



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:36 am GMT

PDB ID : 4O4J
Title : Tubulin-Peloruside A 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 : 2.20 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 : trunk28620
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) : recalc28949

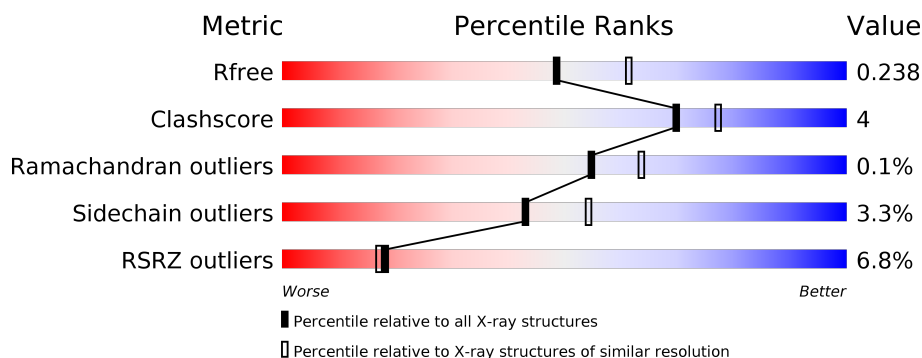
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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>%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>• • •</div> </div> </div>
1	C	451	<div> <div></div> <div>90%</div> <div>6%</div> <div>• •</div> </div>
2	B	445	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• • •</div> </div> </div>
2	D	445	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>•</div> </div> </div>
3	E	143	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>6%</div> <div>14%</div> </div> </div>
4	F	384	<div> <div>32%</div> <div> <div></div> <div>50%</div> <div>16%</div> <div>•</div> <div>31%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MG	C	502	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18124 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	12	0
			3485	2213	587	661	24			
1	C	440	Total	C	N	O	S	0	15	0
			3496	2218	585	667	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	12	0
			3424	2151	581	664	28			
2	D	431	Total	C	N	O	S	0	6	0
			3413	2145	580	659	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	6	0
			1044	645	188	206	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

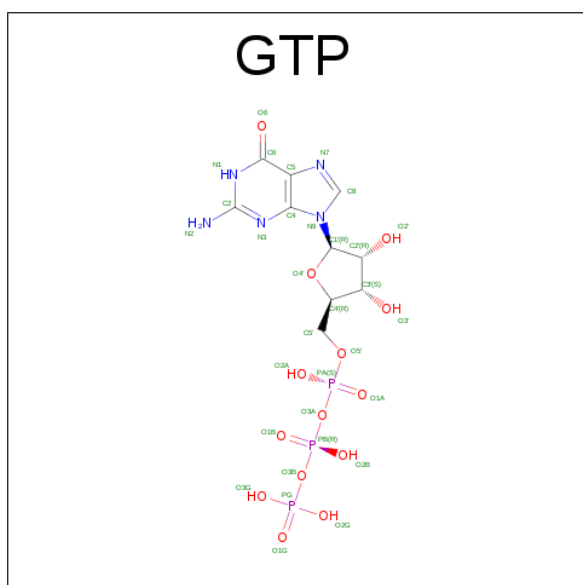
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	265	Total	C	N	O	S	0	1	0
			2179	1409	370	386	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		

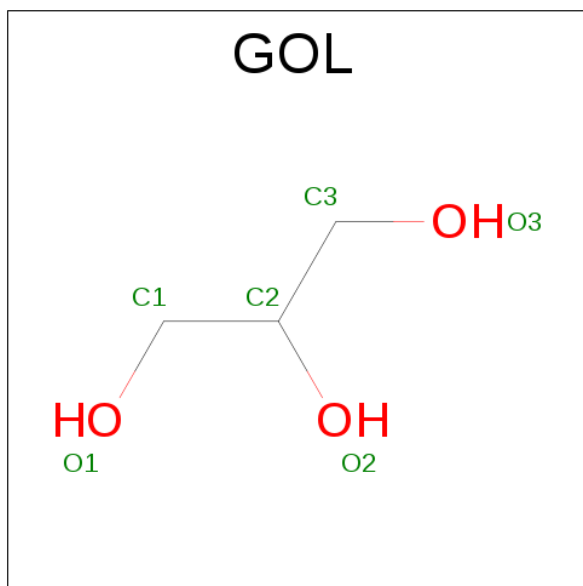
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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		

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

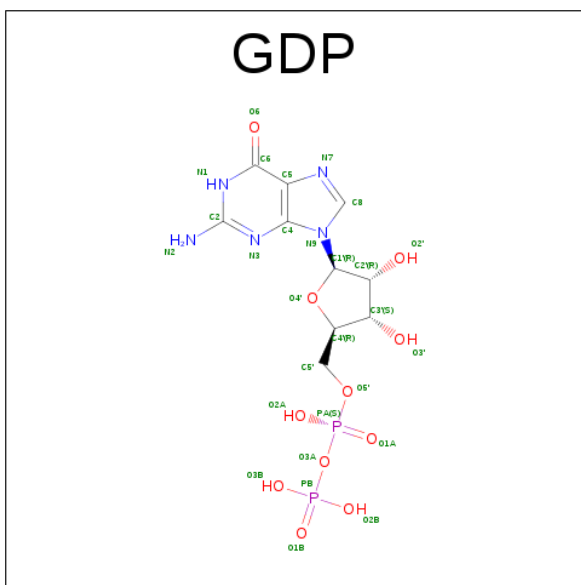
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



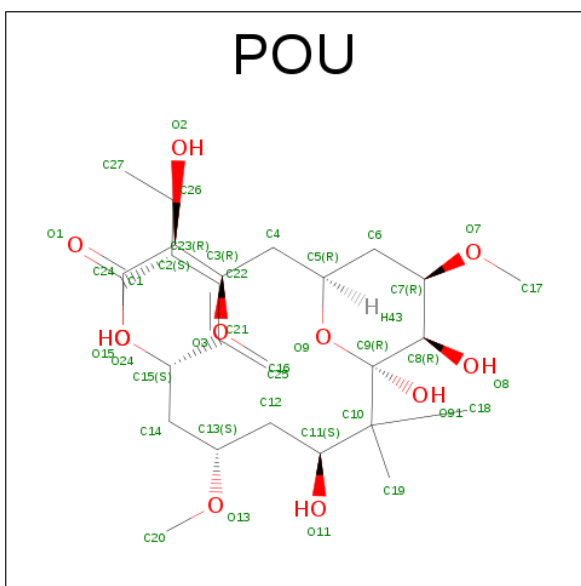
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

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



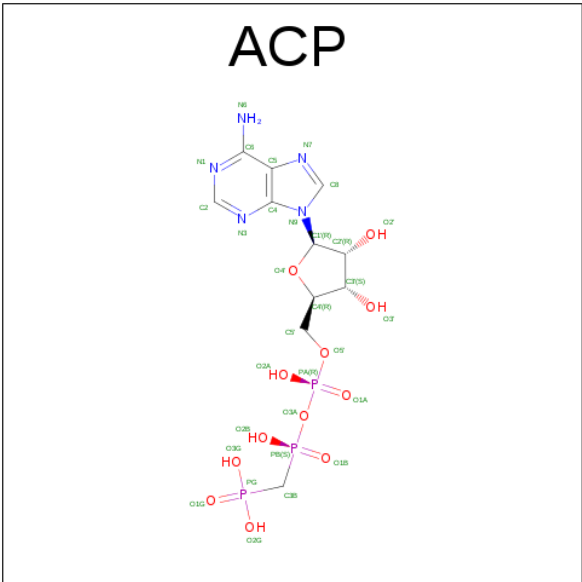
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 10 is PELORUSIDE A (three-letter code: POU) (formula: $C_{27}H_{48}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total 38	C 27	O 11	0	0
10	D	1	Total 38	C 27	O 11	0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

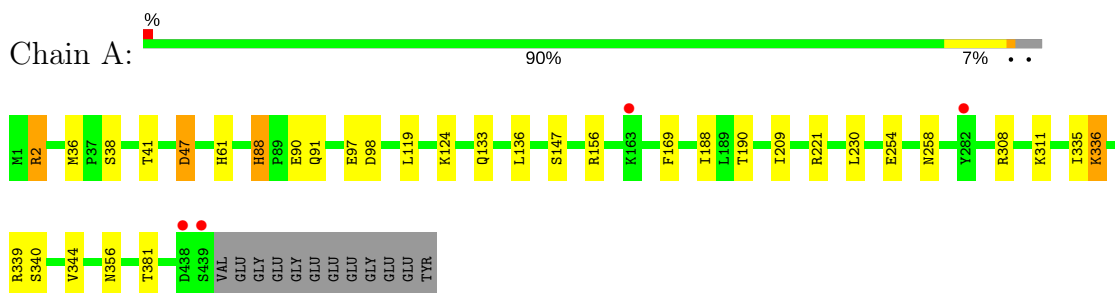
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	191	Total	O	0	0
			191	191		
12	B	210	Total	O	0	0
			210	210		
12	C	264	Total	O	0	0
			264	264		
12	D	116	Total	O	0	0
			116	116		
12	E	43	Total	O	0	0
			43	43		
12	F	21	Total	O	0	0
			21	21		

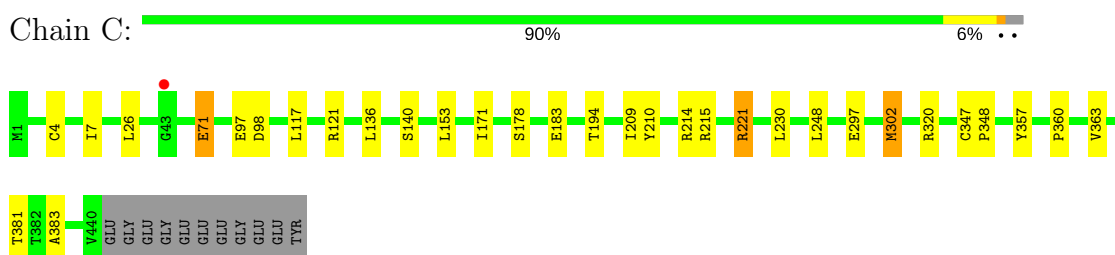
3 Residue-property plots [i](#)

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.

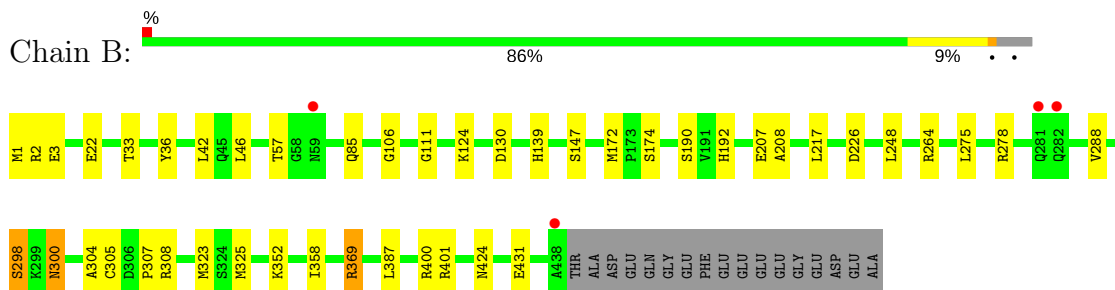
• Molecule 1: Tubulin alpha-1B chain



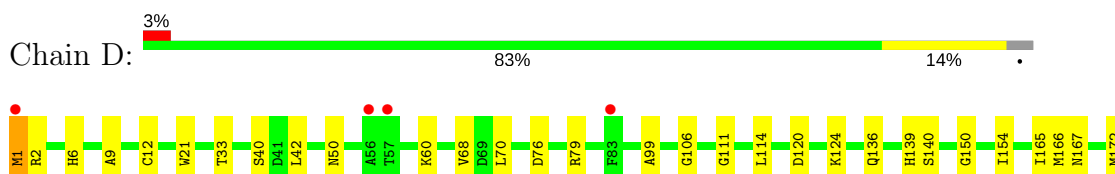
• Molecule 1: Tubulin alpha-1B chain



• Molecule 2: Tubulin beta-2B chain

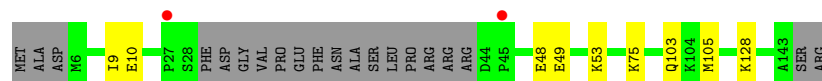
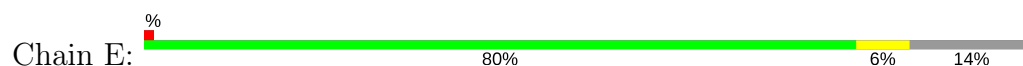


• Molecule 2: Tubulin beta-2B chain

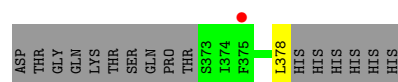
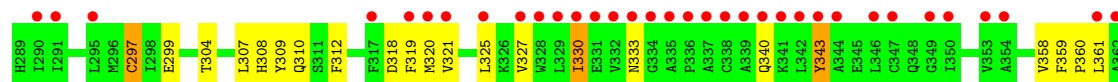
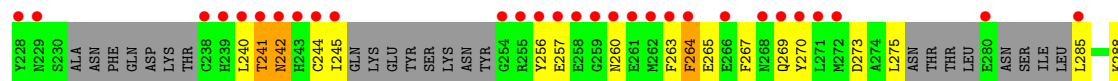
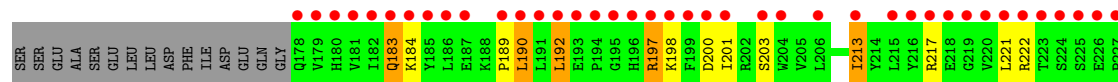
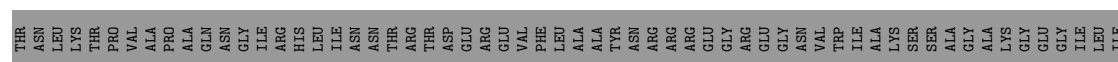
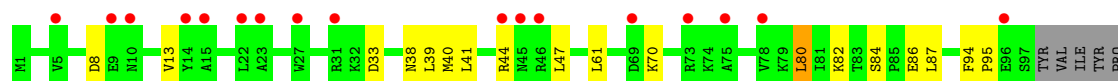




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.37Å 157.84Å 180.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.30 – 2.20 72.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (72.30-2.20) 99.7 (72.30-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.201 , 0.239 0.199 , 0.238	Depositor DCC
R_{free} test set	7566 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18124	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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, CA, POU, GTP, ACP

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	0.29	0/3599	0.47	0/4887
1	C	0.35	0/3619	0.51	0/4917
2	B	0.31	0/3532	0.48	0/4783
2	D	0.27	0/3506	0.45	0/4751
3	E	0.28	0/1071	0.38	0/1423
4	F	0.25	0/2230	0.46	0/3006
All	All	0.30	0/17557	0.47	0/23767

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	3485	0	3436	17	0
1	C	3496	0	3440	22	0
2	B	3424	0	3319	29	0
2	D	3413	0	3310	35	0
3	E	1044	0	1068	4	0
4	F	2179	0	2178	36	0
5	A	32	0	12	1	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	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	38	0	48	3	0
10	D	38	0	48	2	0
11	F	31	0	14	1	0
12	A	191	0	0	1	0
12	B	210	0	0	5	0
12	C	264	0	0	4	0
12	D	116	0	0	2	0
12	E	43	0	0	1	0
12	F	21	0	0	0	0
All	All	18124	0	16917	143	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 (143) 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)
3:E:9:ILE:HG22	3:E:10:GLU:HG3	1.70	0.74
1:C:381:THR:HG22	1:C:383:ALA:H	1.51	0.73
2:B:298:SER:HB3	2:B:307:PRO:HD2	1.71	0.71
2:B:22:GLU:OE2	12:B:802:HOH:O	2.09	0.70
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.23	0.70
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.73	0.68
4:F:61[B]:LEU:HG	4:F:310:GLN:HB2	1.76	0.68
2:D:2:ARG:HH21	2:D:50:ASN:HB2	1.63	0.64
4:F:318:ASP:HB3	4:F:330:ILE:HD12	1.79	0.64
2:D:176:LYS:NZ	2:D:211:ASP:OD1	2.24	0.63
4:F:321:VAL:HG12	4:F:327:VAL:HG22	1.80	0.62
1:A:356:ASN:ND2	12:A:664:HOH:O	2.31	0.62
1:C:297:GLU:OE2	12:C:755:HOH:O	2.16	0.61
3:E:53:LYS:NZ	12:E:217:HOH:O	2.34	0.60
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:VAL:HG22	2:B:323:MET:HE3	1.84	0.59
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.20	0.59
1:A:47:ASP:OD1	1:A:47:ASP:N	2.35	0.58
2:B:217:LEU:O	12:B:795:HOH:O	2.17	0.58
4:F:13:VAL:HA	4:F:343:TYR:HE1	1.69	0.57
2:B:147[A]:SER:HG	2:B:190:SER:HG	1.51	0.57
4:F:269:GLN:O	4:F:273:ASP:N	2.32	0.57
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.40	0.57
4:F:263:PHE:O	4:F:265:GLU:N	2.39	0.56
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.87	0.55
4:F:201:ILE:O	4:F:319:PHE:N	2.32	0.55
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.89	0.55
4:F:242:ASN:N	4:F:242:ASN:OD1	2.40	0.53
2:B:264:ARG:NE	2:B:431[A]:GLU:OE2	2.34	0.53
2:D:136:GLN:HA	2:D:167:ASN:O	2.09	0.52
2:D:76:ASP:OD1	2:D:79:ARG:NH1	2.40	0.52
4:F:242:ASN:O	4:F:245:ILE:N	2.38	0.52
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.92	0.51
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.92	0.51
4:F:201:ILE:HB	4:F:319:PHE:HB2	1.92	0.51
2:D:215:ARG:NH1	12:D:652:HOH:O	2.40	0.51
1:A:97:GLU:HB2	2:B:1:MET:HG2	1.93	0.50
2:D:106:GLY:O	2:D:111:GLY:HA3	2.12	0.50
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.94	0.50
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.94	0.50
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.94	0.49
4:F:190:LEU:HB2	4:F:321:VAL:HG23	1.94	0.49
2:B:106:GLY:O	2:B:111:GLY:HA3	2.13	0.49
2:B:208:ALA:HB2	2:B:304:ALA:N	2.26	0.49
2:D:120:ASP:O	2:D:124:LYS:HG2	2.12	0.49
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.94	0.49
2:B:305:CYS:O	2:B:307:PRO:HD3	2.11	0.49
2:B:300:ASN:O	12:B:798:HOH:O	2.20	0.49
4:F:61[A]:LEU:HD11	4:F:312:PHE:HD2	1.77	0.49
1:A:308:ARG:HG2	1:A:340:SER:HB3	1.95	0.48
2:D:173:PRO:HG2	2:D:187:ALA:HB2	1.95	0.48
2:B:226:ASP:HA	2:B:278:ARG:HD2	1.95	0.48
2:B:42:LEU:HB3	2:B:358:ILE:HD11	1.96	0.48
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.53	0.48
2:B:304:ALA:N	12:B:616:HOH:O	2.46	0.48
1:C:360:PRO:HB2	12:C:787:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:213:ILE:HB	4:F:378:LEU:HB2	1.96	0.48
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.96	0.47
12:B:649:HOH:O	3:E:75:LYS:HD2	2.15	0.47
2:B:226:ASP:OD1	2:B:278:ARG:NH2	2.40	0.47
2:B:248:LEU:HD11	2:B:352:LYS:HB3	1.96	0.47
1:C:221:ARG:HD2	2:D:329:ASP:OD2	2.15	0.47
2:D:277:SER:O	2:D:278:ARG:HB3	2.14	0.47
1:C:97:GLU:HG3	2:D:1:MET:HE3	1.97	0.47
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.15	0.47
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.30	0.46
1:C:381:THR:HG23	12:C:626:HOH:O	2.15	0.46
4:F:86:GLU:OE2	4:F:297:CYS:HA	2.15	0.46
4:F:257:GLU:HB2	4:F:260:ASN:HA	1.98	0.46
2:D:297:ASP:OD2	2:D:299:LYS:NZ	2.37	0.46
4:F:221:LEU:HD21	4:F:267:PHE:CG	2.50	0.46
4:F:80:LEU:O	4:F:84:SER:OG	2.22	0.46
10:D:503:POU:H27	10:D:503:POU:O15	2.16	0.45
10:D:503:POU:H46	10:D:503:POU:H40	1.80	0.45
3:E:128:LYS:HA	3:E:128:LYS:HD3	1.72	0.45
2:D:33:THR:O	2:D:60:LYS:NZ	2.35	0.45
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.71	0.45
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.99	0.45
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.35	0.45
1:A:136[B]:LEU:HD23	1:A:169:PHE:HE2	1.82	0.44
1:A:221:ARG:HG3	2:B:325:MET:HB3	1.99	0.44
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.44
11:F:401:ACP:O2G	11:F:401:ACP:O2B	2.35	0.44
4:F:192:LEU:HA	4:F:270:TYR:CZ	2.53	0.44
1:C:178:SER:HB2	1:C:183:GLU:OE2	2.17	0.44
1:C:26:LEU:HD12	1:C:363[B]:VAL:HG12	2.00	0.44
4:F:61[B]:LEU:CD1	4:F:358:VAL:HG11	2.48	0.44
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.33	0.43
4:F:94:PHE:HA	4:F:95:PRO:HD2	1.88	0.43
1:A:2:ARG:HB3	1:A:133:GLN:HG2	2.00	0.43
2:B:33:THR:HG22	2:B:85:GLN:NE2	2.33	0.43
1:C:140:SER:HA	1:C:171:ILE:HB	2.00	0.43
2:B:275:LEU:HA	2:B:275:LEU:HD23	1.88	0.43
2:D:172:MET:HA	2:D:173:PRO:HD3	1.85	0.43
2:D:305:CYS:SG	2:D:387:LEU:HB2	2.57	0.43
4:F:222:ARG:HB3	4:F:241:THR:OG1	2.17	0.43
2:B:2:ARG:HD2	2:B:130:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:61[B]:LEU:HD11	4:F:358:VAL:HG11	1.99	0.43
2:B:192:HIS:CE1	2:B:424:ASN:HD22	2.36	0.43
4:F:82:LYS:HB2	4:F:82:LYS:HE3	1.71	0.43
10:B:503:POU:H40	10:B:503:POU:H46	1.91	0.43
4:F:304:THR:HG22	4:F:307:LEU:HD12	2.00	0.43
4:F:8:ASP:OD2	4:F:44:ARG:NH1	2.52	0.43
1:C:209:ILE:HD11	1:C:302:MET:HG3	2.00	0.43
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.01	0.43
2:D:40:SER:OG	2:D:42:LEU:HB2	2.19	0.43
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.01	0.42
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.53	0.42
1:C:97:GLU:HG3	2:D:1:MET:HB2	2.02	0.42
1:C:210:TYR:CE2	1:C:214:ARG:HD2	2.55	0.42
2:D:333:LEU:HG	12:D:642:HOH:O	2.20	0.42
1:C:347[A]:CYS:HA	1:C:348:PRO:HD3	1.93	0.42
1:A:88:HIS:ND1	1:A:91:GLN:OE1	2.50	0.42
2:D:191:VAL:O	2:D:195:VAL:HG23	2.19	0.42
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.02	0.42
2:D:150:GLY:O	2:D:154:ILE:HG12	2.20	0.42
4:F:38:ASN:HB3	4:F:359:PHE:CZ	2.55	0.42
2:B:2:ARG:HG3	2:B:3:GLU:OE2	2.20	0.42
4:F:330:ILE:H	4:F:330:ILE:HG13	1.64	0.42
1:C:194[B]:THR:HG21	12:C:617:HOH:O	2.19	0.42
2:D:12:CYS:HB3	2:D:140:SER:HB3	2.02	0.42
1:A:311:LYS:HD3	1:A:344:VAL:HA	2.02	0.41
2:B:124:LYS:HE3	2:B:124:LYS:HB2	1.86	0.41
10:B:503:POU:H27	10:B:503:POU:O15	2.20	0.41
4:F:358:VAL:O	4:F:360:PRO:HD3	2.21	0.41
1:C:221:ARG:HD3	2:D:325:MET:SD	2.61	0.41
4:F:40:MET:HE1	4:F:47:LEU:HG	2.03	0.41
1:C:209:ILE:HG23	1:C:230:LEU:HD23	2.03	0.41
2:D:298:SER:OG	2:D:307:PRO:HD2	2.21	0.41
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.21	0.41
4:F:84:SER:OG	4:F:87:LEU:HB3	2.20	0.41
2:D:9:ALA:HA	2:D:68:VAL:O	2.21	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.04	0.40
10:B:503:POU:H32	10:B:503:POU:H8	1.89	0.40
4:F:183:GLN:HG2	4:F:184:LYS:N	2.36	0.40
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.21	0.40
2:B:369:ARG:HB2	2:B:369:ARG:HE	1.49	0.40
2:D:274:PRO:HB3	2:D:286:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:297:ASP:OD1	2:D:298:SER:N	2.55	0.40
2:D:70:LEU:HD23	2:D:114:LEU:HD22	2.02	0.40
4:F:318:ASP:HB2	4:F:330:ILE:O	2.21	0.40
4:F:307:LEU:HD13	4:F:309:TYR:CE1	2.56	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	449/451 (100%)	440 (98%)	9 (2%)	0	100	100
1	C	453/451 (100%)	441 (97%)	12 (3%)	0	100	100
2	B	438/445 (98%)	430 (98%)	8 (2%)	0	100	100
2	D	435/445 (98%)	421 (97%)	14 (3%)	0	100	100
3	E	125/143 (87%)	123 (98%)	2 (2%)	0	100	100
4	F	253/384 (66%)	239 (94%)	12 (5%)	2 (1%)	22	21
All	All	2153/2319 (93%)	2094 (97%)	57 (3%)	2 (0%)	55	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	264	PHE
4	F	189	PRO

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	382/379 (101%)	372 (97%)	10 (3%)	51	64
1	C	386/379 (102%)	382 (99%)	4 (1%)	80	89
2	B	382/383 (100%)	376 (98%)	6 (2%)	68	81
2	D	378/383 (99%)	372 (98%)	6 (2%)	68	81
3	E	116/127 (91%)	112 (97%)	4 (3%)	42	53
4	F	241/342 (70%)	211 (88%)	30 (12%)	5	4
All	All	1885/1993 (95%)	1825 (97%)	60 (3%)	43	56

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	38	SER
1	A	41	THR
1	A	47	ASP
1	A	88	HIS
1	A	90	GLU
1	A	124	LYS
1	A	188	ILE
1	A	336	LYS
1	A	381	THR
2	B	57	THR
2	B	139	HIS
2	B	298	SER
2	B	300	ASN
2	B	308	ARG
2	B	369	ARG
1	C	71	GLU
1	C	215	ARG
1	C	221	ARG
1	C	302	MET
2	D	1	MET
2	D	139	HIS
2	D	179	ASP
2	D	282	GLN
2	D	284	ARG
2	D	308	ARG
3	E	48	GLU

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Mol	Chain	Res	Type
3	E	49	GLU
3	E	103	GLN
3	E	105	MET
4	F	33	ASP
4	F	70	LYS
4	F	80	LEU
4	F	183	GLN
4	F	190	LEU
4	F	192	LEU
4	F	197	ARG
4	F	198	LYS
4	F	203	SER
4	F	213	ILE
4	F	217	ARG
4	F	240	LEU
4	F	241	THR
4	F	242	ASN
4	F	244	CYS
4	F	256	TYR
4	F	264	PHE
4	F	275	LEU
4	F	285	LEU
4	F	288	LYS
4	F	297	CYS
4	F	299	GLU
4	F	308	HIS
4	F	320	MET
4	F	325	LEU
4	F	330	ILE
4	F	333	ASN
4	F	340	GLN
4	F	343	TYR
4	F	361	LEU

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 molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 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	0.96	1 (3%)	27,54,54	1.82	6 (22%)
8	GOL	A	504	-	5,5,5	0.35	0	5,5,5	0.26	0
9	GDP	B	501	6	25,30,30	1.16	2 (8%)	26,47,47	1.92	6 (23%)
10	POU	B	503	-	35,39,39	2.32	7 (20%)	42,57,57	2.10	11 (26%)
5	GTP	C	501	6	27,34,34	0.95	2 (7%)	27,54,54	1.62	5 (18%)
9	GDP	D	501	-	25,30,30	1.11	2 (8%)	26,47,47	1.96	6 (23%)
10	POU	D	503	-	35,39,39	2.16	6 (17%)	42,57,57	1.92	9 (21%)
11	ACP	F	401	-	27,33,33	1.42	5 (18%)	30,52,52	1.71	4 (13%)

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
8	GOL	A	504	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
10	POU	B	503	-	-	1/54/76/76	0/0/2/2
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	D	501	-	-	0/12/32/32	0/3/3/3
10	POU	D	503	-	-	1/54/76/76	0/0/2/2
11	ACP	F	401	-	-	0/15/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	POU	C2-C1	-5.11	1.39	1.52
10	D	503	POU	C2-C1	-4.96	1.39	1.52
10	B	503	POU	C14-C15	2.01	1.56	1.53
10	B	503	POU	O11-C11	2.10	1.47	1.43
5	C	501	GTP	C2-N1	2.11	1.39	1.35
11	F	401	ACP	PB-O2B	2.21	1.61	1.56
10	D	503	POU	C23-C22	2.21	1.53	1.50
10	B	503	POU	C14-C13	2.23	1.57	1.52
10	B	503	POU	C23-C22	2.55	1.54	1.50
10	D	503	POU	O91-C9	2.65	1.44	1.39
10	B	503	POU	O91-C9	2.66	1.44	1.39
11	F	401	ACP	PG-O3G	2.72	1.61	1.54
5	C	501	GTP	C6-N1	2.80	1.38	1.33
5	A	501	GTP	C6-N1	2.81	1.38	1.33
10	D	503	POU	C14-C13	2.83	1.59	1.52
9	B	501	GDP	C5-C4	2.84	1.46	1.40
11	F	401	ACP	PG-O2G	2.86	1.61	1.54
9	D	501	GDP	C5-C4	2.92	1.47	1.40
11	F	401	ACP	PB-O3A	2.97	1.61	1.58
11	F	401	ACP	C5-C4	3.14	1.47	1.40
9	D	501	GDP	C6-C5	3.47	1.48	1.41
10	D	503	POU	C14-C15	3.76	1.60	1.53
9	B	501	GDP	C6-C5	3.90	1.48	1.41
10	D	503	POU	C22-C21	9.24	1.54	1.33
10	B	503	POU	C22-C21	10.33	1.56	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	POU	C13-C12-C11	-7.69	104.62	114.42
10	D	503	POU	C13-C12-C11	-7.41	104.98	114.42
11	F	401	ACP	N3-C2-N1	-6.05	123.58	128.86
5	A	501	GTP	N3-C2-N1	-5.02	120.12	127.46
5	C	501	GTP	N3-C2-N1	-4.93	120.25	127.46
9	D	501	GDP	C5-C6-N1	-4.01	117.77	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C6-C5-C4	-3.94	116.93	120.84
9	B	501	GDP	C6-C5-C4	-3.68	117.19	120.84
9	B	501	GDP	C5-C6-N1	-3.63	118.32	123.48
5	A	501	GTP	C5-C6-N1	-3.51	118.48	123.48
10	D	503	POU	C3-C4-C5	-3.47	106.62	114.79
11	F	401	ACP	C4-C5-N7	-3.27	106.25	109.41
11	F	401	ACP	PA-O3A-PB	-3.23	121.97	132.39
9	D	501	GDP	N3-C2-N1	-3.05	123.01	127.46
9	B	501	GDP	C4-C5-N7	-3.01	106.50	109.41
10	B	503	POU	C3-C4-C5	-3.00	107.72	114.79
9	D	501	GDP	C4-C5-N7	-2.98	106.53	109.41
9	B	501	GDP	N3-C2-N1	-2.95	123.15	127.46
10	B	503	POU	C26-C23-C24	-2.81	105.74	111.80
5	C	501	GTP	C5-C6-N1	-2.74	119.58	123.48
10	D	503	POU	O91-C9-O9	-2.64	103.20	109.67
5	A	501	GTP	O5'-PA-O1A	-2.47	99.27	109.25
10	B	503	POU	O91-C9-O9	-2.33	103.94	109.67
5	A	501	GTP	C1'-N9-C4	-2.19	122.86	126.64
10	D	503	POU	C26-C23-C24	-2.18	107.10	111.80
11	F	401	ACP	C2'-C3'-C4'	-2.15	98.44	102.62
10	B	503	POU	C25-C21-C22	-2.09	117.60	123.34
10	D	503	POU	O9-C5-C6	2.07	112.80	108.85
5	C	501	GTP	N2-C2-N1	2.08	120.56	117.24
10	B	503	POU	O9-C5-C6	2.09	112.84	108.85
10	B	503	POU	O9-C5-C4	2.12	109.58	105.99
10	B	503	POU	O13-C13-C12	2.31	113.66	108.11
10	D	503	POU	O15-C15-C21	2.54	116.81	109.60
5	C	501	GTP	C6-N1-C2	2.63	119.85	116.06
10	D	503	POU	O13-C13-C12	2.81	114.87	108.11
10	B	503	POU	O15-C15-C14	2.88	113.09	106.62
5	A	501	GTP	C2-N3-C4	2.97	118.62	115.16
10	D	503	POU	O15-C15-C14	3.23	113.87	106.62
10	B	503	POU	O15-C15-C21	3.52	119.58	109.60
5	A	501	GTP	C6-N1-C2	3.64	121.30	116.06
5	C	501	GTP	C2-N3-C4	3.72	119.50	115.16
9	B	501	GDP	C6-N1-C2	4.07	121.91	116.06
10	D	503	POU	C15-O15-C1	4.22	124.79	116.74
9	D	501	GDP	C2-N3-C4	4.33	120.21	115.16
9	D	501	GDP	C6-N1-C2	4.46	122.47	116.06
9	B	501	GDP	C2-N3-C4	4.91	120.89	115.16
10	B	503	POU	C15-O15-C1	5.35	126.93	116.74

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	503	POU	C23-C22-C21-C15
10	D	503	POU	C23-C22-C21-C15

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
10	B	503	POU	3	0
10	D	503	POU	2	0
11	F	401	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%)	-0.22	4 (0%) 84 83	17, 32, 66, 112	0
1	C	440/451 (97%)	-0.28	1 (0%) 94 94	11, 22, 45, 68	0
2	B	428/445 (96%)	-0.18	4 (0%) 84 83	13, 27, 60, 112	2 (0%)
2	D	431/445 (96%)	-0.02	12 (2%) 53 51	18, 44, 77, 102	6 (1%)
3	E	123/143 (86%)	0.10	2 (1%) 72 70	25, 44, 85, 121	0
4	F	265/384 (69%)	2.28	121 (45%) 0 0	39, 79, 123, 153	0
All	All	2126/2319 (91%)	0.15	144 (6%) 18 17	11, 35, 92, 153	8 (0%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	194	PRO	12.5
4	F	182	ILE	10.5
4	F	240	LEU	9.3
4	F	241	THR	9.2
4	F	227	PRO	7.9
4	F	179	VAL	7.9
4	F	195	GLY	7.8
4	F	245	ILE	7.7
1	A	439	SER	7.2
4	F	244	CYS	7.2
4	F	178	GLN	7.0
4	F	192	LEU	6.9
4	F	243	HIS	6.6
4	F	338	CYS	6.6
4	F	44	ARG	6.5
4	F	238	CYS	6.4
4	F	375	PHE	6.2
4	F	184	LYS	6.0
1	A	282	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
4	F	255	ARG	6.0
4	F	258	GLU	5.9
4	F	199	PHE	5.7
4	F	271	LEU	5.7
4	F	201	ILE	5.5
4	F	362	ALA	5.5
4	F	229	ASN	5.4
4	F	183	GLN	5.4
4	F	198	LYS	5.4
4	F	190	LEU	5.3
4	F	75	ALA	5.1
4	F	346	LEU	5.1
4	F	216	TYR	5.0
4	F	180	HIS	4.9
4	F	330	ILE	4.9
4	F	181	VAL	4.9
4	F	221	LEU	4.9
4	F	186	LEU	4.7
4	F	319	PHE	4.7
4	F	225	SER	4.7
2	B	282	GLN	4.6
4	F	361	LEU	4.6
2	D	1	MET	4.6
4	F	242	ASN	4.6
4	F	269	GLN	4.5
4	F	333	ASN	4.5
2	B	281	GLN	4.5
4	F	261	GLU	4.5
4	F	343	TYR	4.4
4	F	340	GLN	4.4
4	F	223	THR	4.4
4	F	73	ARG	4.4
4	F	339	ALA	4.4
4	F	332	VAL	4.3
4	F	280	GLU	4.3
4	F	268	ASN	4.3
4	F	350	ILE	4.2
4	F	353	VAL	4.2
4	F	206	LEU	4.1
4	F	341	LYS	4.1
4	F	256	TYR	4.1
4	F	189	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
4	F	259	GLY	4.1
4	F	239	HIS	4.0
4	F	226	GLU	4.0
4	F	219	GLY	4.0
4	F	45	ASN	3.9
4	F	204	TRP	3.8
4	F	354	ALA	3.8
4	F	185	TYR	3.8
2	B	438	ALA	3.8
4	F	224	SER	3.7
4	F	257	GLU	3.6
4	F	263	PHE	3.6
4	F	218	GLU	3.6
4	F	329	LEU	3.6
4	F	337	ALA	3.5
4	F	328	TRP	3.4
2	D	57	THR	3.3
4	F	291	ILE	3.3
2	D	441	ASP	3.2
4	F	191	LEU	3.2
4	F	342	LEU	3.2
4	F	196	HIS	3.2
4	F	266	GLU	3.2
4	F	213	ILE	3.2
4	F	78	VAL	3.0
4	F	262	MET	3.0
4	F	321	VAL	3.0
4	F	325	LEU	3.0
4	F	193	GLU	3.0
4	F	327	VAL	3.0
4	F	9	GLU	2.9
4	F	46	ARG	2.9
4	F	23	ALA	2.8
3	E	27	PRO	2.8
4	F	290	ILE	2.8
4	F	187	GLU	2.8
4	F	200	ASP	2.8
4	F	320	MET	2.8
2	D	179	ASP	2.7
4	F	220	VAL	2.7
4	F	349	GLY	2.7
4	F	27	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	276	THR	2.6
4	F	96	GLU	2.6
4	F	5	VAL	2.6
4	F	15	ALA	2.6
2	D	277	SER	2.6
4	F	270	TYR	2.6
4	F	336	PRO	2.5
2	D	83	PHE	2.5
1	A	438	ASP	2.5
2	D	418	PHE	2.5
2	B	59	ASN	2.5
4	F	217	ARG	2.4
4	F	222	ARG	2.4
4	F	317	PHE	2.4
4	F	334	GLY	2.4
2	D	390	ARG	2.4
4	F	335	ALA	2.4
4	F	264	PHE	2.3
4	F	22	LEU	2.3
4	F	260	ASN	2.3
4	F	254	GLY	2.3
4	F	347	CYS	2.3
1	C	43	GLY	2.3
4	F	331	GLU	2.3
4	F	344	ALA	2.3
4	F	31	ARG	2.2
4	F	14	TYR	2.2
1	A	163	LYS	2.2
4	F	215	LEU	2.2
4	F	285	LEU	2.2
3	E	45	PRO	2.2
4	F	272	MET	2.2
2	D	283	TYR	2.2
4	F	10	ASN	2.1
4	F	228	TYR	2.1
4	F	295	LEU	2.1
2	D	415	GLU	2.1
4	F	197	ARG	2.1
2	D	56	ALA	2.1
4	F	203	SER	2.0
4	F	69	ASP	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
6	MG	C	502	1/1	0.95	0.14	2.13	18,18,18,18	0
8	GOL	A	504	6/6	0.88	0.22	1.33	57,60,60,62	0
7	CA	A	503	1/1	0.57	0.14	1.22	68,68,68,68	0
10	POU	B	503	38/38	0.90	0.13	0.51	23,44,77,81	0
5	GTP	C	501	32/32	0.99	0.13	0.43	4,13,19,30	0
5	GTP	A	501	32/32	0.98	0.12	0.38	10,17,22,41	0
10	POU	D	503	38/38	0.90	0.16	0.16	35,59,74,77	0
9	GDP	B	501	28/28	0.99	0.14	0.04	11,16,20,22	0
9	GDP	D	501	28/28	0.97	0.11	-0.26	27,36,45,53	0
11	ACP	F	401	31/31	0.78	0.29	-0.86	67,106,145,166	0
6	MG	D	502	1/1	0.57	0.18	-	67,67,67,67	0
6	MG	A	502	1/1	0.96	0.10	-	14,14,14,14	0
6	MG	B	502	1/1	0.99	0.14	-	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.