



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2014 – 03:15 PM BST

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 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>

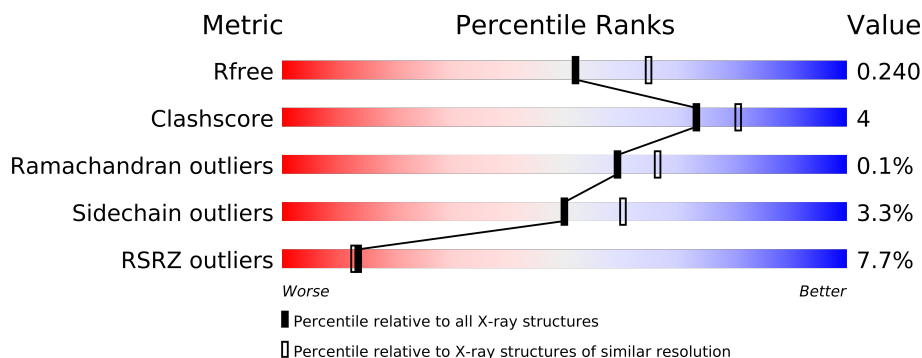
The following versions of software and data (see [references](#)) were used in the production of this report:

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
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 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	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

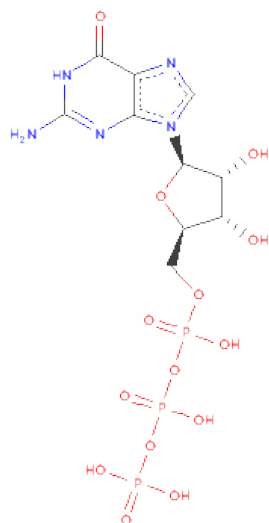
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

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		

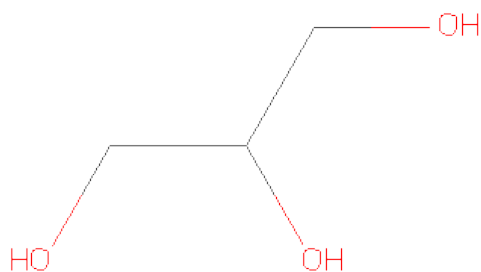
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

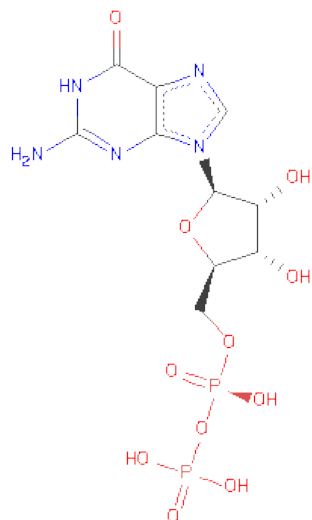
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

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



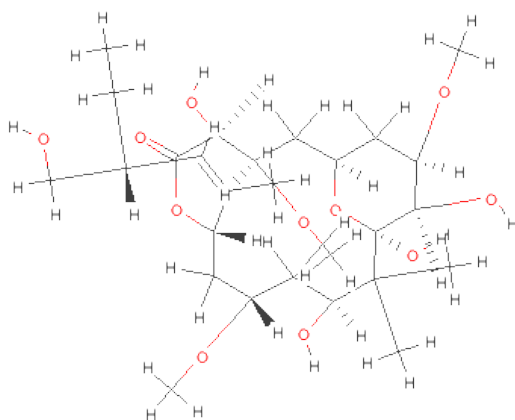
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

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



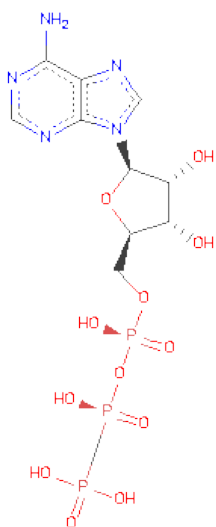
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- 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	C	O	0	0
			38	27	11		
10	D	1	Total	C	O	0	0
			38	27	11		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONICACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

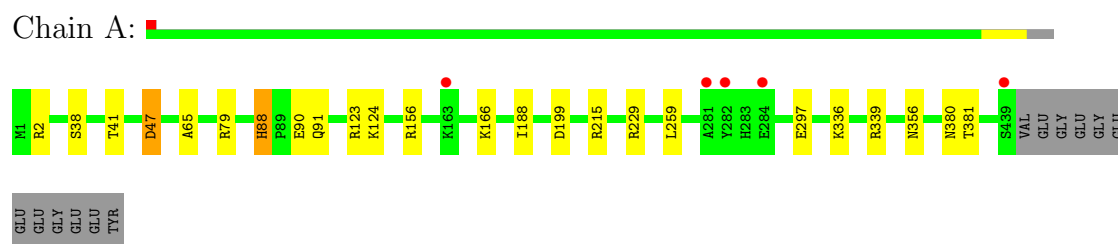
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	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		

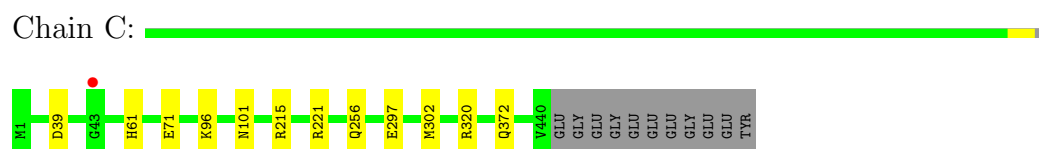
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

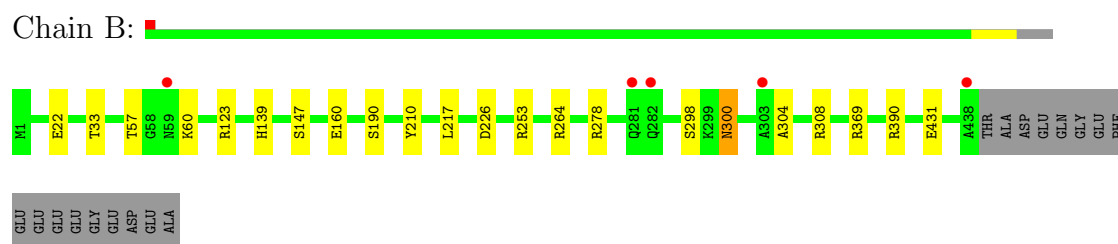
- Molecule 1: Tubulin alpha-1B chain



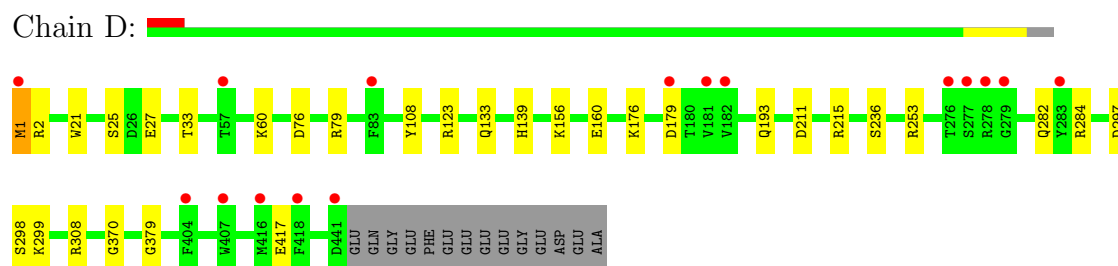
- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta-2B chain

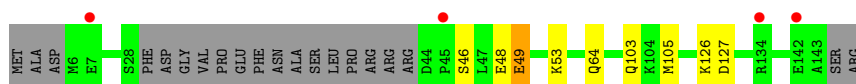


- Molecule 2: Tubulin beta-2B chain



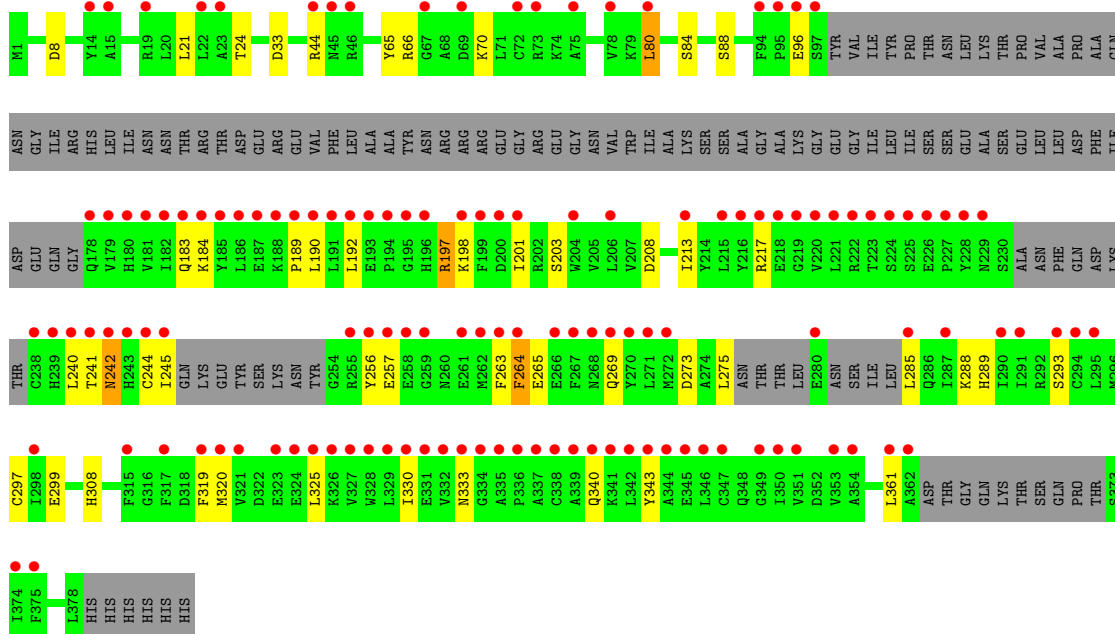
- Molecule 3: Stathmin-4





● Molecule 4: Tubulin-tyrosine ligase

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	104.37Å 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 0.201 , 0.240	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 , 33.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 150728 reflections (0.001%)	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.

5 Model quality

5.1 Standard geometry

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 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	3485	0	0	12	0
1	C	3496	0	0	7	0
2	B	3424	0	0	13	0
2	D	3413	0	0	18	0
3	E	1044	0	0	5	0
4	F	2179	0	0	15	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
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	6	0
12	B	210	0	0	8	0
12	C	264	0	0	5	0
12	D	116	0	0	4	0
12	E	43	0	0	2	0
12	F	21	0	0	1	0
All	All	18124	0	166	73	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 (73) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:253:ARG:NE	12:B:735:HOH:O	2.20	0.72
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.23	0.71
2:B:22:GLU:OE2	12:B:802:HOH:O	2.09	0.70
2:D:176:LYS:NZ	2:D:211:ASP:OD1	2.24	0.70
1:C:372:GLN:NE2	12:C:786:HOH:O	2.25	0.70
4:F:269:GLN:O	4:F:273:ASP:N	2.32	0.63
1:A:156:ARG:NE	12:A:643:HOH:O	2.32	0.62
4:F:201:ILE:O	4:F:319:PHE:N	2.32	0.62
1:A:356:ASN:ND2	12:A:664:HOH:O	2.31	0.62
2:B:264:ARG:NE	2:B:431[A]:GLU:OE2	2.34	0.61
1:C:297:GLU:OE2	12:C:755:HOH:O	2.16	0.61
1:C:39:ASP:OD2	1:C:61:HIS:NE2	2.33	0.60
3:E:53:LYS:NZ	12:E:217:HOH:O	2.34	0.60
2:D:33:THR:O	2:D:60:LYS:NZ	2.35	0.59
2:B:147[A]:SER:OG	2:B:190:SER:OG	2.20	0.59
2:D:123:ARG:NH2	12:D:690:HOH:O	2.36	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:47:ASP:OD1	1:A:47:ASP:N	2.35	0.58
2:D:370:GLY:N	12:D:677:HOH:O	2.36	0.58
2:B:217:LEU:O	12:B:795:HOH:O	2.17	0.58
4:F:242:ASN:O	4:F:245:ILE:N	2.38	0.57
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.37	0.57
1:A:123:ARG:NH1	12:A:722:HOH:O	2.37	0.57
2:D:297:ASP:OD2	2:D:299:LYS:NZ	2.37	0.56
4:F:80:LEU:O	4:F:84:SER:OG	2.22	0.56
4:F:263:PHE:O	4:F:265:GLU:N	2.39	0.56
1:A:79:ARG:NE	12:A:669:HOH:O	2.40	0.55
1:C:256:GLN:NE2	12:C:773:HOH:O	2.39	0.55
2:D:76:ASP:OD1	2:D:79:ARG:NH1	2.40	0.54
2:B:226:ASP:OD1	2:B:278:ARG:NH2	2.40	0.54
2:D:215:ARG:NH1	12:D:652:HOH:O	2.40	0.54
4:F:242:ASN:N	4:F:242:ASN:OD1	2.40	0.53
2:B:123:ARG:NH2	2:B:160:GLU:OE1	2.42	0.53
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.26	0.52
4:F:21:LEU:O	4:F:24:THR:OG1	2.28	0.51
2:B:300:ASN:ND2	12:B:809:HOH:O	2.43	0.51
2:D:156:LYS:NZ	3:E:127:ASP:OD2	2.44	0.51
1:A:229[A]:ARG:NH1	12:A:740:HOH:O	2.43	0.50
4:F:84:SER:O	4:F:88:SER:OG	2.30	0.50
2:B:300:ASN:O	12:B:798:HOH:O	2.20	0.49
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.46	0.49
1:C:101:ASN:ND2	12:C:679:HOH:O	2.46	0.49
2:B:304:ALA:N	12:B:616:HOH:O	2.46	0.48
1:A:65:ALA:O	1:A:91:GLN:NE2	2.46	0.48
4:F:66:ARG:NH1	12:F:501:HOH:O	2.47	0.47
2:B:33:THR:O	2:B:60:LYS:NZ	2.48	0.46
1:C:320:ARG:NH2	12:C:648:HOH:O	2.48	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
2:B:210:TYR:OH	12:B:706:HOH:O	2.21	0.45
1:A:88:HIS:ND1	1:A:91:GLN:OE1	2.50	0.45
4:F:96:GLU:O	4:F:184:LYS:N	2.50	0.45
11:F:401:ACP:O2G	11:F:401:ACP:O2B	2.35	0.44
2:B:390:ARG:NE	12:B:644:HOH:O	2.50	0.44
4:F:201:ILE:N	4:F:319:PHE:O	2.50	0.44
2:D:21:TRP:O	2:D:25:SER:OG	2.34	0.44
4:F:65:TYR:OH	4:F:208:ASP:O	2.35	0.44
2:D:27:GLU:OE1	2:D:236:SER:OG	2.37	0.43
2:D:2:ARG:O	2:D:133:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:289:HIS:O	4:F:293:SER:OG	2.36	0.43
1:A:259:LEU:O	1:A:380:ASN:ND2	2.52	0.43
4:F:8:ASP:OD2	4:F:44:ARG:NH1	2.52	0.43
10:B:503:POU:H46	10:B:503:POU:H40	1.91	0.43
1:A:166:LYS:N	1:A:199:ASP:OD2	2.53	0.42
2:D:253:ARG:NH2	12:D:667:HOH:O	2.53	0.42
10:B:503:POU:H27	10:B:503:POU:O15	2.20	0.41
3:E:46:SER:OG	3:E:49:GLU:OE2	2.38	0.41
2:D:123:ARG:NE	2:D:160:GLU:OE1	2.54	0.41
3:E:64:GLN:NE2	12:E:225:HOH:O	2.53	0.41
1:A:215:ARG:NH2	12:A:732:HOH:O	2.53	0.41
10:B:503:POU:H32	10:B:503:POU:H8	1.89	0.40
2:D:297:ASP:OD1	2:D:298:SER:N	2.55	0.40
1:C:96:LYS:O	2:D:1:MET:N	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	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%)	27	24
All	All	2153/2319 (93%)	2094 (97%)	57 (3%)	2 (0%)	59	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	264	PHE

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Mol	Chain	Res	Type
4	F	189	PRO

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	382/379 (101%)	372 (97%)	10 (3%)	59	70
1	C	386/379 (102%)	382 (99%)	4 (1%)	85	93
2	B	382/383 (100%)	376 (98%)	6 (2%)	75	85
2	D	378/383 (99%)	372 (98%)	6 (2%)	75	85
3	E	116/127 (91%)	112 (97%)	4 (3%)	49	59
4	F	241/342 (70%)	211 (88%)	30 (12%)	7	5
All	All	1885/1993 (95%)	1825 (97%)	60 (3%)	50	62

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

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Mol	Chain	Res	Type
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
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 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 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	34,34,34	1.09	1 (2%)	51,54,54	1.88	11 (21%)
8	GOL	A	504	-	5,5,5	0.34	0	5,5,5	0.27	0
9	GDP	B	501	6	30,30,30	1.48	5 (16%)	44,47,47	3.05	7 (15%)
10	POU	B	503	-	39,39,39	2.50	7 (17%)	57,57,57	2.10	15 (26%)
5	GTP	C	501	6	34,34,34	0.94	1 (2%)	51,54,54	2.43	8 (15%)
9	GDP	D	501	-	30,30,30	1.39	4 (13%)	44,47,47	3.15	7 (15%)
10	POU	D	503	-	39,39,39	2.37	7 (17%)	57,57,57	1.90	13 (22%)
11	ACP	F	401	-	33,33,33	1.52	7 (21%)	52,52,52	1.96	11 (21%)

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	GOL	A	504	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/16/32/32	0/1/3/3
10	POU	B	503	-	-	1/56/76/76	0/0/2/2
5	GTP	C	501	6	-	0/22/38/38	0/1/3/3
9	GDP	D	501	-	-	0/16/32/32	0/1/3/3
10	POU	D	503	-	-	1/56/76/76	0/0/2/2
11	ACP	F	401	-	-	0/20/38/38	0/1/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	POU	C22-C21	10.97	1.56	1.33
10	D	503	POU	C22-C21	9.82	1.54	1.33
10	B	503	POU	C2-C1	-7.95	1.39	1.52
10	D	503	POU	C2-C1	-7.70	1.39	1.52
9	B	501	GDP	C6-C5	4.62	1.48	1.41
9	D	501	GDP	C6-C5	4.13	1.48	1.41
5	A	501	GTP	C2-N3	3.70	1.38	1.33
10	D	503	POU	C14-C15	3.54	1.60	1.53
11	F	401	ACP	PG-O2G	3.51	1.61	1.54
10	D	503	POU	C10-C9	3.39	1.59	1.54
11	F	401	ACP	PG-O3G	3.35	1.61	1.54
11	F	401	ACP	C5-C4	3.14	1.47	1.40
5	C	501	GTP	C2-N3	3.09	1.37	1.33
9	D	501	GDP	C4-N9	-3.01	1.33	1.37
9	D	501	GDP	C5-C4	2.92	1.47	1.40
9	B	501	GDP	C5-C4	2.84	1.46	1.40
10	B	503	POU	C23-C22	2.75	1.54	1.50
11	F	401	ACP	PG-C3B	2.65	1.82	1.79
10	D	503	POU	C14-C13	2.64	1.59	1.52
10	B	503	POU	O91-C9	2.61	1.44	1.39
10	D	503	POU	O91-C9	2.59	1.44	1.39
11	F	401	ACP	PB-C3B	2.57	1.82	1.79
9	B	501	GDP	C4-N9	-2.52	1.34	1.37
11	F	401	ACP	C4-N9	-2.51	1.34	1.37
9	B	501	GDP	C2-N3	2.37	1.36	1.33
10	D	503	POU	C23-C22	2.33	1.53	1.50
9	B	501	GDP	C2-N2	2.31	1.36	1.32
11	F	401	ACP	PB-O2B	2.27	1.61	1.56
10	B	503	POU	C3-C2	-2.13	1.48	1.52
9	D	501	GDP	C2-N2	2.11	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	POU	C14-C13	2.08	1.57	1.52
10	B	503	POU	C10-C9	2.07	1.57	1.54

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C6-C5-N7	17.83	136.54	134.14
9	B	501	GDP	C6-C5-N7	16.13	136.31	134.14
5	C	501	GTP	C6-C5-N7	-14.88	132.14	134.14
5	A	501	GTP	C6-C5-N7	-8.67	132.97	134.14
10	B	503	POU	C12-C11-C10	6.36	121.42	114.79
11	F	401	ACP	N3-C2-N1	-6.13	123.58	128.71
10	D	503	POU	C23-C22-C21	-5.95	119.18	127.17
9	B	501	GDP	N3-C4-N9	5.80	135.42	126.91
10	B	503	POU	C15-O15-C1	5.51	126.93	116.65
9	B	501	GDP	C5-C4-N3	-5.11	118.54	125.94
10	D	503	POU	C12-C11-C10	5.01	120.02	114.79
9	D	501	GDP	N3-C4-N9	4.98	134.21	126.91
11	F	401	ACP	N3-C4-N9	4.95	134.38	125.43
10	B	503	POU	C23-C22-C21	-4.70	120.86	127.17
9	B	501	GDP	O4'-C1'-N9	-4.63	104.13	108.44
10	B	503	POU	O91-C9-C10	-4.63	105.83	110.01
11	F	401	ACP	C2'-C1'-N9	-4.46	101.83	113.27
9	D	501	GDP	C5-C4-N3	-4.38	119.60	125.94
10	D	503	POU	C15-O15-C1	4.36	124.79	116.65
11	F	401	ACP	O4'-C1'-N9	4.20	112.35	108.44
9	B	501	GDP	C2-N3-C4	4.13	120.89	115.09
11	F	401	ACP	C4-C5-N7	-3.82	106.25	109.52
10	D	503	POU	O13-C13-C12	3.69	114.87	106.96
9	D	501	GDP	C2-N3-C4	3.65	120.21	115.09
10	B	503	POU	C13-C12-C11	-3.55	104.62	114.73
9	B	501	GDP	C4-C5-N7	-3.53	106.50	109.52
9	D	501	GDP	C4-C5-N7	-3.49	106.53	109.52
10	B	503	POU	O15-C15-C21	3.48	119.58	109.55
10	D	503	POU	C13-C12-C11	-3.42	104.98	114.73
10	D	503	POU	C3-C4-C5	-3.37	106.62	114.76
11	F	401	ACP	PA-O3A-PB	-3.25	121.97	131.74
10	D	503	POU	O15-C15-C14	3.20	113.87	106.60
5	A	501	GTP	O4'-C1'-N9	-3.19	105.47	108.44
11	F	401	ACP	C5-C4-N3	-3.19	118.76	125.70
11	F	401	ACP	PB-C3B-PG	-3.18	113.04	117.62
5	C	501	GTP	C2-N3-C4	3.14	119.50	115.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	C8-N9-C4	3.13	109.29	106.90
10	B	503	POU	O13-C13-C12	3.13	113.66	106.96
9	D	501	GDP	C8-N9-C4	3.12	109.28	106.90
5	C	501	GTP	C5-C4-N3	-2.98	121.63	125.94
5	C	501	GTP	N3-C4-N9	2.94	131.23	126.91
10	B	503	POU	C3-C4-C5	-2.91	107.72	114.76
10	B	503	POU	O9-C9-C8	2.89	112.89	105.52
10	B	503	POU	O15-C15-C14	2.85	113.09	106.60
5	A	501	GTP	PB-O3B-PG	-2.80	123.46	131.68
10	B	503	POU	O9-C9-C10	2.79	110.03	105.97
9	D	501	GDP	PA-O3A-PB	-2.69	123.79	131.68
10	D	503	POU	O91-C9-C10	-2.66	107.61	110.01
10	D	503	POU	O9-C9-C8	2.64	112.27	105.52
5	A	501	GTP	N3-C4-N9	2.61	130.74	126.91
5	A	501	GTP	O5'-PA-O1A	-2.58	99.27	109.37
10	D	503	POU	O15-C15-C21	2.52	116.81	109.55
5	A	501	GTP	C2-N3-C4	2.51	118.62	115.09
5	C	501	GTP	PA-O3A-PB	-2.47	124.45	131.68
5	A	501	GTP	PA-O3A-PB	-2.46	124.48	131.68
5	A	501	GTP	C5-C4-N3	-2.46	122.39	125.94
5	C	501	GTP	PB-O3B-PG	-2.45	124.49	131.68
5	C	501	GTP	N2-C2-N1	2.45	120.56	117.86
5	A	501	GTP	N7-C8-N9	-2.44	107.45	114.36
5	A	501	GTP	C8-N9-C4	2.44	108.76	106.90
10	B	503	POU	O8-C8-C9	-2.39	110.86	113.26
10	D	503	POU	O9-C9-C10	2.37	109.41	105.97
11	F	401	ACP	C2-N3-C4	2.34	120.67	114.01
10	B	503	POU	C9-O9-C5	2.33	118.31	113.61
10	D	503	POU	C18-C10-C11	-2.26	105.02	109.58
5	A	501	GTP	C1'-N9-C4	-2.19	122.86	126.64
11	F	401	ACP	O2B-PB-C3B	2.17	111.61	106.61
11	F	401	ACP	C2'-C3'-C4'	-2.11	98.44	102.65
10	B	503	POU	C18-C10-C11	-2.11	105.33	109.58
10	D	503	POU	O91-C9-O9	-2.08	103.20	109.12
10	B	503	POU	C25-C21-C22	-2.07	117.60	123.00
5	C	501	GTP	N7-C8-N9	-2.03	108.62	114.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

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

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%)	-0.15	5 (1%) 77 78	17, 32, 66, 112	0
1	C	440/451 (97%)	-0.22	1 (0%) 93 94	11, 22, 45, 68	0
2	B	428/445 (96%)	-0.02	5 (1%) 75 76	13, 27, 60, 112	2 (0%)
2	D	431/445 (96%)	0.16	16 (3%) 39 40	18, 44, 77, 102	6 (1%)
3	E	123/143 (86%)	0.23	4 (3%) 44 45	25, 44, 85, 121	0
4	F	265/384 (69%)	2.32	132 (49%) 1 0	39, 79, 123, 153	0
All	All	2126/2319 (91%)	0.26	163 (7%) 13 13	11, 35, 92, 153	8 (0%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	194	PRO	12.1
4	F	182	ILE	9.2
4	F	192	LEU	7.8
4	F	240	LEU	7.6
4	F	195	GLY	7.6
4	F	179	VAL	7.3
4	F	338	CYS	7.1
4	F	184	LYS	7.1
4	F	227	PRO	7.0
4	F	241	THR	7.0
1	A	439	SER	6.9
4	F	375	PHE	6.8
4	F	178	GLN	6.7
4	F	329	LEU	6.6
4	F	346	LEU	6.5
4	F	183	GLN	6.4
4	F	328	TRP	6.4
4	F	350	ILE	6.1
4	F	330	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
4	F	271	LEU	5.9
4	F	190	LEU	5.9
4	F	44	ARG	5.8
4	F	199	PHE	5.6
4	F	201	ILE	5.6
4	F	245	ILE	5.5
4	F	221	LEU	5.5
4	F	238	CYS	5.4
4	F	75	ALA	5.3
4	F	181	VAL	5.1
4	F	216	TYR	5.1
4	F	354	ALA	5.1
4	F	244	CYS	5.0
4	F	295	LEU	5.0
4	F	291	ILE	5.0
4	F	269	GLN	5.0
4	F	362	ALA	5.0
4	F	186	LEU	4.9
1	A	282	TYR	4.9
4	F	332	VAL	4.9
4	F	255	ARG	4.8
4	F	339	ALA	4.7
4	F	353	VAL	4.7
4	F	180	HIS	4.6
4	F	361	LEU	4.6
4	F	280	GLU	4.5
4	F	321	VAL	4.5
4	F	319	PHE	4.5
4	F	243	HIS	4.4
4	F	198	LYS	4.4
4	F	229	ASN	4.4
4	F	206	LEU	4.4
2	D	1	MET	4.3
4	F	204	TRP	4.3
2	D	276	THR	4.2
4	F	340	GLN	4.2
4	F	189	PRO	4.2
4	F	343	TYR	4.2
4	F	268	ASN	4.1
4	F	333	ASN	4.1
4	F	341	LYS	4.1
4	F	290	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
4	F	219	GLY	3.9
4	F	327	VAL	3.9
4	F	213	ILE	3.9
2	D	277	SER	3.8
4	F	337	ALA	3.7
4	F	325	LEU	3.7
4	F	73	ARG	3.7
2	D	179	ASP	3.7
4	F	191	LEU	3.6
4	F	349	GLY	3.5
4	F	298	ILE	3.5
2	D	83	PHE	3.5
4	F	78	VAL	3.5
4	F	94	PHE	3.5
4	F	218	GLU	3.5
4	F	294	CYS	3.4
4	F	226	GLU	3.4
4	F	239	HIS	3.4
4	F	263	PHE	3.4
4	F	258	GLU	3.4
2	D	418	PHE	3.4
4	F	267	PHE	3.4
2	D	283	TYR	3.4
2	D	404	PHE	3.4
2	D	57	THR	3.3
4	F	262	MET	3.3
2	D	182	VAL	3.3
4	F	317	PHE	3.3
4	F	270	TYR	3.3
4	F	96	GLU	3.3
4	F	320	MET	3.2
4	F	326	LYS	3.2
1	C	43	GLY	3.2
4	F	185	TYR	3.2
4	F	242	ASN	3.2
4	F	256	TYR	3.1
4	F	23	ALA	3.1
4	F	225	SER	3.1
2	D	278	ARG	3.1
4	F	223	THR	3.0
4	F	266	GLU	3.0
3	E	134	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	279	GLY	3.0
4	F	323	GLU	2.9
4	F	187	GLU	2.9
2	B	281	GLN	2.9
2	B	282	GLN	2.8
4	F	200	ASP	2.8
4	F	261	GLU	2.8
2	D	441	ASP	2.7
4	F	220	VAL	2.7
4	F	188	LYS	2.7
4	F	72	CYS	2.7
4	F	264	PHE	2.7
4	F	285	LEU	2.7
4	F	196	HIS	2.6
4	F	193	GLU	2.6
4	F	336	PRO	2.6
1	A	281	ALA	2.6
4	F	345	GLU	2.6
4	F	293	SER	2.6
4	F	351	VAL	2.6
4	F	374	ILE	2.6
4	F	217	ARG	2.6
4	F	342	LEU	2.6
4	F	215	LEU	2.5
4	F	287	ILE	2.5
4	F	224	SER	2.5
4	F	315	PHE	2.5
4	F	15	ALA	2.5
4	F	97	SER	2.5
4	F	347	CYS	2.5
1	A	163	LYS	2.5
4	F	19	ARG	2.5
4	F	331	GLU	2.4
4	F	14	TYR	2.4
4	F	344	ALA	2.4
4	F	222	ARG	2.4
4	F	335	ALA	2.4
4	F	67	GLY	2.4
4	F	80	LEU	2.3
2	D	181	VAL	2.3
3	E	45	PRO	2.3
4	F	257	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	22	LEU	2.2
4	F	45	ASN	2.2
2	B	438	ALA	2.2
2	D	416	MET	2.2
4	F	272	MET	2.2
4	F	228	TYR	2.1
4	F	324	GLU	2.1
3	E	7	GLU	2.1
3	E	142	GLU	2.1
4	F	95	PRO	2.1
2	B	59	ASN	2.1
4	F	69	ASP	2.1
4	F	259	GLY	2.1
2	B	303	ALA	2.1
4	F	46	ARG	2.0
4	F	334	GLY	2.0
1	A	284	GLU	2.0
2	D	407	TRP	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	0.15	2.78	18,18,18,18	0
8	GOL	A	504	6/6	0.24	1.63	57,60,60,62	0
6	MG	B	502	1/1	0.15	1.19	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	POU	D	503	38/38	0.19	1.03	35,59,74,77	0
6	MG	D	502	1/1	0.16	0.77	67,67,67,67	0
5	GTP	C	501	32/32	0.13	0.62	4,13,19,30	0
7	CA	A	503	1/1	0.13	0.46	68,68,68,68	0
5	GTP	A	501	32/32	0.12	0.26	10,17,22,41	0
10	POU	B	503	38/38	0.12	0.22	23,44,77,81	0
9	GDP	B	501	28/28	0.14	0.21	11,16,20,22	0
9	GDP	D	501	28/28	0.10	-0.50	27,36,45,53	0
11	ACP	F	401	31/31	0.27	-0.96	67,106,145,166	0
6	MG	A	502	1/1	0.10	-1.06	14,14,14,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.