



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:30 am GMT

PDB ID : 4X1K
Title : Discovery of cytotoxic Dolastatin 10 analogs with N-terminal modifications
Authors : Parris, K.D.
Deposited on : 2014-11-24
Resolution : 3.50 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 : trunk28620
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) : recalc28949

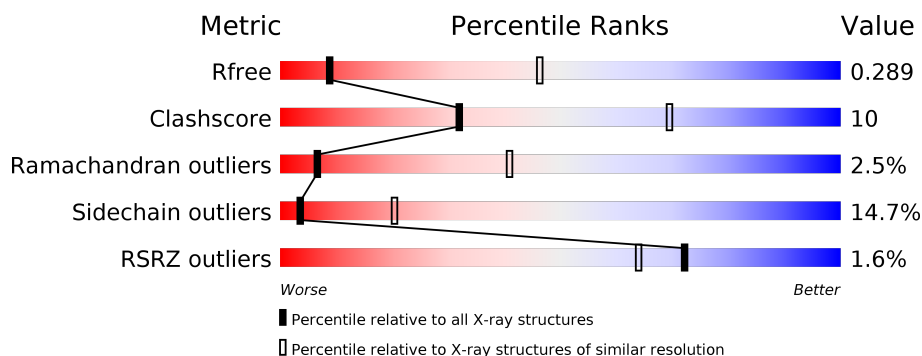
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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>3%</div> <div>61% 29% 5%</div> </div>
1	C	451	<div> <div>%</div> <div>63% 28% 5%</div> </div>
2	B	445	<div> <div>3%</div> <div>63% 27% 5%</div> </div>
2	D	445	<div> <div></div> <div>64% 29%</div> </div>
3	E	142	<div> <div>%</div> <div>61% 21% 5% 13%</div> </div>

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
4	GTP	A	600	-	-	-	X
5	MG	C	601	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14713 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3363	2132	572	638	21			
1	C	430	Total	C	N	O	S	0	2	0
			3351	2124	569	635	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3342	2100	568	649	25			
2	D	430	Total	C	N	O	S	0	1	0
			3369	2112	578	655	24			

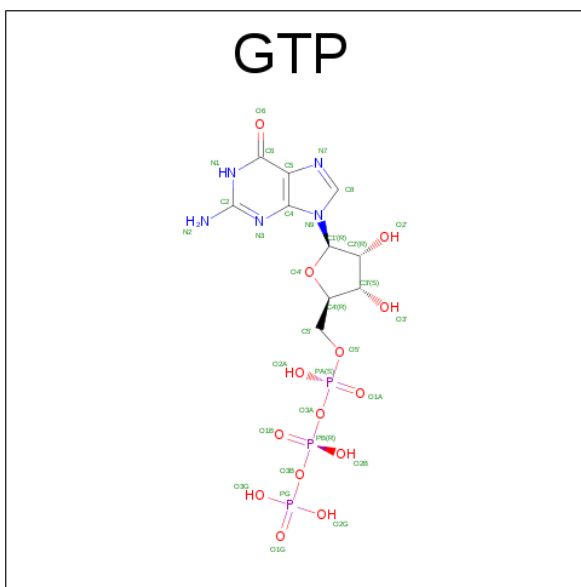
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1008	626	184	195	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

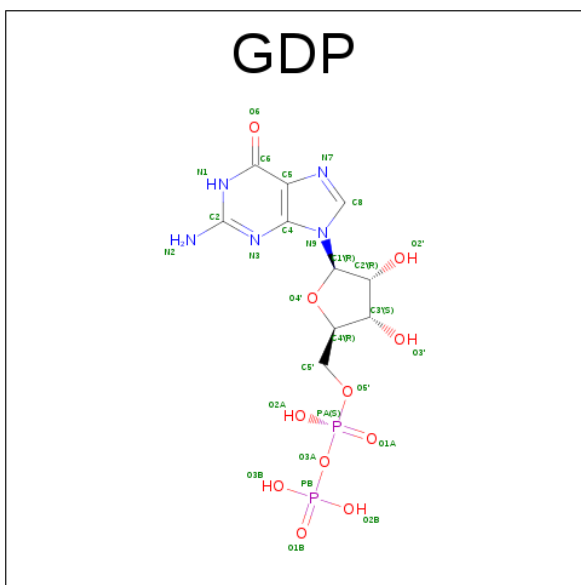


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

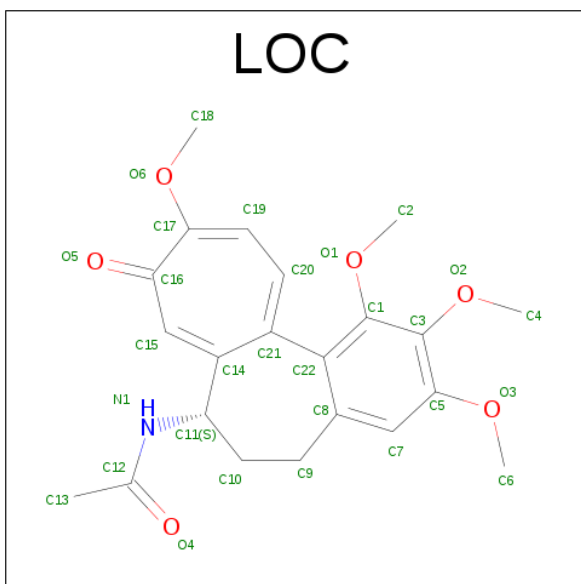
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 7 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]ethanamide (three-letter code: LOC) (formula: C₂₂H₂₅NO₆).



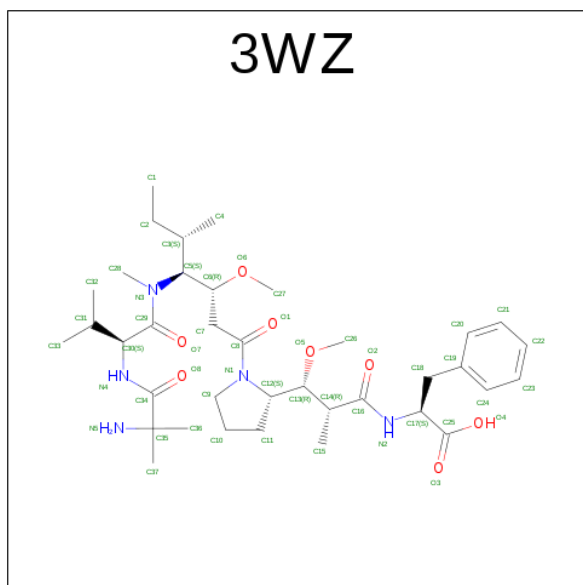
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			29	22	1	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			29	22	1	6		

- Molecule 8 is 2-methyl-L-alanyl-N-[(3R,4S,5S)-1-{(2S)-2-[(1R,2R)-3-{[(1S)-1-carboxy-2-phenylethyl]amino}-1-methoxy-2-methyl-3-oxopropyl]pyrrolidin-1-yl}-3-methoxy-5-methyl-1-oxoheptan-4-yl]-N-methyl-L-valinamide (three-letter code: 3WZ) (formula: C₃₇H₆₁N₅O₈).

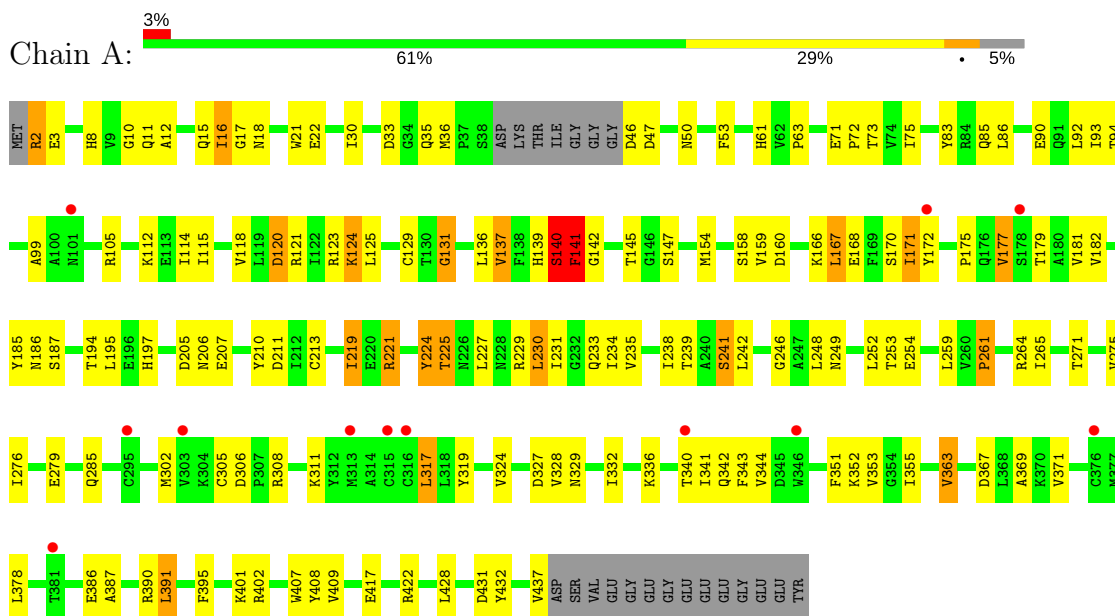


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			50	37	5	8		
8	D	1	Total	C	N	O	0	0
			50	37	5	8		

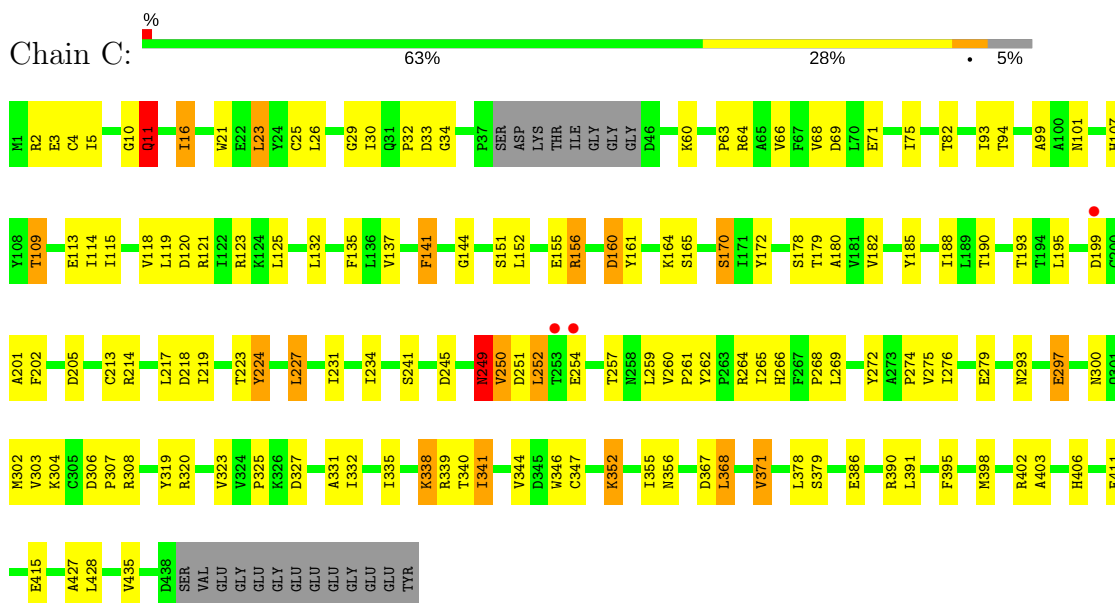
3 Residue-property plots

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.

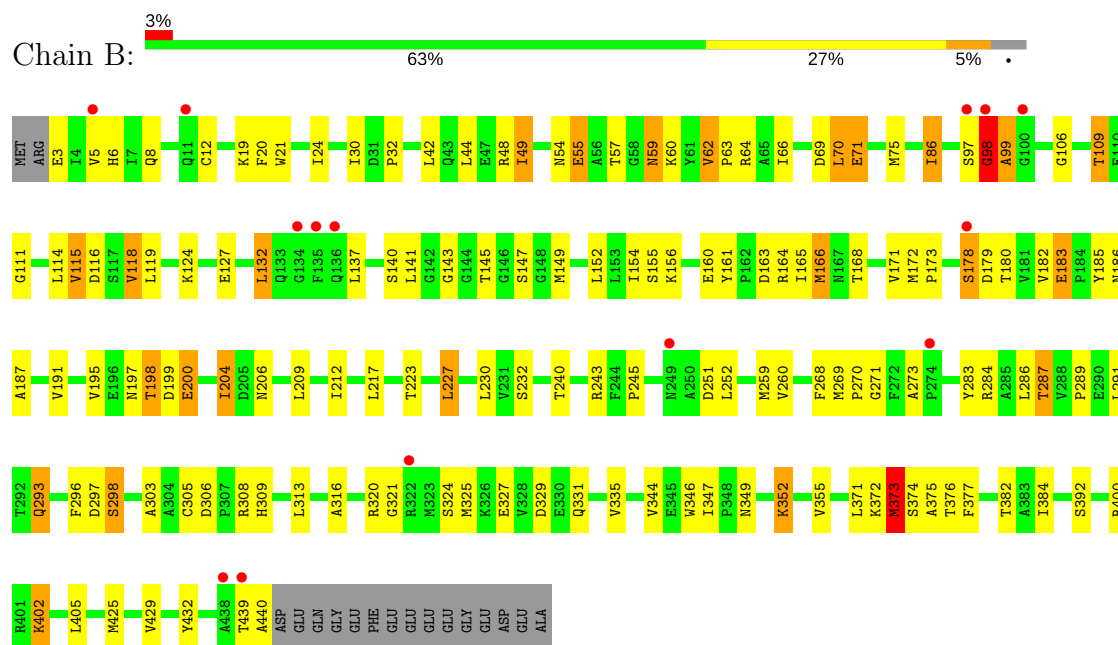
• Molecule 1: Tubulin alpha chain



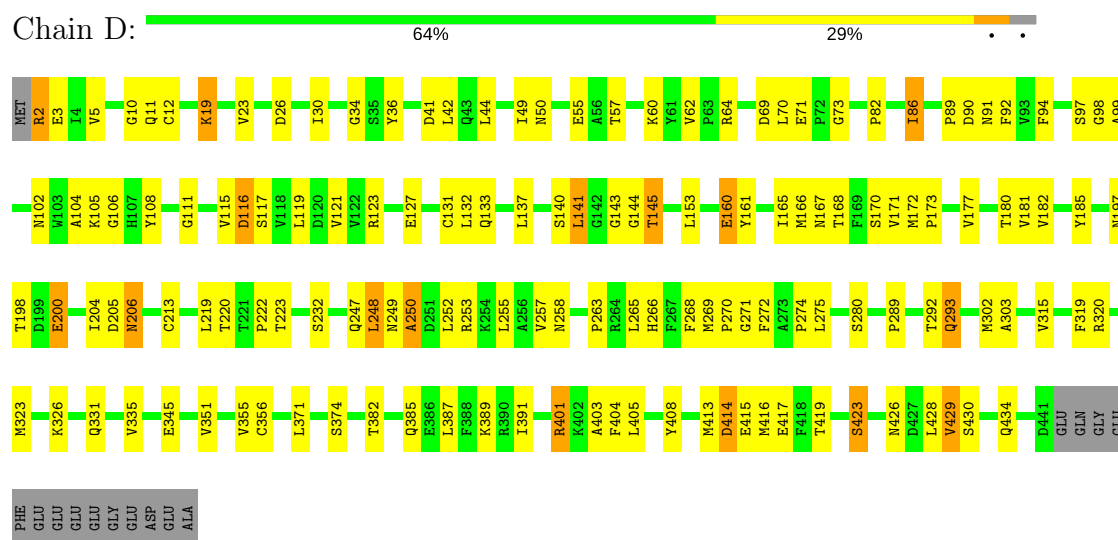
• Molecule 1: Tubulin alpha chain



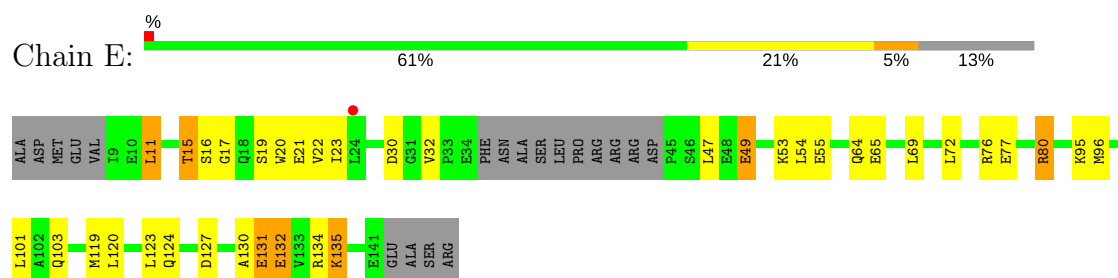
- Molecule 2: Tubulin beta chain



- Molecule 2: Tubulin beta chain



- Molecule 3: Stathmin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.73Å 128.30Å 254.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.45 – 3.50 46.04 – 3.01	Depositor EDS
% Data completeness (in resolution range)	92.1 (45.45-3.50) 82.3 (46.04-3.01)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.200 , 0.263 0.216 , 0.289	Depositor DCC
R_{free} test set	1371 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	115.6	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 108.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14713	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: GTP, LOC, MG, GDP, 3WZ

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	0.51	0/3440	0.76	0/4671
1	C	0.53	0/3432	0.79	0/4662
2	B	0.53	0/3417	0.82	1/4634 (0.0%)
2	D	0.54	0/3446	0.80	2/4670 (0.0%)
3	E	0.50	0/1019	0.75	0/1355
All	All	0.53	0/14754	0.79	3/19992 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	248	LEU	C-N-CA	6.53	138.01	121.70
2	D	249	ASN	C-N-CA	6.32	137.51	121.70
2	B	98	GLY	N-CA-C	5.41	126.63	113.10

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	3363	0	3274	71	0
1	C	3351	0	3258	70	0
2	B	3342	0	3198	77	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3369	0	3237	71	0
3	E	1008	0	1022	17	0
4	A	32	0	12	1	0
4	C	32	0	12	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	1	0
6	D	28	0	12	3	0
7	B	29	0	25	1	0
7	D	29	0	25	2	0
8	B	50	0	60	0	0
8	D	50	0	60	0	0
All	All	14713	0	14207	291	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 10.

All (291) 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)
1:C:338:LYS:HD3	1:C:340:THR:HG22	1.26	1.16
1:C:338:LYS:HD3	1:C:340:THR:CG2	1.92	0.99
1:C:338:LYS:CD	1:C:340:THR:HG22	1.95	0.97
1:A:33:ASP:HA	1:A:85:GLN:HB3	1.56	0.86
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.59	0.83
2:D:247:GLN:HE22	2:D:355:VAL:H	1.28	0.80
1:C:155:GLU:HB3	3:E:101:LEU:HD21	1.66	0.76
2:B:30:ILE:HG22	2:B:86:ILE:HD11	1.66	0.76
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.69	0.73
1:A:248:LEU:HB2	3:E:19:SER:HB3	1.70	0.73
1:A:246:GLY:HA2	3:E:17:GLY:HA3	1.70	0.71
2:B:200:GLU:HB3	2:B:268:PHE:HE1	1.57	0.70
1:A:158:SER:HB2	1:A:197:HIS:HD2	1.56	0.70
2:B:69:ASP:HA	2:B:145:THR:HG21	1.74	0.69
2:B:166:MET:HB3	2:B:198:THR:HG22	1.75	0.69
1:A:175:PRO:HA	1:A:179:THR:HG21	1.75	0.67
2:D:12:CYS:SG	2:D:171:VAL:HG11	2.35	0.67
1:C:241:SER:HA	1:C:250:VAL:HB	1.77	0.66
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.77	0.66
2:B:402:LYS:HB3	2:B:405:LEU:HD22	1.75	0.66
2:D:401:ARG:HE	2:D:403:ALA:HB2	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASN:HD21	3:E:22:VAL:HG11	1.61	0.65
1:A:259:LEU:O	1:A:261:PRO:HD3	1.96	0.65
3:E:11:LEU:HB2	3:E:20:TRP:HA	1.76	0.65
1:A:387:ALA:HA	1:A:390:ARG:HE	1.60	0.65
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.79	0.65
2:B:382:THR:HA	2:B:432:TYR:HD2	1.63	0.64
1:C:319:TYR:HB3	1:C:323:VAL:HG21	1.80	0.64
1:C:5:ILE:HD12	1:C:135:PHE:CE2	2.33	0.64
2:D:106:GLY:O	2:D:111:GLY:HA3	1.97	0.64
2:B:331:GLN:O	2:B:335:VAL:HG23	1.97	0.64
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.80	0.64
2:D:253:ARG:O	2:D:257:VAL:HG23	1.97	0.64
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.79	0.64
2:D:272:PHE:CE1	2:D:374:SER:HB2	2.33	0.63
2:B:48:ARG:HH11	2:B:245:PRO:HA	1.63	0.63
2:D:19:LYS:O	2:D:23:VAL:HG23	1.99	0.63
2:D:293:GLN:HE22	2:D:331:GLN:HE21	1.47	0.63
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.79	0.62
2:B:320:ARG:HB2	2:B:374:SER:HB3	1.81	0.62
2:B:179:ASP:HB2	1:C:352:LYS:HG2	1.83	0.61
2:D:250:ALA:HA	7:D:502:LOC:H6B	1.82	0.61
2:B:382:THR:HA	2:B:432:TYR:CD2	2.35	0.60
1:C:276:ILE:HD11	1:C:371:VAL:HG22	1.83	0.60
1:C:308:ARG:NH1	1:C:340:THR:HG21	2.16	0.60
1:A:225:THR:O	1:A:229:ARG:HG2	2.01	0.60
1:C:195:LEU:HD21	1:C:428:LEU:HD13	1.85	0.59
2:B:204:ILE:HD13	2:B:270:PRO:HG2	1.84	0.59
1:A:177:VAL:HG21	1:A:206:ASN:HB3	1.84	0.59
2:B:273:ALA:HB3	2:B:375:ALA:HB3	1.84	0.59
2:D:50:ASN:O	2:D:64:ARG:NH2	2.35	0.58
2:B:200:GLU:HB3	2:B:268:PHE:CE1	2.38	0.58
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.39	0.58
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.86	0.57
1:C:141:PHE:CE1	1:C:170:SER:HB2	2.40	0.57
2:B:352:LYS:HE3	7:B:502:LOC:O5	2.04	0.57
2:D:36:TYR:CZ	2:D:44:LEU:HD11	2.39	0.57
1:A:317:LEU:HD12	1:A:353:VAL:HG22	1.87	0.57
2:D:133:GLN:HE21	2:D:252:LEU:H	1.52	0.57
1:A:311:LYS:HD3	1:A:344:VAL:HG12	1.87	0.56
2:B:293:GLN:HE22	2:B:331:GLN:HE21	1.52	0.56
2:B:313:LEU:HA	2:B:344:VAL:HG22	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:389:LYS:HG3	2:D:429:VAL:HG11	1.87	0.56
1:C:346:TRP:HZ2	1:C:435:VAL:HG22	1.69	0.56
3:E:130:ALA:HB1	3:E:134:ARG:HH12	1.72	0.55
1:A:15:GLN:HA	1:A:18:ASN:HD22	1.71	0.55
1:A:136:LEU:HD11	1:A:252:LEU:HD21	1.88	0.55
1:A:53:PHE:HB3	1:A:61:HIS:HB3	1.89	0.54
1:A:158:SER:CB	1:A:197:HIS:HD2	2.20	0.54
2:B:191:VAL:O	2:B:195:VAL:HG23	2.08	0.54
2:B:259:MET:HE2	2:B:316:ALA:HB2	1.90	0.54
1:C:3:GLU:HG2	1:C:64:ARG:CZ	2.37	0.54
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.42	0.54
2:B:140:SER:HA	2:B:171:VAL:HG22	1.90	0.54
1:A:154:MET:HG3	1:A:194:THR:HG23	1.89	0.54
1:C:297:GLU:HB3	1:C:300:ASN:HD22	1.73	0.54
1:C:259:LEU:O	1:C:261:PRO:HD3	2.08	0.53
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.90	0.53
1:A:140:SER:HA	1:A:171:ILE:HG22	1.91	0.53
2:D:102:ASN:HB3	2:D:105:LYS:HB2	1.89	0.53
1:A:112:LYS:HE3	3:E:54:LEU:HB3	1.91	0.53
1:A:276:ILE:HG23	1:A:369:ALA:HB3	1.89	0.53
2:D:200:GLU:HB2	2:D:268:PHE:CE1	2.43	0.53
2:B:71:GLU:HB3	2:B:98:GLY:HA2	1.91	0.53
1:C:260:VAL:HG12	1:C:262:TYR:O	2.09	0.53
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.91	0.53
2:D:319:PHE:HB2	2:D:355:VAL:HG22	1.91	0.53
1:A:249:ASN:HD22	1:A:254:GLU:HB3	1.74	0.53
2:B:3:GLU:HB2	2:B:132:LEU:HA	1.90	0.52
1:A:207:GLU:O	1:A:210:TYR:HB3	2.09	0.52
2:B:305:CYS:SG	2:B:384:ILE:HA	2.49	0.52
1:C:119:LEU:HD13	1:C:156:ARG:HE	1.73	0.52
1:A:235:VAL:HA	1:A:238:ILE:HD12	1.92	0.52
1:C:266:HIS:O	1:C:268:PRO:HD3	2.09	0.52
2:D:71:GLU:HG2	2:D:98:GLY:HA2	1.92	0.52
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.45	0.52
2:B:106:GLY:O	2:B:111:GLY:HA3	2.09	0.52
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.44	0.52
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.92	0.52
2:D:62:VAL:HG23	2:D:86:ILE:O	2.10	0.52
2:D:274:PRO:HD3	2:D:374:SER:HA	1.92	0.52
1:A:182:VAL:O	1:A:185:TYR:HB2	2.10	0.52
2:B:206:ASN:HA	2:B:209:LEU:HB2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:CYS:HA	1:C:217:LEU:HB2	1.93	0.51
1:C:188:ILE:HD13	1:C:395:PHE:HB2	1.93	0.51
2:B:141:LEU:HD12	2:B:172:MET:SD	2.51	0.51
1:A:12:ALA:O	1:A:16:ILE:HB	2.11	0.51
3:E:11:LEU:HD23	3:E:21:GLU:HB2	1.92	0.51
1:A:123:ARG:HH12	1:A:160:ASP:HB3	1.75	0.51
2:B:425:MET:O	2:B:429:VAL:HG23	2.09	0.51
2:D:171:VAL:HA	2:D:204:ILE:O	2.10	0.51
2:B:344:VAL:HG21	2:B:347:ILE:HD12	1.92	0.51
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.93	0.51
2:D:30:ILE:HD11	2:D:49:ILE:HD11	1.93	0.50
2:B:54:ASN:HD21	2:B:64:ARG:HD3	1.76	0.50
2:B:143:GLY:O	2:B:147:SER:HB3	2.12	0.50
2:B:371:LEU:H	2:B:371:LEU:HD23	1.77	0.50
1:A:230:LEU:HD23	1:A:234:ILE:HD11	1.94	0.50
1:A:3:GLU:HG3	1:A:129:CYS:SG	2.51	0.50
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.94	0.50
2:D:133:GLN:NE2	2:D:252:LEU:H	2.10	0.50
1:C:249:ASN:HB2	1:C:355:ILE:H	1.77	0.50
2:D:166:MET:HG3	2:D:198:THR:HG22	1.92	0.49
1:A:159:VAL:HG11	3:E:47:LEU:HB2	1.93	0.49
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.47	0.49
1:C:320:ARG:HB3	1:C:356:ASN:HB3	1.95	0.49
2:D:116:ASP:HA	2:D:119:LEU:HD12	1.95	0.49
2:D:34:GLY:HA3	2:D:60:LYS:HE3	1.94	0.49
1:A:142:GLY:HA2	1:A:186:ASN:HB2	1.94	0.49
2:B:259:MET:CE	2:B:316:ALA:HB2	2.43	0.49
2:D:141:LEU:HG	2:D:170:SER:HB3	1.95	0.49
1:A:340:THR:O	1:A:340:THR:HG22	2.13	0.49
3:E:132:GLU:HA	3:E:135:LYS:HB3	1.95	0.49
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.94	0.48
3:E:49:GLU:HG3	3:E:53:LYS:HE2	1.95	0.48
1:A:139:HIS:CE1	1:A:170:SER:HB3	2.48	0.48
1:A:213:CYS:HB3	1:A:219:ILE:HD12	1.95	0.48
1:A:16:ILE:HD11	1:A:231:ILE:HD13	1.94	0.48
2:B:286:LEU:HD23	2:B:291:LEU:HD12	1.95	0.48
2:B:271:GLY:HA3	2:B:377:PHE:HB3	1.96	0.48
1:C:179:THR:HG22	1:C:180:ALA:H	1.78	0.48
2:D:5:VAL:HG23	2:D:132:LEU:CD1	2.43	0.48
1:C:252:LEU:C	1:C:254:GLU:H	2.16	0.48
1:C:202:PHE:HE2	1:C:378:LEU:HD22	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:LEU:HD21	2:B:156:LYS:HB3	1.95	0.48
2:B:217:LEU:HD11	2:B:230:LEU:HD21	1.96	0.48
2:B:346:TRP:HB3	2:B:440:ALA:HB2	1.96	0.48
1:A:407:TRP:HZ2	2:B:260:VAL:HB	1.78	0.47
1:C:66:VAL:HG12	1:C:68:VAL:HG23	1.95	0.47
1:A:265:ILE:HD11	1:A:431:ASP:HB3	1.95	0.47
2:B:137:LEU:HD23	2:B:154:ILE:HD11	1.95	0.47
2:D:213:CYS:HB3	2:D:219:LEU:HD12	1.96	0.47
2:D:423:SER:HA	2:D:426:ASN:HB2	1.94	0.47
2:B:21:TRP:CE3	2:B:24:ILE:HD11	2.50	0.47
1:A:167:LEU:HD13	1:A:252:LEU:HD22	1.96	0.47
2:B:12:CYS:CB	2:B:140:SER:HB3	2.45	0.47
1:C:224:TYR:HA	1:C:227:LEU:HD12	1.96	0.47
2:B:179:ASP:HB2	1:C:352:LYS:HE3	1.96	0.47
1:A:305:CYS:HB2	1:A:386:GLU:HB2	1.95	0.47
2:B:71:GLU:HB3	2:B:98:GLY:CA	2.45	0.47
2:D:220:THR:O	2:D:222:PRO:HD3	2.15	0.46
2:B:114:LEU:HB3	2:B:149:MET:HE3	1.97	0.46
1:C:160:ASP:HB3	1:C:161:TYR:CD1	2.51	0.46
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.98	0.46
1:A:229:ARG:HD2	1:A:363:VAL:HG21	1.98	0.46
1:C:119:LEU:CD1	1:C:156:ARG:HE	2.29	0.46
1:A:2:ARG:N	1:A:131:GLY:O	2.48	0.46
1:A:224:TYR:HA	1:A:227:LEU:HD12	1.98	0.46
2:B:155:SER:HB2	3:E:76:ARG:HH22	1.80	0.46
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.34	0.46
2:B:119:LEU:HD23	2:B:160:GLU:OE1	2.16	0.45
2:D:272:PHE:HE1	2:D:374:SER:HB2	1.81	0.45
2:D:185:TYR:HD1	2:D:408:TYR:CE1	2.34	0.45
1:A:238:ILE:HG12	1:A:378:LEU:HD21	1.99	0.45
2:B:70:LEU:HD11	2:B:111:GLY:HA2	1.96	0.45
1:C:151[A]:SER:HB3	1:C:190:THR:HG1	1.81	0.45
1:C:275:VAL:HG13	1:C:368:LEU:HD11	1.98	0.45
1:C:241:SER:OG	1:C:252:LEU:HB2	2.16	0.45
2:D:414:ASP:OD1	2:D:417:GLU:HB2	2.17	0.45
2:D:320:ARG:HA	2:D:356:CYS:O	2.16	0.45
1:A:137:VAL:HG23	1:A:168:GLU:HA	1.99	0.45
2:B:19:LYS:HB3	2:B:232:SER:HB3	1.99	0.44
1:C:202:PHE:CE2	1:C:268:PRO:HG2	2.52	0.44
3:E:130:ALA:HB1	3:E:134:ARG:NH1	2.31	0.44
1:A:15:GLN:O	1:A:18:ASN:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:HA	1:A:36:MET:HB3	1.98	0.44
2:D:5:VAL:HG23	2:D:132:LEU:HD13	2.00	0.44
2:D:387:LEU:O	2:D:391:ILE:HG12	2.16	0.44
1:A:158:SER:HB2	1:A:197:HIS:CD2	2.45	0.44
2:B:44:LEU:HD23	2:B:49:ILE:HD13	1.98	0.44
2:D:89:PRO:HA	2:D:92:PHE:CD1	2.52	0.44
1:A:12:ALA:HA	4:A:600:GTP:C5	2.52	0.44
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.51	0.44
2:D:69:ASP:HA	2:D:145:THR:HG21	1.99	0.44
2:D:104:ALA:HB2	2:D:413:MET:SD	2.58	0.44
1:A:239:THR:HA	1:A:242:LEU:HD12	1.99	0.44
2:B:115:VAL:HG22	2:B:119:LEU:HD13	1.99	0.44
2:D:108:TYR:CE2	3:E:130:ALA:HA	2.52	0.44
2:B:12:CYS:HB3	2:B:140:SER:HB3	2.00	0.44
1:C:231:ILE:HA	1:C:234:ILE:HD12	2.00	0.43
1:C:23:LEU:HA	1:C:26:LEU:HD12	2.00	0.43
1:C:25:CYS:O	1:C:30:ILE:N	2.51	0.43
1:C:69:ASP:CB	1:C:75:ILE:HD12	2.48	0.43
2:D:2:ARG:HB3	2:D:131:CYS:O	2.17	0.43
2:B:173:PRO:HG3	2:B:187:ALA:HB2	1.99	0.43
1:C:331:ALA:O	1:C:335:ILE:HG12	2.19	0.43
2:D:315:VAL:HB	2:D:351:VAL:HG13	2.01	0.43
1:A:395:PHE:CE2	1:A:422:ARG:HB2	2.54	0.43
2:B:54:ASN:HB2	2:B:62:VAL:HG13	2.01	0.43
1:C:205:ASP:HB2	1:C:303:VAL:HG13	2.01	0.43
2:D:10:GLY:HA3	6:D:501:GDP:O1B	2.19	0.43
2:D:206:ASN:HD21	6:D:501:GDP:HN22	1.65	0.43
2:D:91:ASN:HA	2:D:121:VAL:HG11	1.99	0.43
3:E:131:GLU:HG2	3:E:134:ARG:HH21	1.82	0.43
2:B:70:LEU:HD11	2:B:111:GLY:CA	2.48	0.43
2:B:182:VAL:O	2:B:185:TYR:HB2	2.18	0.43
2:D:181:VAL:HG21	2:D:404:PHE:CZ	2.53	0.43
2:B:209:LEU:HB3	2:B:227:LEU:HG	2.01	0.43
2:B:384:ILE:HG22	2:B:432:TYR:CE2	2.54	0.43
1:C:346:TRP:CZ2	1:C:435:VAL:HG22	2.52	0.43
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.99	0.43
2:B:289:PRO:O	2:B:293:GLN:HG2	2.18	0.43
1:C:182:VAL:O	1:C:185:TYR:HB2	2.18	0.43
1:C:93:ILE:HG21	1:C:118:VAL:HG22	2.00	0.43
2:D:123:ARG:O	2:D:127:GLU:HG2	2.18	0.43
2:D:173:PRO:HB3	6:D:501:GDP:O3'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:382:THR:O	2:D:385:GLN:HG2	2.18	0.43
2:D:70:LEU:HD21	2:D:111:GLY:HA2	2.00	0.43
2:B:306:ASP:O	2:B:309:HIS:HB2	2.19	0.43
1:C:411:GLU:OE2	1:C:411:GLU:HA	2.19	0.43
1:A:195:LEU:HD21	1:A:264:ARG:NH1	2.33	0.42
2:D:263:PRO:O	2:D:266:HIS:HD2	2.01	0.42
1:A:319:TYR:HB2	1:A:355:ILE:HG12	2.00	0.42
1:C:11:GLN:HB2	1:C:11:GLN:HE21	1.72	0.42
1:A:83:TYR:HD2	1:A:86:LEU:HD22	1.83	0.42
2:B:55:GLU:HG2	2:B:59:ASN:O	2.19	0.42
1:A:93:ILE:HG21	1:A:118:VAL:HG22	2.01	0.42
1:A:329:ASN:HA	1:A:332:ILE:HB	2.02	0.42
1:C:132:LEU:HD23	1:C:164:LYS:HE3	2.01	0.42
1:C:107:HIS:O	1:C:152:LEU:HD22	2.19	0.42
1:C:340:THR:CG2	1:C:341:ILE:N	2.83	0.42
1:C:386:GLU:O	1:C:390:ARG:HB2	2.19	0.42
2:B:206:ASN:HD21	6:B:501:GDP:HN22	1.67	0.42
1:C:214:ARG:O	1:C:218:ASP:HA	2.20	0.42
2:B:149:MET:O	2:B:152:LEU:HB3	2.20	0.42
2:B:154:ILE:HG22	2:B:197:ASN:HB3	2.02	0.42
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.01	0.42
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.54	0.42
1:A:17:GLY:O	1:A:21:TRP:HD1	2.03	0.41
1:A:221:ARG:HG2	2:B:325:MET:HB3	2.01	0.41
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.01	0.41
2:D:160:GLU:HB3	2:D:161:TYR:CE1	2.55	0.41
3:E:77:GLU:HA	3:E:80:ARG:HB2	2.03	0.41
2:B:165:ILE:HG22	2:B:252:LEU:HD23	2.01	0.41
1:C:99:ALA:HB3	1:C:144:GLY:HA3	2.01	0.41
2:D:289:PRO:O	2:D:293:GLN:HB2	2.20	0.41
1:A:120:ASP:O	1:A:124:LYS:HD2	2.20	0.41
2:B:321:GLY:HA3	2:B:373:MET:HA	2.01	0.41
1:C:195:LEU:HD12	1:C:266:HIS:HE1	1.84	0.41
1:C:69:ASP:HB2	1:C:75:ILE:HD12	2.02	0.41
1:A:241:SER:HB3	1:A:248:LEU:O	2.21	0.41
1:C:340:THR:HG23	1:C:341:ILE:N	2.34	0.41
1:C:93:ILE:HD13	1:C:118:VAL:HA	2.02	0.41
1:C:180:ALA:HA	7:D:502:LOC:O5	2.21	0.41
2:D:70:LEU:O	2:D:98:GLY:N	2.53	0.41
1:C:201:ALA:H	1:C:266:HIS:HD2	1.69	0.41
2:D:5:VAL:HG13	2:D:64:ARG:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PHE:O	1:A:147:SER:HB3	2.21	0.41
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.03	0.41
1:A:428:LEU:O	1:A:432:TYR:HD1	2.04	0.41
2:B:183:GLU:HA	2:B:186:ASN:HD22	1.86	0.41
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.56	0.41
2:B:243:ARG:HH22	2:B:320:ARG:HH12	1.69	0.41
1:A:324:VAL:O	1:A:328:VAL:HG23	2.21	0.41
2:B:114:LEU:O	2:B:118:VAL:HG23	2.21	0.41
2:B:5:VAL:HG13	2:B:66:ILE:HD13	2.02	0.41
2:B:97:SER:O	2:B:99:ALA:N	2.51	0.41
1:C:16:ILE:HD11	1:C:231:ILE:HD13	2.03	0.41
2:D:180:THR:HG22	2:D:182:VAL:HG22	2.03	0.41
1:A:329:ASN:ND2	3:E:22:VAL:HG11	2.34	0.41
1:C:264:ARG:HH22	1:C:427:ALA:HB3	1.86	0.40
2:D:331:GLN:O	2:D:335:VAL:HG23	2.21	0.40
2:B:160:GLU:HB3	2:B:161:TYR:CD1	2.56	0.40
2:D:140:SER:HA	2:D:171:VAL:HG13	2.03	0.40
1:A:140:SER:HB2	1:A:141:PHE:H	1.70	0.40
1:A:99:ALA:HA	1:A:105:ARG:HG2	2.03	0.40
1:C:398:MET:HB3	1:C:403:ALA:HB3	2.03	0.40
1:C:101:ASN:HD22	2:D:258:ASN:HD21	1.68	0.40
1:A:185:TYR:HD1	1:A:408:TYR:CE1	2.39	0.40
1:C:234:ILE:HG12	1:C:272:TYR:HB2	2.04	0.40
2:D:69:ASP:HB3	2:D:94:PHE:CD1	2.56	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	425/451 (94%)	364 (86%)	51 (12%)	10 (2%)	7 42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	428/451 (95%)	363 (85%)	53 (12%)	12 (3%)	6	39
2	B	426/445 (96%)	366 (86%)	47 (11%)	13 (3%)	5	37
2	D	429/445 (96%)	381 (89%)	40 (9%)	8 (2%)	9	47
3	E	119/142 (84%)	108 (91%)	9 (8%)	2 (2%)	11	49
All	All	1827/1934 (94%)	1582 (87%)	200 (11%)	45 (2%)	6	41

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	73	THR
1	A	341	ILE
2	B	60	LYS
2	B	98	GLY
2	B	109	THR
1	C	10	GLY
1	C	109	THR
1	C	249	ASN
2	D	82	PRO
2	D	115	VAL
2	D	250	ALA
3	E	32	VAL
1	A	10	GLY
1	A	72	PRO
1	A	115	ILE
1	A	131	GLY
2	B	57	THR
2	B	99	ALA
2	B	298	SER
2	B	373	MET
1	C	11	GLN
1	C	29	GLY
1	C	250	VAL
2	D	73	GLY
1	A	140	SER
1	A	261	PRO
1	C	115	ILE
2	D	144	GLY
3	E	15	THR
1	A	141	PHE
2	B	178	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	283	TYR
2	B	284	ARG
2	D	97	SER
2	B	32	PRO
1	C	265	ILE
1	C	279	GLU
1	C	325	PRO
1	C	32	PRO
1	C	341	ILE
2	D	143	GLY
2	B	183	GLU
2	D	271	GLY
2	B	115	VAL

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	362/378 (96%)	303 (84%)	59 (16%)	3	15
1	C	359/378 (95%)	304 (85%)	55 (15%)	3	19
2	B	364/383 (95%)	315 (86%)	49 (14%)	4	24
2	D	369/383 (96%)	325 (88%)	44 (12%)	6	28
3	E	107/125 (86%)	84 (78%)	23 (22%)	1	6
All	All	1561/1647 (95%)	1331 (85%)	230 (15%)	3	20

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	16	ILE
1	A	22	GLU
1	A	35	GLN
1	A	46	ASP
1	A	47	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	50	ASN
1	A	71	GLU
1	A	75	ILE
1	A	90	GLU
1	A	92	LEU
1	A	94	THR
1	A	114	ILE
1	A	120	ASP
1	A	121	ARG
1	A	124	LYS
1	A	125	LEU
1	A	137	VAL
1	A	140	SER
1	A	141	PHE
1	A	145	THR
1	A	166	LYS
1	A	167	LEU
1	A	171	ILE
1	A	177	VAL
1	A	181	VAL
1	A	187	SER
1	A	211	ASP
1	A	219	ILE
1	A	221	ARG
1	A	224	TYR
1	A	225	THR
1	A	230	LEU
1	A	233	GLN
1	A	241	SER
1	A	253	THR
1	A	271	THR
1	A	275	VAL
1	A	279	GLU
1	A	285	GLN
1	A	302	MET
1	A	306	ASP
1	A	308	ARG
1	A	317	LEU
1	A	327	ASP
1	A	336	LYS
1	A	342	GLN
1	A	343	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	351	PHE
1	A	352	LYS
1	A	363	VAL
1	A	367	ASP
1	A	371	VAL
1	A	391	LEU
1	A	401	LYS
1	A	402	ARG
1	A	409	VAL
1	A	417	GLU
1	A	437	VAL
2	B	20	PHE
2	B	42	LEU
2	B	49	ILE
2	B	55	GLU
2	B	59	ASN
2	B	62	VAL
2	B	70	LEU
2	B	71	GLU
2	B	75	MET
2	B	86	ILE
2	B	109	THR
2	B	116	ASP
2	B	118	VAL
2	B	124	LYS
2	B	127	GLU
2	B	132	LEU
2	B	163	ASP
2	B	164	ARG
2	B	166	MET
2	B	178	SER
2	B	180	THR
2	B	198	THR
2	B	199	ASP
2	B	200	GLU
2	B	204	ILE
2	B	212	ILE
2	B	223	THR
2	B	227	LEU
2	B	240	THR
2	B	251	ASP
2	B	287	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	293	GLN
2	B	296	PHE
2	B	297	ASP
2	B	298	SER
2	B	308	ARG
2	B	324	SER
2	B	327	GLU
2	B	329	ASP
2	B	349	ASN
2	B	352	LYS
2	B	355	VAL
2	B	372	LYS
2	B	373	MET
2	B	376	THR
2	B	392	SER
2	B	400	ARG
2	B	402	LYS
2	B	439	THR
1	C	2	ARG
1	C	4[A]	CYS
1	C	4[B]	CYS
1	C	11	GLN
1	C	16	ILE
1	C	23	LEU
1	C	33	ASP
1	C	71	GLU
1	C	82	THR
1	C	94	THR
1	C	109	THR
1	C	113	GLU
1	C	114	ILE
1	C	120	ASP
1	C	121	ARG
1	C	123	ARG
1	C	125	LEU
1	C	137	VAL
1	C	141	PHE
1	C	156	ARG
1	C	160	ASP
1	C	165	SER
1	C	170	SER
1	C	178	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	193	THR
1	C	199	ASP
1	C	219	ILE
1	C	223	THR
1	C	224	TYR
1	C	227	LEU
1	C	245	ASP
1	C	249	ASN
1	C	251	ASP
1	C	252	LEU
1	C	257	THR
1	C	269	LEU
1	C	293	ASN
1	C	297	GLU
1	C	302	MET
1	C	304	LYS
1	C	306	ASP
1	C	307	PRO
1	C	327	ASP
1	C	332	ILE
1	C	338	LYS
1	C	339	ARG
1	C	344	VAL
1	C	347	CYS
1	C	352	LYS
1	C	367	ASP
1	C	368	LEU
1	C	371	VAL
1	C	379	SER
1	C	402	ARG
1	C	415	GLU
2	D	2	ARG
2	D	3	GLU
2	D	11	GLN
2	D	19	LYS
2	D	26	ASP
2	D	41	ASP
2	D	42	LEU
2	D	55	GLU
2	D	57	THR
2	D	86	ILE
2	D	90	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	116	ASP
2	D	117	SER
2	D	141	LEU
2	D	145	THR
2	D	153	LEU
2	D	160	GLU
2	D	167	ASN
2	D	177	VAL
2	D	197	ASN
2	D	200	GLU
2	D	206	ASN
2	D	223	THR
2	D	248	LEU
2	D	255	LEU
2	D	265	LEU
2	D	275	LEU
2	D	280	SER
2	D	293	GLN
2	D	323	MET
2	D	326	LYS
2	D	345	GLU
2	D	371	LEU
2	D	401	ARG
2	D	405	LEU
2	D	414	ASP
2	D	415	GLU
2	D	416	MET
2	D	419	THR
2	D	423	SER
2	D	428	LEU
2	D	429	VAL
2	D	430	SER
2	D	434	GLN
3	E	11	LEU
3	E	15	THR
3	E	16	SER
3	E	23	ILE
3	E	30	ASP
3	E	49	GLU
3	E	55	GLU
3	E	64	GLN
3	E	65	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	69	LEU
3	E	72	LEU
3	E	80	ARG
3	E	95	LYS
3	E	96	MET
3	E	103	GLN
3	E	119	MET
3	E	120	LEU
3	E	123	LEU
3	E	124	GLN
3	E	127	ASP
3	E	131	GLU
3	E	132	GLU
3	E	135	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	28	HIS
1	A	50	ASN
1	A	61	HIS
1	A	91	GLN
1	A	139	HIS
1	A	197	HIS
1	A	249	ASN
1	A	301	GLN
2	B	8	GLN
2	B	14	ASN
2	B	54	ASN
2	B	139	HIS
2	B	193	GLN
2	B	206	ASN
2	B	229	HIS
2	B	293	GLN
2	B	309	HIS
2	B	385	GLN
2	B	424	ASN
2	B	433	GLN
2	B	436	GLN
1	C	8	HIS
1	C	11	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	50	ASN
1	C	61	HIS
1	C	107	HIS
1	C	266	HIS
1	C	300	ASN
1	C	380	ASN
2	D	6	HIS
2	D	14	ASN
2	D	133	GLN
2	D	136	GLN
2	D	139	HIS
2	D	193	GLN
2	D	197	ASN
2	D	206	ASN
2	D	247	GLN
2	D	258	ASN
2	D	266	HIS
2	D	293	GLN
2	D	300	ASN
2	D	331	GLN
2	D	394	GLN
2	D	424	ASN
2	D	426	ASN
2	D	433	GLN
3	E	12	ASN
3	E	111	ASN
3	E	115	HIS

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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GTP	A	600	5	27,34,34	0.99	2 (7%)	27,54,54	2.20	4 (14%)
6	GDP	B	501	-	25,30,30	1.19	2 (8%)	26,47,47	2.36	4 (15%)
7	LOC	B	502	-	30,31,31	0.91	2 (6%)	27,44,44	0.52	0
8	3WZ	B	503	-	44,51,51	1.12	2 (4%)	46,72,72	1.30	4 (8%)
4	GTP	C	600	5	27,34,34	1.01	2 (7%)	27,54,54	2.21	4 (14%)
6	GDP	D	501	-	25,30,30	0.95	1 (4%)	26,47,47	2.25	5 (19%)
7	LOC	D	502	-	30,31,31	0.88	1 (3%)	27,44,44	0.63	1 (3%)
8	3WZ	D	503	-	44,51,51	1.02	2 (4%)	46,72,72	1.41	9 (19%)

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
4	GTP	A	600	5	-	0/18/38/38	0/3/3/3
6	GDP	B	501	-	-	0/12/32/32	0/3/3/3
7	LOC	B	502	-	-	0/10/25/25	0/3/3/3
8	3WZ	B	503	-	-	0/66/82/82	0/2/2/2
4	GTP	C	600	5	-	0/18/38/38	0/3/3/3
6	GDP	D	501	-	-	0/12/32/32	0/3/3/3
7	LOC	D	502	-	-	0/10/25/25	0/3/3/3
8	3WZ	D	503	-	-	0/66/82/82	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	502	LOC	C15-C16	2.37	1.44	1.39
4	C	600	GTP	C6-C5	2.48	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	LOC	C15-C16	2.54	1.44	1.39
4	A	600	GTP	C6-C5	2.56	1.46	1.41
7	B	502	LOC	C14-C11	2.70	1.57	1.52
4	A	600	GTP	C6-N1	3.14	1.38	1.33
4	C	600	GTP	C6-N1	3.26	1.39	1.33
6	B	501	GDP	C6-N1	3.36	1.39	1.33
6	D	501	GDP	C6-N1	3.66	1.39	1.33
8	D	503	3WZ	C6-C5	4.02	1.59	1.52
6	B	501	GDP	C6-C5	4.09	1.49	1.41
8	B	503	3WZ	C5-N3	4.52	1.57	1.47
8	D	503	3WZ	C5-N3	4.95	1.58	1.47
8	B	503	3WZ	C6-C5	5.17	1.61	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	GDP	C5-C6-N1	-8.17	111.85	123.48
4	A	600	GTP	C5-C6-N1	-8.05	112.02	123.48
4	C	600	GTP	C5-C6-N1	-8.05	112.02	123.48
6	D	501	GDP	C5-C6-N1	-7.95	112.16	123.48
6	B	501	GDP	C6-C5-C4	-3.57	117.29	120.84
8	D	503	3WZ	O7-C29-C30	-2.99	114.38	120.09
4	A	600	GTP	C6-C5-C4	-2.95	117.91	120.84
4	C	600	GTP	C6-C5-C4	-2.84	118.02	120.84
4	C	600	GTP	N3-C2-N1	-2.77	123.41	127.46
6	D	501	GDP	N3-C2-N1	-2.76	123.42	127.46
8	D	503	3WZ	C15-C14-C16	-2.74	103.19	108.67
6	D	501	GDP	C6-C5-C4	-2.65	118.21	120.84
4	A	600	GTP	N3-C2-N1	-2.62	123.64	127.46
6	B	501	GDP	N3-C2-N1	-2.52	123.78	127.46
8	D	503	3WZ	C14-C16-N2	-2.43	112.70	116.65
8	D	503	3WZ	O8-C34-C35	-2.39	115.78	120.57
8	D	503	3WZ	C17-N2-C16	-2.09	119.97	123.16
6	D	501	GDP	C2-N3-C4	-2.07	112.74	115.16
7	D	502	LOC	C10-C11-N1	2.03	113.82	110.05
8	B	503	3WZ	C37-C35-C34	2.33	111.67	108.21
8	B	503	3WZ	C30-C29-N3	2.39	123.61	118.61
8	D	503	3WZ	C29-C30-N4	2.50	113.82	107.96
8	D	503	3WZ	C28-N3-C29	2.73	131.04	122.41
8	D	503	3WZ	C31-C30-C29	3.06	116.82	110.70
8	B	503	3WZ	O5-C13-C14	3.22	113.54	105.81
8	D	503	3WZ	C30-C29-N3	3.24	125.39	118.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	503	3WZ	C5-N3-C29	4.79	133.58	120.27
6	D	501	GDP	C6-N1-C2	6.40	125.27	116.06
4	C	600	GTP	C6-N1-C2	6.41	125.28	116.06
4	A	600	GTP	C6-N1-C2	6.46	125.36	116.06
6	B	501	GDP	C6-N1-C2	6.54	125.47	116.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GTP	1	0
6	B	501	GDP	1	0
7	B	502	LOC	1	0
6	D	501	GDP	3	0
7	D	502	LOC	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	429/451 (95%)	-0.14	12 (2%) 53 45	118, 157, 210, 234	0
1	C	430/451 (95%)	-0.37	3 (0%) 87 82	100, 132, 175, 197	1 (0%)
2	B	428/445 (96%)	-0.16	14 (3%) 47 39	108, 144, 181, 202	2 (0%)
2	D	430/445 (96%)	-0.41	0 100 100	93, 124, 158, 185	2 (0%)
3	E	123/142 (86%)	-0.46	1 (0%) 86 79	127, 160, 208, 215	0
All	All	1840/1934 (95%)	-0.29	30 (1%) 72 64	93, 142, 190, 234	5 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	24	LEU	5.1
2	B	438	ALA	5.0
1	A	340	THR	4.4
2	B	439	THR	3.7
2	B	135	PHE	3.7
1	A	316	CYS	3.6
2	B	178	SER	3.4
2	B	136	GLN	3.4
2	B	134	GLY	3.3
2	B	5	VAL	3.0
1	A	346	TRP	2.9
1	A	101	ASN	2.8
1	C	253	THR	2.8
1	A	172	TYR	2.7
1	A	303	VAL	2.7
1	A	178	SER	2.6
1	A	381	THR	2.5
1	A	313	MET	2.5
2	B	322	ARG	2.5
1	C	254	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	315	CYS	2.3
2	B	97	SER	2.3
1	A	295	CYS	2.3
2	B	274	PRO	2.2
2	B	249	ASN	2.2
1	C	199	ASP	2.2
2	B	100	GLY	2.2
2	B	98	GLY	2.1
2	B	11	GLN	2.1
1	A	376	CYS	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(\AA^2)	Q<0.9
4	GTP	A	600	32/32	0.90	0.48	1.26	141,151,161,161	0
6	GDP	D	501	28/28	0.90	0.29	1.22	110,117,129,130	0
5	MG	C	601	1/1	0.99	0.41	1.01	92,92,92,92	0
7	LOC	D	502	29/29	0.93	0.35	0.61	123,139,142,144	0
8	3WZ	D	503	50/50	0.90	0.26	0.48	109,139,162,172	0
4	GTP	C	600	32/32	0.92	0.30	0.46	112,116,120,122	0
6	GDP	B	501	28/28	0.92	0.32	0.27	122,136,140,143	0
7	LOC	B	502	29/29	0.91	0.31	-0.08	153,162,166,167	0
8	3WZ	B	503	50/50	0.89	0.25	-0.13	147,163,172,175	0
5	MG	A	601	1/1	0.87	0.40	-0.26	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.