



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2017 – 01:55 AM EDT

PDB ID : 4YJ2
Title : Crystal structure of tubulin bound to MI-181
Authors : McNamara, D.E.; Torres, J.Z.; Yeates, T.O.
Deposited on : unknown
Resolution : 2.60 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-20029824
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-20029824

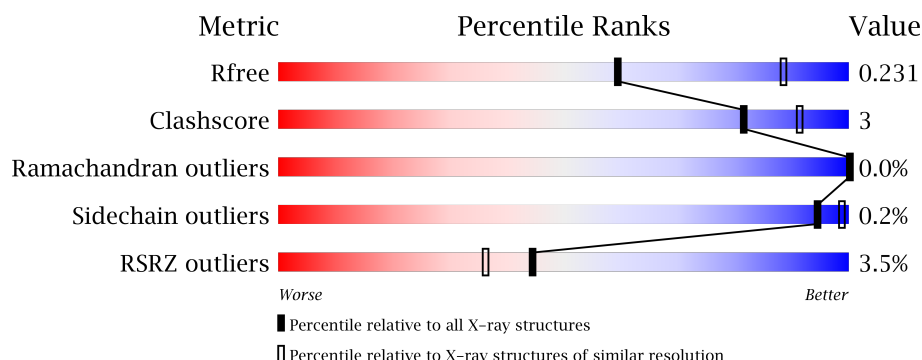
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



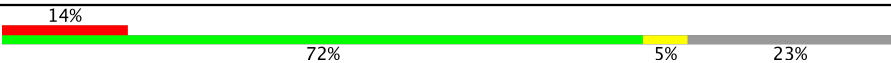
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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>90%</div> <div>7%</div> <div>.</div> </div>
1	C	451	<div> <div>%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
2	B	445	<div> <div>%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
2	D	445	<div> <div>2%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
3	E	143	<div> <div>%</div> <div>80%</div> <div>5%</div> <div>15%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	4ED	D	503[A]	-	-	-	X
11	MES	B	506	-	-	-	X
12	IMD	C	504	-	-	-	X
8	GOL	A	504	-	-	-	X
8	GOL	A	505	-	-	-	X
8	GOL	C	503	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17335 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	437	Total	C	N	O	S	0	1	0
			3420	2167	581	650	22			
1	C	440	Total	C	N	O	S	0	2	0
			3445	2180	584	658	23			

- 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	0	2	0
			3336	2098	569	642	27			
2	D	421	Total	C	N	O	S	0	10	0
			3379	2127	572	652	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	0	0
			1003	619	182	197	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

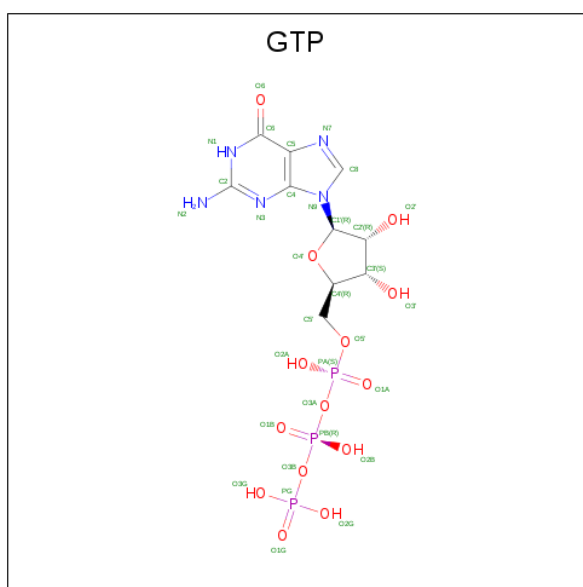
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	296	Total	C	N	O	S	0	0	0
			2417	1564	401	440	12			

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		

Continued on next page...

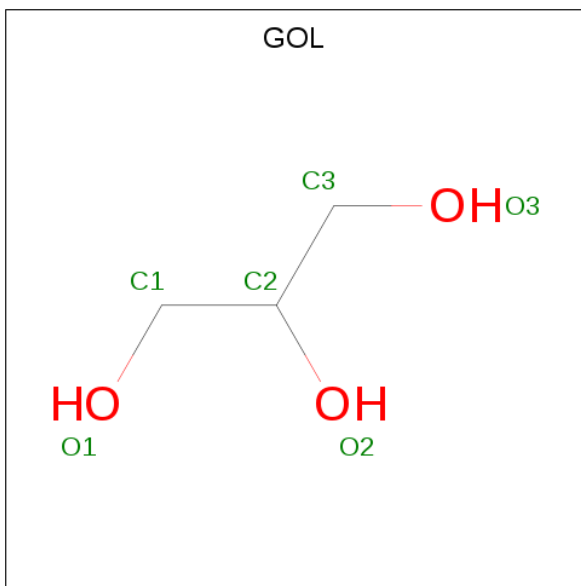
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

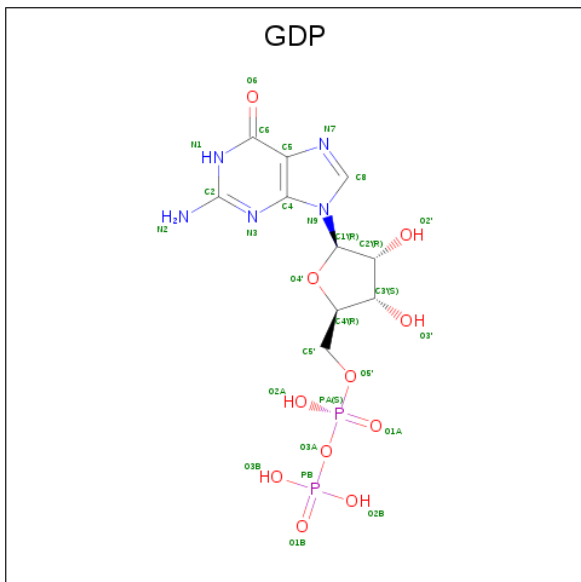
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



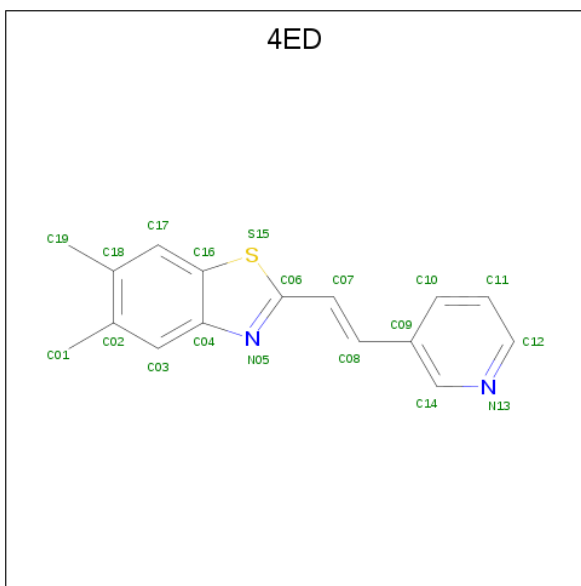
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		

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



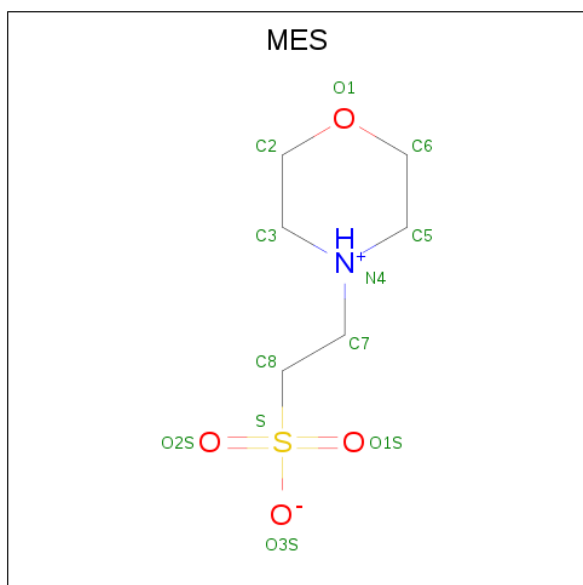
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 5,6-dimethyl-2-[(E)-2-(pyridin-3-yl)ethenyl]-1,3-benzothiazole (three-letter code: 4ED) (formula: $C_{16}H_{14}N_2S$).



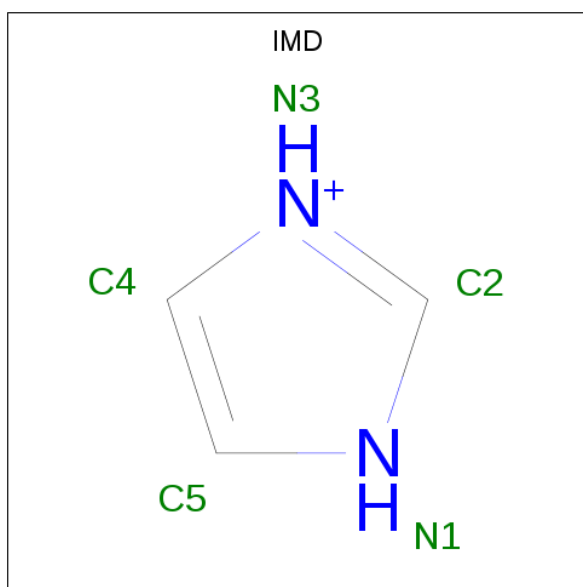
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	S	0	0
			19	16	2	1		
10	D	1	Total	C	N	S	0	1
			19	16	2	1		

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



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

- 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	0	0
			5	3	2		

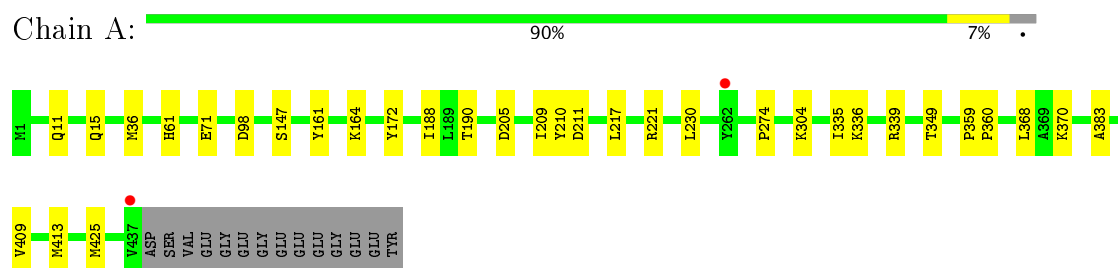
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	23	Total	O	0	0
			23	23		
13	B	30	Total	O	0	0
			30	30		
13	C	47	Total	O	0	0
			47	47		
13	D	9	Total	O	0	1
			9	9		
13	F	2	Total	O	0	0
			2	2		

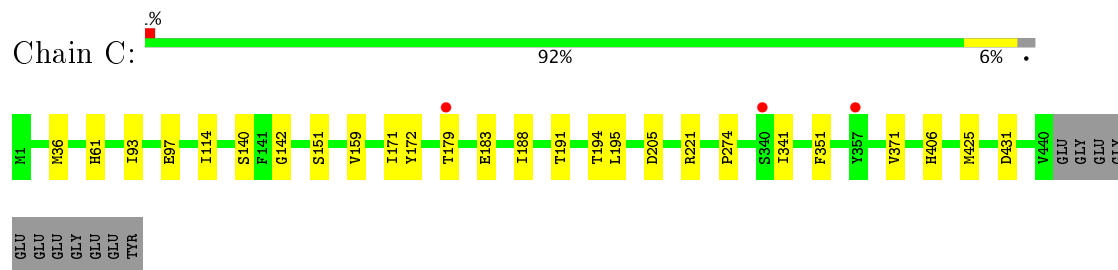
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

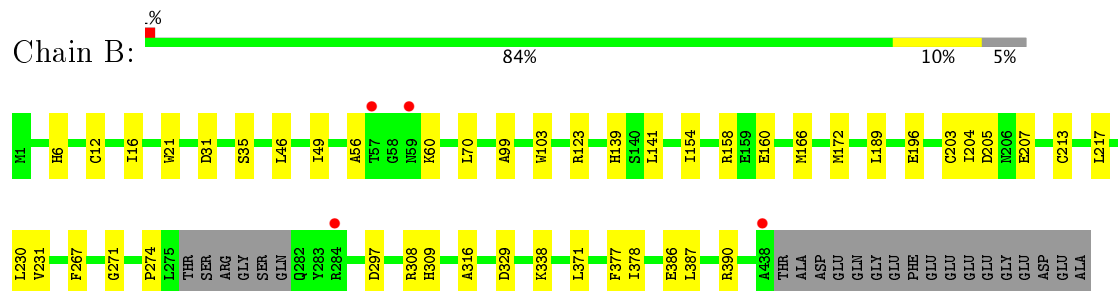
- Molecule 1: Tubulin alpha-1B chain



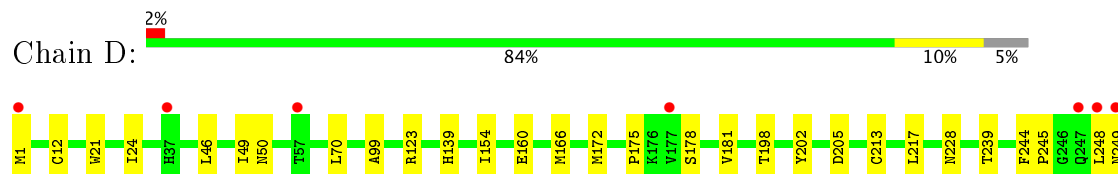
- Molecule 1: Tubulin alpha-1B chain

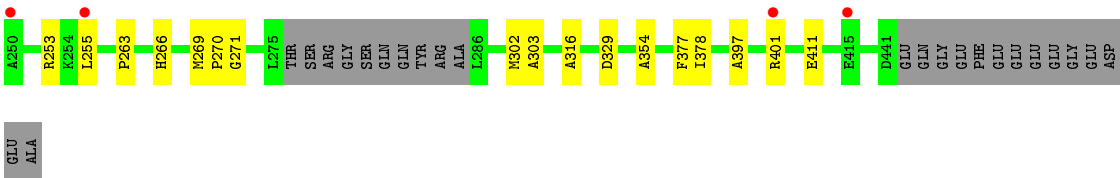


- Molecule 2: Tubulin beta-2B chain

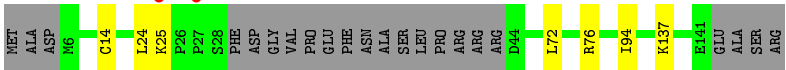
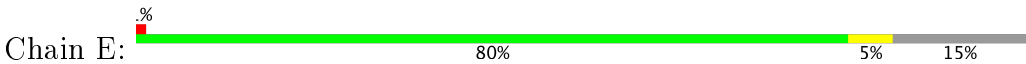


- Molecule 2: Tubulin beta-2B chain

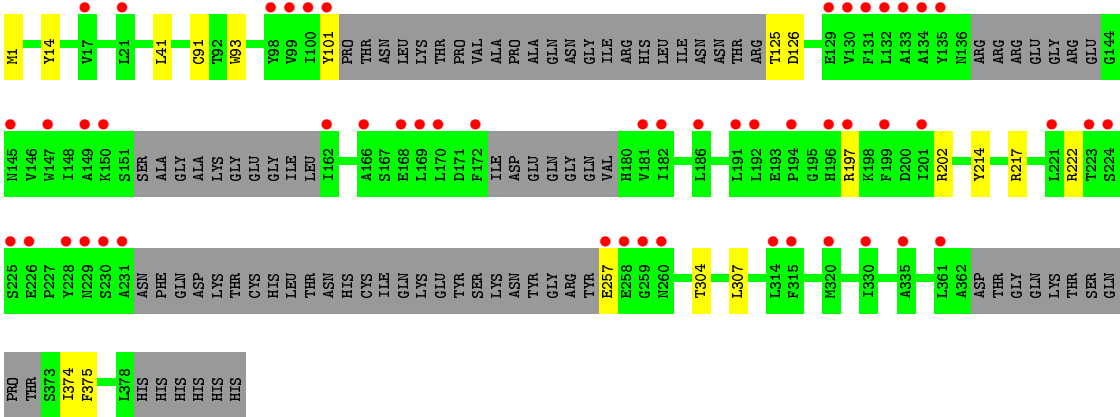




• Molecule 3: Stathmin-4



• Molecule 4: 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	104.83Å 157.65Å 181.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.72 – 2.60 90.72 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (90.72-2.60) 99.8 (90.72-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.62Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.188 , 0.231 0.188 , 0.231	Depositor DCC
R_{free} test set	9259 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17335	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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 [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, IMD, CA, 4ED, GTP, 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	0.21	0/3501	0.37	0/4753
1	C	0.21	0/3529	0.38	0/4791
2	B	0.22	0/3416	0.36	0/4626
2	D	0.21	0/3460	0.36	0/4688
3	E	0.20	0/1012	0.31	0/1344
4	F	0.21	0/2469	0.35	0/3334
All	All	0.21	0/17387	0.36	0/23536

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	3420	0	3339	22	0
1	C	3445	0	3357	16	0
2	B	3336	0	3220	27	0
2	D	3379	0	3261	29	0
3	E	1003	0	1019	5	0
4	F	2417	0	2403	10	0
5	A	32	0	12	3	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	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	12	0	16	2	0
8	B	6	0	8	0	0
8	C	6	0	8	0	0
8	D	6	0	8	2	0
9	B	28	0	12	1	0
9	D	28	0	12	2	0
10	B	19	0	14	1	0
10	D	19	0	14	3	0
11	B	24	0	24	2	0
12	C	5	0	5	1	0
13	A	23	0	0	0	0
13	B	30	0	0	0	0
13	C	47	0	0	0	0
13	D	9	0	0	0	0
13	F	2	0	0	0	0
All	All	17335	0	16744	101	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 (101) 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:D:253:ARG:HH11	8:D:504:GOL:HO3	1.37	0.70
2:D:253:ARG:NH1	8:D:504:GOL:O3	2.26	0.68
1:C:179:THR:HB	2:D:248[B]:LEU:HD13	1.75	0.67
1:A:383:ALA:HA	8:A:505:GOL:H31	1.78	0.65
4:F:217:ARG:HE	4:F:374:ILE:HA	1.63	0.63
2:D:202:TYR:OH	10:D:503[A]:4ED:H7	2.01	0.61
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.83	0.60
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.83	0.60
2:D:397:ALA:O	2:D:401:ARG:NH1	2.37	0.58
2:B:297:ASP:HA	11:B:506:MES:H62	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.86	0.58
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.86	0.57
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.87	0.57
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.87	0.57
4:F:101:TYR:HD2	4:F:126:ASP:HB3	1.70	0.57
1:C:97:GLU:OE2	2:D:253:ARG:NH2	2.39	0.56
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.88	0.56
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.89	0.54
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.41	0.54
1:A:274:PRO:HA	8:A:504:GOL:H32	1.89	0.54
2:B:207:GLU:OE1	2:B:390:ARG:NH1	2.41	0.53
2:D:46:LEU:HA	2:D:49:ILE:HB	1.90	0.53
2:D:175:PRO:HA	2:D:178:SER:HB2	1.91	0.53
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.40	0.52
2:D:269[A]:MET:HG3	2:D:303:ALA:HB3	1.90	0.52
2:D:248[B]:LEU:HD23	2:D:354:ALA:HB2	1.91	0.52
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.90	0.52
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.91	0.52
2:D:1:MET:N	2:D:50:ASN:OD1	2.43	0.52
2:D:123:ARG:NH2	2:D:160:GLU:OE1	2.43	0.52
1:A:360:PRO:O	1:A:370:LYS:NZ	2.41	0.51
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.92	0.51
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.93	0.51
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.91	0.51
1:A:221:ARG:HH21	2:B:329:ASP:HB3	1.76	0.51
4:F:202:ARG:HB2	4:F:222:ARG:HH21	1.75	0.50
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.92	0.50
1:A:349:THR:HB	3:E:25:LYS:HB3	1.94	0.50
1:A:359:PRO:HB2	1:A:370:LYS:HZ2	1.77	0.49
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.93	0.49
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.47	0.49
1:A:11:GLN:HB3	5:A:501:GTP:O2A	2.13	0.49
2:B:205:ASP:OD2	2:B:390:ARG:NH2	2.45	0.48
1:C:431:ASP:HB3	12:C:504:IMD:H4	1.95	0.48
2:B:217:LEU:HD11	2:B:230:LEU:HD21	1.96	0.48
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.49	0.48
2:B:308:ARG:HH21	11:B:506:MES:H52	1.78	0.48
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.96	0.48
1:A:147:SER:HB2	1:A:190:THR:HB	1.95	0.47
2:B:271:GLY:HA3	2:B:377:PHE:HB3	1.97	0.47
2:B:31:ASP:OD1	2:B:35:SER:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:271:GLY:HA3	2:D:377:PHE:HB3	1.97	0.46
10:B:504:4ED:H3	10:B:504:4ED:H12	1.64	0.46
2:D:228:ASN:OD1	9:D:501:GDP:N1	2.37	0.46
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.98	0.46
1:C:142:GLY:HA3	1:C:183:GLU:OE2	2.17	0.45
2:B:154:ILE:HG23	2:B:166:MET:HG2	1.99	0.45
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.34	0.45
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.97	0.45
1:C:151:SER:HA	1:C:194:THR:HG22	1.99	0.45
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.52	0.44
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.34	0.44
2:D:249[B]:ASN:HB3	2:D:255[B]:LEU:HD12	1.99	0.44
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.57	0.44
2:B:274:PRO:HD2	2:B:371:LEU:HD13	1.99	0.44
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.99	0.44
4:F:91:CYS:O	4:F:93:TRP:N	2.46	0.44
2:B:338:LYS:HE2	4:F:1:MET:HB3	1.99	0.44
2:D:198:THR:OG1	2:D:266:HIS:NE2	2.48	0.44
2:B:141:LEU:HD12	2:B:172:MET:SD	2.57	0.44
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.53	0.43
2:D:411:GLU:HA	3:E:137:LYS:HD2	2.00	0.43
1:A:409:VAL:HA	1:A:413:MET:O	2.19	0.43
2:B:158:ARG:NH1	2:B:196:GLU:O	2.51	0.43
2:D:172:MET:HB2	2:D:205:ASP:HA	2.00	0.43
1:A:210:TYR:OH	1:A:221:ARG:NH1	2.51	0.43
2:B:123:ARG:NE	2:B:160:GLU:OE2	2.51	0.43
2:B:213:CYS:HA	2:B:217:LEU:HB2	2.01	0.43
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.01	0.43
1:C:221:ARG:NE	2:D:329:ASP:OD2	2.52	0.43
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.53	0.43
10:D:503[A]:4ED:H3	10:D:503[A]:4ED:H12	1.64	0.43
2:B:46:LEU:HA	2:B:49:ILE:HB	2.01	0.42
2:B:56:ALA:HB3	2:B:60:LYS:HB2	2.01	0.42
2:B:309:HIS:ND1	2:B:386:GLU:OE1	2.50	0.42
2:D:244[A]:PHE:HA	2:D:245[A]:PRO:HD3	1.88	0.42
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.02	0.41
1:A:98:ASP:HB2	5:A:501:GTP:O3G	2.20	0.41
1:C:140:SER:HA	1:C:171:ILE:HB	2.02	0.41
3:E:72:LEU:O	3:E:76:ARG:HG2	2.20	0.41
2:B:204:ILE:HD13	2:B:231:VAL:HG13	2.02	0.41
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:125:THR:HA	4:F:126:ASP:HA	1.68	0.41
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.55	0.41
1:C:341:ILE:HD13	1:C:351:PHE:HZ	1.85	0.41
2:D:239:THR:HG22	10:D:503[A]:4ED:H9	2.01	0.41
1:A:188:ILE:HG13	1:A:425:MET:HG3	2.03	0.40
2:D:270:PRO:HB2	2:D:302:MET:HB2	2.03	0.40
1:A:161:TYR:HB3	1:A:164:LYS:HD3	2.04	0.40
1:C:159:VAL:HA	3:E:94:ILE:HG23	2.03	0.40
1:C:191:THR:O	1:C:195:LEU:HB2	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	436/451 (97%)	421 (97%)	15 (3%)	0	100	100
1	C	440/451 (98%)	430 (98%)	10 (2%)	0	100	100
2	B	420/445 (94%)	408 (97%)	12 (3%)	0	100	100
2	D	427/445 (96%)	416 (97%)	10 (2%)	1 (0%)	51	76
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	282/384 (73%)	268 (95%)	14 (5%)	0	100	100
All	All	2122/2319 (92%)	2059 (97%)	62 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	181	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/379 (97%)	369 (100%)	0	100	100
1	C	373/379 (98%)	373 (100%)	0	100	100
2	B	367/383 (96%)	366 (100%)	1 (0%)	94	98
2	D	372/383 (97%)	371 (100%)	1 (0%)	94	98
3	E	109/127 (86%)	108 (99%)	1 (1%)	82	93
4	F	266/342 (78%)	266 (100%)	0	100	100
All	All	1856/1993 (93%)	1853 (100%)	3 (0%)	94	99

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	139	HIS
2	D	139	HIS
3	E	14	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 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	0.95	1 (3%)	27,54,54	1.70	4 (14%)
8	GOL	A	504	-	5,5,5	0.34	0	5,5,5	0.28	0
8	GOL	A	505	-	5,5,5	0.33	0	5,5,5	0.28	0
9	GDP	B	501	6	25,30,30	1.17	2 (8%)	26,47,47	1.99	6 (23%)
10	4ED	B	504	-	20,21,21	1.10	1 (5%)	23,29,29	1.38	4 (17%)
11	MES	B	505	-	12,12,12	2.14	1 (8%)	14,16,16	2.40	8 (57%)
11	MES	B	506	-	12,12,12	2.17	1 (8%)	14,16,16	2.64	8 (57%)
8	GOL	B	507	-	5,5,5	0.35	0	5,5,5	0.26	0
5	GTP	C	501	6	27,34,34	0.93	1 (3%)	27,54,54	1.63	4 (14%)
8	GOL	C	503	-	5,5,5	0.36	0	5,5,5	0.25	0
12	IMD	C	504	-	3,5,5	0.55	0	4,5,5	0.59	0
9	GDP	D	501	6	25,30,30	1.15	2 (8%)	26,47,47	2.00	6 (23%)
10	4ED	D	503[A]	-	20,21,21	1.07	1 (5%)	23,29,29	1.40	4 (17%)
8	GOL	D	504	-	5,5,5	0.36	0	5,5,5	0.24	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
8	GOL	A	504	-	-	0/4/4/4	0/0/0/0
8	GOL	A	505	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	4ED	B	504	-	-	0/3/5/5	0/3/3/3
11	MES	B	505	-	-	0/6/14/14	0/1/1/1
11	MES	B	506	-	-	0/6/14/14	0/1/1/1
8	GOL	B	507	-	-	0/4/4/4	0/0/0/0
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
12	IMD	C	504	-	-	0/0/0/0	0/1/1/1
9	GDP	D	501	6	-	0/12/32/32	0/3/3/3
10	4ED	D	503[A]	-	-	0/3/5/5	0/3/3/3
8	GOL	D	504	-	-	0/4/4/4	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	506	MES	C8-S	-7.24	1.66	1.77
11	B	505	MES	C8-S	-7.15	1.66	1.77
5	C	501	GTP	C6-N1	3.00	1.38	1.33
9	B	501	GDP	C5-C4	3.00	1.47	1.40
9	D	501	GDP	C5-C4	3.01	1.47	1.40
5	A	501	GTP	C6-N1	3.01	1.38	1.33
10	D	503[A]	4ED	C06-S15	3.36	1.78	1.73
10	B	504	4ED	C06-S15	3.49	1.78	1.73
9	D	501	GDP	C6-C5	3.78	1.48	1.41
9	B	501	GDP	C6-C5	3.86	1.48	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.05	120.08	127.46
5	C	501	GTP	N3-C2-N1	-4.93	120.26	127.46
9	B	501	GDP	C6-C5-C4	-4.03	116.84	120.84
9	D	501	GDP	C5-C6-N1	-3.91	117.92	123.48
9	D	501	GDP	C6-C5-C4	-3.74	117.12	120.84
9	B	501	GDP	C5-C6-N1	-3.72	118.19	123.48
9	B	501	GDP	N3-C2-N1	-3.31	122.62	127.46
11	B	506	MES	C2-C3-N4	-3.24	105.57	110.11
9	D	501	GDP	N3-C2-N1	-3.22	122.76	127.46
11	B	506	MES	C6-C5-N4	-3.01	105.89	110.11
9	D	501	GDP	C4-C5-N7	-2.93	106.58	109.41
11	B	505	MES	C6-C5-N4	-2.92	106.01	110.11
9	B	501	GDP	C4-C5-N7	-2.88	106.63	109.41
5	C	501	GTP	C5-C6-N1	-2.82	119.47	123.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C6-N1	-2.76	119.55	123.48
11	B	505	MES	C2-C3-N4	-2.40	106.74	110.11
10	D	503[A]	4ED	C03-C04-N05	-2.34	123.97	130.75
10	B	504	4ED	C03-C04-N05	-2.31	124.05	130.75
11	B	505	MES	C7-N4-C5	2.39	117.37	111.26
10	B	504	4ED	C06-N05-C04	2.62	110.01	104.43
10	D	503[A]	4ED	C06-N05-C04	2.62	110.02	104.43
11	B	505	MES	C7-N4-C3	2.66	118.07	111.26
11	B	506	MES	O3S-S-C8	2.68	109.36	106.06
5	C	501	GTP	C6-N1-C2	2.70	119.95	116.06
5	A	501	GTP	C6-N1-C2	2.73	119.98	116.06
11	B	505	MES	O2S-S-C8	2.77	109.17	106.79
10	B	504	4ED	C17-C16-S15	2.80	130.00	124.84
10	D	503[A]	4ED	C17-C16-S15	2.84	130.08	124.84
11	B	505	MES	O3S-S-C8	2.87	109.59	106.06
11	B	506	MES	O2S-S-C8	3.01	109.38	106.79
11	B	506	MES	C7-N4-C3	3.04	119.05	111.26
11	B	506	MES	C7-N4-C5	3.05	119.08	111.26
10	D	503[A]	4ED	C16-C04-N05	3.15	115.30	108.04
10	B	504	4ED	C16-C04-N05	3.16	115.33	108.04
11	B	506	MES	O1S-S-C8	3.27	109.60	106.79
11	B	505	MES	O1S-S-C8	3.96	110.19	106.79
11	B	505	MES	C5-N4-C3	4.11	118.19	108.87
5	C	501	GTP	C2-N3-C4	4.18	120.04	115.16
5	A	501	GTP	C2-N3-C4	4.35	120.24	115.16
9	B	501	GDP	C6-N1-C2	4.40	122.39	116.06
9	D	501	GDP	C6-N1-C2	4.43	122.43	116.06
9	D	501	GDP	C2-N3-C4	4.92	120.90	115.16
9	B	501	GDP	C2-N3-C4	5.04	121.04	115.16
11	B	506	MES	C5-N4-C3	5.11	120.45	108.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	3	0
8	A	504	GOL	1	0
8	A	505	GOL	1	0
9	B	501	GDP	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	504	4ED	1	0
11	B	506	MES	2	0
12	C	504	IMD	1	0
9	D	501	GDP	2	0
10	D	503[A]	4ED	3	0
8	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	437/451 (96%)	-0.09	2 (0%) 90 89	47, 70, 104, 124	0
1	C	440/451 (97%)	0.06	3 (0%) 87 85	35, 54, 87, 113	0
2	B	422/445 (94%)	0.02	4 (0%) 84 81	44, 64, 103, 143	0
2	D	421/445 (94%)	0.03	11 (2%) 56 49	49, 80, 120, 137	0
3	E	121/143 (84%)	0.13	2 (1%) 70 65	55, 85, 120, 133	0
4	F	296/384 (77%)	0.90	52 (17%) 2 1	57, 98, 162, 179	0
All	All	2137/2319 (92%)	0.14	74 (3%) 44 36	35, 72, 120, 179	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	132	LEU	8.0
4	F	259	GLY	6.6
4	F	169	LEU	6.3
1	C	179	THR	5.7
4	F	231	ALA	4.8
4	F	130	VAL	4.6
4	F	170	LEU	4.4
4	F	226	GLU	4.4
4	F	228	TYR	4.3
2	D	249[A]	ASN	4.1
2	D	57	THR	4.1
4	F	223	THR	4.0
4	F	229	ASN	3.8
4	F	182	ILE	3.7
4	F	131	PHE	3.7
4	F	199	PHE	3.7
1	A	262	TYR	3.6
2	D	401	ARG	3.5
4	F	101	TYR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	57	THR	3.4
4	F	258	GLU	3.4
4	F	133	ALA	3.4
2	B	284	ARG	3.3
2	D	248[A]	LEU	3.3
4	F	260	ASN	3.2
4	F	99	VAL	3.2
4	F	162	ILE	3.1
4	F	147	TRP	3.1
1	A	437	VAL	3.1
4	F	181	VAL	3.1
2	B	438	ALA	3.1
4	F	17	VAL	3.0
4	F	149	ALA	3.0
4	F	134	ALA	3.0
4	F	166	ALA	3.0
4	F	192	LEU	2.9
2	D	247[A]	GLN	2.9
1	C	340	SER	2.9
2	D	415	GLU	2.9
4	F	145	ASN	2.8
4	F	150	LYS	2.8
4	F	225	SER	2.8
4	F	224	SER	2.8
4	F	230	SER	2.8
2	D	1	MET	2.8
4	F	361	LEU	2.8
4	F	186	LEU	2.7
4	F	129	GLU	2.6
4	F	197	ARG	2.6
2	D	37	HIS	2.6
1	C	357	TYR	2.6
4	F	314	LEU	2.5
4	F	135	TYR	2.5
4	F	168	GLU	2.5
4	F	335	ALA	2.4
4	F	100	ILE	2.4
4	F	191	LEU	2.4
4	F	320	MET	2.4
3	E	27	PRO	2.4
2	B	59	ASN	2.3
4	F	98	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	177	VAL	2.3
4	F	21	LEU	2.3
4	F	172	PHE	2.3
4	F	315	PHE	2.3
4	F	257	GLU	2.3
4	F	194	PRO	2.2
4	F	221	LEU	2.2
4	F	330	ILE	2.2
2	D	255[A]	LEU	2.2
4	F	201	ILE	2.2
3	E	25	LYS	2.2
4	F	196	HIS	2.2
2	D	250[A]	ALA	2.1

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
11	MES	B	506	12/12	0.75	0.33	7.43	113,119,158,159	0
8	GOL	A	505	6/6	0.81	0.44	5.58	97,101,108,111	0
8	GOL	A	504	6/6	0.86	0.25	2.80	86,87,88,90	0
12	IMD	C	504	5/5	0.93	0.23	2.77	79,79,80,82	0
8	GOL	C	503	6/6	0.90	0.55	2.76	93,100,102,104	0
10	4ED	D	503[A]	19/19	0.83	0.48	2.55	39,51,59,61	19
8	GOL	D	504	6/6	0.89	0.20	1.29	70,72,76,77	0
11	MES	B	505	12/12	0.95	0.17	0.51	56,77,89,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GTP	A	501	32/32	0.98	0.16	0.45	44,55,63,76	0
5	GTP	C	501	32/32	0.97	0.19	0.38	42,48,67,76	0
8	GOL	B	507	6/6	0.89	0.20	0.17	88,90,92,92	0
10	4ED	B	504	19/19	0.97	0.18	0.17	47,57,62,64	0
9	GDP	D	501	28/28	0.96	0.17	0.04	63,74,84,135	0
9	GDP	B	501	28/28	0.98	0.18	-0.10	34,46,53,55	0
7	CA	C	502	1/1	0.99	0.13	-0.34	86,86,86,86	0
6	MG	C	505	1/1	0.98	0.14	-0.72	46,46,46,46	0
7	CA	A	503	1/1	0.89	0.09	-1.25	95,95,95,95	0
6	MG	A	502	1/1	0.98	0.10	-2.09	56,56,56,56	0
7	CA	B	503	1/1	0.87	0.20	-	101,101,101,101	0
6	MG	B	502	1/1	0.98	0.14	-	42,42,42,42	0
6	MG	D	502	1/1	0.70	0.10	-	87,87,87,87	0

6.5 Other polymers ⓘ

There are no such residues in this entry.