



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:38 PM GMT

PDB ID : 4TV8
Title : Tubulin-Maytansine complex
Authors : Prota, A.E.; Bargsten, K.; Diaz, J.F.; Marsh, M.; Cuevas, C.; Liniger, M.; Neuhaus, C.; Andreu, J.M.; Altmann, K.H.; Steinmetz, M.O.
Deposited on : 2014-06-26
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

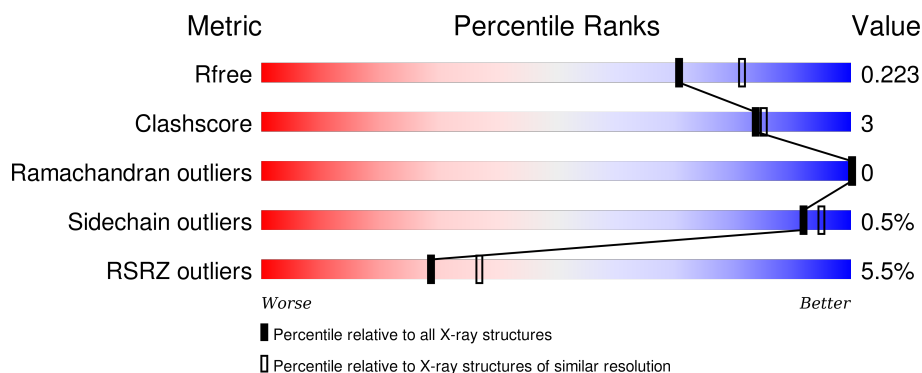
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div></div> <div>88% 8% .</div> </div>
1	C	451	<div> <div></div> <div>88% 9% .</div> </div>
2	B	445	<div> <div>2%</div> <div>89% 7% .</div> </div>
2	D	445	<div> <div>4%</div> <div>87% 8% 5%</div> </div>
3	E	143	<div> <div></div> <div>77% 8% 15%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a red segment labeled '22%', a green segment labeled '80%', a yellow segment labeled '7%', and a grey segment labeled '13%'. The segments are stacked horizontally to represent the distribution of quality metrics.

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
8	GOL	C	503	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18278 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	436	Total	C	N	O	S	0	7	0
			3433	2175	580	654	24			
1	C	440	Total	C	N	O	S	0	11	0
			3483	2208	585	665	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	4	0
			3365	2116	572	650	27			
2	D	422	Total	C	N	O	S	0	3	0
			3326	2091	563	644	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	1	0
			1006	621	182	198	5			

There are 2 discrepancies between the modelled and reference sequences:

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

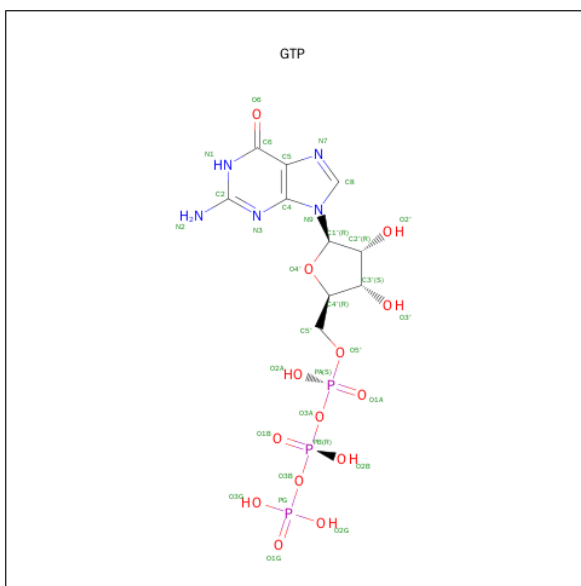
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	335	Total	C	N	O	S	0	2	0
			2763	1776	473	500	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

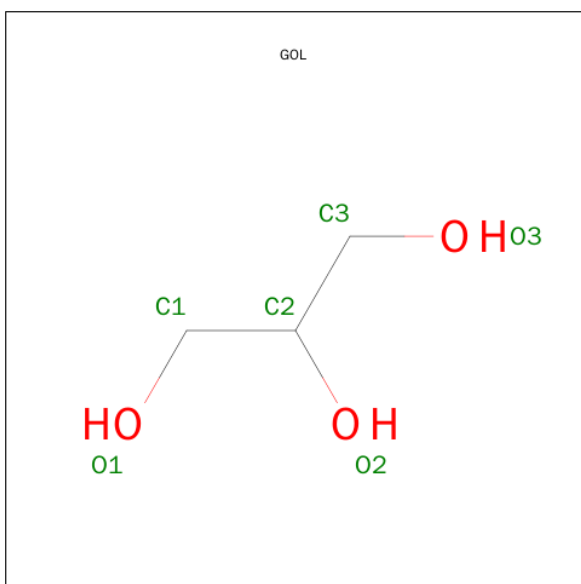
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	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).

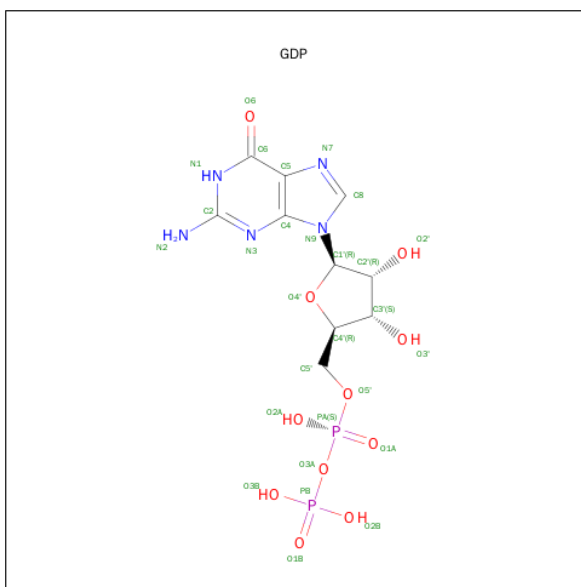
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



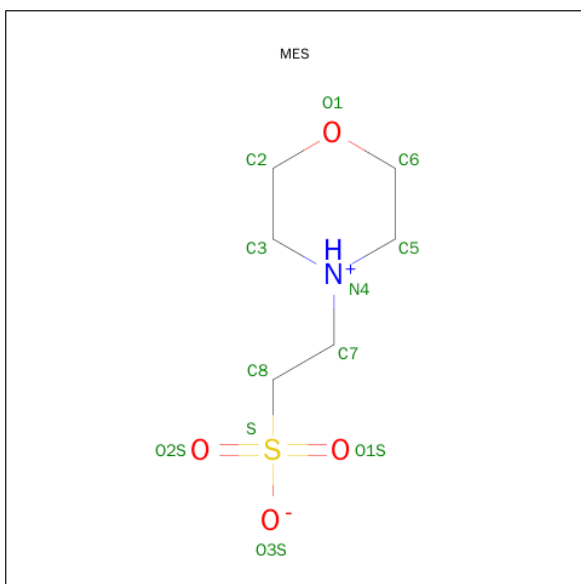
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

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



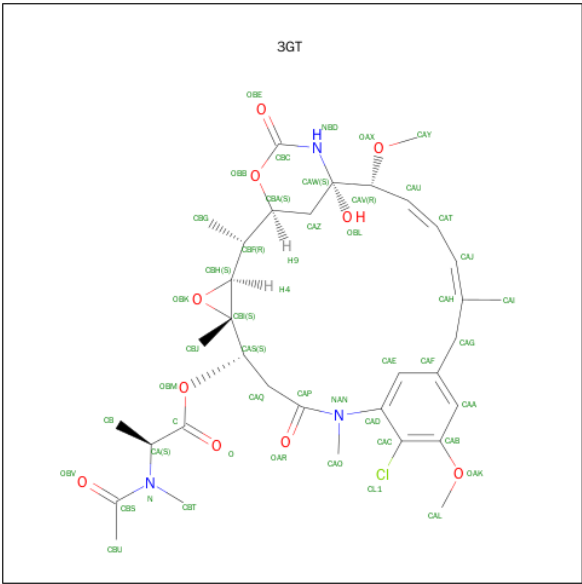
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



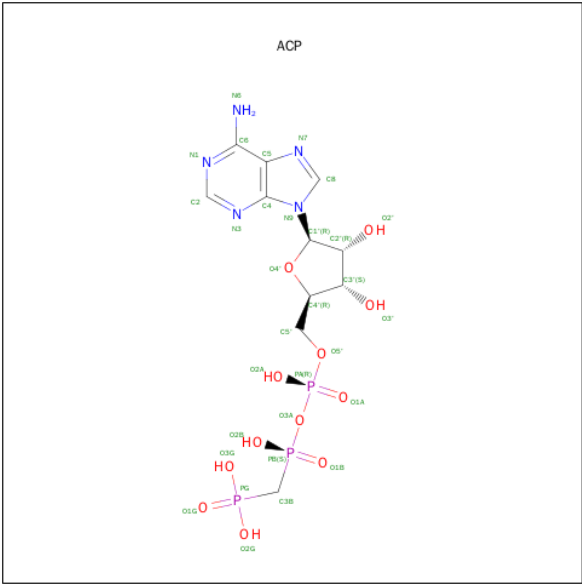
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (3beta,4beta,5beta,10beta,11E,13E)-maytansine (three-letter code: 3GT) (formula: C₃₄H₄₆ClN₃O₁₀).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	Cl	N	O	0	0
			48	34	1	3	10		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

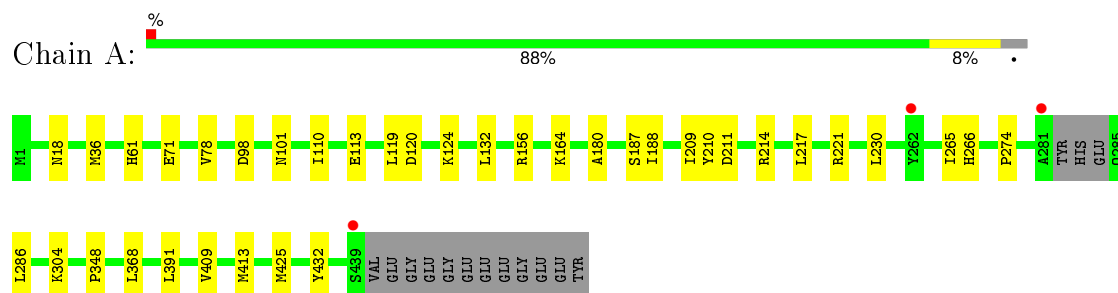
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	134	Total 134	O 134	0	0
13	B	113	Total 113	O 113	0	0
13	C	252	Total 252	O 252	0	0
13	D	97	Total 97	O 97	0	0
13	E	30	Total 30	O 30	0	0
13	F	45	Total 45	O 45	0	0

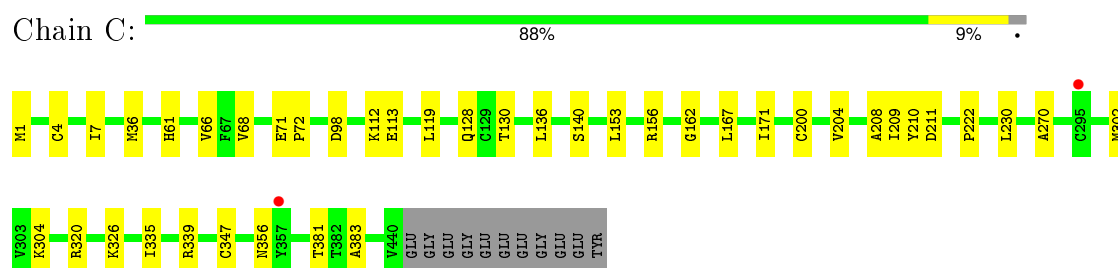
3 Residue-property plots [i](#)

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

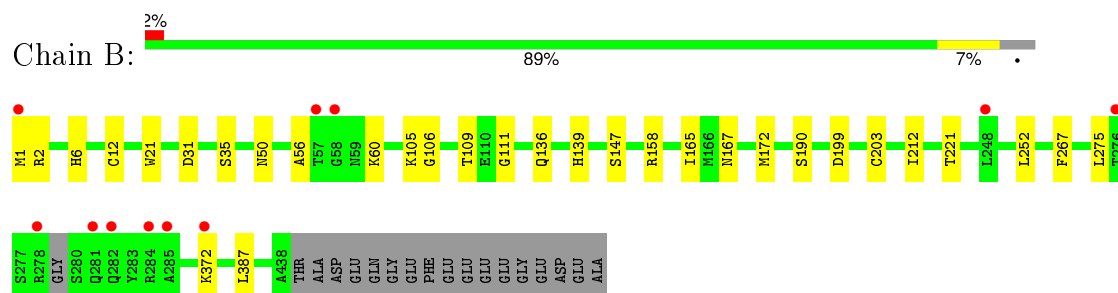
- Molecule 1: Tubulin alpha-1B chain



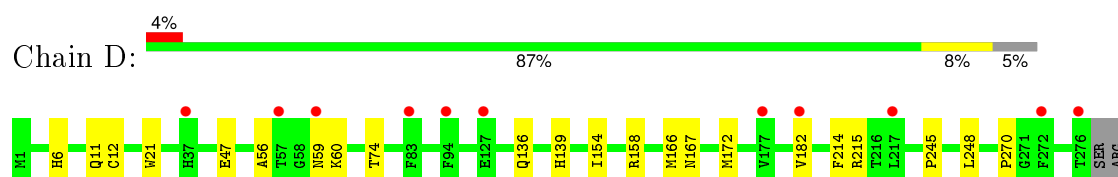
- Molecule 1: Tubulin alpha-1B chain

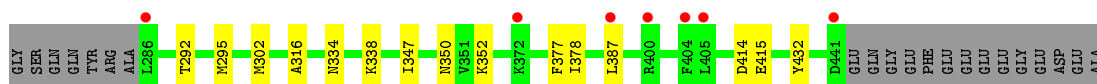


- Molecule 2: Tubulin beta-2B chain

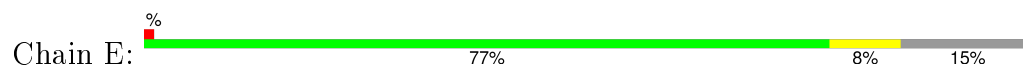


- Molecule 2: Tubulin beta-2B chain

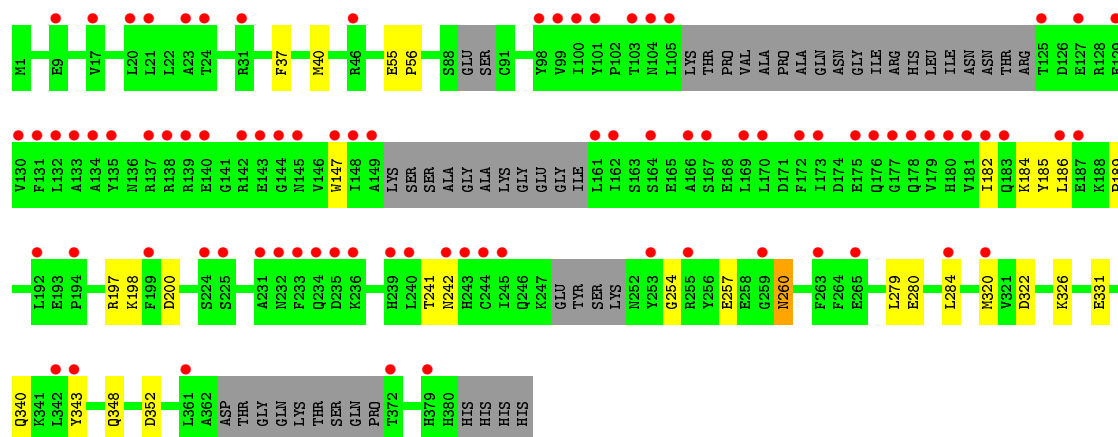




● Molecule 3: Stathmin-4



● Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.86Å 155.57Å 180.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.42 – 2.10 78.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (62.42-2.10) 99.8 (78.10-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.189 , 0.218 0.199 , 0.223	Depositor DCC
R_{free} test set	8416 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 169451 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18278	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, CA, 3GT, GTP, ACP, MES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/3527	0.39	0/4786
1	C	0.23	0/3594	0.40	0/4882
2	B	0.22	0/3451	0.38	0/4674
2	D	0.22	0/3408	0.38	0/4617
3	E	0.21	0/1017	0.32	0/1349
4	F	0.21	0/2830	0.37	0/3823
All	All	0.22	0/17827	0.38	0/24131

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3433	0	3364	20	0
1	C	3483	0	3415	24	0
2	B	3365	0	3243	19	0
2	D	3326	0	3213	19	0
3	E	1006	0	1026	7	0
4	F	2763	0	2740	16	0
5	A	32	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	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
7	C	1	0	0	0	0
8	A	6	0	8	0	0
8	C	6	0	8	0	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	12	0	13	3	0
11	D	48	0	46	2	0
12	F	31	0	14	3	0
13	A	134	0	0	1	0
13	B	113	0	0	2	0
13	C	252	0	0	2	0
13	D	97	0	0	1	0
13	E	30	0	0	1	0
13	F	45	0	0	0	0
All	All	18278	0	17138	105	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 3.

All (105) 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:147[A]:SER:HG	2:B:190:SER:HG	1.32	0.77
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.67	0.76
1:C:381:THR:HG22	1:C:383:ALA:H	1.53	0.74
1:A:18:ASN:HD21	1:A:78:VAL:HG13	1.60	0.66
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.76	0.65
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.80	0.62
2:D:248:LEU:HD11	2:D:352:LYS:HB3	1.83	0.61
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.83	0.60
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.82	0.60
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.34	0.59
2:B:221:THR:HG21	1:C:326:LYS:HA	1.84	0.59
3:E:64:GLN:NE2	13:E:222:HOH:O	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:NH1	13:B:658:HOH:O	2.38	0.57
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.37	0.57
2:B:158:ARG:CZ	10:B:505:MES:H21	2.35	0.56
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.30	0.56
2:D:432:TYR:OH	13:D:686:HOH:O	2.16	0.56
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.88	0.56
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.25	0.55
1:A:71:GLU:O	13:A:609:HOH:O	2.18	0.54
4:F:348:GLN:NE2	4:F:352:ASP:OD2	2.41	0.53
1:C:128:GLN:NE2	13:C:602:HOH:O	2.40	0.53
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.89	0.53
1:C:162:GLY:N	13:C:601:HOH:O	2.42	0.53
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.90	0.53
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.43	0.53
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.28	0.52
2:B:31:ASP:OD1	2:B:35:SER:N	2.40	0.52
2:B:372:LYS:NZ	13:B:601:HOH:O	2.41	0.52
2:B:1:MET:SD	2:B:50:ASN:ND2	2.83	0.52
1:C:320:ARG:HA	1:C:356:ASN:O	2.10	0.52
12:F:401:ACP:O2G	12:F:401:ACP:O1B	2.29	0.51
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.92	0.51
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.92	0.51
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.93	0.50
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.93	0.50
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.51	0.50
4:F:147:TRP:HB3	4:F:182:ILE:HD11	1.94	0.50
1:A:348:PRO:HB3	3:E:27:PRO:HD3	1.94	0.50
1:C:140:SER:HA	1:C:171:ILE:HB	1.94	0.50
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.44	0.50
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.93	0.49
4:F:241:THR:OG1	12:F:401:ACP:O3'	2.22	0.49
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.47	0.49
4:F:184:LYS:NZ	4:F:185:TYR:O	2.45	0.49
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.93	0.49
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.96	0.48
1:A:120:ASP:OD2	1:A:124:LYS:NZ	2.40	0.48
4:F:189:PRO:HA	4:F:322:ASP:HA	1.95	0.48
11:D:502:3GT:H42	11:D:502:3GT:H20	1.96	0.47
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.55	0.47
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.97	0.47
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.79	0.47
2:B:212:ILE:HG23	2:B:275:LEU:HD13	1.96	0.47
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.98	0.46
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.97	0.46
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.15	0.46
2:D:56:ALA:HB3	2:D:60:LYS:HB2	1.98	0.45
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.34	0.45
2:B:136:GLN:HA	2:B:167:ASN:O	2.16	0.45
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.52	0.45
2:D:214:PHE:HD2	2:D:215:ARG:HG3	1.81	0.45
4:F:331:GLU:OE2	12:F:401:ACP:O2G	2.35	0.44
2:B:199:ASP:OD2	10:B:505:MES:H52	2.17	0.44
1:A:132:LEU:O	1:A:164:LYS:NZ	2.44	0.44
3:E:127:ASP:O	3:E:131:GLU:HG2	2.18	0.44
1:C:1:MET:HB3	1:C:130:THR:OG1	2.17	0.44
1:A:110:ILE:O	1:A:113:GLU:HG2	2.17	0.44
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.99	0.43
2:D:414:ASP:OD1	2:D:415:GLU:N	2.51	0.43
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.99	0.43
2:B:199:ASP:OD1	10:B:505:MES:H32	2.18	0.43
2:D:292:THR:O	2:D:295:MET:HG2	2.18	0.43
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.00	0.43
2:B:106:GLY:O	2:B:111:GLY:HA3	2.19	0.43
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.99	0.43
11:D:502:3GT:H3	11:D:502:3GT:H5	1.56	0.43
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.43
3:E:52:LYS:HE3	3:E:52:LYS:HB2	1.84	0.43
4:F:279:LEU:HG	4:F:284[B]:LEU:HG	2.01	0.43
2:D:136:GLN:HA	2:D:167:ASN:O	2.17	0.43
1:C:204:VAL:HG22	1:C:302:MET:HE3	2.01	0.42
1:C:208:ALA:HB2	1:C:304:LYS:HG2	2.02	0.42
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.42
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.55	0.42
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.01	0.42
4:F:254:GLY:H	4:F:260:ASN:ND2	2.19	0.41
1:A:101:ASN:ND2	1:A:180:ALA:HB2	2.35	0.41
2:D:295:MET:HE2	2:D:377:PHE:HB2	2.02	0.41
2:B:105:LYS:HA	2:B:109:THR:OG1	2.20	0.41
3:E:74:GLU:O	3:E:77:GLU:HG2	2.20	0.41
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.56	0.41
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:334:ASN:OD1	2:D:338:LYS:HE3	2.21	0.41
4:F:37:PHE:CE1	4:F:40:MET:HB2	2.55	0.41
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.03	0.41
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.52	0.41
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.40
3:E:101:LEU:O	3:E:105:MET:HG2	2.21	0.40
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	2.04	0.40
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.56	0.40
4:F:55:GLU:HA	4:F:56:PRO:HD2	1.97	0.40
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.20	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	439/451 (97%)	432 (98%)	7 (2%)	0	100	100
1	C	449/451 (100%)	441 (98%)	8 (2%)	0	100	100
2	B	427/445 (96%)	420 (98%)	7 (2%)	0	100	100
2	D	421/445 (95%)	412 (98%)	9 (2%)	0	100	100
3	E	118/143 (82%)	118 (100%)	0	0	100	100
4	F	325/384 (85%)	315 (97%)	10 (3%)	0	100	100
All	All	2179/2319 (94%)	2138 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	374/379 (99%)	373 (100%)	1 (0%)	94	97
1	C	382/379 (101%)	380 (100%)	2 (0%)	92	95
2	B	370/383 (97%)	369 (100%)	1 (0%)	94	97
2	D	368/383 (96%)	365 (99%)	3 (1%)	86	91
3	E	110/127 (87%)	109 (99%)	1 (1%)	84	89
4	F	304/342 (89%)	301 (99%)	3 (1%)	82	87
All	All	1908/1993 (96%)	1897 (99%)	11 (1%)	92	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
2	B	139	HIS
1	C	347[A]	CYS
1	C	347[B]	CYS
2	D	59	ASN
2	D	139	HIS
2	D	182	VAL
3	E	124	GLN
4	F	242	ASN
4	F	260	ASN
4	F	326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	301	GLN
4	F	260	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 8 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	1.16	2 (8%)	34,54,54	1.85	7 (20%)
8	GOL	A	504	-	5,5,5	0.34	0	5,5,5	0.23	0
9	GDP	B	501	6	23,30,30	1.18	2 (8%)	30,47,47	1.76	6 (20%)
10	MES	B	505	-	11,12,12	0.54	0	14,16,16	1.49	1 (7%)
5	GTP	C	501	6	25,34,34	1.15	2 (8%)	34,54,54	1.84	8 (23%)
8	GOL	C	503	-	5,5,5	0.35	0	5,5,5	0.23	0
9	GDP	D	501	6	23,30,30	1.18	2 (8%)	30,47,47	1.83	6 (20%)
11	3GT	D	502	-	47,51,51	1.67	7 (14%)	52,77,77	1.99	11 (21%)
12	ACP	F	401	-	25,33,33	1.45	5 (20%)	31,52,52	1.85	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	0/18/38/38	0/3/3/3
8	GOL	A	504	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
10	MES	B	505	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
8	GOL	C	503	-	-	0/4/4/4	0/0/0/0
9	GDP	D	501	6	-	0/12/32/32	0/3/3/3
11	3GT	D	502	-	-	0/56/84/84	0/0/4/4
12	ACP	F	401	-	-	0/15/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	502	3GT	CAD-NAN	-2.49	1.40	1.44
11	D	502	3GT	OBK-CBI	-2.40	1.42	1.45
11	D	502	3GT	OBB-CBA	-2.23	1.43	1.46
12	F	401	ACP	PB-O2B	2.26	1.61	1.56
12	F	401	ACP	PG-O2G	2.75	1.61	1.54
12	F	401	ACP	PG-O3G	2.90	1.61	1.54
5	C	501	GTP	C5-C4	3.02	1.47	1.40
9	B	501	GDP	C5-C4	3.03	1.47	1.40
9	D	501	GDP	C5-C4	3.05	1.47	1.40
5	A	501	GTP	C5-C4	3.06	1.47	1.40
12	F	401	ACP	C5-C4	3.09	1.47	1.40
12	F	401	ACP	PB-O3A	3.11	1.61	1.58
11	D	502	3GT	CAC-CL1	3.16	1.79	1.72
9	B	501	GDP	C6-C5	3.62	1.48	1.41
5	A	501	GTP	C6-C5	3.66	1.48	1.41
9	D	501	GDP	C6-C5	3.68	1.48	1.41
5	C	501	GTP	C6-C5	3.68	1.48	1.41
11	D	502	3GT	CBI-CBH	4.41	1.52	1.47
11	D	502	3GT	OBM-C	5.10	1.46	1.34
11	D	502	3GT	OBB-CBC	6.50	1.45	1.35

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	401	ACP	N3-C2-N1	-6.64	123.81	128.89
11	D	502	3GT	CBI-CBH-CBF	-6.55	114.10	124.30
12	F	401	ACP	PA-O3A-PB	-4.43	120.28	132.73
5	A	501	GTP	C5-C6-N1	-4.25	117.77	123.59
5	C	501	GTP	C5-C6-N1	-4.23	117.80	123.59
9	D	501	GDP	C5-C6-N1	-4.17	117.89	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	C5-C6-N1	-3.93	118.22	123.59
5	C	501	GTP	PA-O3A-PB	-3.65	122.49	132.73
5	A	501	GTP	PA-O3A-PB	-3.61	122.58	132.73
5	C	501	GTP	C6-C5-C4	-3.40	116.83	120.90
9	B	501	GDP	C6-C5-C4	-3.38	116.86	120.90
12	F	401	ACP	C2'-C1'-N9	-3.38	109.13	114.29
5	C	501	GTP	N3-C2-N1	-3.30	122.42	127.44
5	A	501	GTP	C6-C5-C4	-3.29	116.96	120.90
5	A	501	GTP	C4-C5-N7	-3.25	106.49	109.48
9	D	501	GDP	C6-C5-C4	-3.24	117.02	120.90
5	A	501	GTP	N3-C2-N1	-3.24	122.52	127.44
9	D	501	GDP	C4-C5-N7	-3.21	106.52	109.48
5	C	501	GTP	C4-C5-N7	-3.19	106.54	109.48
9	B	501	GDP	C4-C5-N7	-3.14	106.59	109.48
12	F	401	ACP	C4-C5-N7	-3.10	106.62	109.48
11	D	502	3GT	OBK-CBH-CBI	-3.10	57.43	59.87
9	B	501	GDP	N3-C2-N1	-3.09	122.73	127.44
9	D	501	GDP	N3-C2-N1	-3.06	122.79	127.44
11	D	502	3GT	CAS-OBM-C	-3.04	113.00	118.12
9	D	501	GDP	PA-O3A-PB	-2.76	123.41	132.67
9	B	501	GDP	PA-O3A-PB	-2.63	123.86	132.67
5	A	501	GTP	PB-O3B-PG	-2.52	124.21	132.67
11	D	502	3GT	OAK-CAB-CAA	-2.45	120.03	124.21
5	C	501	GTP	PB-O3B-PG	-2.19	125.33	132.67
11	D	502	3GT	OBM-C-O	-2.06	119.65	123.89
11	D	502	3GT	CAE-CAD-CAC	-2.00	119.48	122.41
5	C	501	GTP	O3G-PG-O2G	2.03	115.12	107.38
11	D	502	3GT	CAO-NAN-CAP	2.38	123.35	119.11
11	D	502	3GT	CBJ-CBI-CAS	2.63	120.93	115.17
11	D	502	3GT	OAK-CAB-CAC	3.20	119.71	115.48
10	B	505	MES	O2S-S-C8	3.46	109.85	106.91
11	D	502	3GT	OBM-C-CA	4.40	120.15	110.63
9	B	501	GDP	C6-N1-C2	4.62	122.35	115.94
9	D	501	GDP	C6-N1-C2	4.74	122.52	115.94
5	A	501	GTP	C6-N1-C2	4.92	122.77	115.94
5	C	501	GTP	C6-N1-C2	4.99	122.86	115.94
11	D	502	3GT	CBI-OBK-CBH	6.71	64.42	60.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
9	B	501	GDP	1	0
10	B	505	MES	3	0
5	C	501	GTP	1	0
9	D	501	GDP	1	0
11	D	502	3GT	2	0
12	F	401	ACP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	436/451 (96%)	0.11	3 (0%) 89 91	42, 60, 95, 133	0
1	C	440/451 (97%)	0.27	2 (0%) 91 93	36, 48, 76, 111	0
2	B	427/445 (95%)	0.31	11 (2%) 59 66	36, 56, 96, 139	2 (0%)
2	D	422/445 (94%)	0.25	18 (4%) 39 48	43, 67, 100, 139	3 (0%)
3	E	121/143 (84%)	0.40	2 (1%) 73 78	49, 73, 111, 128	0
4	F	335/384 (87%)	1.23	84 (25%) 1 1	51, 85, 161, 181	0
All	All	2181/2319 (94%)	0.40	120 (5%) 29 37	36, 62, 113, 181	5 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	8.6
4	F	182	ILE	7.5
4	F	233	PHE	7.5
4	F	100	ILE	7.2
4	F	105	LEU	6.1
4	F	134	ALA	5.9
4	F	103	THR	5.8
4	F	132	LEU	5.8
4	F	161	LEU	5.8
4	F	234	GLN	5.5
4	F	99	VAL	5.2
4	F	232	ASN	5.2
4	F	181	VAL	5.1
4	F	125	THR	5.1
4	F	133	ALA	5.0
4	F	138	ARG	4.9
4	F	244	CYS	4.9
4	F	130	VAL	4.8
4	F	172	PHE	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	282	GLN	4.5
4	F	131	PHE	4.4
4	F	231	ALA	4.3
4	F	177	GLY	4.2
4	F	166	ALA	4.2
4	F	372	THR	4.1
4	F	253	TYR	4.1
4	F	147	TRP	4.1
4	F	167	SER	4.0
4	F	101	TYR	4.0
4	F	98	TYR	3.9
4	F	236	LYS	3.9
4	F	178	GLN	3.9
4	F	142	ARG	3.9
3	E	139	LEU	3.8
4	F	104	ASN	3.8
4	F	143	GLU	3.8
4	F	179	VAL	3.8
2	D	276	THR	3.8
4	F	145	ASN	3.8
4	F	162	ILE	3.8
2	B	1	MET	3.7
2	B	57	THR	3.6
4	F	240	LEU	3.6
4	F	135	TYR	3.5
2	B	281	GLN	3.4
1	A	262	TYR	3.4
2	B	58	GLY	3.4
4	F	129	GLU	3.4
4	F	235	ASP	3.3
4	F	139	ARG	3.3
2	D	405	LEU	3.3
4	F	169	LEU	3.3
4	F	186	LEU	3.3
2	B	276	THR	3.2
2	B	285	ALA	3.2
2	B	248	LEU	3.2
2	B	278	ARG	3.1
1	A	439	SER	3.1
2	B	284	ARG	3.1
4	F	144	GLY	3.1
4	F	259	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	357	TYR	3.0
2	D	404	PHE	3.0
4	F	148	ILE	2.9
4	F	224	SER	2.9
4	F	225	SER	2.9
4	F	245	ILE	2.9
4	F	24	THR	2.9
4	F	183	GLN	2.9
4	F	239	HIS	2.8
2	D	57	THR	2.8
2	D	217	LEU	2.8
4	F	20	LEU	2.8
2	D	400	ARG	2.7
4	F	140	GLU	2.6
2	D	94	PHE	2.6
4	F	284[A]	LEU	2.6
4	F	170	LEU	2.6
4	F	149	ALA	2.6
2	D	59	ASN	2.6
4	F	361	LEU	2.5
4	F	255	ARG	2.5
4	F	180	HIS	2.5
2	D	286	LEU	2.5
2	D	182	VAL	2.5
4	F	23	ALA	2.5
4	F	176	GLN	2.5
4	F	175	GLU	2.5
4	F	320	MET	2.4
2	D	37	HIS	2.4
4	F	46	ARG	2.4
1	A	281	ALA	2.4
4	F	137	ARG	2.4
4	F	17	VAL	2.4
4	F	9	GLU	2.4
2	D	272	PHE	2.3
4	F	342	LEU	2.3
2	D	83	PHE	2.3
3	E	25	LYS	2.3
2	D	177	VAL	2.3
4	F	127	GLU	2.3
2	D	387	LEU	2.3
1	C	295[A]	CYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	372	LYS	2.3
2	D	372	LYS	2.3
4	F	194	PRO	2.2
4	F	265	GLU	2.2
4	F	192	LEU	2.2
4	F	187	GLU	2.2
4	F	21	LEU	2.1
4	F	379	HIS	2.1
2	D	441	ASP	2.1
4	F	242	ASN	2.1
4	F	343	TYR	2.1
4	F	263	PHE	2.1
4	F	31	ARG	2.1
4	F	199	PHE	2.0
4	F	164	SER	2.0
2	D	127	GLU	2.0
4	F	243	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	GOL	C	503	6/6	0.94	0.21	3.27	77,79,82,82	0
10	MES	B	505	12/12	0.95	0.14	1.04	57,65,77,82	0
11	3GT	D	502	48/48	0.90	0.20	0.84	80,89,105,188	0
5	GTP	A	501	32/32	0.98	0.13	0.43	37,44,49,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	GOL	A	504	6/6	0.77	0.14	0.41	86,87,90,92	0
9	GDP	B	501	28/28	0.98	0.16	0.32	32,43,47,50	0
7	CA	A	503	1/1	0.89	0.12	0.26	85,85,85,85	0
5	GTP	C	501	32/32	0.98	0.13	0.07	30,37,41,46	0
9	GDP	D	501	28/28	0.94	0.13	0.00	56,64,74,85	0
7	CA	C	504	1/1	0.99	0.12	-0.48	67,67,67,67	0
12	ACP	F	401	31/31	0.80	0.14	-1.15	87,97,167,172	0
6	MG	C	502	1/1	0.96	0.13	-	41,41,41,41	0
7	CA	B	504	1/1	0.68	0.30	-	115,115,115,115	0
6	MG	D	503	1/1	0.86	0.09	-	62,62,62,62	0
6	MG	B	502	1/1	0.96	0.26	-	39,39,39,39	0
7	CA	B	503	1/1	0.94	0.08	-	101,101,101,101	0
6	MG	A	502	1/1	0.97	0.09	-	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.