



Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 03:23 PM BST

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

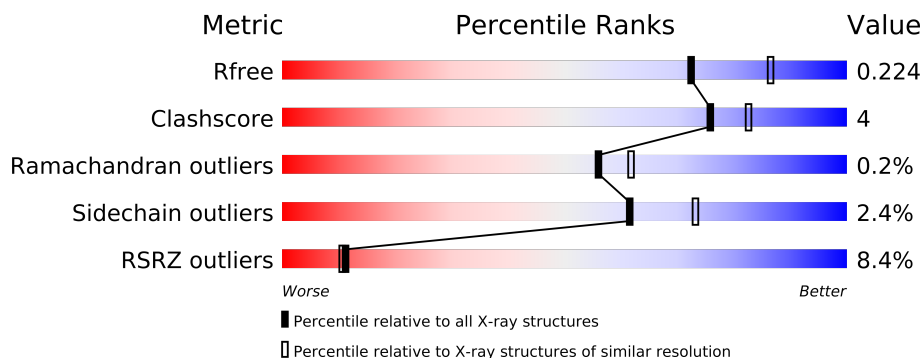
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable23004
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23004

1 Overall quality at a glance

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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
2	B	445	
2	D	445	
3	E	143	
4	F	384	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	EP	D	504	-	X
6	MG	B	502	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	MG	C	502	-	X
7	CA	B	505	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18663 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	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

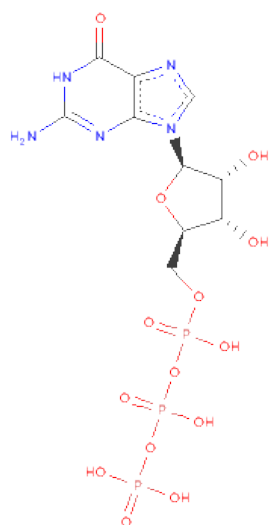
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

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		

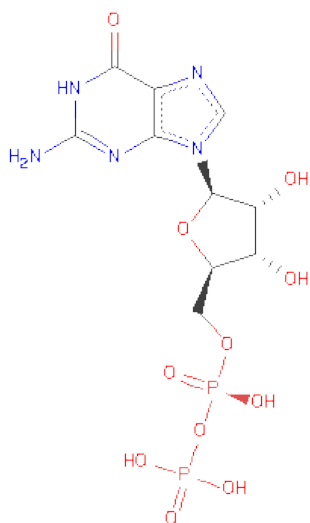
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

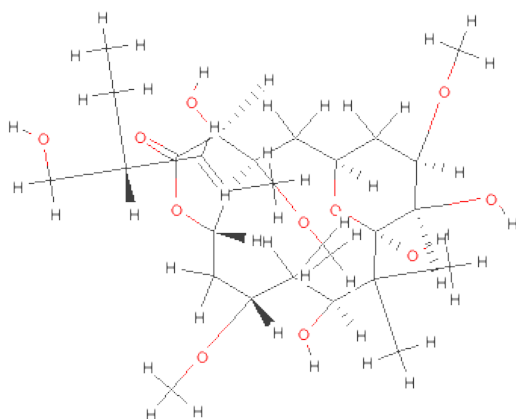
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	1	Total	Ca	0	0
			1	1		

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



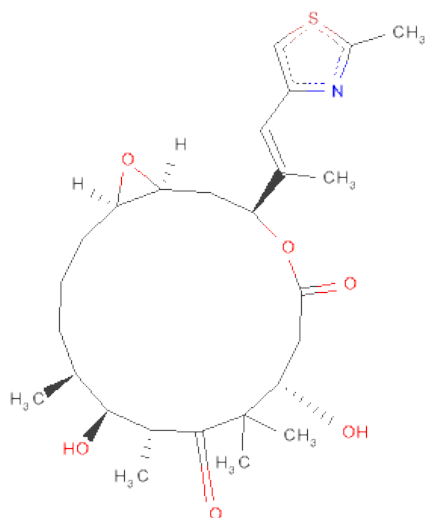
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is PELORUSIDE A (three-letter code: POU) (formula: C₂₇H₄₈O₁₁).



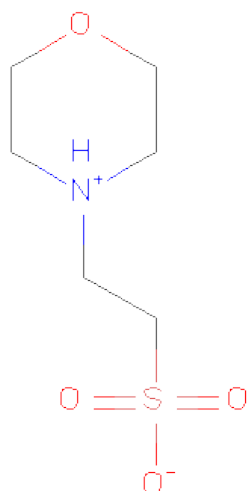
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			38	27	11		
9	D	1	Total	C	O	0	0
			38	27	11		

- 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	0	0
			34	26	1	6	1		
10	D	1	Total	C	N	O	S	0	0
			34	26	1	6	1		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

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.

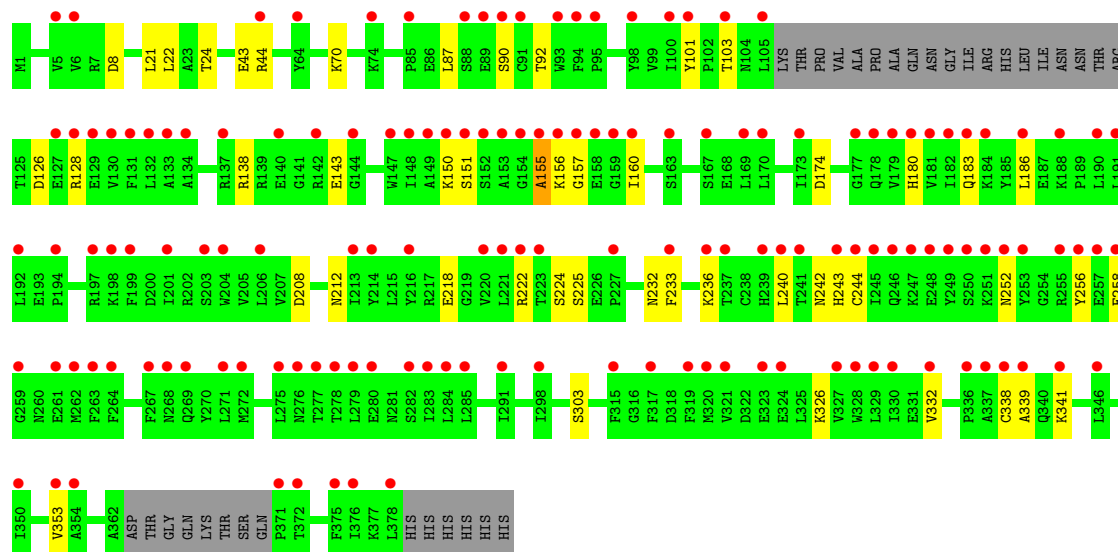
- Molecule 1: Tubulin alpha-1B chain

Chain A: 



● Molecule 4: Tubulin-tyrosine ligase

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.40Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.186 , 0.224 0.187 , 0.224	Depositor DCC
R_{free} test set	7513 reflections (5.02%)	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 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3489	0	0	12	0
1	C	3536	0	0	10	0
2	B	3435	0	0	16	0
2	D	3411	0	0	12	0
3	E	1046	0	0	1	0
4	F	2902	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	B	38	0	48	1	0
9	D	38	0	48	3	0
10	B	34	0	39	1	0
10	D	34	0	39	0	0
11	B	12	0	12	3	0
12	A	130	0	0	6	0
12	B	127	0	0	3	0
12	C	204	0	0	3	0
12	D	44	0	0	3	0
12	E	30	0	0	0	0
12	F	26	0	0	1	0
All	All	18663	0	234	72	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (72) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:138:ARG:NH1	4:F:143:GLU:OE1	2.20	0.75
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
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	0.64
4:F:101:TYR:N	4:F:126:ASP:OD1	2.31	0.63
1:C:356[A]:ASN:ND2	12:C:643:HOH:O	2.35	0.59
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.37	0.58
1:A:438:ASP:N	1:A:438:ASP:OD1	2.38	0.57
4:F:225:SER:OG	4:F:252:ASN:O	2.23	0.57
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.23	0.56
4:F:155:ALA:O	4:F:157:GLY:N	2.39	0.56
2:D:185:TYR:OH	2:D:398:MET:O	2.23	0.55
2:D:397:ALA:O	2:D:401:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:283:HIS:N	12:A:636:HOH:O	2.39	0.54
2:B:158:ARG:CZ	11:B:507:MES:H21	2.37	0.54
4:F:151:SER:OG	4:F:180:HIS:NE2	2.40	0.54
4:F:242:ASN:O	4:F:244:CYS:N	2.42	0.53
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.27	0.53
4:F:92:THR:O	4:F:326:LYS:NZ	2.43	0.52
1:C:211[A]:ASP:OD2	1:C:304:LYS:NZ	2.42	0.52
2:B:311:ARG:NH1	12:B:638:HOH:O	2.43	0.51
2:B:253:ARG:NH2	11:B:507:MES:O2S	2.44	0.51
1:C:60:LYS:NZ	1:C:85:GLN:O	2.43	0.50
2:B:179:ASP:O	1:C:352:LYS:NZ	2.45	0.50
4:F:150:LYS:NZ	4:F:183:GLN:OE1	2.45	0.49
4:F:160:ILE:O	4:F:236:LYS:NZ	2.46	0.49
2:D:279:GLY:N	12:D:627:HOH:O	2.45	0.49
1:A:203:MET:N	12:A:604:HOH:O	2.45	0.49
2:D:309:HIS:O	2:D:436:GLN:NE2	2.46	0.49
4:F:43:GLU:OE2	4:F:43:GLU:N	2.46	0.49
4:F:332:VAL:N	12:F:416:HOH:O	2.46	0.48
1:A:402:ARG:NE	1:A:415:GLU:OE2	2.47	0.48
1:A:263:PRO:O	1:A:266:HIS:ND1	2.47	0.47
1:C:229:ARG:NH2	12:C:780:HOH:O	2.47	0.47
2:D:167:ASN:ND2	12:D:619:HOH:O	2.48	0.47
2:B:2:ARG:O	2:B:133:GLN:NE2	2.48	0.47
1:A:40:LYS:N	12:A:704:HOH:O	2.49	0.46
2:B:199:ASP:OD2	11:B:507:MES:H52	2.15	0.46
2:B:132:LEU:O	2:B:164:ARG:NH1	2.49	0.46
1:A:2:ARG:NH2	12:A:728:HOH:O	2.50	0.45
9:D:503:POU:H46	9:D:503:POU:H40	1.85	0.45
4:F:103:THR:N	4:F:174:ASP:OD2	2.50	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
4:F:87:LEU:O	4:F:90:SER:OG	2.35	0.44
4:F:338:CYS:SG	4:F:339:ALA:N	2.91	0.43
1:C:285:GLN:NE2	12:C:772:HOH:O	2.50	0.43
1:A:259:LEU:O	1:A:380:ASN:ND2	2.52	0.43
2:B:277:SER:N	12:B:627:HOH:O	2.52	0.43
1:C:39:ASP:OD2	1:C:61:HIS:NE2	2.52	0.43
1:C:41:THR:O	1:C:41:THR:OG1	2.36	0.43
9:D:503:POU:H27	9:D:503:POU:O15	2.19	0.42
2:B:303:ALA:O	2:B:305:CYS:N	2.53	0.42
2:D:176:LYS:NZ	2:D:211:ASP:OD1	2.53	0.42
1:A:101:ASN:ND2	12:A:658:HOH:O	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.37	0.42
2:D:142:GLY:O	2:D:186:ASN:ND2	2.52	0.42
1:A:229:ARG:NH1	12:A:646:HOH:O	2.53	0.41
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.53	0.41
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.54	0.41
2:B:236:SER:O	2:B:243:ARG:NH2	2.54	0.41
4:F:208:ASP:OD1	4:F:212:ASN:N	2.54	0.41
4:F:21:LEU:O	4:F:24:THR:OG1	2.38	0.41
1:A:308:ARG:NH1	4:F:303:SER:O	2.54	0.41
2:D:432:TYR:OH	12:D:644:HOH:O	2.21	0.41
9:B:503:POU:O8	9:B:503:POU:H17	2.21	0.41
2:B:159:GLU:OE2	12:B:696:HOH:O	2.22	0.40
2:B:229:HIS:ND1	10:B:504:EP:H321	2.37	0.40
2:B:152:LEU:O	2:B:155[B]:SER:OG	2.39	0.40
9:D:503:POU:H45	9:D:503:POU:H12	1.84	0.40
2:D:139:HIS:ND1	2:D:146:GLY:O	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	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%)	56	62
3	E	125/143 (87%)	120 (96%)	5 (4%)	0	100	100
4	F	353/384 (92%)	314 (89%)	35 (10%)	4 (1%)	21	16
All	All	2264/2319 (98%)	2169 (96%)	90 (4%)	5 (0%)	56	62

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 ⓘ

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%)	80	89
1	C	393/379 (104%)	387 (98%)	6 (2%)	76	86
2	B	385/383 (100%)	373 (97%)	12 (3%)	52	63
2	D	378/383 (99%)	370 (98%)	8 (2%)	66	78
3	E	116/127 (91%)	113 (97%)	3 (3%)	59	70
4	F	322/342 (94%)	309 (96%)	13 (4%)	42	51
All	All	1977/1993 (99%)	1930 (98%)	47 (2%)	61	73

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

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Mol	Chain	Res	Type
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
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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 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	34,34,34	1.00	1 (2%)	51,54,54	2.12	8 (15%)
8	GDP	B	501	6	30,30,30	1.45	4 (13%)	44,47,47	3.41	7 (15%)
9	POU	B	503	-	39,39,39	2.24	4 (10%)	57,57,57	1.96	16 (28%)
10	EP	B	504	-	36,36,36	1.42	4 (11%)	50,53,53	2.98	16 (32%)
11	MES	B	507	-	12,12,12	2.11	1 (8%)	16,16,16	2.13	3 (18%)
5	GTP	C	501	6	34,34,34	0.96	1 (2%)	51,54,54	2.04	9 (17%)
8	GDP	D	501	6	30,30,30	1.45	4 (13%)	44,47,47	3.52	7 (15%)
9	POU	D	503	-	39,39,39	2.41	6 (15%)	57,57,57	1.99	14 (24%)
10	EP	D	504	-	36,36,36	1.46	5 (13%)	50,53,53	2.93	16 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	0/22/38/38	0/1/3/3
8	GDP	B	501	6	-	0/16/32/32	0/1/3/3
9	POU	B	503	-	-	1/56/76/76	0/0/2/2
10	EP	B	504	-	-	1/49/55/55	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MES	B	507	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/22/38/38	0/1/3/3
8	GDP	D	501	6	-	0/16/32/32	0/1/3/3
9	POU	D	503	-	-	1/56/76/76	0/0/2/2
10	EP	D	504	-	-	1/49/55/55	0/1/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	503	POU	C22-C21	10.05	1.54	1.33
9	B	503	POU	C22-C21	9.28	1.53	1.33
9	D	503	POU	C2-C1	-8.02	1.38	1.52
9	B	503	POU	C2-C1	-7.73	1.39	1.52
11	B	507	MES	C8-S	-6.43	1.66	1.78
8	B	501	GDP	C6-C5	4.60	1.48	1.41
10	D	504	EP	C27-C24	4.54	1.53	1.46
8	D	501	GDP	C6-C5	4.49	1.48	1.41
10	B	504	EP	C27-C24	4.49	1.53	1.46
10	D	504	EP	O2-C75	3.98	1.46	1.34
10	B	504	EP	O2-C75	3.95	1.46	1.34
5	A	501	GTP	C2-N3	3.88	1.38	1.33
5	C	501	GTP	C2-N3	3.69	1.38	1.33
10	D	504	EP	C10-C5	3.57	1.36	1.33
8	D	501	GDP	C4-N9	-3.28	1.33	1.37
9	B	503	POU	C9-C8	3.21	1.56	1.52
8	B	501	GDP	C5-C4	3.01	1.47	1.40
8	B	501	GDP	C4-N9	-3.00	1.33	1.37
9	D	503	POU	O91-C9	3.00	1.45	1.39
10	B	504	EP	C10-C5	3.00	1.35	1.33
8	D	501	GDP	C5-C4	2.98	1.47	1.40
10	B	504	EP	C59-C68	-2.66	1.52	1.56
10	D	504	EP	C59-C68	-2.63	1.52	1.56
9	D	503	POU	C10-C9	2.43	1.57	1.54
8	B	501	GDP	C2-N2	2.23	1.35	1.32
8	D	501	GDP	C2-N2	2.22	1.35	1.32
9	D	503	POU	C12-C11	-2.18	1.50	1.53
9	D	503	POU	C14-C15	2.16	1.57	1.53
9	B	503	POU	C14-C15	2.11	1.57	1.53
10	D	504	EP	C13-S1	2.08	1.74	1.70

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C6-C5-N7	20.72	136.93	134.14
8	B	501	GDP	C6-C5-N7	19.96	136.83	134.14
10	B	504	EP	C12-C13-S1	-12.99	107.49	109.63
10	D	504	EP	C12-C13-S1	-12.97	107.50	109.63
5	A	501	GTP	C6-C5-N7	-11.49	132.59	134.14
5	C	501	GTP	C6-C5-N7	-10.74	132.69	134.14
10	B	504	EP	C32-C27-C24	-7.11	114.36	123.55
10	D	504	EP	C32-C27-C24	-6.80	114.75	123.55
11	B	507	MES	C5-N4-C3	6.54	122.72	109.75
10	D	504	EP	C27-O26-C24	6.44	65.10	60.72
10	B	504	EP	C27-O26-C24	6.43	65.09	60.72
10	B	504	EP	C21-C24-C27	-6.12	114.46	125.05
10	D	504	EP	C21-C24-C27	-5.90	114.86	125.05
9	D	503	POU	C23-C22-C21	-5.76	119.43	127.17
9	B	503	POU	C23-C22-C21	-5.62	119.62	127.17
9	B	503	POU	C15-O15-C1	5.29	126.53	116.65
9	D	503	POU	O91-C9-C10	-5.00	105.50	110.01
9	D	503	POU	C12-C11-C10	4.98	119.98	114.79
8	B	501	GDP	N3-C4-N9	4.90	134.09	126.91
8	D	501	GDP	N3-C4-N9	4.81	133.96	126.91
8	B	501	GDP	C5-C4-N3	-4.71	119.12	125.94
9	D	503	POU	C15-O15-C1	4.69	125.40	116.65
10	B	504	EP	O26-C27-C32	-4.59	110.27	116.59
8	D	501	GDP	C5-C4-N3	-4.42	119.54	125.94
10	D	504	EP	O26-C27-C32	-4.31	110.66	116.59
9	B	503	POU	O13-C13-C12	4.22	116.01	106.96
9	B	503	POU	O91-C9-C10	-4.09	106.32	110.01
8	B	501	GDP	C2-N3-C4	4.08	120.83	115.09
10	D	504	EP	C10-C12-N20	-4.00	117.25	124.01
10	B	504	EP	C16-C15-S1	-3.97	114.78	120.12
8	D	501	GDP	C2-N3-C4	3.89	120.56	115.09
9	B	503	POU	O15-C15-C21	3.79	120.49	109.55
5	C	501	GTP	C2-N3-C4	3.79	120.42	115.09
8	B	501	GDP	C4-C5-N7	-3.70	106.35	109.52
10	D	504	EP	O26-C24-C21	-3.66	107.72	116.05
9	D	503	POU	C13-C12-C11	-3.63	104.39	114.73
5	C	501	GTP	C5-C4-N3	-3.58	120.75	125.94
8	D	501	GDP	C4-C5-N7	-3.58	106.46	109.52
10	B	504	EP	O26-C24-C21	-3.55	107.98	116.05
10	D	504	EP	C16-C15-S1	-3.54	115.36	120.12
9	B	503	POU	O13-C13-C14	3.52	114.51	106.96
10	B	504	EP	C10-C12-N20	-3.52	118.07	124.01
5	A	501	GTP	C2-N3-C4	3.49	119.99	115.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C4-N3	-3.43	120.97	125.94
5	C	501	GTP	N3-C4-N9	3.42	131.93	126.91
10	B	504	EP	C13-C12-N20	3.36	118.05	110.83
5	A	501	GTP	PA-O3A-PB	-3.31	121.98	131.68
10	D	504	EP	C13-C12-N20	3.28	117.87	110.83
5	A	501	GTP	N3-C4-N9	3.24	131.66	126.91
9	D	503	POU	O15-C15-C21	3.19	118.74	109.55
9	D	503	POU	C3-C4-C5	-3.13	107.21	114.76
9	D	503	POU	O13-C13-C12	3.12	113.65	106.96
10	B	504	EP	C16-C15-N20	3.12	132.22	124.07
10	D	504	EP	O26-C24-C27	-3.10	57.44	59.65
10	B	504	EP	O26-C24-C27	-3.09	57.45	59.65
10	B	504	EP	O26-C27-C24	-3.07	57.46	59.65
10	D	504	EP	O26-C27-C24	-3.06	57.47	59.65
9	B	503	POU	C3-C2-C1	-3.04	104.26	109.96
8	D	501	GDP	PA-O3A-PB	-3.01	122.85	131.68
10	D	504	EP	O2-C75-C72	2.98	117.17	111.43
9	D	503	POU	O9-C9-C8	2.91	112.94	105.52
10	B	504	EP	O2-C75-C72	2.87	116.96	111.43
5	C	501	GTP	PB-O3B-PG	-2.86	123.31	131.68
10	D	504	EP	C16-C15-N20	2.85	131.52	124.07
5	A	501	GTP	PB-O3B-PG	-2.82	123.40	131.68
8	B	501	GDP	PA-O3A-PB	-2.82	123.41	131.68
11	B	507	MES	C8-C7-N4	-2.79	107.66	112.44
5	C	501	GTP	PA-O3A-PB	-2.72	123.72	131.68
8	D	501	GDP	C8-N9-C4	2.66	108.93	106.90
9	D	503	POU	O15-C15-C14	2.66	112.65	106.60
9	B	503	POU	C25-C21-C22	-2.59	116.24	123.00
9	D	503	POU	O9-C9-C10	2.57	109.70	105.97
9	B	503	POU	O15-C15-C14	2.55	112.40	106.60
10	B	504	EP	C21-C3-C5	-2.49	110.07	113.62
9	B	503	POU	O9-C9-C10	2.46	109.55	105.97
9	B	503	POU	C12-C11-C10	2.36	117.25	114.79
10	D	504	EP	C53-C51-C47	-2.32	108.17	112.36
9	B	503	POU	O9-C5-C6	2.30	114.02	109.44
10	B	504	EP	C68-C72-C75	-2.29	105.00	111.44
5	A	501	GTP	N2-C2-N1	2.28	120.37	117.86
5	C	501	GTP	N2-C2-N1	2.21	120.29	117.86
10	D	504	EP	C21-C3-C5	-2.21	110.46	113.62
10	B	504	EP	C53-C51-C47	-2.19	108.40	112.36
5	C	501	GTP	N7-C8-N9	-2.14	108.30	114.36
5	A	501	GTP	N7-C8-N9	-2.11	108.39	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	O4'-C1'-N9	-2.11	106.48	108.44
9	B	503	POU	C3-C4-C5	-2.10	109.70	114.76
9	B	503	POU	C18-C10-C11	-2.10	105.35	109.58
9	D	503	POU	C25-C21-C22	-2.08	117.56	123.00
9	B	503	POU	O9-C9-C8	2.08	110.83	105.52
9	D	503	POU	O9-C5-C6	2.08	113.57	109.44
8	B	501	GDP	C8-N9-C4	2.05	108.46	106.90
10	D	504	EP	C68-C72-C75	-2.03	105.73	111.44
11	B	507	MES	C2-C3-N4	2.03	112.56	109.96
9	D	503	POU	O91-C9-O9	-2.02	103.38	109.12
9	B	503	POU	C13-C12-C11	-2.00	109.02	114.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	439/451 (97%)	0.07	2 (0%)	88 90	31, 48, 83, 158	0
1	C	440/451 (97%)	0.11	2 (0%)	88 90	25, 38, 66, 97	0
2	B	428/445 (96%)	0.22	8 (1%)	64 64	25, 44, 83, 159	2 (0%)
2	D	431/445 (96%)	0.38	22 (5%)	27 27	35, 67, 103, 140	6 (1%)
3	E	123/143 (86%)	0.40	5 (4%)	35 36	38, 65, 107, 137	0
4	F	351/384 (91%)	2.11	147 (41%)	1 0	51, 110, 185, 210	0
All	All	2212/2319 (95%)	0.51	186 (8%)	11 10	25, 54, 140, 210	8 (0%)

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	89	GLU	12.5
2	B	280	SER	11.6
4	F	133	ALA	11.4
2	D	283	TYR	11.4
4	F	177	GLY	11.0
4	F	284[A]	LEU	9.8
4	F	173	ILE	9.4
4	F	190	LEU	8.3
1	A	282	TYR	8.0
4	F	240	LEU	7.8
4	F	178	GLN	7.6
4	F	103	THR	7.6
2	B	279	GLY	7.5
4	F	199	PHE	7.5
4	F	160	ILE	7.1
4	F	155	ALA	6.8
4	F	170	LEU	6.8
4	F	278	THR	6.7
4	F	201	ILE	6.5

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Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	6.5
4	F	241	THR	6.5
4	F	353[A]	VAL	6.4
4	F	220[A]	VAL	6.3
2	B	283	TYR	6.2
4	F	372	THR	6.0
4	F	279	LEU	5.8
4	F	338	CYS	5.7
4	F	243	HIS	5.7
4	F	320	MET	5.6
4	F	156	LYS	5.5
4	F	181	VAL	5.5
4	F	251	LYS	5.4
4	F	157	GLY	5.3
4	F	134	ALA	5.2
4	F	186	LEU	5.2
4	F	277[A]	THR	5.2
4	F	158	GLU	5.1
4	F	371	PRO	5.1
4	F	154	GLY	5.0
4	F	330	ILE	5.0
4	F	256	TYR	4.9
4	F	206	LEU	4.8
4	F	153	ALA	4.7
4	F	246	GLN	4.6
4	F	223	THR	4.6
4	F	337	ALA	4.6
4	F	194	PRO	4.6
4	F	271[A]	LEU	4.6
4	F	263	PHE	4.5
4	F	101	TYR	4.5
2	B	285	ALA	4.4
4	F	204	TRP	4.4
4	F	244	CYS	4.4
4	F	148	ILE	4.3
2	B	282	GLN	4.3
4	F	245	ILE	4.2
4	F	236	LYS	4.2
4	F	283	ILE	4.2
4	F	137	ARG	4.2
4	F	319	PHE	4.1
3	E	6	MET	4.1

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Mol	Chain	Res	Type	RSRZ
4	F	259	GLY	4.1
4	F	268	ASN	4.1
4	F	327	VAL	4.1
2	B	1	MET	4.0
4	F	192	LEU	4.0
4	F	150	LYS	4.0
4	F	285	LEU	4.0
4	F	183	GLN	4.0
4	F	328	TRP	4.0
4	F	132	LEU	4.0
4	F	339	ALA	4.0
4	F	336	PRO	4.0
4	F	375	PHE	4.0
4	F	130	VAL	4.0
4	F	221	LEU	4.0
4	F	280	GLU	3.9
2	D	400	ARG	3.9
4	F	105	LEU	3.8
4	F	252	ASN	3.8
4	F	332	VAL	3.7
4	F	90	SER	3.7
4	F	317	PHE	3.7
4	F	191	LEU	3.7
4	F	184	LYS	3.6
4	F	267	PHE	3.6
4	F	239	HIS	3.5
4	F	269	GLN	3.5
4	F	182	ILE	3.4
4	F	247	LYS	3.3
4	F	151	SER	3.3
4	F	321	VAL	3.3
4	F	142	ARG	3.2
4	F	248	GLU	3.2
4	F	159	GLY	3.2
4	F	6	VAL	3.2
4	F	95	PRO	3.2
4	F	376	ILE	3.1
4	F	147	TRP	3.1
2	D	397	ALA	3.1
4	F	198	LYS	3.1
4	F	179	VAL	3.1
4	F	144	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
4	F	85	PRO	3.0
4	F	264	PHE	3.0
4	F	329	LEU	3.0
4	F	140	GLU	3.0
4	F	258	GLU	3.0
4	F	261	GLU	3.0
4	F	197	ARG	3.0
2	D	429	VAL	2.9
4	F	233	PHE	2.9
4	F	167	SER	2.9
2	D	384[A]	ILE	2.9
4	F	131	PHE	2.9
4	F	128	ARG	2.9
4	F	203	SER	2.8
4	F	149	ALA	2.8
4	F	272	MET	2.8
4	F	291	ILE	2.8
4	F	129	GLU	2.8
4	F	93	TRP	2.8
2	D	94	PHE	2.8
4	F	253	TYR	2.8
2	D	157	ILE	2.8
4	F	350	ILE	2.8
2	D	388	PHE	2.7
2	D	304	ALA	2.7
4	F	255[A]	ARG	2.7
2	B	284	ARG	2.7
2	D	248	LEU	2.7
4	F	346	LEU	2.7
3	E	24	LEU	2.7
1	C	357	TYR	2.7
2	D	187	ALA	2.7
4	F	64	TYR	2.6
4	F	188	LYS	2.6
4	F	216	TYR	2.6
2	D	121	VAL	2.6
2	D	177	VAL	2.6
4	F	222	ARG	2.6
3	E	140	LYS	2.5
2	D	282	GLN	2.5
3	E	143	ALA	2.5
4	F	354	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
4	F	227	PRO	2.5
4	F	169	LEU	2.5
4	F	237	THR	2.5
2	D	401	ARG	2.5
1	C	302[A]	MET	2.4
4	F	250	SER	2.4
2	D	204	ILE	2.4
4	F	98	TYR	2.4
2	D	179	ASP	2.4
4	F	127	GLU	2.4
4	F	262	MET	2.4
2	D	307	PRO	2.4
4	F	323	GLU	2.4
4	F	341	LYS	2.4
4	F	88	SER	2.4
4	F	282	SER	2.4
2	D	404	PHE	2.4
4	F	5	VAL	2.3
1	A	439	SER	2.3
4	F	275[A]	LEU	2.3
4	F	44	ARG	2.2
4	F	94	PHE	2.2
2	B	57	THR	2.2
4	F	180	HIS	2.2
4	F	163	SER	2.2
4	F	378[A]	LEU	2.1
3	E	28	SER	2.1
4	F	152	SER	2.1
4	F	91	CYS	2.1
4	F	100	ILE	2.1
4	F	324	GLU	2.1
4	F	257	GLU	2.1
4	F	315	PHE	2.1
4	F	74	LYS	2.1
4	F	298	ILE	2.1
4	F	213	ILE	2.1
2	D	220	THR	2.1
2	D	396	THR	2.1
4	F	214	TYR	2.1
4	F	276	ASN	2.0
2	D	172	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	MG	C	502	1/1	0.18	5.73	36,36,36,36	0
7	CA	B	505	1/1	0.20	4.60	97,97,97,97	0
10	EP	D	504	34/34	0.31	3.52	49,67,73,82	0
6	MG	B	502	1/1	0.22	2.71	24,24,24,24	0
9	POU	D	503	38/38	0.28	1.49	43,84,113,114	0
7	CA	A	503	1/1	0.16	1.26	66,66,66,66	0
8	GDP	B	501	28/28	0.17	0.56	23,29,36,39	0
7	CA	B	506	1/1	0.19	0.52	99,99,99,99	0
11	MES	B	507	12/12	0.14	0.42	51,61,73,81	0
5	GTP	C	501	32/32	0.14	0.34	17,27,40,53	0
9	POU	B	503	38/38	0.12	-0.16	37,56,88,96	0
5	GTP	A	501	32/32	0.14	-0.17	24,32,39,49	0
6	MG	A	502	1/1	0.13	-0.26	33,33,33,33	0
10	EP	B	504	34/34	0.15	-0.35	53,68,78,108	0
8	GDP	D	501	28/28	0.13	-0.40	40,59,72,75	0
6	MG	D	502	1/1	0.06	-	64,64,64,64	0

6.5 Other polymers ⓘ

There are no such residues in this entry.