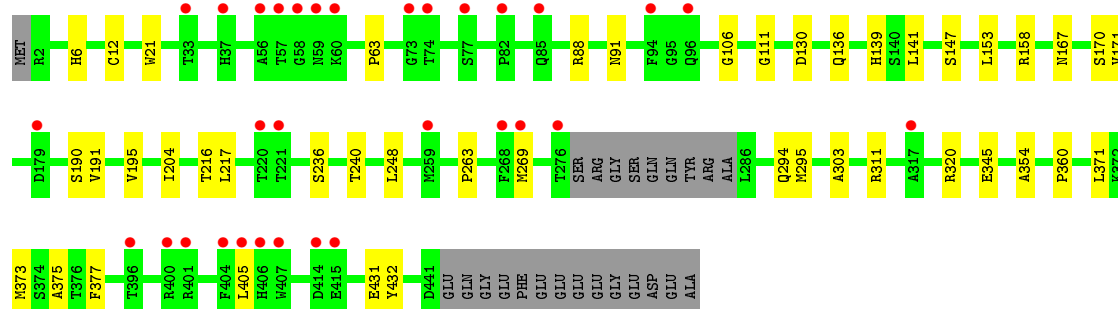


- Molecule 2: Tubulin beta-2B chain

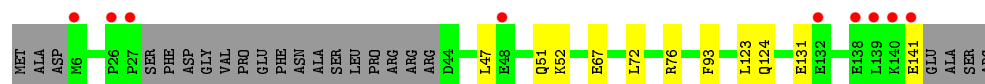
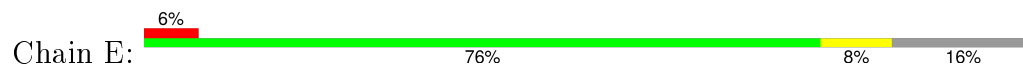


- Molecule 2: Tubulin beta-2B chain

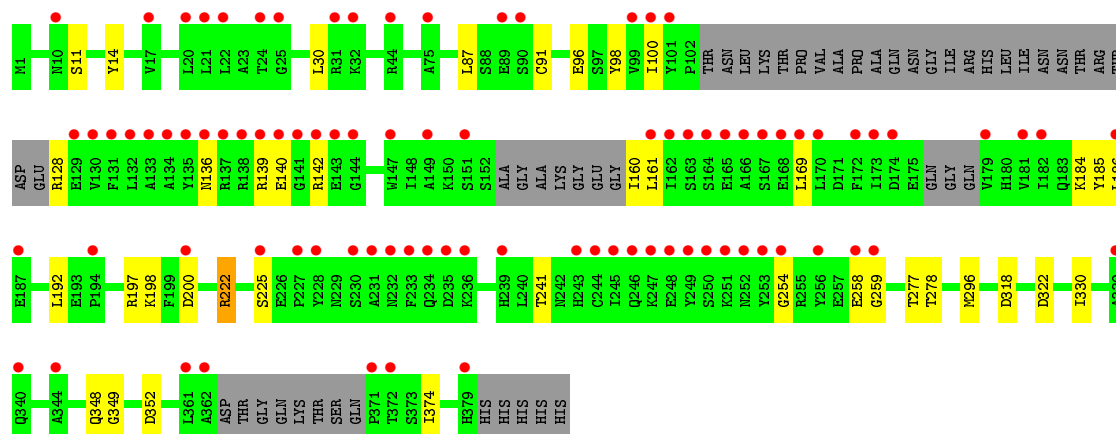




● Molecule 3: Stathmin-4



● Molecule 4: TUBULIN-TYROSINE LIGASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.40Å 157.36Å 180.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 2.30 49.55 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.55-2.30) 95.1 (49.55-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.160 , 0.195 0.171 , 0.198	Depositor DCC
R_{free} test set	1655 reflections (1.28%)	DCC
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 157606 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18021	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MG, CL, CA, GTP, ACP, 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	0.38	0/3582	0.53	0/4860
1	C	0.47	0/3565	0.57	0/4840
2	B	0.43	0/3405	0.54	0/4611
2	D	0.35	0/3405	0.48	0/4613
3	E	0.39	0/1029	0.48	0/1365
4	F	0.31	0/2823	0.47	0/3812
All	All	0.39	0/17809	0.52	0/24101

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3480	0	3415	23	0
1	C	3469	0	3392	28	0
2	B	3326	0	3219	28	0
2	D	3326	0	3208	27	0
3	E	1011	0	1035	5	0
4	F	2760	0	2741	21	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	C	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
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	2	0
10	B	24	0	24	3	0
11	F	31	0	14	1	0
12	A	89	0	0	3	0
12	B	97	0	0	10	0
12	C	181	0	0	4	0
12	D	43	0	0	4	0
12	E	19	0	0	0	0
12	F	35	0	0	4	0
All	All	18021	0	17096	131	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 4.

All (131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:432:TYR:OH	12:D:625:HOH:O	1.92	0.88
9:D:501:GDP:O1B	12:D:627:HOH:O	1.91	0.86
4:F:160:ILE:N	12:F:528:HOH:O	2.13	0.81
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.63	0.80
1:C:1:MET:O	12:C:724:HOH:O	2.01	0.78
2:B:163:ASP:OD1	12:B:665:HOH:O	2.05	0.74
2:B:221:THR:O	12:B:673:HOH:O	2.06	0.73
2:D:311[B]:ARG:NH2	2:D:345:GLU:OE1	2.21	0.72
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.20	0.72
2:D:240[B]:THR:HG21	2:D:320:ARG:HD2	1.71	0.72
4:F:30:LEU:O	12:F:521:HOH:O	2.08	0.71
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.74	0.69
1:A:3:GLU:OE2	12:A:687:HOH:O	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:OD2	12:A:669:HOH:O	2.12	0.67
4:F:200:ASP:OD1	4:F:222:ARG:NH2	2.25	0.67
2:B:179:ASP:OD2	12:B:683:HOH:O	2.12	0.66
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.27	0.66
2:B:421:ALA:O	12:B:670:HOH:O	2.15	0.64
2:D:431:GLU:OE1	12:D:614:HOH:O	2.14	0.63
11:F:402:ACP:O2G	11:F:402:ACP:O1B	2.18	0.60
1:C:438:ASP:OD1	12:C:725:HOH:O	2.15	0.60
1:C:18:ASN:OD1	12:C:748:HOH:O	2.17	0.60
4:F:140:GLU:HA	4:F:142:ARG:HH21	1.67	0.59
2:B:136:GLN:OE1	12:B:687:HOH:O	2.17	0.58
1:C:96:LYS:NZ	2:D:130:ASP:OD1	2.34	0.58
4:F:14:TYR:OH	12:F:508:HOH:O	2.06	0.57
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.86	0.57
1:C:210:TYR:CE1	1:C:214:ARG:HD2	2.40	0.57
1:A:209:ILE:HD11	1:A:302[A]:MET:SD	2.45	0.57
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.87	0.56
1:A:132:LEU:O	1:A:164:LYS:NZ	2.38	0.55
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.41	0.55
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.41	0.55
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.89	0.54
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.42	0.54
4:F:96:GLU:OE1	4:F:98:TYR:OH	2.25	0.53
1:A:386:GLU:O	1:A:390[A]:ARG:HD3	2.09	0.52
10:B:504:MES:H51	12:B:649:HOH:O	2.09	0.51
2:D:106:GLY:O	2:D:111:GLY:HA3	2.11	0.51
2:B:22:GLU:OE2	12:B:690:HOH:O	2.19	0.51
1:C:107:HIS:HD2	1:C:151[A]:SER:OG	1.94	0.51
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.93	0.50
2:D:216:THR:HG22	2:D:217:LEU:HD23	1.94	0.50
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.27	0.50
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.77	0.49
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.95	0.49
1:C:430:LYS:HE2	1:C:434:GLU:OE1	2.13	0.49
2:D:295:MET:HE3	2:D:375:ALA:HB1	1.94	0.49
2:D:294:GLN:OE1	12:D:631:HOH:O	2.20	0.49
4:F:161:LEU:HD23	4:F:169:LEU:HD23	1.94	0.48
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.94	0.48
4:F:100:ILE:HG23	4:F:128:ARG:HG3	1.95	0.48
2:D:147[B]:SER:OG	2:D:190:SER:OG	2.22	0.48
1:C:204:VAL:HG22	1:C:302[B]:MET:HE1	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.32	0.48
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.49	0.48
1:A:218:ASP:HB2	12:A:669:HOH:O	2.13	0.48
9:B:501:GDP:O2B	12:B:639:HOH:O	2.20	0.48
1:C:320:ARG:HA	1:C:356:ASN:O	2.14	0.47
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.96	0.47
2:D:236:SER:O	2:D:240[B]:THR:HG23	2.14	0.47
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.97	0.47
2:B:106:GLY:O	2:B:111:GLY:HA3	2.15	0.47
4:F:186:LEU:HD21	4:F:322:ASP:HB3	1.97	0.47
2:B:141:LEU:HD12	2:B:172:MET:SD	2.55	0.46
1:C:244:PHE:CG	1:C:358:GLN:HG3	2.51	0.46
1:C:209:ILE:HD11	1:C:302[A]:MET:HG3	1.98	0.46
2:B:248:LEU:HD23	2:B:354:ALA:HB2	1.97	0.46
2:B:48:ARG:NH1	2:B:244:PHE:O	2.49	0.46
4:F:87:LEU:O	4:F:91:CYS:HB2	2.15	0.46
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.98	0.46
1:C:244:PHE:CD1	1:C:358:GLN:HG3	2.51	0.45
1:A:3:GLU:O	1:A:133:GLN:HG2	2.18	0.44
1:A:34:GLY:HA3	1:A:60:LYS:HG3	2.00	0.44
2:B:136:GLN:HA	2:B:167:ASN:O	2.18	0.44
1:C:104:ALA:HB2	1:C:413:MET:SD	2.57	0.44
3:E:72:LEU:O	3:E:76:ARG:HG2	2.18	0.44
2:D:88:ARG:NH1	2:D:91:ASN:OD1	2.46	0.44
1:A:174:ALA:HA	1:A:175:PRO:HD3	1.88	0.44
2:B:295:MET:HE3	2:B:375:ALA:HB1	2.00	0.44
2:D:147[A]:SER:HB2	2:D:190:SER:HG	1.82	0.44
2:D:136:GLN:HA	2:D:167:ASN:O	2.18	0.44
1:A:262:TYR:HA	1:A:263:PRO:HD3	1.88	0.44
1:A:230:LEU:O	1:A:234:ILE:HD12	2.17	0.43
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.33	0.43
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.99	0.43
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.52	0.43
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.01	0.43
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.00	0.43
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.43
2:D:191:VAL:O	2:D:195:VAL:HG23	2.19	0.42
4:F:254:GLY:HA2	4:F:259:GLY:O	2.19	0.42
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.00	0.42
4:F:318:ASP:OD2	12:F:529:HOH:O	2.21	0.42
2:D:141:LEU:HD21	2:D:170:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.00	0.42
1:C:89:PRO:O	12:C:710:HOH:O	2.21	0.42
1:A:141:PHE:O	1:A:147:SER:HB3	2.20	0.42
2:B:431:GLU:OE1	12:B:656:HOH:O	2.22	0.42
1:A:77:GLU:HA	1:A:80:THR:HG22	2.02	0.42
4:F:277:THR:HG22	4:F:278:THR:H	1.85	0.42
2:B:270:PRO:HG2	2:B:302:MET:HB2	2.02	0.42
2:D:171:VAL:HA	2:D:204:ILE:O	2.20	0.42
2:B:164:ARG:HD2	12:B:668:HOH:O	2.19	0.42
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.26	0.42
3:E:47:LEU:HD11	3:E:51:GLN:HE21	1.84	0.41
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.02	0.41
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.37	0.41
3:E:52:LYS:HE2	3:E:52:LYS:HB3	1.70	0.41
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.60	0.41
2:D:405:LEU:HD12	2:D:405:LEU:HA	1.87	0.41
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.56	0.41
1:C:164:LYS:HB2	1:C:164:LYS:HE2	1.82	0.41
2:B:308:ARG:HH11	10:B:504:MES:H71	1.85	0.41
4:F:330:ILE:HA	4:F:330:ILE:HD13	1.83	0.41
1:C:346:TRP:CZ3	1:C:347[B]:CYS:SG	3.13	0.41
1:C:163:LYS:HE3	3:E:93:PHE:CD2	2.56	0.41
4:F:258:GLU:HA	4:F:259:GLY:HA2	1.71	0.41
4:F:136:ASN:HA	4:F:139:ARG:HB3	2.02	0.41
4:F:184:LYS:HE2	4:F:184:LYS:HB3	1.92	0.41
2:B:31:ASP:OD2	2:B:35:SER:HB2	2.21	0.41
2:B:298:SER:HA	2:B:301:MET:HG3	2.03	0.41
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.56	0.40
1:A:69:ASP:O	1:A:94:THR:HA	2.20	0.40
2:B:308:ARG:NH1	10:B:504:MES:H71	2.36	0.40
2:B:56:ALA:HB3	2:B:60:LYS:HB2	2.04	0.40
1:A:220:GLU:HB3	2:B:326:LYS:HD3	2.02	0.40
2:B:181:VAL:HG21	2:B:404:PHE:CZ	2.57	0.40
2:B:275:LEU:HA	2:B:275:LEU:HD23	1.93	0.40
2:D:360:PRO:HG2	2:D:371:LEU:HD12	2.04	0.40
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.54	0.40

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	446/451 (99%)	437 (98%)	8 (2%)	1 (0%)	52	64
1	C	445/451 (99%)	433 (97%)	12 (3%)	0	100	100
2	B	420/445 (94%)	409 (97%)	11 (3%)	0	100	100
2	D	420/445 (94%)	415 (99%)	5 (1%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	326/384 (85%)	318 (98%)	8 (2%)	0	100	100
All	All	2176/2319 (94%)	2130 (98%)	45 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	LYS

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	379/379 (100%)	376 (99%)	3 (1%)	86	94
1	C	378/379 (100%)	370 (98%)	8 (2%)	61	78
2	B	367/383 (96%)	362 (99%)	5 (1%)	74	86
2	D	367/383 (96%)	364 (99%)	3 (1%)	86	94
3	E	111/127 (87%)	107 (96%)	4 (4%)	42	57
4	F	304/342 (89%)	298 (98%)	6 (2%)	63	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1906/1993 (96%)	1877 (98%)	29 (2%)	72 85

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	84	ARG
1	A	221	ARG
2	B	77	SER
2	B	86	ILE
2	B	139	HIS
2	B	178	SER
2	B	414	ASP
1	C	1	MET
1	C	71	GLU
1	C	221	ARG
1	C	284	GLU
1	C	302[A]	MET
1	C	302[B]	MET
1	C	361	THR
1	C	381	THR
2	D	139	HIS
2	D	153	LEU
2	D	373	MET
3	E	67	GLU
3	E	124	GLN
3	E	131	GLU
3	E	141	GLU
4	F	11	SER
4	F	192	LEU
4	F	197	ARG
4	F	222	ARG
4	F	225	SER
4	F	296	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	107	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 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 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	25,34,34	0.79	1 (4%)	34,54,54	1.80	8 (23%)
9	GDP	B	501	7	23,30,30	1.09	2 (8%)	30,47,47	1.94	7 (23%)
10	MES	B	503	-	11,12,12	0.62	0	14,16,16	3.15	6 (42%)
10	MES	B	504	-	11,12,12	0.66	0	14,16,16	2.40	7 (50%)
5	GTP	C	501	6	25,34,34	0.89	1 (4%)	34,54,54	1.68	6 (17%)
9	GDP	D	501	7	23,30,30	1.11	2 (8%)	30,47,47	1.90	8 (26%)
11	ACP	F	402	6	25,33,33	1.92	7 (28%)	31,52,52	1.82	4 (12%)

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
9	GDP	B	501	7	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MES	B	503	-	-	0/6/14/14	0/1/1/1
10	MES	B	504	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
9	GDP	D	501	7	-	0/12/32/32	0/3/3/3
11	ACP	F	402	6	-	0/15/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	PB-O2B	-3.31	1.48	1.56
11	F	402	ACP	PG-O2G	-2.55	1.48	1.54
11	F	402	ACP	PG-O3G	2.25	1.60	1.54
5	A	501	GTP	C6-N1	2.32	1.37	1.33
5	C	501	GTP	C6-N1	2.63	1.38	1.33
9	B	501	GDP	C5-C4	2.64	1.46	1.40
9	D	501	GDP	C5-C4	2.89	1.47	1.40
11	F	402	ACP	PB-O3A	2.93	1.61	1.58
11	F	402	ACP	C5-C4	3.23	1.47	1.40
9	D	501	GDP	C6-C5	3.24	1.47	1.41
9	B	501	GDP	C6-C5	3.44	1.48	1.41
11	F	402	ACP	PB-O1B	3.88	1.61	1.51
11	F	402	ACP	PG-O1G	4.94	1.61	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	402	ACP	N3-C2-N1	-6.60	123.84	128.89
10	B	503	MES	O1S-S-C8	-5.98	101.80	106.91
5	A	501	GTP	N3-C2-N1	-5.22	119.49	127.44
5	C	501	GTP	N3-C2-N1	-4.74	120.23	127.44
11	F	402	ACP	PA-O3A-PB	-4.60	119.80	132.73
9	B	501	GDP	C6-C5-C4	-4.40	115.64	120.90
9	D	501	GDP	C5-C6-N1	-4.17	117.88	123.59
9	B	501	GDP	C1'-N9-C4	-3.84	121.16	126.94
9	B	501	GDP	N3-C2-N1	-3.50	122.12	127.44
9	D	501	GDP	C6-C5-C4	-3.47	116.75	120.90
9	B	501	GDP	C5-C6-N1	-3.45	118.88	123.59
5	C	501	GTP	C5-C6-N1	-3.26	119.13	123.59
9	D	501	GDP	PA-O3A-PB	-3.26	121.73	132.67
5	A	501	GTP	C5-C6-N1	-3.22	119.18	123.59
9	D	501	GDP	N3-C2-N1	-3.13	122.68	127.44
5	A	501	GTP	C1'-N9-C4	-3.10	122.26	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C4-C5-N7	-3.10	106.63	109.48
11	F	402	ACP	C4-C5-N7	-3.03	106.69	109.48
5	A	501	GTP	PA-O3A-PB	-2.98	124.35	132.73
9	B	501	GDP	C4-C5-N7	-2.95	106.77	109.48
5	C	501	GTP	PB-O3B-PG	-2.86	123.06	132.67
5	C	501	GTP	PA-O3A-PB	-2.71	125.13	132.73
5	C	501	GTP	C1'-N9-C4	-2.61	123.01	126.94
11	F	402	ACP	C2'-C1'-N9	-2.32	110.74	114.29
10	B	504	MES	C6-C5-N4	-2.28	106.67	110.12
9	D	501	GDP	C1'-N9-C4	-2.24	123.56	126.94
5	A	501	GTP	PB-O3B-PG	-2.20	125.28	132.67
5	A	501	GTP	C6-C5-C4	-2.15	118.33	120.90
10	B	504	MES	C2-C3-N4	-2.03	107.04	110.12
9	D	501	GDP	O3A-PA-O5'	-2.03	97.55	102.94
9	B	501	GDP	PA-O3A-PB	-2.02	125.89	132.67
10	B	503	MES	C2-C3-N4	-2.02	107.07	110.12
5	A	501	GTP	O2G-PG-O3B	2.01	114.23	105.09
10	B	503	MES	C7-N4-C3	2.13	116.73	111.27
10	B	503	MES	C7-N4-C5	2.41	117.44	111.27
10	B	504	MES	C7-N4-C3	2.75	118.31	111.27
10	B	504	MES	C7-N4-C5	2.81	118.48	111.27
10	B	504	MES	O2S-S-C8	3.07	109.52	106.91
10	B	504	MES	O1S-S-C8	3.15	109.59	106.91
5	C	501	GTP	C6-N1-C2	3.40	120.66	115.94
5	A	501	GTP	C6-N1-C2	3.77	121.17	115.94
10	B	503	MES	C5-N4-C3	4.30	118.22	108.90
9	D	501	GDP	C6-N1-C2	4.87	122.70	115.94
9	B	501	GDP	C6-N1-C2	4.90	122.74	115.94
10	B	504	MES	C5-N4-C3	5.40	120.58	108.90
10	B	503	MES	O2S-S-C8	7.85	113.60	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	501	GDP	1	0
10	B	504	MES	3	0
9	D	501	GDP	2	0
11	F	402	ACP	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	439/451 (97%)	0.09	14 (3%) 51 60	34, 52, 84, 126	0
1	C	440/451 (97%)	-0.24	2 (0%) 91 94	27, 40, 66, 83	0
2	B	422/445 (94%)	-0.04	13 (3%) 52 62	29, 48, 81, 130	1 (0%)
2	D	421/445 (94%)	0.27	31 (7%) 17 25	33, 60, 91, 119	4 (0%)
3	E	120/143 (83%)	0.14	9 (7%) 17 24	40, 65, 97, 113	0
4	F	336/384 (87%)	1.04	89 (26%) 1 1	43, 75, 134, 159	0
All	All	2178/2319 (93%)	0.18	158 (7%) 18 25	27, 54, 100, 159	5 (0%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	7.4
4	F	173	ILE	7.2
4	F	130	VAL	7.2
4	F	372	THR	6.9
2	D	57	THR	6.6
4	F	169	LEU	6.5
4	F	134	ALA	6.2
4	F	244	CYS	6.2
1	A	439	SER	6.1
4	F	89	GLU	6.1
2	B	57	THR	6.0
4	F	233	PHE	6.0
4	F	253	TYR	5.9
4	F	251	LYS	5.9
4	F	129	GLU	5.6
4	F	234	GLN	5.5
4	F	231	ALA	5.5
4	F	232	ASN	5.4
4	F	161	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	5.3
4	F	143	GLU	5.3
4	F	142	ARG	5.3
4	F	135	TYR	5.3
4	F	137	ARG	5.2
2	B	59	ASN	5.2
4	F	182	ILE	4.9
4	F	250	SER	4.9
2	D	276	THR	4.8
4	F	170	LEU	4.8
4	F	167	SER	4.7
4	F	133	ALA	4.6
4	F	131	PHE	4.5
2	B	277	SER	4.4
2	B	58	GLY	4.4
4	F	179	VAL	4.3
4	F	90	SER	4.2
2	D	94	PHE	4.2
4	F	99	VAL	4.1
4	F	166	ALA	4.1
4	F	245	ILE	4.1
4	F	165	GLU	4.0
4	F	20	LEU	4.0
2	D	37	HIS	4.0
4	F	252	ASN	3.9
4	F	235	ASP	3.9
3	E	139	LEU	3.9
4	F	248	GLU	3.9
4	F	132	LEU	3.9
2	B	33	THR	3.8
3	E	26	PRO	3.8
4	F	371	PRO	3.8
1	C	440	VAL	3.7
1	C	340	SER	3.7
2	D	59	ASN	3.7
2	D	400	ARG	3.7
4	F	362	ALA	3.7
4	F	138	ARG	3.7
4	F	186	LEU	3.6
4	F	136	ASN	3.6
2	D	56	ALA	3.5
4	F	100	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	438	ALA	3.4
4	F	227	PRO	3.4
4	F	344	ALA	3.4
2	D	179	ASP	3.4
2	D	407	TRP	3.3
4	F	230	SER	3.3
2	B	276	THR	3.3
4	F	101	TYR	3.3
2	B	82	PRO	3.2
2	D	33	THR	3.2
4	F	10	ASN	3.2
4	F	151	SER	3.1
4	F	361	LEU	3.1
4	F	256	TYR	3.1
4	F	236	LYS	3.1
1	A	42	ILE	3.0
2	B	37	HIS	3.1
1	A	280	LYS	3.0
4	F	339	ALA	2.9
4	F	22	LEU	2.9
4	F	174	ASP	2.9
4	F	247	LYS	2.9
2	D	414	ASP	2.8
4	F	31	ARG	2.8
2	D	401	ARG	2.8
4	F	144	GLY	2.8
1	A	171	ILE	2.7
4	F	25	GLY	2.7
4	F	194	PRO	2.7
3	E	27	PRO	2.7
4	F	140	GLU	2.7
4	F	200	ASP	2.7
2	D	405	LEU	2.7
1	A	41	THR	2.7
2	B	56	ALA	2.6
4	F	243	HIS	2.6
4	F	379	HIS	2.6
4	F	172	PHE	2.6
2	B	437	ASP	2.6
3	E	140	LYS	2.6
2	D	85	GLN	2.6
2	B	41	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	225	SER	2.6
4	F	181	VAL	2.6
1	A	345	ASP	2.6
2	D	220	THR	2.6
4	F	75	ALA	2.6
4	F	17	VAL	2.6
4	F	162	ILE	2.5
4	F	228	TYR	2.5
3	E	6	MET	2.5
2	D	58	GLY	2.5
4	F	239	HIS	2.5
4	F	258	GLU	2.5
1	A	346	TRP	2.5
4	F	149	ALA	2.4
4	F	24	THR	2.4
3	E	48	GLU	2.4
4	F	147	TRP	2.4
2	D	406	HIS	2.4
4	F	340	GLN	2.4
2	B	38	GLY	2.4
4	F	141	GLY	2.4
2	D	82	PRO	2.4
4	F	254	GLY	2.3
2	D	404	PHE	2.3
4	F	187	GLU	2.3
4	F	139	ARG	2.3
4	F	163	SER	2.3
1	A	12	ALA	2.3
4	F	246	GLN	2.3
4	F	21	LEU	2.3
2	D	269	MET	2.3
2	D	317	ALA	2.2
1	A	283	HIS	2.2
4	F	164	SER	2.2
4	F	168	GLU	2.2
2	D	415	GLU	2.2
4	F	32	LYS	2.2
2	D	60	LYS	2.1
4	F	259	GLY	2.1
2	D	73	GLY	2.1
1	A	37	PRO	2.1
1	A	364	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	77	SER	2.1
2	D	74	THR	2.1
2	D	268	PHE	2.1
1	A	262	TYR	2.1
3	E	132	GLU	2.1
3	E	141	GLU	2.1
2	D	396	THR	2.0
3	E	138	GLU	2.0
1	A	9	VAL	2.0
2	D	96	GLN	2.0
2	D	221	THR	2.0
2	D	259	MET	2.0
4	F	44	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
10	MES	B	504	12/12	0.86	0.22	4.83	86,90,112,117	0
10	MES	B	503	12/12	0.97	0.14	0.76	43,48,68,72	0
6	MG	C	502	1/1	0.84	0.17	0.70	33,33,33,33	0
5	GTP	C	501	32/32	0.98	0.13	0.03	25,29,34,44	0
9	GDP	B	501	28/28	0.99	0.14	-0.11	24,37,41,44	0
9	GDP	D	501	28/28	0.96	0.11	-0.18	45,54,64,69	0
5	GTP	A	501	32/32	0.98	0.18	-0.25	27,35,42,58	0
7	CA	B	502	1/1	0.93	0.11	-1.07	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	CL	C	504	1/1	0.87	0.10	-1.12	68,68,68,68	0
11	ACP	F	402	31/31	0.90	0.15	-1.30	69,82,133,139	0
7	CA	A	503	1/1	0.97	0.05	-1.67	65,65,65,65	0
6	MG	F	401	1/1	0.89	0.04	-2.75	68,68,68,68	0
7	CA	C	503	1/1	0.95	0.04	-4.87	50,50,50,50	0
6	MG	A	502	1/1	0.88	0.12	-	36,36,36,36	0
7	CA	B	505	1/1	0.97	0.13	-	44,44,44,44	0
8	CL	A	504	1/1	0.83	0.10	-	74,74,74,74	0
7	CA	D	502	1/1	0.88	0.07	-	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.