Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:13 PM GMT

PDB ID	:	4O4L
Title	:	Tubulin-Peloruside A-Epothilone 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 ①) were used in the production of this report:

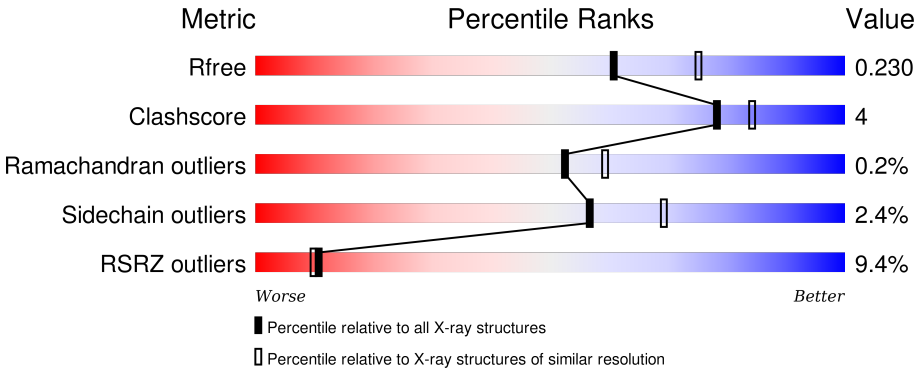
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 <=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	90% 7%
1	C	451	89% 8%
2	B	445	87% 9%
2	D	445	4% 86% 11%
3	E	143	4% 82% 14%

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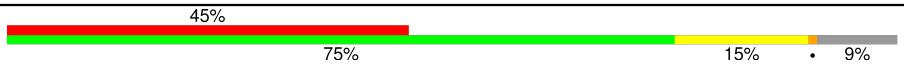
Mol	Chain	Length	Quality of chain
4	F	384	

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	EP	D	504	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18663 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	13	0
			3489	2217	585	662	25			
1	C	440	Total	C	N	O	S	0	22	0
			3536	2245	588	676	27			

- 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	15	0
			3435	2164	580	662	29			
2	D	431	Total	C	N	O	S	0	6	0
			3411	2143	580	660	28			

- 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
			1046	647	188	205	6			

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

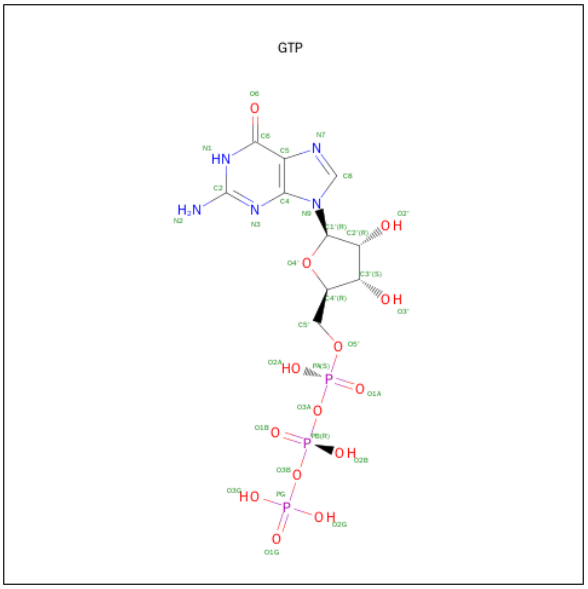
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	351	Total	C	N	O	S	0	9	0
			2902	1870	490	528	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		

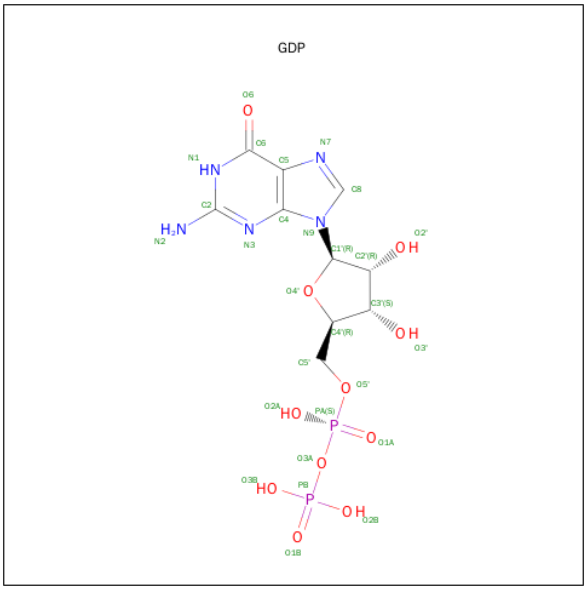
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

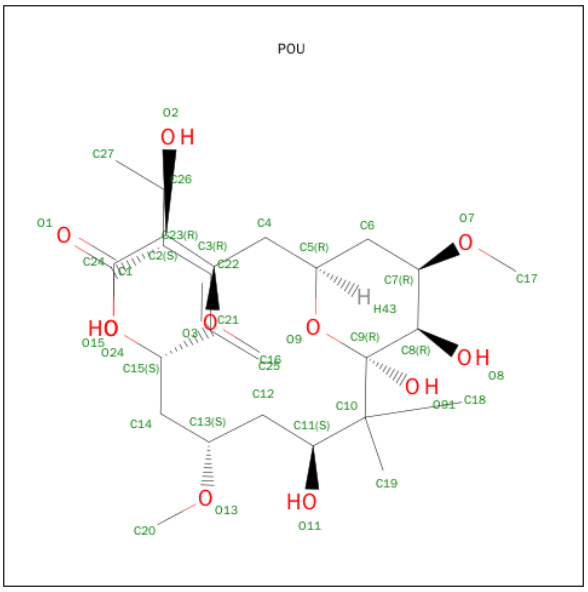
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Ca 2 2	0	0
7	A	1	Total Ca 1 1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



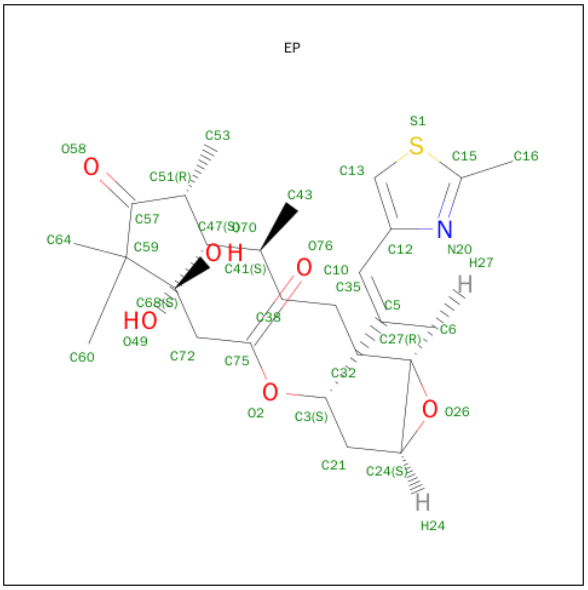
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0
8	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 9 is PELORUSIDE A (three-letter code: POU) (formula: $C_{27}H_{48}O_{11}$).



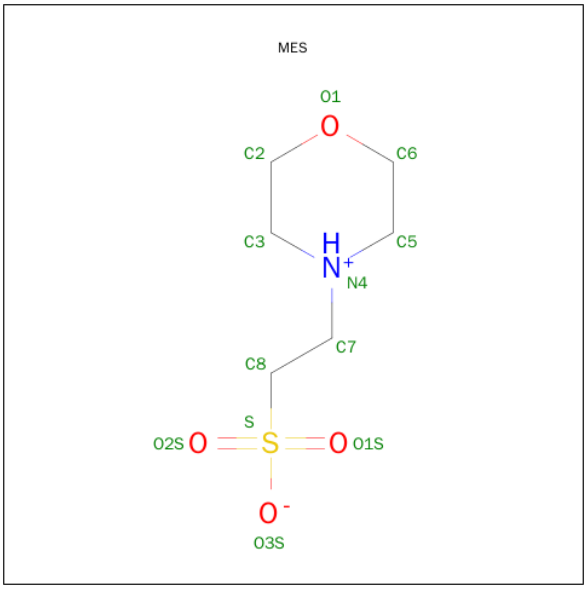
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 38 27 11	0	0
9	D	1	Total C O 38 27 11	0	0

- Molecule 10 is EPOTHILONE A (three-letter code: EP) (formula: $C_{26}H_{39}NO_6S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C N O S 34 26 1 6 1	0	0
10	D	1	Total C N O S 34 26 1 6 1	0	0

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 12 is water.

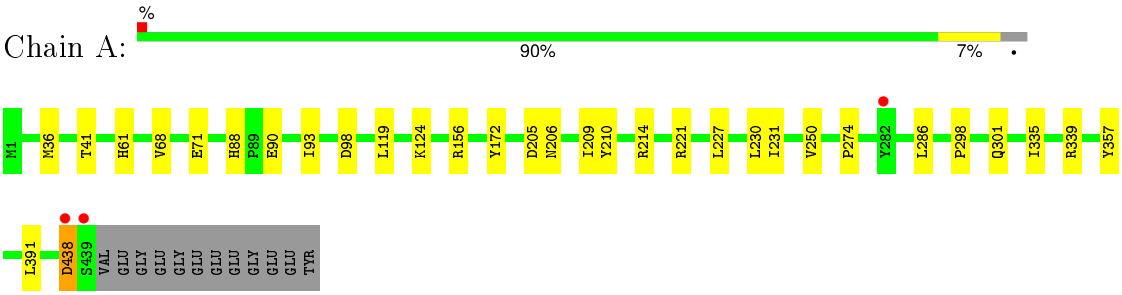
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	130	Total	O	0	0
			130	130		
12	B	127	Total	O	0	0
			127	127		
12	C	204	Total	O	0	0
			204	204		
12	D	44	Total	O	0	0
			44	44		
12	E	30	Total	O	0	0
			30	30		
12	F	26	Total	O	0	0
			26	26		

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.

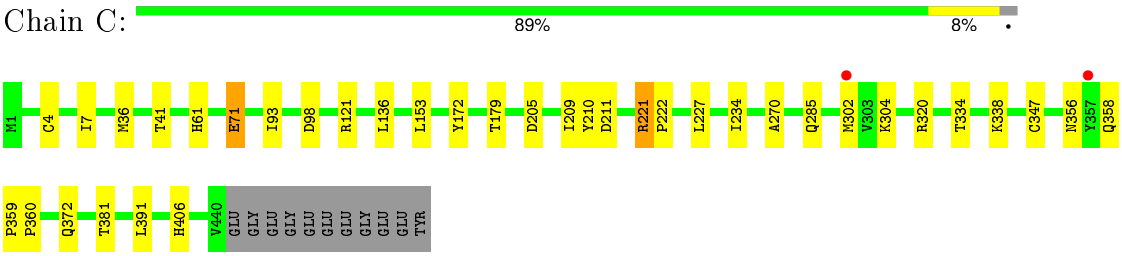
- Molecule 1: Tubulin alpha-1B chain

Chain A:



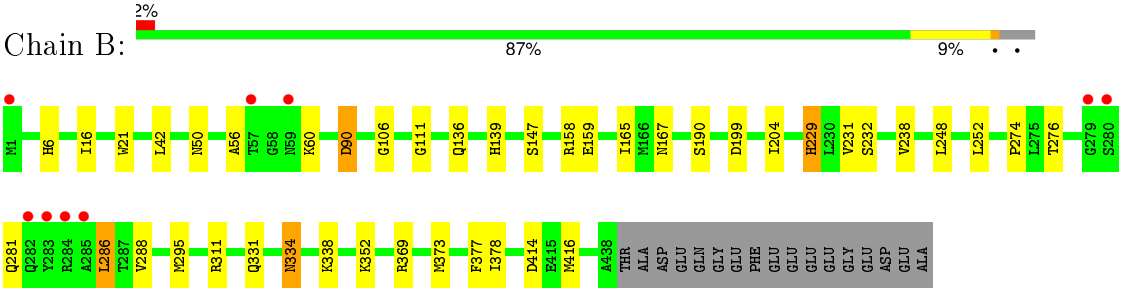
- Molecule 1: Tubulin alpha-1B chain

Chain C:



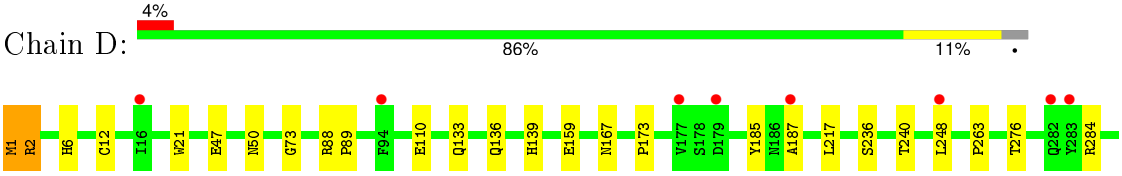
- Molecule 2: Tubulin beta-2B chain

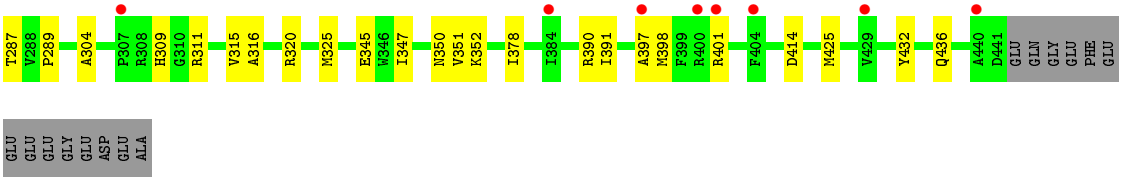
Chain B:



- Molecule 2: Tubulin beta-2B chain

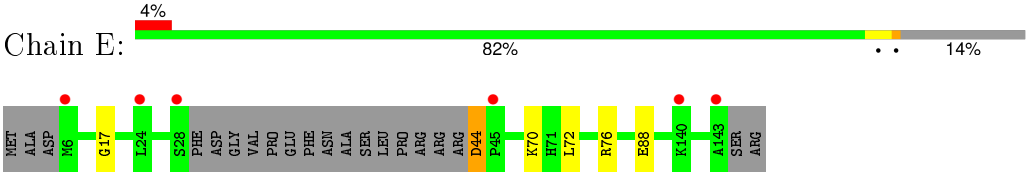
Chain D:





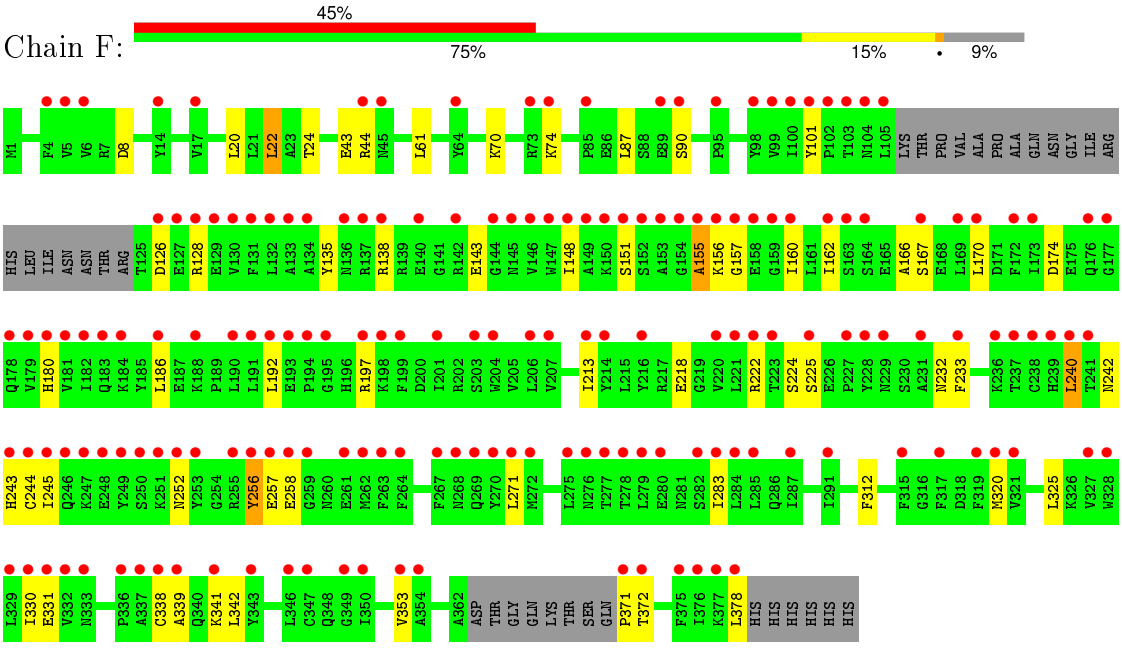
- Molecule 3: Stathmin-4

Chain E:



- Molecule 4: Tubulin-tyrosine ligase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.40Å 156.33Å 180.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.10 – 2.20 78.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (59.10-2.20) 99.9 (78.23-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.186 , 0.224 0.197 , 0.230	Depositor DCC
R_{free} test set	7516 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 149694 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18663	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, CA, POU, GTP, MES, EP

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	0.22	0/3606	0.42	0/4896
1	C	0.23	0/3678	0.43	0/4997
2	B	0.23	0/3552	0.42	0/4809
2	D	0.22	0/3504	0.40	0/4748
3	E	0.21	0/1073	0.36	0/1425
4	F	0.21	0/2992	0.41	0/4042
All	All	0.22	0/18405	0.41	0/24917

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

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	3489	0	3442	18	0
1	C	3536	0	3485	22	0
2	B	3435	0	3355	23	0
2	D	3411	0	3306	28	0
3	E	1046	0	1072	3	0
4	F	2902	0	2921	33	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
7	B	2	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	1	0
9	B	38	0	48	1	0
9	D	38	0	48	3	0
10	B	34	0	39	1	0
10	D	34	0	39	2	0
11	B	12	0	12	2	0
12	A	130	0	0	0	0
12	B	127	0	0	2	0
12	C	204	0	0	2	0
12	D	44	0	0	2	0
12	E	30	0	0	0	0
12	F	26	0	0	0	0
All	All	18663	0	17815	128	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 (128) 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:286:LEU:HD13	2:B:373:MET:HG2	1.65	0.76
4:F:138:ARG:NH1	4:F:143:GLU:OE1	2.20	0.74
2:D:240[B]:THR:HG21	2:D:320:ARG:HD2	1.69	0.73
2:D:311:ARG:NH1	2:D:436:GLN:O	2.22	0.73
2:B:90:ASP:OD1	2:B:90:ASP:N	2.21	0.72
2:B:248:LEU:HD21	2:B:352:LYS:HB3	1.74	0.69
3:E:44:ASP:OD1	3:E:44:ASP:N	2.24	0.68
2:D:276:THR:OG1	2:D:284:ARG:NH1	2.31	0.63
4:F:74:LYS:HZ3	4:F:331:GLU:HB3	1.63	0.63
4:F:213:ILE:HB	4:F:378[A]:LEU:HB2	1.83	0.61
4:F:320:MET:HG2	4:F:330:ILE:HD11	1.83	0.59
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.20	0.59
2:D:173:PRO:HG2	2:D:187:ALA:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:157:GLY:HA3	4:F:245:ILE:HD11	1.85	0.59
1:C:356[A]:ASN:ND2	12:C:643:HOH:O	2.35	0.59
4:F:213:ILE:HB	4:F:378[B]:LEU:HB2	1.85	0.58
4:F:101:TYR:N	4:F:126:ASP:OD1	2.31	0.58
2:B:286:LEU:HD12	2:B:286:LEU:H	1.69	0.58
1:A:438:ASP:OD1	1:A:438:ASP:N	2.38	0.57
4:F:225:SER:OG	4:F:252:ASN:O	2.23	0.57
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.37	0.56
2:D:315:VAL:HB	2:D:351:VAL:HG22	1.87	0.56
1:C:270:ALA:HB3	1:C:302[B]:MET:HE2	1.88	0.55
2:D:397:ALA:O	2:D:401:ARG:NH1	2.40	0.55
4:F:283:ILE:HD11	4:F:325:LEU:HD22	1.90	0.54
2:B:158:ARG:CZ	11:B:507:MES:H21	2.37	0.54
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.23	0.53
4:F:155:ALA:O	4:F:157:GLY:N	2.39	0.53
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.43	0.53
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.90	0.53
2:B:334:ASN:HB2	2:B:338:LYS:HD2	1.89	0.53
4:F:74:LYS:NZ	4:F:331:GLU:HB3	2.23	0.52
1:A:88:HIS:CE1	1:A:90:GLU:HB2	2.43	0.52
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.91	0.52
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.91	0.52
2:D:304:ALA:HB3	2:D:390:ARG:HH12	1.76	0.51
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.91	0.51
4:F:138:ARG:HB3	4:F:143:GLU:HB2	1.92	0.51
2:D:391:ILE:HB	2:D:425:MET:HE2	1.93	0.51
2:D:248:LEU:HD21	2:D:352:LYS:HB3	1.92	0.50
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.51	0.50
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.94	0.50
2:D:185:TYR:OH	2:D:398:MET:O	2.23	0.50
4:F:162:ILE:HD11	4:F:240:LEU:HD23	1.94	0.50
2:D:1:MET:SD	2:D:50:ASN:HB2	2.51	0.50
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.94	0.50
2:B:311:ARG:NH1	12:B:638:HOH:O	2.43	0.49
1:C:334:THR:O	1:C:338:LYS:HG2	2.13	0.49
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.47	0.49
2:D:309:HIS:O	2:D:436:GLN:NE2	2.46	0.49
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.94	0.48
1:A:68[B]:VAL:HG12	1:A:93:ILE:HB	1.93	0.48
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.13	0.48
2:D:2:ARG:HG3	2:D:133:GLN:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.94	0.48
1:C:320:ARG:HG3	1:C:360:PRO:HG3	1.96	0.48
3:E:72:LEU:O	3:E:76:ARG:HG2	2.13	0.48
4:F:151:SER:HG	4:F:180:HIS:CD2	2.32	0.47
4:F:192:LEU:HB3	4:F:197:ARG:HG3	1.97	0.47
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.97	0.47
2:B:136:GLN:HA	2:B:167:ASN:O	2.14	0.47
4:F:371:PRO:HA	4:F:372:THR:HA	1.72	0.47
2:D:167:ASN:ND2	12:D:619:HOH:O	2.48	0.47
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.50	0.46
2:B:295[B]:MET:HG2	2:B:377:PHE:HB2	1.96	0.46
4:F:148:ILE:HG13	4:F:162:ILE:HG12	1.97	0.46
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.50	0.46
4:F:242:ASN:O	4:F:244:CYS:N	2.42	0.46
4:F:160:ILE:HD12	4:F:240:LEU:HD13	1.98	0.46
2:B:274:PRO:HG3	2:B:286:LEU:HD23	1.97	0.46
2:D:136:GLN:HA	2:D:167:ASN:O	2.14	0.46
2:B:199:ASP:OD2	11:B:507:MES:H52	2.15	0.46
1:A:90:GLU:HG2	1:A:124:LYS:NZ	2.31	0.45
1:C:211[A]:ASP:OD2	1:C:304:LYS:NZ	2.42	0.45
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.98	0.45
9:D:503:POU:H46	9:D:503:POU:H40	1.85	0.45
4:F:167:SER:HA	4:F:170:LEU:HG	1.98	0.45
2:D:217:LEU:HD22	10:D:504:EP:H721	1.98	0.45
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.50	0.45
4:F:8:ASP:OD2	4:F:44:ARG:NH1	2.51	0.45
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.99	0.44
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.99	0.44
2:B:106:GLY:O	2:B:111:GLY:HA3	2.18	0.44
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.53	0.44
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.00	0.44
4:F:338:CYS:SG	4:F:339:ALA:N	2.91	0.43
1:A:209[B]:ILE:HD12	1:A:227:LEU:HB3	2.00	0.43
1:C:210:TYR:CE1	1:C:222:PRO:HG2	2.52	0.43
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.37	0.43
1:C:285:GLN:NE2	12:C:772:HOH:O	2.50	0.43
4:F:339:ALA:HB3	4:F:342:LEU:HD12	2.01	0.43
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.00	0.43
1:C:41:THR:OG1	1:C:41:THR:O	2.36	0.43
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.59	0.42
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:87:LEU:O	4:F:90:SER:OG	2.35	0.42
9:D:503:POU:H27	9:D:503:POU:O15	2.19	0.42
2:D:284:ARG:HD3	10:D:504:EP:H161	2.00	0.42
4:F:135:TYR:CZ	4:F:166:ALA:HB2	2.55	0.42
1:A:206:ASN:OD1	1:A:209[B]:ILE:HD11	2.19	0.42
2:D:304:ALA:HB3	2:D:390:ARG:NH1	2.35	0.42
2:B:238[B]:VAL:HG22	2:B:378:ILE:HD11	2.01	0.42
1:C:406:HIS:CD2	2:D:263:PRO:HD3	2.55	0.41
2:D:316:ALA:HB3	2:D:378:ILE:HB	2.02	0.41
4:F:61:LEU:HD11	4:F:312:PHE:HD2	1.85	0.41
4:F:8:ASP:HB2	4:F:43:GLU:HA	2.01	0.41
4:F:256:TYR:HB2	4:F:257:GLU:OE2	2.20	0.41
2:B:50[B]:ASN:ND2	2:B:50[B]:ASN:H	2.19	0.41
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.55	0.41
2:D:287:THR:HB	2:D:289:PRO:HD2	2.00	0.41
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	2.02	0.41
1:C:358[B]:GLN:HA	1:C:359:PRO:HD3	1.92	0.41
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.92	0.41
4:F:271[A]:LEU:HA	4:F:271[A]:LEU:HD12	1.87	0.41
1:C:209:ILE:HD11	1:C:302[A]:MET:HG3	2.03	0.41
2:B:288:VAL:HG12	2:B:331:GLN:HG3	2.03	0.41
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.03	0.41
4:F:22:LEU:HA	4:F:22:LEU:HD12	1.96	0.41
2:D:432:TYR:OH	12:D:644:HOH:O	2.21	0.41
9:B:503:POU:H17	9:B:503:POU:O8	2.21	0.41
2:B:159:GLU:OE2	12:B:696:HOH:O	2.22	0.40
4:F:242:ASN:HB2	4:F:245:ILE:HD12	2.03	0.40
2:D:88:ARG:HA	2:D:89:PRO:HD2	1.87	0.40
2:D:236:SER:O	2:D:240[B]:THR:HG23	2.21	0.40
2:B:229:HIS:ND1	10:B:504:EP:H321	2.37	0.40
9:D:503:POU:H45	9:D:503:POU:H12	1.84	0.40
4:F:20:LEU:O	4:F:24:THR:HG23	2.22	0.40
1:A:298:PRO:HA	1:A:301:GLN:CD	2.42	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	450/451 (100%)	436 (97%)	14 (3%)	0	100	100
1	C	460/451 (102%)	452 (98%)	8 (2%)	0	100	100
2	B	441/445 (99%)	427 (97%)	14 (3%)	0	100	100
2	D	435/445 (98%)	420 (97%)	14 (3%)	1 (0%)	52	59
3	E	125/143 (87%)	120 (96%)	5 (4%)	0	100	100
4	F	353/384 (92%)	314 (89%)	35 (10%)	4 (1%)	17	14
All	All	2264/2319 (98%)	2169 (96%)	90 (4%)	5 (0%)	52	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	156	LYS
4	F	243	HIS
4	F	155	ALA
4	F	232	ASN
2	D	73	GLY

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	383/379 (101%)	378 (99%)	5 (1%)	76	87
1	C	393/379 (104%)	387 (98%)	6 (2%)	72	84
2	B	385/383 (100%)	373 (97%)	12 (3%)	47	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	378/383 (99%)	370 (98%)	8 (2%)	61 74
3	E	116/127 (91%)	113 (97%)	3 (3%)	54 66
4	F	322/342 (94%)	309 (96%)	13 (4%)	38 47
All	All	1977/1993 (99%)	1930 (98%)	47 (2%)	57 69

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	71	GLU
1	A	221	ARG
1	A	250	VAL
1	A	438	ASP
2	B	42	LEU
2	B	90	ASP
2	B	139	HIS
2	B	229	HIS
2	B	232	SER
2	B	276	THR
2	B	281	GLN
2	B	286	LEU
2	B	334	ASN
2	B	369	ARG
2	B	414	ASP
2	B	416	MET
1	C	71	GLU
1	C	179	THR
1	C	221	ARG
1	C	347[A]	CYS
1	C	347[B]	CYS
1	C	381	THR
2	D	1	MET
2	D	2	ARG
2	D	47	GLU
2	D	110	GLU
2	D	139	HIS
2	D	159	GLU
2	D	345	GLU
2	D	414	ASP
3	E	44	ASP
3	E	70	LYS

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Mol	Chain	Res	Type
3	E	88	GLU
4	F	22	LEU
4	F	70	LYS
4	F	186	LEU
4	F	218	GLU
4	F	222	ARG
4	F	224	SER
4	F	233	PHE
4	F	240	LEU
4	F	256	TYR
4	F	258	GLU
4	F	341	LYS
4	F	353[A]	VAL
4	F	353[B]	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
2	B	293	GLN

5.3.3 RNA (i)

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 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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	0.95	1 (4%)	34,54,54	1.62	5 (14%)
8	GDP	B	501	6	23,30,30	1.20	2 (8%)	30,47,47	1.76	7 (23%)
9	POU	B	503	-	36,39,39	2.04	4 (11%)	33,57,57	1.88	9 (27%)
10	EP	B	504	-	32,36,36	1.28	3 (9%)	35,53,53	2.42	11 (31%)
11	MES	B	507	-	11,12,12	0.61	0	14,16,16	2.29	3 (21%)
5	GTP	C	501	6	25,34,34	0.94	1 (4%)	34,54,54	1.63	5 (14%)
8	GDP	D	501	6	23,30,30	1.18	2 (8%)	30,47,47	1.87	8 (26%)
9	POU	D	503	-	36,39,39	2.22	6 (16%)	33,57,57	2.17	9 (27%)
10	EP	D	504	-	32,36,36	1.30	4 (12%)	35,53,53	2.36	11 (31%)

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	GDP	B	501	6	-	0/12/32/32	0/3/3/3
9	POU	B	503	-	-	1/54/76/76	0/0/2/2
10	EP	B	504	-	-	1/49/55/55	0/1/3/3
11	MES	B	507	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
8	GDP	D	501	6	-	0/12/32/32	0/3/3/3
9	POU	D	503	-	-	1/54/76/76	0/0/2/2
10	EP	D	504	-	-	1/49/55/55	0/1/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	503	POU	C2-C1	-4.85	1.38	1.52
9	B	503	POU	C2-C1	-4.68	1.39	1.52
9	D	503	POU	C12-C11	-2.21	1.50	1.53
10	D	504	EP	C59-C57	-2.01	1.51	1.54
10	B	504	EP	C13-S1	2.01	1.73	1.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	503	POU	C14-C13	2.05	1.57	1.52
10	D	504	EP	C13-S1	2.16	1.74	1.70
9	B	503	POU	C14-C15	2.16	1.57	1.53
9	D	503	POU	C14-C15	2.21	1.57	1.53
5	A	501	GTP	C6-N1	2.92	1.38	1.33
5	C	501	GTP	C6-N1	2.93	1.38	1.33
8	D	501	GDP	C5-C4	2.98	1.47	1.40
8	B	501	GDP	C5-C4	3.01	1.47	1.40
9	B	503	POU	C9-C8	3.15	1.56	1.53
9	D	503	POU	O91-C9	3.18	1.45	1.39
8	D	501	GDP	C6-C5	3.65	1.48	1.41
8	B	501	GDP	C6-C5	3.74	1.48	1.41
10	B	504	EP	O2-C75	4.01	1.46	1.34
10	D	504	EP	O2-C75	4.04	1.46	1.34
10	B	504	EP	C27-C24	4.22	1.53	1.46
10	D	504	EP	C27-C24	4.26	1.53	1.46
9	B	503	POU	C22-C21	9.10	1.53	1.33
9	D	503	POU	C22-C21	9.85	1.54	1.33

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	503	POU	C13-C12-C11	-7.83	104.39	114.35
10	B	504	EP	C32-C27-C24	-6.69	114.36	123.40
10	D	504	EP	C32-C27-C24	-6.40	114.75	123.40
5	C	501	GTP	N3-C2-N1	-5.06	119.73	127.44
5	A	501	GTP	N3-C2-N1	-4.79	120.14	127.44
9	B	503	POU	C13-C12-C11	-4.20	109.02	114.35
10	B	504	EP	O26-C27-C32	-4.19	110.27	116.59
8	D	501	GDP	C5-C6-N1	-4.17	117.88	123.59
10	D	504	EP	O26-C24-C27	-4.07	57.44	59.66
10	B	504	EP	O26-C24-C27	-4.05	57.45	59.66
10	B	504	EP	O26-C27-C24	-4.03	57.46	59.66
8	B	501	GDP	C5-C6-N1	-4.03	118.08	123.59
10	D	504	EP	O26-C27-C24	-4.02	57.47	59.66
10	D	504	EP	O26-C27-C32	-3.94	110.66	116.59
5	A	501	GTP	PA-O3A-PB	-3.83	121.98	132.73
10	D	504	EP	O26-C24-C21	-3.72	107.72	116.36
10	B	504	EP	O26-C24-C21	-3.61	107.98	116.36
8	D	501	GDP	C6-C5-C4	-3.59	116.61	120.90
8	B	501	GDP	C6-C5-C4	-3.41	116.82	120.90
8	B	501	GDP	C4-C5-N7	-3.40	106.35	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	501	GDP	C4-C5-N7	-3.28	106.46	109.48
5	C	501	GTP	PA-O3A-PB	-3.21	123.72	132.73
10	B	504	EP	C68-C72-C75	-3.20	105.00	112.35
5	C	501	GTP	C5-C6-N1	-3.16	119.27	123.59
9	D	503	POU	C3-C4-C5	-3.11	107.21	114.93
8	D	501	GDP	N3-C2-N1	-3.10	122.72	127.44
8	B	501	GDP	N3-C2-N1	-3.02	122.84	127.44
5	A	501	GTP	C5-C6-N1	-2.98	119.51	123.59
8	D	501	GDP	PA-O3A-PB	-2.93	122.85	132.67
10	D	504	EP	C68-C72-C75	-2.88	105.73	112.35
5	C	501	GTP	PB-O3B-PG	-2.79	123.31	132.67
5	A	501	GTP	PB-O3B-PG	-2.76	123.40	132.67
8	B	501	GDP	PA-O3A-PB	-2.76	123.41	132.67
9	B	503	POU	C25-C21-C22	-2.70	116.24	123.31
10	B	504	EP	C21-C3-C5	-2.55	110.07	113.72
10	D	504	EP	C53-C51-C47	-2.39	108.17	112.37
9	B	503	POU	C26-C23-C24	-2.35	106.73	111.80
10	D	504	EP	C21-C3-C5	-2.28	110.46	113.72
10	B	504	EP	C53-C51-C47	-2.26	108.40	112.37
9	D	503	POU	C23-C22-C21	-2.20	119.43	126.60
9	D	503	POU	C25-C21-C22	-2.20	117.56	123.31
8	D	501	GDP	C2'-C1'-N9	-2.18	110.96	114.29
8	D	501	GDP	C1'-N9-C4	-2.18	123.65	126.94
9	B	503	POU	C23-C22-C21	-2.14	119.62	126.60
9	D	503	POU	C17-O7-C7	-2.11	108.35	114.09
9	B	503	POU	C3-C4-C5	-2.11	109.70	114.93
8	B	501	GDP	C1'-N9-C4	-2.04	123.86	126.94
9	D	503	POU	O9-C5-C6	2.33	113.57	108.85
9	B	503	POU	O9-C5-C6	2.56	114.02	108.85
11	B	507	MES	O1S-S-C8	2.74	109.24	106.91
10	B	504	EP	O2-C75-C72	2.80	116.96	111.54
10	D	504	EP	C16-C15-N20	2.91	131.52	123.88
10	D	504	EP	O2-C75-C72	2.91	117.17	111.54
5	A	501	GTP	C6-N1-C2	2.91	119.98	115.94
9	B	503	POU	O15-C15-C14	3.00	112.40	106.28
9	D	503	POU	O15-C15-C14	3.13	112.65	106.28
10	B	504	EP	C16-C15-N20	3.17	132.22	123.88
9	D	503	POU	O15-C15-C21	3.19	118.74	109.44
5	C	501	GTP	C6-N1-C2	3.19	120.37	115.94
11	B	507	MES	O2S-S-C8	3.33	109.75	106.91
9	B	503	POU	O15-C15-C21	3.79	120.49	109.44
9	D	503	POU	C15-O15-C1	3.97	125.40	116.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	503	POU	C15-O15-C1	4.49	126.53	116.87
8	B	501	GDP	C6-N1-C2	4.59	122.31	115.94
8	D	501	GDP	C6-N1-C2	4.86	122.68	115.94
11	B	507	MES	C5-N4-C3	6.38	122.72	108.90
10	B	504	EP	C27-O26-C24	6.57	65.09	60.69
10	D	504	EP	C27-O26-C24	6.57	65.10	60.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	504	EP	C5-C10-C12-N20
10	D	504	EP	C5-C10-C12-N20
9	B	503	POU	C23-C22-C21-C15
9	D	503	POU	C23-C22-C21-C15

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
9	B	503	POU	1	0
10	B	504	EP	1	0
11	B	507	MES	2	0
8	D	501	GDP	1	0
9	D	503	POU	3	0
10	D	504	EP	2	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, 95^{th} 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%)	0.04	3 (0%) 89 88	31, 48, 83, 158	0
1	C	440/451 (97%)	0.11	2 (0%) 91 91	25, 38, 66, 97	0
2	B	428/445 (96%)	0.22	9 (2%) 67 65	25, 44, 83, 159	2 (0%)
2	D	431/445 (96%)	0.26	16 (3%) 45 44	35, 67, 103, 140	6 (1%)
3	E	123/143 (86%)	0.40	6 (4%) 33 33	38, 65, 107, 137	0
4	F	351/384 (91%)	2.58	173 (49%) 0 0	51, 110, 185, 210	0
All	All	2212/2319 (95%)	0.56	209 (9%) 11 10	25, 54, 140, 210	8 (0%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	133	ALA	16.3
4	F	173	ILE	15.2
4	F	89	GLU	12.3
4	F	177	GLY	12.0
2	B	280	SER	11.8
4	F	134	ALA	10.9
4	F	284[A]	LEU	10.6
2	D	283	TYR	10.2
4	F	101	TYR	10.1
4	F	178	GLN	8.9
2	B	283	TYR	8.7
4	F	137	ARG	8.4
4	F	181	VAL	8.2
4	F	240	LEU	8.0
2	B	279	GLY	7.8
4	F	251	LYS	7.8
4	F	249	TYR	7.6
4	F	241	THR	7.4
4	F	160	ILE	7.3

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Mol	Chain	Res	Type	RSRZ
4	F	194	PRO	7.1
4	F	199	PHE	7.1
1	A	282	TYR	7.0
4	F	256	TYR	7.0
4	F	190	LEU	6.8
4	F	132	LEU	6.6
4	F	243	HIS	6.5
4	F	156	LYS	6.5
4	F	330	ILE	6.5
4	F	170	LEU	6.3
4	F	130	VAL	6.3
4	F	246	GLN	6.3
4	F	155	ALA	6.2
4	F	103	THR	6.2
4	F	252	ASN	6.2
4	F	277[A]	THR	6.2
4	F	253	TYR	6.2
4	F	250	SER	6.0
4	F	353[A]	VAL	5.9
4	F	338	CYS	5.9
4	F	278	THR	5.8
4	F	285	LEU	5.8
4	F	245	ILE	5.8
4	F	128	ARG	5.7
4	F	223	THR	5.6
4	F	158	GLU	5.6
4	F	206	LEU	5.5
4	F	154	GLY	5.4
4	F	220[A]	VAL	5.3
4	F	147	TRP	5.2
4	F	320	MET	5.2
4	F	201	ILE	5.2
4	F	271[A]	LEU	5.2
4	F	247	LYS	5.2
4	F	236	LYS	5.2
4	F	319	PHE	5.1
4	F	186	LEU	5.1
4	F	204	TRP	5.1
4	F	150	LYS	5.1
4	F	192	LEU	5.1
4	F	244	CYS	5.1
4	F	129	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
4	F	100	ILE	4.9
4	F	179	VAL	4.8
4	F	259	GLY	4.8
4	F	336	PRO	4.8
4	F	337	ALA	4.8
4	F	131	PHE	4.8
4	F	153	ALA	4.7
4	F	105	LEU	4.7
4	F	191	LEU	4.7
4	F	327	VAL	4.7
4	F	375	PHE	4.7
4	F	279	LEU	4.6
4	F	157	GLY	4.6
4	F	182	ILE	4.5
4	F	180	HIS	4.5
4	F	184	LYS	4.5
4	F	332	VAL	4.5
4	F	149	ALA	4.5
4	F	263	PHE	4.5
4	F	144	GLY	4.4
2	B	282	GLN	4.4
4	F	317	PHE	4.4
4	F	159	GLY	4.4
4	F	239	HIS	4.3
2	D	177	VAL	4.3
4	F	127	GLU	4.3
4	F	233	PHE	4.3
4	F	169	LEU	4.2
4	F	257	GLU	4.2
4	F	148	ILE	4.2
4	F	376	ILE	4.2
4	F	275[A]	LEU	4.2
4	F	372	THR	4.2
4	F	102	PRO	4.1
4	F	6	VAL	4.1
4	F	98	TYR	4.1
4	F	151	SER	4.1
4	F	183	GLN	4.0
4	F	258	GLU	4.0
4	F	339	ALA	3.9
4	F	138	ARG	3.9
4	F	255[A]	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
4	F	283	ILE	3.9
4	F	248	GLU	3.8
4	F	197	ARG	3.8
2	D	404	PHE	3.8
4	F	136	ASN	3.8
4	F	280	GLU	3.7
4	F	328	TRP	3.6
4	F	371	PRO	3.6
4	F	269	GLN	3.6
4	F	329	LEU	3.6
4	F	261	GLU	3.6
4	F	291	ILE	3.6
4	F	272	MET	3.5
4	F	99	VAL	3.5
4	F	350	ILE	3.5
4	F	162	ILE	3.4
4	F	203	SER	3.4
4	F	321	VAL	3.3
4	F	164	SER	3.3
4	F	268	ASN	3.3
4	F	140	GLU	3.3
4	F	237	THR	3.3
2	D	248	LEU	3.3
2	B	285	ALA	3.3
4	F	163	SER	3.3
4	F	44	ARG	3.2
1	A	439	SER	3.2
4	F	152	SER	3.2
2	D	400	ARG	3.2
4	F	198	LYS	3.2
1	A	438	ASP	3.2
2	B	57	THR	3.2
4	F	90	SER	3.1
2	D	429	VAL	3.0
4	F	267	PHE	3.0
4	F	346	LEU	3.0
2	D	397	ALA	3.0
2	D	179	ASP	2.9
2	B	284	ARG	2.9
4	F	146	VAL	2.9
4	F	104	ASN	2.9
4	F	142	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	17	VAL	2.9
4	F	195	GLY	2.9
4	F	221	LEU	2.8
4	F	167	SER	2.8
4	F	343	TYR	2.7
2	D	401	ARG	2.7
2	B	1	MET	2.7
4	F	176	GLN	2.7
4	F	64	TYR	2.7
4	F	73	ARG	2.7
4	F	207	VAL	2.7
4	F	227	PRO	2.7
4	F	276	ASN	2.6
4	F	262	MET	2.6
2	D	187	ALA	2.6
4	F	231	ALA	2.6
4	F	216	TYR	2.6
1	C	357	TYR	2.6
3	E	45	PRO	2.6
4	F	270	TYR	2.6
3	E	28	SER	2.5
4	F	45	ASN	2.5
4	F	238	CYS	2.5
4	F	214	TYR	2.5
4	F	341	LYS	2.5
2	D	307	PRO	2.5
4	F	5	VAL	2.5
2	B	59	ASN	2.4
4	F	333	ASN	2.4
4	F	222	ARG	2.4
3	E	24	LEU	2.4
4	F	193	GLU	2.4
4	F	377	LYS	2.4
4	F	225	SER	2.3
4	F	282	SER	2.3
2	D	94	PHE	2.3
1	C	302[A]	MET	2.3
4	F	315	PHE	2.3
4	F	95	PRO	2.3
2	D	440	ALA	2.3
4	F	378[A]	LEU	2.3
4	F	228	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	349	GLY	2.3
4	F	85	PRO	2.3
2	D	16	ILE	2.3
4	F	264	PHE	2.3
4	F	213	ILE	2.2
3	E	140	LYS	2.2
4	F	188	LYS	2.1
4	F	287	ILE	2.1
4	F	172	PHE	2.1
4	F	347	CYS	2.1
4	F	354	ALA	2.1
4	F	14	TYR	2.1
3	E	6	MET	2.1
2	D	282	GLN	2.1
3	E	143	ALA	2.1
4	F	4	PHE	2.1
2	D	384[A]	ILE	2.1
4	F	331	GLU	2.0
4	F	229	ASN	2.0
4	F	74	LYS	2.0
4	F	145	ASN	2.0
4	F	126	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, 95^{th} 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	EP	D	504	34/34	0.90	0.25	2.61	49,67,73,82	0
9	POU	D	503	38/38	0.88	0.30	1.33	43,84,113,114	0
7	CA	A	503	1/1	0.98	0.15	1.16	66,66,66,66	0
8	GDP	B	501	28/28	0.98	0.19	0.73	23,29,36,39	0
11	MES	B	507	12/12	0.94	0.14	0.23	51,61,73,81	0
5	GTP	C	501	32/32	0.98	0.14	0.16	17,27,40,53	0
9	POU	B	503	38/38	0.92	0.13	0.08	37,56,88,96	0
5	GTP	A	501	32/32	0.98	0.14	-0.09	24,32,39,49	0
10	EP	B	504	34/34	0.87	0.17	-0.27	53,68,78,108	0
8	GDP	D	501	28/28	0.96	0.14	-0.46	40,59,72,75	0
6	MG	D	502	1/1	0.97	0.06	-	64,64,64,64	0
6	MG	C	502	1/1	0.90	0.19	-	36,36,36,36	0
6	MG	B	502	1/1	0.96	0.23	-	24,24,24,24	0
7	CA	B	505	1/1	0.75	0.20	-	97,97,97,97	0
6	MG	A	502	1/1	0.98	0.13	-	33,33,33,33	0
7	CA	B	506	1/1	0.80	0.21	-	99,99,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.