



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2017 – 02:33 PM EDT

PDB ID : 5GON
Title : Structures of a beta-lactam bridged analogue in complex with tubulin
Authors : Zhou, L.; Liu, Y.; Cheng, L.; Wang, Y.
Deposited on : 2016-07-28
Resolution : 2.48 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

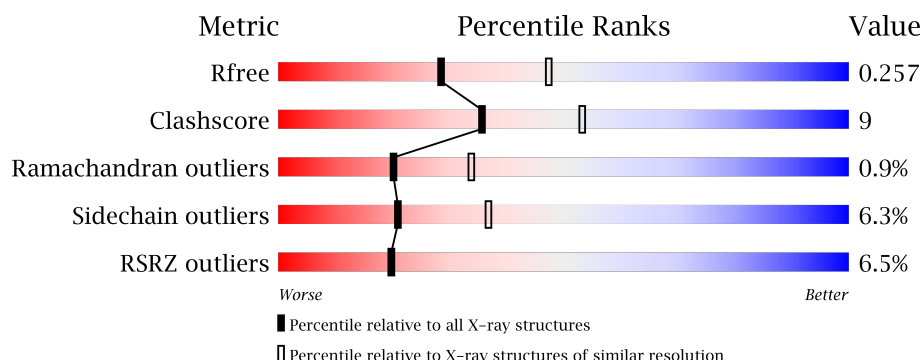
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4719 (2.50-2.46)
Clashscore	112137	5483 (2.50-2.46)
Ramachandran outliers	110173	5388 (2.50-2.46)
Sidechain outliers	110143	5390 (2.50-2.46)
RSRZ outliers	101464	4754 (2.50-2.46)

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	440	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>•</div> </div> </div>
1	C	440	<div> <div>87%</div> <div>12%</div> <div>•</div> </div>
2	B	431	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>••</div> </div> </div>
2	D	431	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>••</div> </div> </div>
3	E	136	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	378	

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
12	IMD	C	509	-	-	-	X
12	IMD	C	510	-	-	-	X
6	MG	A	502	-	-	-	X
6	MG	C	504	-	-	-	X
7	GOL	A	504	-	-	-	X
7	GOL	B	503	-	-	-	X
7	GOL	B	504	-	-	-	X
7	GOL	B	505	-	-	X	X
7	GOL	C	502	-	-	-	X
7	GOL	C	506	-	-	-	X
7	GOL	C	507	-	-	-	X
7	GOL	D	504	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17847 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	13	0
			3488	2217	585	661	25			
1	C	440	Total	C	N	O	S	0	11	0
			3489	2209	588	668	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	1	11	0
			3374	2126	568	653	27			
2	D	421	Total	C	N	O	S	0	4	0
			3326	2094	562	642	28			

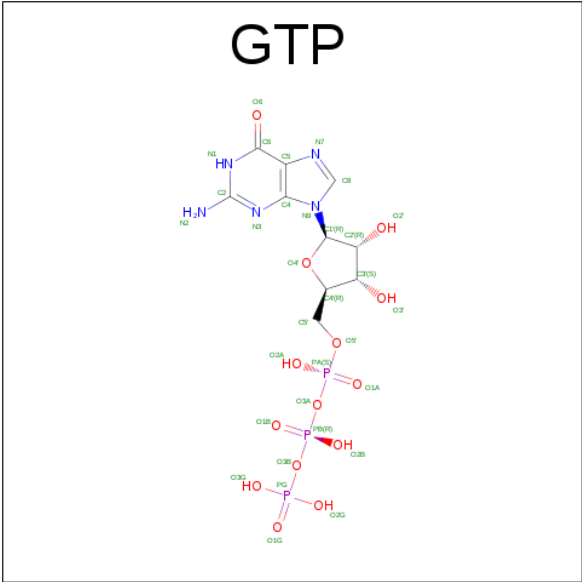
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	3	0
			1016	628	183	199	6			

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	319	Total	C	N	O	S	0	5	0
			2633	1706	436	477	14			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

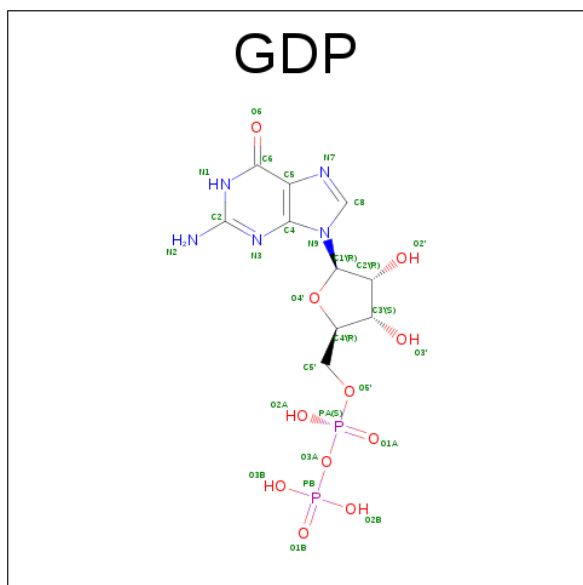


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

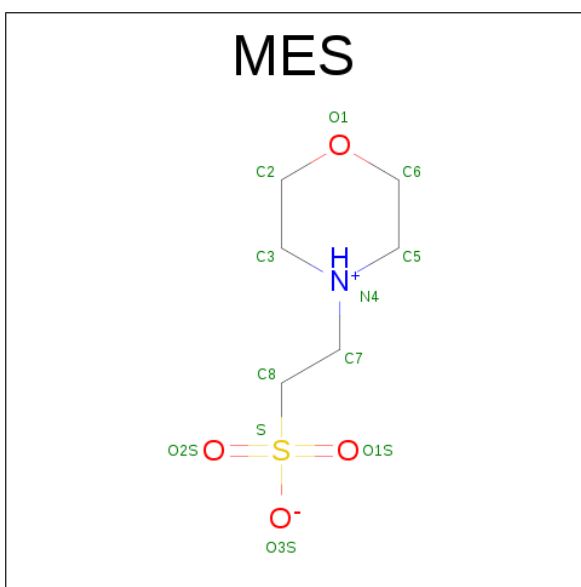
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Ca 1 1	0	0
8	A	1	Total Ca 1 1	0	0
8	C	1	Total Ca 1 1	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



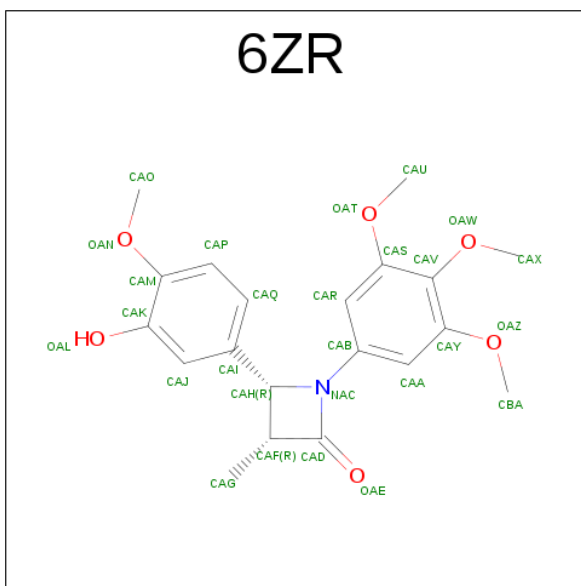
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O P 28 10 5 11 2	0	0
9	D	1	Total C N O P 28 10 5 11 2	0	0

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



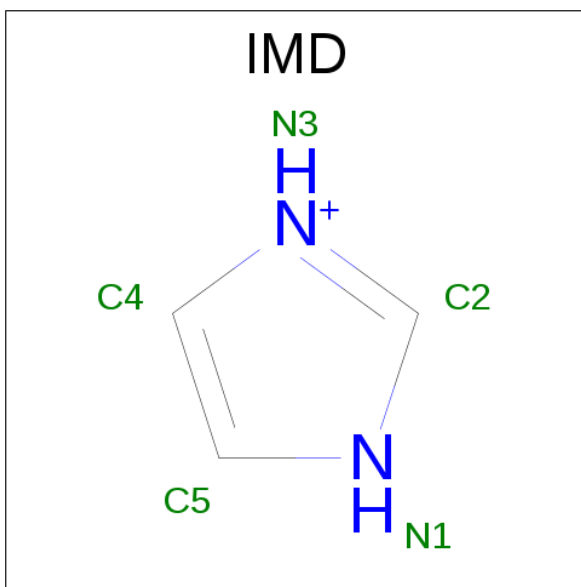
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (3R,4R)-4-(4-methoxy-3-oxidanyl-phenyl)-3-methyl-1-(3,4,5-trimethoxyphenyl)azetidin-2-one (three-letter code: 6ZR) (formula: $C_{20}H_{23}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			27	20	1	6		

- Molecule 12 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C N 5 3 2	0	0
12	C	1	Total C N 5 3 2	0	0
12	C	1	Total C N 5 3 2	0	0

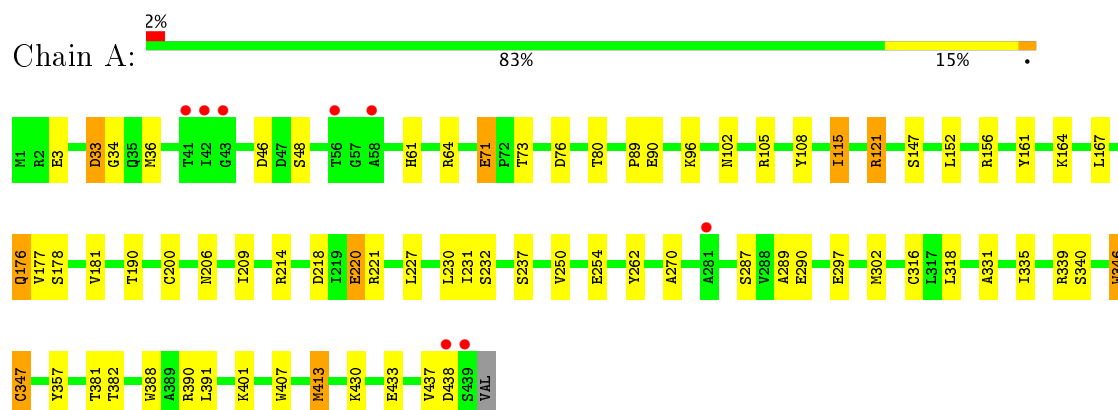
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	44	Total O 44 44	0	0
13	B	52	Total O 52 52	0	0
13	C	110	Total O 110 110	0	0
13	D	25	Total O 25 25	0	0
13	E	16	Total O 16 16	0	0
13	F	20	Total O 20 20	0	0

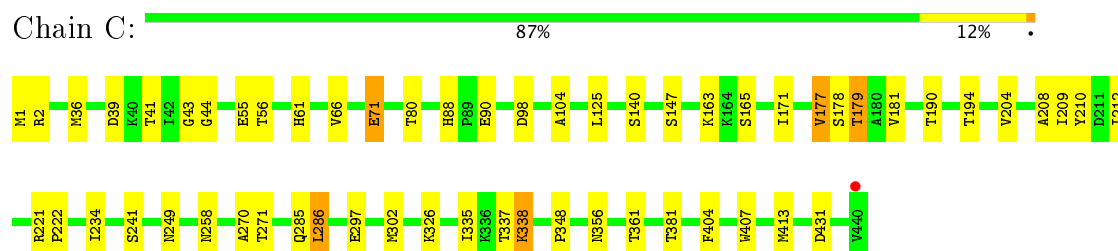
3 Residue-property plots [i](#)

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

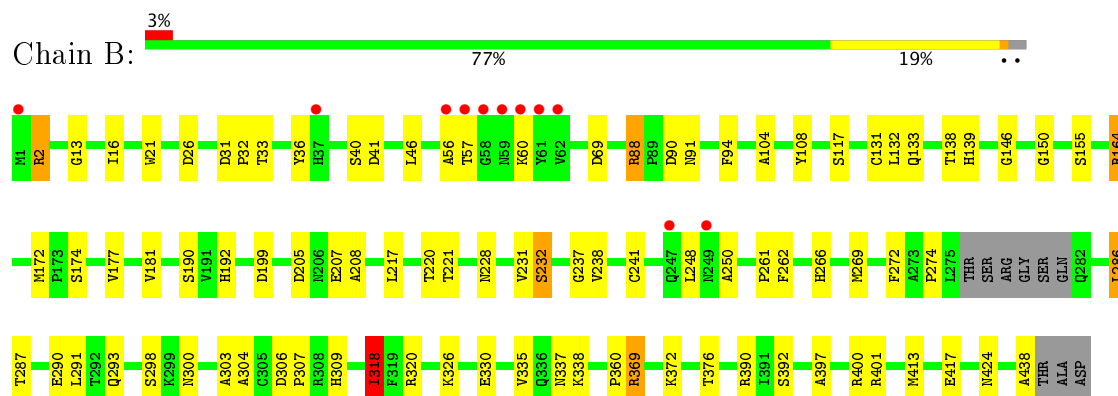
- Molecule 1: Tubulin alpha-1B chain



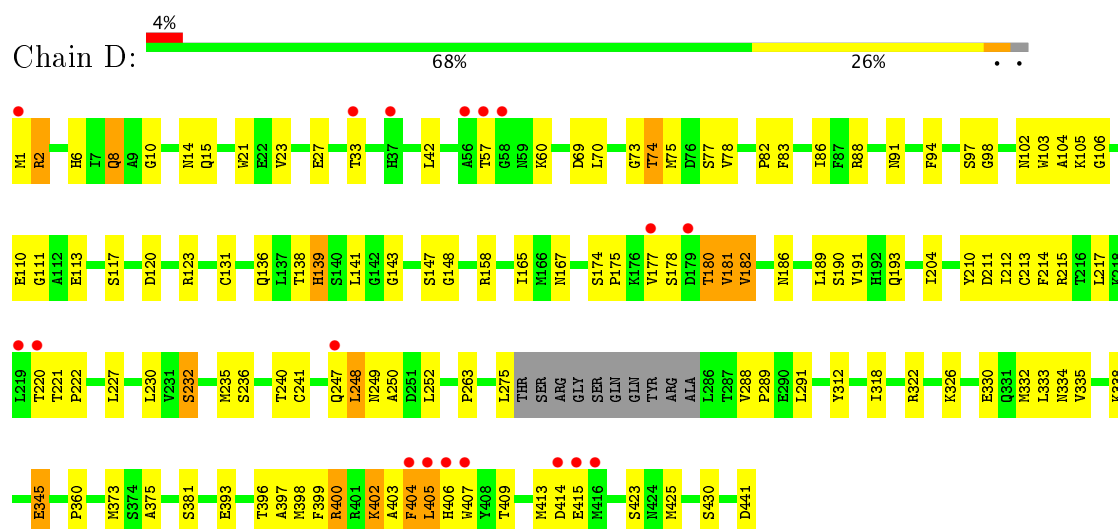
- Molecule 1: Tubulin alpha-1B chain



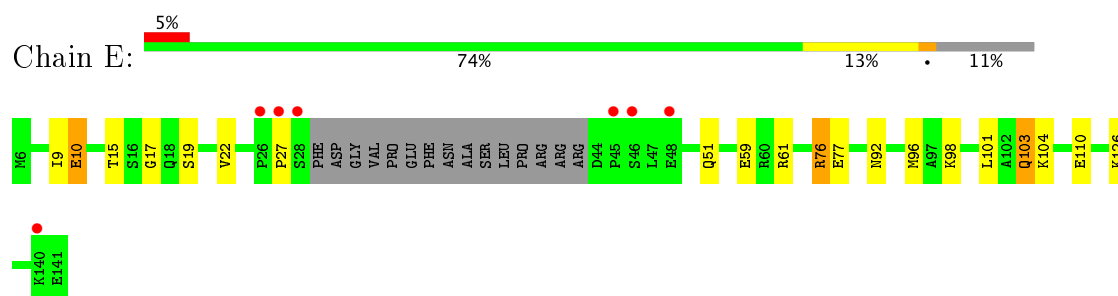
- Molecule 2: Tubulin beta-2B chain



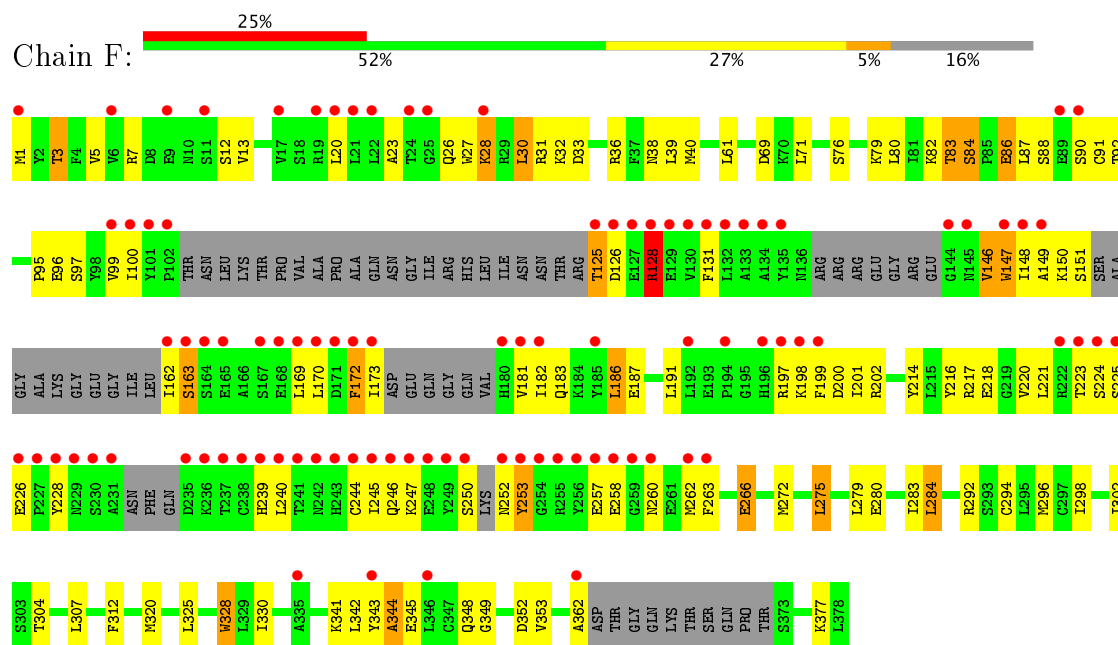
- Molecule 2: Tubulin beta-2B chain



- Molecule 3: Stathmin-4



- Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.51Å 156.46Å 181.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.60 – 2.48 49.71 – 2.48	Depositor EDS
% Data completeness (in resolution range)	92.9 (118.60-2.48) 92.9 (49.71-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.257 0.205 , 0.257	Depositor DCC
R_{free} test set	4912 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17847	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 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, IMD, CA, GTP, MES, 6ZR

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	0.75	3/3605 (0.1%)	0.75	1/4895 (0.0%)
1	C	0.88	1/3597 (0.0%)	0.82	0/4885
2	B	0.81	1/3478 (0.0%)	0.78	2/4710 (0.0%)
2	D	0.74	2/3411 (0.1%)	0.78	2/4622 (0.0%)
3	E	0.77	0/1033	0.81	2/1370 (0.1%)
4	F	0.82	5/2704 (0.2%)	0.77	2/3650 (0.1%)
All	All	0.80	12/17828 (0.1%)	0.78	9/24132 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	42	LEU	C-N	9.96	1.56	1.34
2	D	360	PRO	C-N	9.08	1.54	1.34
4	F	226	GLU	CD-OE1	-8.86	1.16	1.25
4	F	27	TRP	CD2-CE2	6.11	1.48	1.41
1	A	346	TRP	CD2-CE2	5.96	1.48	1.41
1	A	388	TRP	CD2-CE2	5.86	1.48	1.41
1	A	407	TRP	CD2-CE2	5.75	1.48	1.41
1	C	407	TRP	CD2-CE2	5.61	1.48	1.41
4	F	147	TRP	CD2-CE2	5.42	1.47	1.41
2	B	21	TRP	CD2-CE2	5.25	1.47	1.41
4	F	128	ARG	NE-CZ	5.18	1.39	1.33
4	F	328	TRP	CD2-CE2	5.12	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	405	LEU	CB-CG-CD1	-9.60	94.67	111.00
2	D	2	ARG	NE-CZ-NH1	-7.99	116.31	120.30
3	E	61	ARG	NE-CZ-NH1	7.42	124.01	120.30
4	F	36	ARG	NE-CZ-NH1	5.63	123.11	120.30
3	E	76	ARG	NE-CZ-NH1	-5.61	117.50	120.30
2	B	318	ILE	CB-CA-C	-5.61	100.39	111.60
1	A	121	ARG	NE-CZ-NH1	5.56	123.08	120.30
4	F	186	LEU	CB-CG-CD1	5.32	120.05	111.00
2	B	172	MET	CG-SD-CE	5.16	108.46	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	249	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3488	0	3441	40	0
1	C	3489	0	3413	43	0
2	B	3374	0	3270	71	0
2	D	3326	0	3221	78	0
3	E	1016	0	1041	11	0
4	F	2633	0	2631	80	0
5	A	32	0	12	0	0
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
6	F	1	0	0	0	0
7	A	18	0	24	1	0
7	B	18	0	24	12	0
7	C	24	0	32	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	12	0	16	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	12	0	13	1	0
11	B	27	0	0	3	0
12	C	15	0	15	4	0
13	A	44	0	0	2	0
13	B	52	0	0	0	0
13	C	110	0	0	3	0
13	D	25	0	0	1	0
13	E	16	0	0	0	0
13	F	20	0	0	0	0
All	All	17847	0	17189	321	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 9.

All (321) 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)
4:F:240:LEU:HD23	4:F:245:ILE:HD12	1.30	1.13
2:B:320:ARG:HH11	7:B:505:GOL:H11	1.05	1.10
4:F:1:MET:HG2	4:F:28:LYS:HD2	1.19	1.09
2:B:320:ARG:NH1	7:B:505:GOL:H11	1.68	1.06
4:F:320:MET:HG2	4:F:330:ILE:HD11	1.34	1.05
4:F:240:LEU:CD2	4:F:245:ILE:HD12	1.99	0.93
4:F:163:SER:HB2	4:F:169:LEU:HG	1.47	0.93
4:F:240:LEU:HD23	4:F:245:ILE:CD1	1.99	0.93
1:A:214:ARG:NH1	1:A:220:GLU:O	2.01	0.93
4:F:149:ALA:HB2	4:F:182:ILE:HG12	1.55	0.89
2:D:180:THR:HG22	2:D:181:VAL:N	1.88	0.88
1:C:221:ARG:NH1	7:C:505:GOL:O3	2.07	0.87
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.56	0.86
2:D:2:ARG:NH1	2:D:131:CYS:SG	2.49	0.86
4:F:320:MET:CG	4:F:330:ILE:HD11	2.07	0.84
2:B:306:ASP:HB3	2:B:309:HIS:CD2	2.12	0.84
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.11	0.82
4:F:1:MET:CG	4:F:28:LYS:HD2	2.07	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:87:LEU:O	4:F:91:CYS:HB3	1.78	0.82
2:D:180:THR:HG22	2:D:181:VAL:H	1.42	0.81
4:F:342:LEU:O	4:F:344:ALA:N	2.13	0.81
4:F:82:LYS:NZ	4:F:97:SER:O	2.13	0.81
2:B:320:ARG:HH11	7:B:505:GOL:C1	1.91	0.80
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.44	0.80
4:F:170:LEU:O	4:F:173:ILE:CD1	2.29	0.80
1:C:210:TYR:OH	1:C:221:ARG:NH2	2.15	0.79
2:D:402:LYS:HB3	2:D:405:LEU:HD22	1.63	0.79
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.18	0.78
4:F:199:PHE:HB3	4:F:223:THR:HG22	1.63	0.78
4:F:31:ARG:HE	4:F:32:LYS:H	1.32	0.78
4:F:1:MET:HG2	4:F:28:LYS:CD	2.09	0.78
4:F:240:LEU:CD2	4:F:245:ILE:CD1	2.59	0.76
1:C:286:LEU:H	1:C:286:LEU:HD12	1.50	0.76
2:B:306:ASP:HB3	2:B:309:HIS:HD2	1.52	0.75
7:C:506:GOL:O1	13:C:601:HOH:O	2.04	0.74
2:B:401:ARG:HE	7:B:503:GOL:H2	1.53	0.74
2:B:56:ALA:HB3	2:B:60:LYS:H	1.53	0.74
4:F:263:PHE:CE2	4:F:341:LYS:HE3	2.23	0.71
4:F:39:LEU:HD13	4:F:61:LEU:HD22	1.72	0.71
2:D:88:ARG:NH1	2:D:91:ASN:OD1	2.24	0.71
1:A:209[A]:ILE:HG22	1:A:227:LEU:HD23	1.72	0.70
2:B:192:HIS:CD2	2:B:424[B]:ASN:HD22	2.10	0.70
1:C:39:ASP:OD2	1:C:55:GLU:OE2	2.10	0.70
1:C:1:MET:O	13:C:602:HOH:O	2.10	0.70
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.73	0.69
4:F:170:LEU:O	4:F:173:ILE:HD13	1.92	0.69
4:F:125:THR:HG22	4:F:126:ASP:HA	1.75	0.68
2:B:2:ARG:HH11	2:B:2:ARG:HG3	1.59	0.68
1:C:66:VAL:HG23	1:C:125:LEU:HD11	1.74	0.67
3:E:9:ILE:HG22	3:E:10:GLU:N	2.09	0.67
1:A:46:ASP:N	1:A:46:ASP:OD1	2.29	0.66
2:B:338:LYS:HG3	2:B:338:LYS:O	1.96	0.66
1:C:165:SER:OG	12:C:510:IMD:H2	1.96	0.65
4:F:61:LEU:HD21	4:F:312:PHE:CD1	2.31	0.65
2:B:360:PRO:HG3	7:B:505:GOL:H2	1.78	0.64
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.15	0.64
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.30	0.64
2:B:326:LYS:O	2:B:330:GLU:HG3	1.98	0.64
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.32	0.63
4:F:61:LEU:HD21	4:F:312:PHE:CE1	2.33	0.62
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.35	0.62
2:B:2:ARG:NH1	2:B:2:ARG:HG3	2.14	0.61
3:E:9:ILE:HG22	3:E:10:GLU:H	1.65	0.61
4:F:149:ALA:HA	4:F:181:VAL:O	2.00	0.61
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.36	0.60
4:F:100:ILE:HA	4:F:126:ASP:HB2	1.83	0.60
4:F:100:ILE:HA	4:F:126:ASP:CB	2.31	0.60
2:D:403:ALA:O	2:D:405:LEU:CD1	2.49	0.60
2:D:396:THR:O	2:D:400:ARG:HG2	2.02	0.60
4:F:201:ILE:HG12	4:F:221:LEU:CD2	2.32	0.59
1:A:220:GLU:CD	1:A:221:ARG:H	2.05	0.59
2:D:402:LYS:HB3	2:D:405:LEU:CD2	2.32	0.59
2:D:210:TYR:CE1	2:D:222:PRO:HG3	2.36	0.59
4:F:349:GLY:O	4:F:353[A]:VAL:HG22	2.02	0.59
4:F:149:ALA:CB	4:F:182:ILE:HG12	2.30	0.59
1:A:262:TYR:CE1	1:A:346:TRP:CH2	2.91	0.58
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.85	0.58
11:B:508:6ZR:CAX	11:B:508:6ZR:OAZ	2.51	0.58
1:C:209:ILE:HD11	1:C:302:MET:HE2	1.85	0.57
2:D:241:CYS:SG	2:D:318:ILE:HD12	2.44	0.57
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.17	0.57
4:F:169:LEU:O	4:F:172:PHE:HB2	2.05	0.57
1:A:390:ARG:NH2	13:A:602:HOH:O	2.37	0.56
2:D:104:ALA:HB2	2:D:413:MET:SD	2.45	0.56
2:D:393:GLU:O	2:D:396:THR:HG22	2.06	0.56
2:D:120:ASP:OD1	2:D:123:ARG:NH1	2.38	0.56
2:D:82:PRO:O	2:D:83:PHE:HB2	2.06	0.56
2:B:40:SER:OG	2:B:41:ASP:N	2.40	0.55
3:E:51:GLN:HA	3:E:51:GLN:OE1	2.07	0.55
4:F:96:GLU:OE2	4:F:147:TRP:HH2	1.89	0.55
2:D:414:ASP:OD1	2:D:415:GLU:N	2.40	0.55
2:D:334:ASN:OD1	2:D:338:LYS:HE2	2.07	0.55
4:F:320:MET:HG2	4:F:330:ILE:CD1	2.23	0.55
4:F:198:LYS:HZ3	4:F:228:TYR:HE1	1.53	0.54
4:F:200:ASP:HB3	4:F:320:MET:SD	2.47	0.54
2:D:174:SER:O	2:D:178:SER:HB2	2.08	0.54
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.90	0.54
2:D:180:THR:CG2	2:D:181:VAL:H	2.08	0.54
2:B:401:ARG:HE	7:B:503:GOL:C2	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:SER:OG	2:D:148:GLY:N	2.42	0.53
4:F:201:ILE:HG12	4:F:221:LEU:HD21	1.91	0.53
1:C:177:VAL:HG12	7:C:505:GOL:H32	1.89	0.53
4:F:99:VAL:HG22	4:F:181:VAL:HG12	1.91	0.53
2:D:402:LYS:CB	2:D:405:LEU:HD22	2.38	0.53
2:D:248:LEU:HD23	2:D:250:ALA:HB2	1.91	0.52
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.91	0.52
4:F:199:PHE:CD1	4:F:221:LEU:HD22	2.44	0.52
2:D:291:LEU:HG	2:D:375:ALA:HB2	1.91	0.52
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.91	0.52
2:B:287:THR:OG1	2:B:290:GLU:HG3	2.09	0.51
2:D:97:SER:HB2	2:D:110:GLU:OE1	2.09	0.51
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.93	0.51
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.40	0.51
1:A:287:SER:OG	1:A:290:GLU:HG3	2.11	0.51
2:D:403:ALA:O	2:D:405:LEU:HD13	2.10	0.51
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.92	0.51
12:C:509:IMD:C2	7:D:504:GOL:H2	2.41	0.51
4:F:170:LEU:O	4:F:173:ILE:HD11	2.11	0.51
1:A:237:SER:O	13:A:601:HOH:O	2.18	0.51
12:C:509:IMD:H2	7:D:504:GOL:H2	1.93	0.50
2:B:104:ALA:HB2	2:B:413:MET:SD	2.51	0.50
1:A:250[B]:VAL:HG22	1:A:254:GLU:OE1	2.11	0.50
2:D:191:VAL:HG11	2:D:425:MET:HG3	1.92	0.50
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.93	0.50
4:F:3:THR:O	4:F:38:ASN:HB2	2.11	0.50
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.93	0.50
2:B:272:PHE:HZ	7:B:505:GOL:HO2	1.54	0.49
4:F:148:ILE:HD13	4:F:162:ILE:HG13	1.94	0.49
2:D:210:TYR:CE1	2:D:222:PRO:CG	2.96	0.49
4:F:262:MET:CG	4:F:266:GLU:HG2	2.42	0.49
1:A:90:GLU:O	1:A:121:ARG:HD2	2.13	0.49
3:E:103:GLN:HG3	3:E:104:LYS:N	2.27	0.49
2:B:269:MET:HG2	2:B:303:ALA:HB3	1.94	0.49
2:D:263:PRO:HD2	13:D:618:HOH:O	2.12	0.49
2:B:272:PHE:CE1	7:B:505:GOL:O2	2.67	0.48
1:C:39:ASP:OD1	1:C:41:THR:OG1	2.31	0.48
1:C:209:ILE:HD11	1:C:302:MET:CE	2.43	0.48
2:D:10:GLY:O	2:D:14:ASN:ND2	2.40	0.48
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.37	0.48
2:B:261:PRO:HG2	2:B:262:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:248:LEU:CD2	2:D:250:ALA:HB2	2.44	0.48
2:D:404:PHE:HE1	2:D:407:TRP:CE2	2.32	0.48
2:D:33:THR:O	2:D:60:LYS:HD2	2.14	0.48
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.49	0.48
1:A:430:LYS:O	1:A:433:GLU:HB3	2.14	0.48
2:B:205:ASP:OD2	2:B:390:ARG:NH1	2.41	0.48
2:B:146:GLY:O	2:B:150:GLY:HA3	2.13	0.48
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.96	0.48
2:D:175:PRO:HA	2:D:178:SER:HB2	1.96	0.48
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.29	0.48
1:A:347:CYS:N	3:E:27:PRO:HB3	2.29	0.47
1:A:177:VAL:HG21	1:A:206:ASN:HB3	1.95	0.47
2:D:180:THR:HG22	2:D:182:VAL:H	1.79	0.47
2:D:143:GLY:O	2:D:186:ASN:ND2	2.47	0.47
4:F:96:GLU:OE2	4:F:147:TRP:CH2	2.67	0.47
1:A:176:GLN:CD	1:A:176:GLN:H	2.18	0.47
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.95	0.47
4:F:240:LEU:CD2	4:F:245:ILE:HD13	2.42	0.47
4:F:26:GLN:HE22	4:F:362:ALA:H	1.62	0.47
1:A:297:GLU:OE2	1:A:339:ARG:NH1	2.48	0.47
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.46	0.47
1:A:289:ALA:HA	1:A:331:ALA:HB2	1.96	0.47
1:C:190:THR:O	1:C:194[B]:THR:HG23	2.14	0.47
4:F:150:LYS:O	4:F:151:SER:HB3	2.15	0.46
2:B:2:ARG:HH11	2:B:2:ARG:CG	2.24	0.46
2:B:181:VAL:HG22	1:C:258:ASN:OD1	2.15	0.46
2:D:110:GLU:HA	2:D:113:GLU:HG2	1.97	0.46
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.97	0.46
2:D:322:ARG:O	2:D:373:MET:CE	2.63	0.46
2:B:272:PHE:O	2:B:300:ASN:HB3	2.15	0.46
4:F:95:PRO:HB2	4:F:183:GLN:HG2	1.97	0.46
2:B:397:ALA:O	2:B:400:ARG:NH2	2.45	0.46
2:D:102:ASN:HB3	2:D:105:LYS:HD2	1.97	0.46
2:D:103:TRP:HD1	2:D:147:SER:OG	1.97	0.46
2:B:241:CYS:O	2:B:250:ALA:HB3	2.15	0.46
1:C:204:VAL:HG22	1:C:302:MET:SD	2.55	0.46
3:E:9:ILE:CG2	3:E:10:GLU:N	2.77	0.46
1:C:104:ALA:HB2	1:C:413:MET:SD	2.55	0.46
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.51	0.46
11:B:508:6ZR:CAO	11:B:508:6ZR:OAL	2.63	0.46
1:C:1:MET:C	1:C:2:ARG:HG2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:GLY:O	2:D:111:GLY:HA3	2.15	0.46
4:F:292:ARG:O	4:F:296:MET:HB2	2.16	0.46
1:A:102:ASN:HB3	1:A:105:ARG:HB3	1.97	0.46
2:B:360:PRO:HG3	7:B:505:GOL:C2	2.45	0.45
2:B:306:ASP:HA	2:B:307:PRO:HD3	1.76	0.45
1:C:181:VAL:HG21	1:C:404:PHE:CZ	2.51	0.45
2:B:56:ALA:CB	2:B:60:LYS:HB2	2.46	0.45
2:D:27:GLU:OE1	2:D:236:SER:OG	2.29	0.45
4:F:61:LEU:HD21	4:F:312:PHE:HD1	1.80	0.45
2:B:192:HIS:HD2	2:B:424[B]:ASN:HD22	1.57	0.45
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.97	0.45
2:D:332:MET:O	2:D:335:VAL:HG12	2.16	0.45
2:D:139:HIS:CE1	2:D:141:LEU:CD2	3.00	0.45
2:B:318:ILE:CD1	2:B:376:THR:HB	2.47	0.45
2:D:405:LEU:CD1	2:D:405:LEU:N	2.80	0.45
1:C:234:ILE:HD13	1:C:302:MET:HE3	1.98	0.45
4:F:246:GLN:HA	4:F:250:SER:HB2	1.99	0.45
2:B:287:THR:O	2:B:290:GLU:N	2.46	0.45
3:E:9:ILE:CG2	3:E:10:GLU:H	2.29	0.45
4:F:275[B]:LEU:HD23	4:F:275[B]:LEU:HA	1.64	0.45
7:C:505:GOL:O1	2:D:247:GLN:OE1	2.30	0.44
4:F:128:ARG:O	4:F:131:PHE:HB3	2.16	0.44
2:B:56:ALA:HB3	2:B:60:LYS:N	2.26	0.44
3:E:92:ASN:ND2	3:E:96:MET:HE2	2.32	0.44
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.86	0.44
1:C:39:ASP:OD2	1:C:55:GLU:CD	2.55	0.44
1:A:115:ILE:HD13	1:A:152:LEU:HG	2.00	0.44
2:B:192:HIS:CE1	2:B:424[A]:ASN:OD1	2.70	0.44
2:D:139:HIS:CE1	2:D:141:LEU:HD21	2.52	0.44
4:F:262:MET:HG3	4:F:266:GLU:HG2	1.98	0.44
4:F:325:LEU:HD23	4:F:325:LEU:HA	1.77	0.44
4:F:5:VAL:HG12	4:F:30:LEU:HB2	1.98	0.44
2:B:2:ARG:HB3	2:B:133:GLN:NE2	2.32	0.44
4:F:7:ARG:HD3	4:F:40:MET:CE	2.48	0.44
2:B:274:PRO:HB3	2:B:286:LEU:HD22	2.00	0.44
2:D:180:THR:CG2	2:D:181:VAL:N	2.58	0.44
2:D:227:LEU:O	2:D:230:LEU:HB2	2.17	0.44
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	2.00	0.44
2:B:164:ARG:HA	2:B:164:ARG:HD3	1.76	0.44
4:F:247:LYS:HA	4:F:253:TYR:HE2	1.83	0.44
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:GLY:HA2	1:C:55:GLU:HB2	1.99	0.44
4:F:149:ALA:O	4:F:150:LYS:HD2	2.17	0.44
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.44
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.99	0.44
2:B:31:ASP:C	2:B:33:THR:H	2.21	0.44
2:B:272:PHE:CE1	7:B:505:GOL:H32	2.53	0.44
1:C:140:SER:HA	1:C:171:ILE:HB	1.99	0.44
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.53	0.43
2:B:318:ILE:HD11	2:B:376:THR:HB	2.00	0.43
2:B:318:ILE:HG12	11:B:508:6ZR:CAX	2.48	0.43
2:B:56:ALA:N	2:B:60:LYS:O	2.49	0.43
4:F:146:VAL:HG13	4:F:187:GLU:OE2	2.18	0.43
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.33	0.43
1:C:234:ILE:HD13	1:C:302:MET:CE	2.48	0.43
4:F:26:GLN:HE22	4:F:362:ALA:HB3	1.83	0.43
1:C:163:LYS:HG2	7:C:507:GOL:O2	2.18	0.43
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.54	0.43
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.99	0.43
2:D:326:LYS:O	2:D:330:GLU:HG3	2.18	0.43
2:D:312:TYR:CD1	2:D:381:SER:HB2	2.54	0.43
2:D:75:MET:O	2:D:78:VAL:HB	2.18	0.43
1:A:115:ILE:HD11	1:A:156:ARG:HG3	2.01	0.43
4:F:198:LYS:NZ	4:F:239:HIS:HA	2.33	0.43
1:A:270:ALA:HB3	1:A:302[A]:MET:HG3	2.01	0.43
2:B:174:SER:OG	2:B:207:GLU:OE1	2.31	0.43
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.48	0.43
2:B:69:ASP:O	2:B:94:PHE:HA	2.19	0.43
2:D:210:TYR:CD1	2:D:222:PRO:HG3	2.53	0.43
2:D:333:LEU:HA	2:D:333:LEU:HD23	1.84	0.43
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.34	0.43
2:B:199:ASP:O	2:B:266:HIS:HB2	2.19	0.42
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.59	0.42
1:C:147:SER:HB2	1:C:190:THR:HB	1.99	0.42
2:B:2:ARG:HA	2:B:131:CYS:O	2.20	0.42
2:B:181:VAL:HG12	1:C:348:PRO:CG	2.50	0.42
2:B:31:ASP:OD1	2:B:33:THR:OG1	2.18	0.42
2:D:69:ASP:O	2:D:94:PHE:HA	2.18	0.42
2:D:83:PHE:O	2:D:86:ILE:HG22	2.19	0.42
1:C:208:ALA:O	1:C:212:ILE:HG13	2.20	0.42
4:F:284[A]:LEU:HD12	4:F:284[A]:LEU:HA	1.87	0.42
4:F:71:LEU:HD11	4:F:294:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:201:ILE:HG12	4:F:221:LEU:HD23	2.00	0.42
4:F:214:TYR:CE2	4:F:353[B]:VAL:HG11	2.54	0.42
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.44	0.42
2:D:136:GLN:HA	2:D:167:ASN:O	2.19	0.42
2:D:103:TRP:NE1	2:D:148:GLY:HA2	2.35	0.42
4:F:280:GLU:HA	4:F:284[A]:LEU:HB2	2.01	0.42
1:A:33:ASP:OD1	1:A:33:ASP:N	2.52	0.42
2:B:286:LEU:HD23	2:B:291:LEU:HD23	2.02	0.42
2:D:235:MET:HE2	2:D:235:MET:HB3	1.88	0.42
2:D:406:HIS:CE1	2:D:407:TRP:HD1	2.37	0.42
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.54	0.42
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.42
1:A:335:ILE:HG23	1:A:339:ARG:HG3	2.02	0.42
2:B:221:THR:HG21	1:C:326:LYS:HB2	2.01	0.42
2:D:322:ARG:O	2:D:373:MET:HE1	2.20	0.42
4:F:186:LEU:HD21	4:F:328:TRP:CE2	2.55	0.42
4:F:79:LYS:O	4:F:83:THR:HB	2.20	0.42
1:A:289:ALA:HA	1:A:331:ALA:CB	2.50	0.41
2:B:272:PHE:CZ	7:B:505:GOL:O2	2.67	0.41
1:C:43:GLY:HA2	1:C:56:THR:O	2.20	0.41
2:D:345:GLU:H	2:D:345:GLU:CD	2.24	0.41
2:D:405:LEU:HA	2:D:405:LEU:HD12	1.89	0.41
2:B:2:ARG:HD2	2:B:2:ARG:H	1.86	0.41
2:B:237:GLY:HA2	7:B:505:GOL:H12	2.03	0.41
4:F:216:TYR:OH	4:F:345:GLU:OE1	2.26	0.41
4:F:80:LEU:O	4:F:84:SER:HB2	2.20	0.41
2:B:192:HIS:NE2	2:B:424[A]:ASN:OD1	2.53	0.41
1:C:431:ASP:HB3	12:C:508:IMD:H2	2.01	0.41
2:B:228:ASN:O	2:B:232:SER:HB2	2.20	0.41
2:B:88:ARG:O	2:B:91:ASN:HB2	2.21	0.41
2:D:240:THR:HB	2:D:318:ILE:HD13	2.02	0.41
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.39	0.41
1:A:401:LYS:HE3	2:B:438:ALA:HB1	2.02	0.41
1:C:337:THR:OG1	1:C:338:LYS:HD2	2.20	0.41
4:F:223:THR:O	4:F:260:ASN:HB3	2.20	0.41
1:C:356[A]:ASN:OD1	13:C:603:HOH:O	2.21	0.41
2:D:402:LYS:O	2:D:405:LEU:HD13	2.19	0.41
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.02	0.41
2:D:330:GLU:O	2:D:334:ASN:HB2	2.20	0.41
3:E:101:LEU:HA	3:E:101:LEU:HD12	1.90	0.41
1:A:34:GLY:O	1:A:61:HIS:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASP:O	1:A:80[A]:THR:HG22	2.21	0.41
2:B:88:ARG:HH12	2:B:90:ASP:HB2	1.86	0.41
2:D:212:ILE:HG23	2:D:275:LEU:HD13	2.02	0.41
2:B:164:ARG:O	10:B:507:MES:H71	2.22	0.40
2:D:180:THR:HG22	2:D:181:VAL:HG12	2.03	0.40
2:D:211:ASP:OD1	2:D:211:ASP:N	2.53	0.40
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.51	0.40
4:F:198:LYS:HE2	4:F:198:LYS:HB2	1.75	0.40
1:C:179:THR:HG23	5:C:503:GTP:H3'	2.02	0.40
1:A:382:THR:O	7:A:504:GOL:H2	2.22	0.40
2:D:74:THR:O	2:D:78:VAL:HG23	2.22	0.40
2:D:70:LEU:O	2:D:98:GLY:HA2	2.21	0.40
4:F:221:LEU:HD23	4:F:221:LEU:HA	1.87	0.40
4:F:86:GLU:O	4:F:87:LEU:HD23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	450/440 (102%)	431 (96%)	19 (4%)	0	100	100
1	C	449/440 (102%)	437 (97%)	12 (3%)	0	100	100
2	B	429/431 (100%)	409 (95%)	18 (4%)	2 (0%)	32	51
2	D	421/431 (98%)	395 (94%)	18 (4%)	8 (2%)	9	14
3	E	120/136 (88%)	111 (92%)	8 (7%)	1 (1%)	22	37
4	F	307/378 (81%)	264 (86%)	34 (11%)	9 (3%)	5	7
All	All	2176/2256 (96%)	2047 (94%)	109 (5%)	20 (1%)	20	34

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	177	VAL
2	D	399	PHE
4	F	343	TYR
2	B	337	ASN
2	D	181	VAL
2	D	214	PHE
2	D	398	MET
2	D	402	LYS
4	F	128	ARG
2	B	369	ARG
2	D	73	GLY
2	D	180	THR
4	F	90	SER
4	F	225	SER
3	E	10	GLU
4	F	23	ALA
4	F	88	SER
4	F	92	THR
4	F	272	MET
4	F	344	ALA

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	383/371 (103%)	365 (95%)	18 (5%)	30	52
1	C	382/371 (103%)	369 (97%)	13 (3%)	42	67
2	B	375/372 (101%)	350 (93%)	25 (7%)	19	33
2	D	368/372 (99%)	342 (93%)	26 (7%)	17	30
3	E	112/122 (92%)	103 (92%)	9 (8%)	14	25
4	F	293/336 (87%)	261 (89%)	32 (11%)	7	13
All	All	1913/1944 (98%)	1790 (94%)	123 (6%)	21	36

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	48	SER
1	A	71	GLU
1	A	89	PRO
1	A	96	LYS
1	A	115	ILE
1	A	176	GLN
1	A	178	SER
1	A	181	VAL
1	A	218	ASP
1	A	220	GLU
1	A	232	SER
1	A	340	SER
1	A	347	CYS
1	A	381	THR
1	A	413	MET
1	A	437	VAL
1	A	438	ASP
2	B	2	ARG
2	B	26	ASP
2	B	57	THR
2	B	88	ARG
2	B	117	SER
2	B	132	LEU
2	B	139	HIS
2	B	155[A]	SER
2	B	155[B]	SER
2	B	164	ARG
2	B	177	VAL
2	B	190	SER
2	B	217	LEU
2	B	220	THR
2	B	232	SER
2	B	238	VAL
2	B	248	LEU
2	B	286	LEU
2	B	293	GLN
2	B	298	SER
2	B	318	ILE
2	B	335	VAL
2	B	369	ARG
2	B	372	LYS
2	B	392	SER

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Mol	Chain	Res	Type
1	C	71	GLU
1	C	80	THR
1	C	177	VAL
1	C	178	SER
1	C	179	THR
1	C	241	SER
1	C	285	GLN
1	C	286	LEU
1	C	297	GLU
1	C	335	ILE
1	C	338	LYS
1	C	361	THR
1	C	381	THR
2	D	1	MET
2	D	8	GLN
2	D	15	GLN
2	D	57	THR
2	D	74	THR
2	D	77	SER
2	D	117	SER
2	D	138	THR
2	D	139	HIS
2	D	158	ARG
2	D	182	VAL
2	D	190	SER
2	D	204	ILE
2	D	215	ARG
2	D	220	THR
2	D	221[A]	THR
2	D	221[B]	THR
2	D	232	SER
2	D	248	LEU
2	D	345	GLU
2	D	400	ARG
2	D	404	PHE
2	D	409	THR
2	D	423	SER
2	D	430	SER
2	D	441	ASP
3	E	15	THR
3	E	19	SER
3	E	22	VAL

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Mol	Chain	Res	Type
3	E	59	GLU
3	E	76	ARG
3	E	77	GLU
3	E	98	LYS
3	E	103	GLN
3	E	110	GLU
4	F	3	THR
4	F	12	SER
4	F	13	VAL
4	F	20	LEU
4	F	28	LYS
4	F	30	LEU
4	F	33	ASP
4	F	69	ASP
4	F	76[A]	SER
4	F	76[B]	SER
4	F	83	THR
4	F	84	SER
4	F	86	GLU
4	F	125	THR
4	F	146	VAL
4	F	163	SER
4	F	172	PHE
4	F	191	LEU
4	F	202	ARG
4	F	217	ARG
4	F	220	VAL
4	F	224	SER
4	F	244	CYS
4	F	252	ASN
4	F	253	TYR
4	F	258	GLU
4	F	266	GLU
4	F	275[A]	LEU
4	F	275[B]	LEU
4	F	284[A]	LEU
4	F	284[B]	LEU
4	F	377	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	301	GLN
2	B	192	HIS
2	B	309	HIS
2	D	101	ASN
2	D	406	HIS
3	E	92	ASN
4	F	26	GLN
4	F	145	ASN
4	F	196	HIS
4	F	239	HIS
4	F	243	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 8 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	A	501	6	27,34,34	1.02	2 (7%)	27,54,54	1.75	8 (29%)
7	GOL	A	503	-	5,5,5	0.50	0	5,5,5	0.37	0
7	GOL	A	504	-	5,5,5	0.84	0	5,5,5	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	A	506	-	5,5,5	0.53	0	5,5,5	0.77	0
9	GDP	B	501	6	25,30,30	1.39	3 (12%)	26,47,47	1.83	6 (23%)
7	GOL	B	503	-	5,5,5	0.47	0	5,5,5	1.04	0
7	GOL	B	504	-	5,5,5	0.57	0	5,5,5	0.29	0
7	GOL	B	505	-	5,5,5	0.62	0	5,5,5	0.37	0
10	MES	B	507	-	12,12,12	2.09	1 (8%)	14,16,16	3.77	7 (50%)
11	6ZR	B	508	-	28,29,29	2.20	7 (25%)	38,42,42	2.58	13 (34%)
7	GOL	C	502	-	5,5,5	0.92	0	5,5,5	0.59	0
5	GTP	C	503	6	27,34,34	1.19	1 (3%)	27,54,54	2.03	7 (25%)
7	GOL	C	505	-	5,5,5	0.59	0	5,5,5	0.57	0
7	GOL	C	506	-	5,5,5	0.51	0	5,5,5	0.54	0
7	GOL	C	507	-	5,5,5	0.90	0	5,5,5	0.73	0
12	IMD	C	508	-	3,5,5	0.50	0	4,5,5	0.47	0
12	IMD	C	509	-	3,5,5	0.43	0	4,5,5	0.95	0
12	IMD	C	510	-	3,5,5	0.45	0	4,5,5	0.58	0
9	GDP	D	501	6	25,30,30	1.25	2 (8%)	26,47,47	1.93	6 (23%)
7	GOL	D	503	-	5,5,5	0.50	0	5,5,5	0.26	0
7	GOL	D	504	-	5,5,5	0.29	0	5,5,5	0.43	0

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
7	GOL	A	503	-	-	0/4/4/4	0/0/0/0
7	GOL	A	504	-	-	0/4/4/4	0/0/0/0
7	GOL	A	506	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
7	GOL	B	503	-	-	0/4/4/4	0/0/0/0
7	GOL	B	504	-	-	0/4/4/4	0/0/0/0
7	GOL	B	505	-	-	0/4/4/4	0/0/0/0
10	MES	B	507	-	-	0/6/14/14	0/1/1/1
11	6ZR	B	508	-	-	0/16/32/32	0/3/3/3
7	GOL	C	502	-	-	0/4/4/4	0/0/0/0
5	GTP	C	503	6	-	0/18/38/38	0/3/3/3
7	GOL	C	505	-	-	0/4/4/4	0/0/0/0
7	GOL	C	506	-	-	0/4/4/4	0/0/0/0
7	GOL	C	507	-	-	0/4/4/4	0/0/0/0
12	IMD	C	508	-	-	0/0/0/0	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	IMD	C	509	-	-	0/0/0/0	0/1/1/1
12	IMD	C	510	-	-	0/0/0/0	0/1/1/1
9	GDP	D	501	6	-	0/12/32/32	0/3/3/3
7	GOL	D	503	-	-	0/4/4/4	0/0/0/0
7	GOL	D	504	-	-	0/4/4/4	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	507	MES	C8-S	-6.84	1.67	1.77
11	B	508	6ZR	CAB-NAC	-5.86	1.32	1.43
11	B	508	6ZR	CAF-CAH	-5.42	1.50	1.57
11	B	508	6ZR	CAI-CAH	-4.47	1.45	1.51
9	B	501	GDP	C2'-C1'	-3.71	1.47	1.53
5	A	501	GTP	C2'-C1'	-2.37	1.49	1.53
9	B	501	GDP	C4-N3	-2.14	1.32	1.35
11	B	508	6ZR	CAH-NAC	-2.09	1.46	1.48
5	C	503	GTP	C6-C5	2.04	1.45	1.41
11	B	508	6ZR	CAG-CAF	2.10	1.57	1.53
11	B	508	6ZR	CAK-CAM	2.35	1.43	1.40
9	B	501	GDP	C6-C5	2.57	1.46	1.41
5	A	501	GTP	C6-C5	2.74	1.46	1.41
9	D	501	GDP	C5-C4	2.88	1.47	1.40
11	B	508	6ZR	CAD-NAC	3.80	1.43	1.37
9	D	501	GDP	C6-C5	4.34	1.49	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	508	6ZR	OAN-CAM-CAP	-6.13	114.08	124.37
11	B	508	6ZR	CAH-NAC-CAD	-4.31	90.84	95.27
10	B	507	MES	C6-C5-N4	-4.02	104.48	110.11
11	B	508	6ZR	CAU-OAT-CAS	-3.97	111.83	117.54
5	C	503	GTP	C6-C5-C4	-3.96	116.91	120.84
9	D	501	GDP	C6-C5-C4	-3.93	116.94	120.84
5	C	503	GTP	N3-C2-N1	-3.88	121.79	127.46
9	B	501	GDP	C6-C5-C4	-3.77	117.09	120.84
9	D	501	GDP	C4-C5-N7	-3.77	105.77	109.41
5	A	501	GTP	C5-C6-N1	-3.75	118.15	123.48
11	B	508	6ZR	OAW-CAV-CAS	-3.62	114.97	120.12
9	D	501	GDP	C5-C6-N1	-3.13	119.02	123.48
9	B	501	GDP	C4-C5-N7	-3.06	106.45	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	N3-C2-N1	-3.01	123.06	127.46
9	D	501	GDP	N3-C2-N1	-2.76	123.43	127.46
5	A	501	GTP	C6-C5-C4	-2.69	118.17	120.84
10	B	507	MES	C2-C3-N4	-2.61	106.45	110.11
11	B	508	6ZR	CBA-OAZ-CAY	-2.61	113.78	117.54
5	C	503	GTP	C4-C5-N7	-2.50	107.00	109.41
5	A	501	GTP	C4-C5-N7	-2.44	107.05	109.41
9	B	501	GDP	C5-C6-N1	-2.43	120.03	123.48
10	B	507	MES	O2S-S-O1S	-2.42	105.47	113.86
11	B	508	6ZR	CAA-CAY-CAV	-2.41	117.44	120.22
5	C	503	GTP	C1'-N9-C4	-2.34	122.59	126.64
5	A	501	GTP	N3-C2-N1	-2.21	124.23	127.46
5	C	503	GTP	C5-C6-N1	-2.07	120.54	123.48
10	B	507	MES	O3S-S-C8	-2.01	103.58	106.06
5	A	501	GTP	C4'-O4'-C1'	2.13	112.03	109.77
11	B	508	6ZR	CAA-CAB-NAC	2.30	121.59	119.40
11	B	508	6ZR	CAQ-CAI-CAJ	2.32	121.49	118.79
5	C	503	GTP	C6-N1-C2	2.48	119.62	116.06
10	B	507	MES	O2S-S-C8	2.51	108.94	106.79
11	B	508	6ZR	OAW-CAV-CAY	2.63	123.87	120.12
5	A	501	GTP	O3G-PG-O2G	2.72	118.59	107.61
11	B	508	6ZR	OAZ-CAY-CAV	2.91	120.34	115.22
11	B	508	6ZR	CAB-NAC-CAH	2.94	135.19	130.31
9	B	501	GDP	C6-N1-C2	3.13	120.57	116.06
5	A	501	GTP	C6-N1-C2	3.26	120.75	116.06
10	B	507	MES	C5-N4-C3	3.28	116.29	108.87
9	D	501	GDP	C6-N1-C2	3.58	121.21	116.06
5	A	501	GTP	C2-N3-C4	3.59	119.35	115.16
9	D	501	GDP	C2-N3-C4	4.68	120.62	115.16
11	B	508	6ZR	CAI-CAH-NAC	4.74	121.13	115.77
9	B	501	GDP	C2-N3-C4	4.89	120.87	115.16
5	C	503	GTP	C2-N3-C4	6.53	122.78	115.16
11	B	508	6ZR	OAN-CAM-CAK	8.18	124.52	114.55
10	B	507	MES	O1S-S-C8	11.78	116.91	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	504	GOL	1	0
7	B	503	GOL	2	0
7	B	505	GOL	10	0
10	B	507	MES	1	0
11	B	508	6ZR	3	0
5	C	503	GTP	1	0
7	C	505	GOL	3	0
7	C	506	GOL	1	0
7	C	507	GOL	2	0
12	C	508	IMD	1	0
12	C	509	IMD	2	0
12	C	510	IMD	1	0
7	D	504	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	439/440 (99%)	0.05	8 (1%) 69 70	18, 38, 62, 99	0
1	C	440/440 (100%)	-0.42	1 (0%) 94 95	10, 23, 43, 59	0
2	B	422/431 (97%)	-0.08	11 (2%) 56 58	12, 33, 66, 99	1 (0%)
2	D	421/431 (97%)	0.18	18 (4%) 36 38	22, 45, 73, 93	2 (0%)
3	E	121/136 (88%)	0.18	7 (5%) 24 24	20, 44, 76, 96	0
4	F	319/378 (84%)	1.53	96 (30%) 1 0	27, 62, 143, 176	0
All	All	2162/2256 (95%)	0.18	141 (6%) 20 20	10, 39, 79, 176	3 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	13.3
4	F	256	TYR	12.0
4	F	252	ASN	11.9
4	F	253	TYR	9.2
4	F	243	HIS	8.8
4	F	249	TYR	8.6
4	F	250	SER	8.5
4	F	231	ALA	8.4
4	F	245	ILE	8.2
4	F	241	THR	8.0
4	F	255	ARG	7.9
4	F	238	CYS	7.7
4	F	230	SER	7.6
4	F	229	ASN	7.5
4	F	237	THR	7.5
4	F	247	LYS	7.5
4	F	225	SER	7.3
4	F	240	LEU	7.2
4	F	235	ASP	7.1

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Mol	Chain	Res	Type	RSRZ
4	F	130	VAL	6.9
4	F	257	GLU	6.8
4	F	236	LYS	6.8
4	F	242	ASN	6.8
4	F	224	SER	6.7
4	F	239	HIS	6.7
4	F	254	GLY	6.6
4	F	149	ALA	6.5
1	A	439	SER	6.4
4	F	100	ILE	6.4
4	F	248	GLU	6.4
4	F	169	LEU	6.1
4	F	246	GLN	6.0
4	F	133	ALA	6.0
2	D	57	THR	5.8
4	F	259	GLY	5.8
2	B	57	THR	5.6
4	F	228	TYR	5.4
4	F	227	PRO	5.3
2	B	1	MET	5.1
4	F	172	PHE	5.0
4	F	162	ILE	5.0
4	F	134	ALA	5.0
4	F	21	LEU	4.7
4	F	182	ILE	4.7
4	F	258	GLU	4.6
4	F	260	ASN	4.6
3	E	27	PRO	4.6
4	F	199	PHE	4.4
4	F	125	THR	4.4
2	B	59	ASN	4.3
4	F	147	TRP	4.3
1	A	42	ILE	4.2
4	F	168	GLU	4.2
2	D	177	VAL	4.0
3	E	28	SER	4.0
2	D	219	LEU	3.9
4	F	198	LYS	3.8
4	F	181	VAL	3.8
4	F	99	VAL	3.8
4	F	226	GLU	3.8
4	F	194	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	247	GLN	3.7
2	B	249	ASN	3.6
4	F	20	LEU	3.6
4	F	223	THR	3.6
4	F	343	TYR	3.6
2	D	406	HIS	3.5
4	F	101	TYR	3.4
4	F	24	THR	3.3
4	F	129	GLU	3.3
2	B	37	HIS	3.3
4	F	196	HIS	3.3
4	F	197	ARG	3.2
4	F	222	ARG	3.2
2	D	58	GLY	3.2
4	F	163	SER	3.2
4	F	90	SER	3.1
4	F	19	ARG	3.1
1	C	440	VAL	3.1
4	F	128	ARG	3.1
4	F	102	PRO	3.0
2	D	405	LEU	3.0
4	F	165	GLU	3.0
4	F	17	VAL	3.0
4	F	167	SER	3.0
2	D	37	HIS	3.0
4	F	362	ALA	2.9
2	B	58	GLY	2.9
4	F	145	ASN	2.9
3	E	45	PRO	2.8
2	D	56	ALA	2.8
4	F	89	GLU	2.8
4	F	170	LEU	2.8
4	F	148	ILE	2.8
1	A	281	ALA	2.8
4	F	25	GLY	2.7
4	F	185	TYR	2.7
4	F	173	ILE	2.7
4	F	192	LEU	2.7
4	F	9	GLU	2.6
2	D	33	THR	2.6
4	F	180	HIS	2.6
2	B	56	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	132	LEU	2.6
4	F	171	ASP	2.6
2	D	179	ASP	2.5
1	A	438	ASP	2.5
3	E	140	LYS	2.5
2	D	1	MET	2.5
4	F	127	GLU	2.4
4	F	263	PHE	2.4
2	D	407	TRP	2.4
4	F	28	LYS	2.4
4	F	135	TYR	2.4
2	B	247	GLN	2.4
2	B	60	LYS	2.4
4	F	131	PHE	2.3
1	A	41	THR	2.3
4	F	11	SER	2.3
4	F	1	MET	2.3
2	D	416	MET	2.3
3	E	26	PRO	2.3
2	D	220	THR	2.2
4	F	164	SER	2.2
4	F	335	ALA	2.2
2	D	404	PHE	2.2
2	D	415	GLU	2.2
4	F	262	MET	2.1
4	F	144	GLY	2.1
1	A	58	ALA	2.1
4	F	6	VAL	2.1
4	F	22	LEU	2.1
3	E	48	GLU	2.1
1	A	56	THR	2.0
2	B	62	VAL	2.0
3	E	46	SER	2.0
2	B	61	TYR	2.0
4	F	346	LEU	2.0
2	D	414	ASP	2.0
4	F	126	ASP	2.0
1	A	43	GLY	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	GOL	B	505	6/6	0.84	0.48	12.04	54,55,62,68	0
7	GOL	C	506	6/6	0.90	0.31	9.64	47,52,65,65	0
7	GOL	B	503	6/6	0.88	0.38	8.01	42,49,52,72	0
6	MG	A	502	1/1	0.97	0.33	7.22	37,37,37,37	0
7	GOL	B	504	6/6	0.65	0.33	7.03	53,62,69,71	0
6	MG	C	504	1/1	0.91	0.34	6.74	38,38,38,38	0
12	IMD	C	510	5/5	0.83	0.28	4.94	56,64,66,67	0
7	GOL	C	502	6/6	0.76	0.30	4.77	46,52,64,67	0
7	GOL	A	504	6/6	0.81	0.29	4.54	56,71,73,79	0
7	GOL	D	504	6/6	0.89	0.29	4.26	51,53,65,77	0
12	IMD	C	509	5/5	0.86	0.23	3.48	64,66,73,76	0
7	GOL	C	507	6/6	0.88	0.19	2.14	34,47,48,57	0
7	GOL	A	503	6/6	0.93	0.19	1.46	47,56,58,59	0
7	GOL	C	505	6/6	0.86	0.33	1.32	61,65,73,81	0
7	GOL	A	506	6/6	0.80	0.22	0.97	52,63,69,73	0
5	GTP	C	503	32/32	0.98	0.15	0.89	12,16,20,22	0
9	GDP	B	501	28/28	0.99	0.15	0.32	13,18,21,24	0
11	6ZR	B	508	27/27	0.93	0.16	-0.10	35,47,53,58	0
10	MES	B	507	12/12	0.97	0.12	-0.16	26,38,47,52	0
5	GTP	A	501	32/32	0.99	0.19	-0.22	18,23,30,33	0
9	GDP	D	501	28/28	0.97	0.13	-0.38	33,42,57,61	0
8	CA	A	505	1/1	0.95	0.06	-2.08	59,59,59,59	0
6	MG	F	401	1/1	0.77	0.83	-	86,86,86,86	0
6	MG	B	502	1/1	0.98	0.34	-	16,16,16,16	0
12	IMD	C	508	5/5	0.95	0.21	-	32,35,36,42	0
8	CA	C	501	1/1	0.96	0.06	-	82,82,82,82	0
6	MG	D	502	1/1	0.95	0.12	-	40,40,40,40	0
7	GOL	D	503	6/6	0.76	0.44	-	74,81,86,87	0
8	CA	B	506	1/1	0.95	0.09	-	81,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.