



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:35 am GMT

PDB ID : 5LOV
Title : DZ-2384 tubulin complex
Authors : Prota, A.E.; Steinmetz, M.O.; Shore, G.C.; Brouhard, G.; Roulston, A.
Deposited on : 2016-08-10
Resolution : 2.40 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

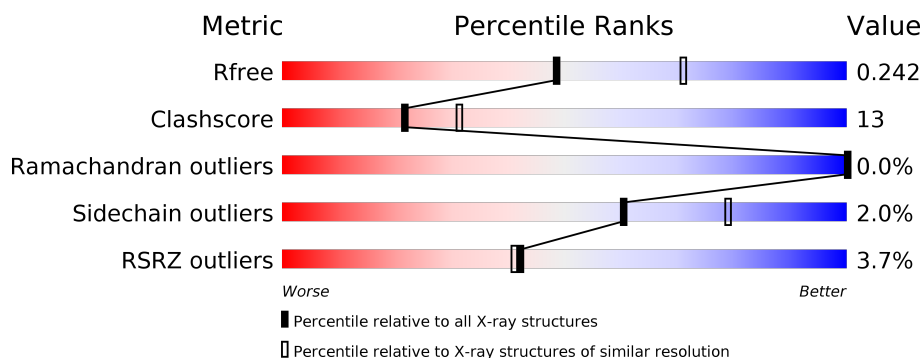
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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>13%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>•</div> </div> </div>
1	C	451	<div> <div></div> <div> <div></div> <div>80%</div> <div>17%</div> <div>•</div> </div> </div>
2	B	445	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>28%</div> <div>6%</div> </div> </div>
2	D	445	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>30%</div> <div>• 5%</div> </div> </div>
3	E	143	<div> <div></div> <div> <div></div> <div>67%</div> <div>15%</div> <div>18%</div> </div> </div>
4	F	384	<div> <div>13%</div> <div> <div></div> <div>51%</div> <div>26%</div> <div>•</div> <div>22%</div> </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
6	MG	B	503	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17322 atoms, of which 49 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	6	0
			3442	2185	582	652	23			
1	C	437	Total	C	N	O	S	0	7	0
			3442	2182	581	655	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	417	Total	C	N	O	S	0	2	0
			3287	2068	558	634	27			
2	D	422	Total	C	N	O	S	0	2	0
			3323	2089	563	644	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	117	Total	C	N	O	S	0	0	0
			970	599	177	190	4			

There are 2 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

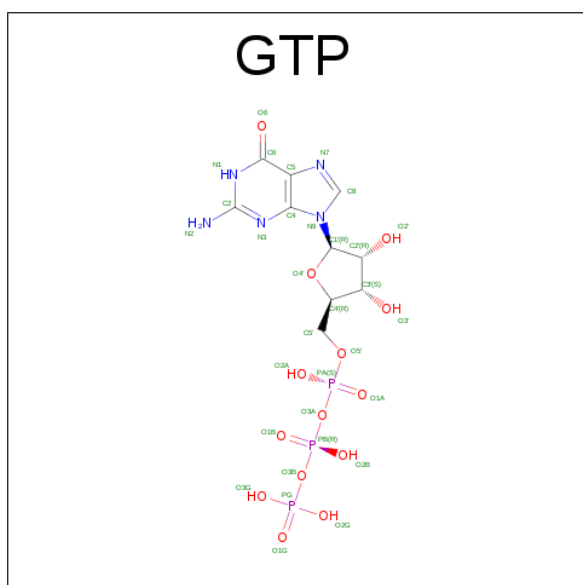
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	298	Total	C	N	O	S	0	5	0
			2460	1596	409	443	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		

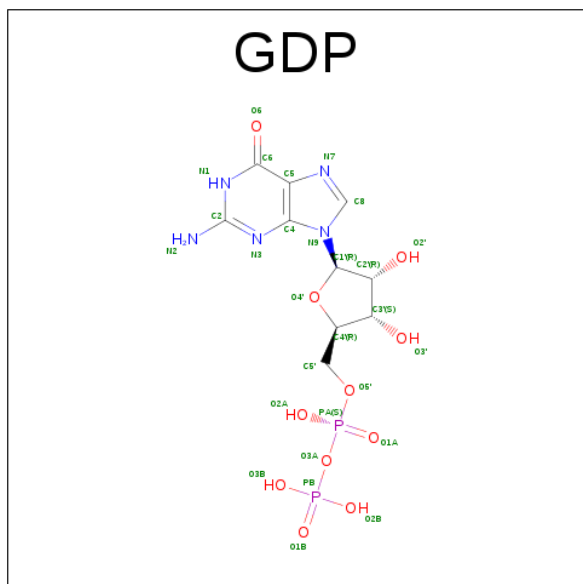
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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	C	1	Total	Mg	0	0
			1	1		

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

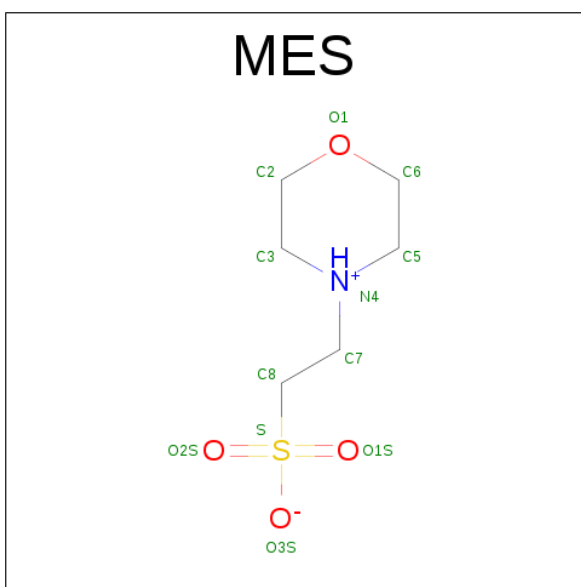
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



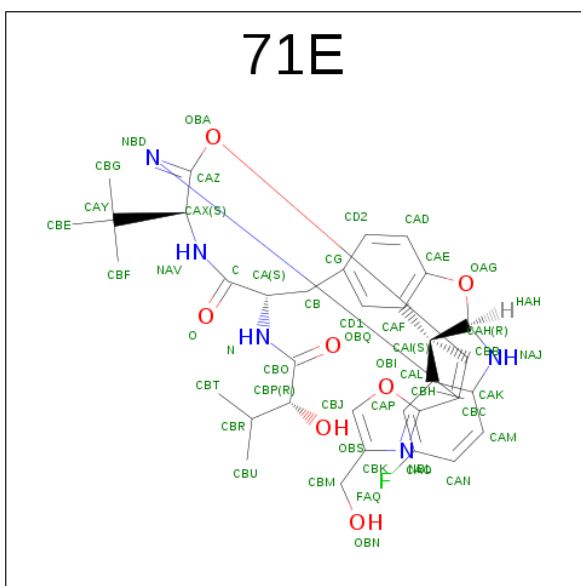
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



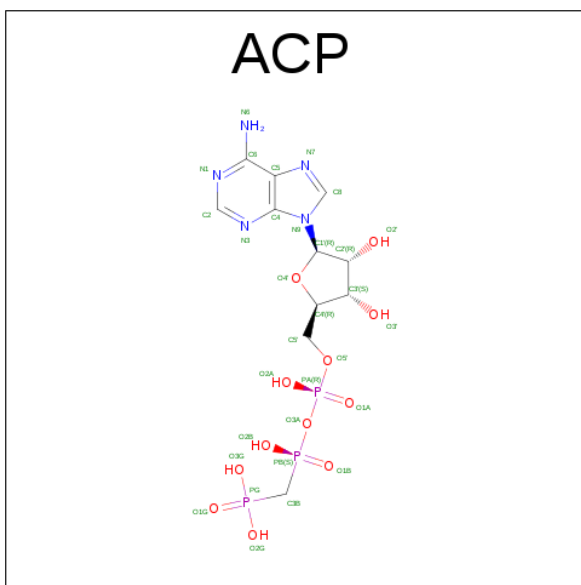
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 10 is DZ 2384 (three-letter code: 71E) (formula: $\text{C}_{34}\text{H}_{36}\text{FN}_5\text{O}_7$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	C	1	Total	C	F	H	N	O	0	0
			83	34	1	36	5	7		

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



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

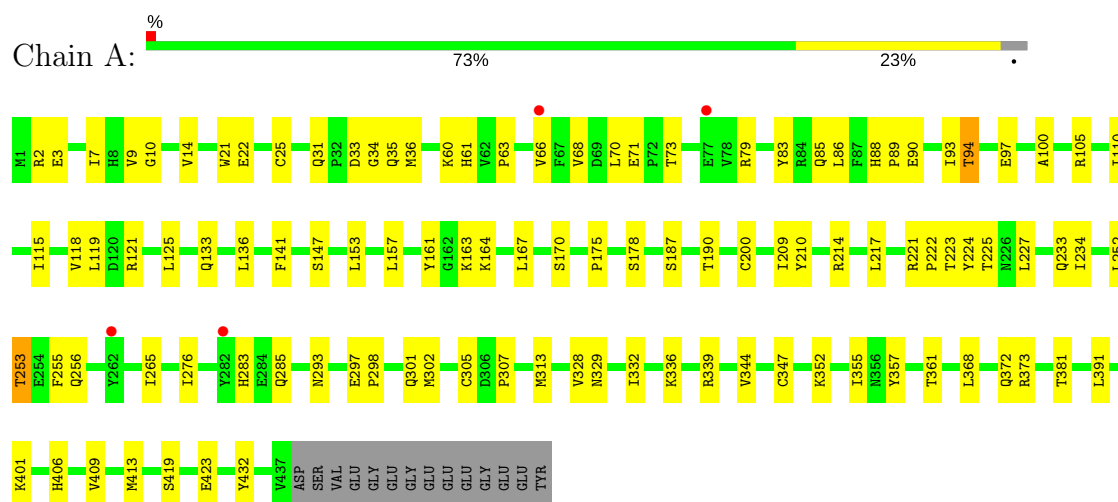
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	32	Total O 32 32	0	0
12	B	30	Total O 30 30	0	0
12	C	66	Total O 66 66	0	0
12	D	7	Total O 7 7	0	0

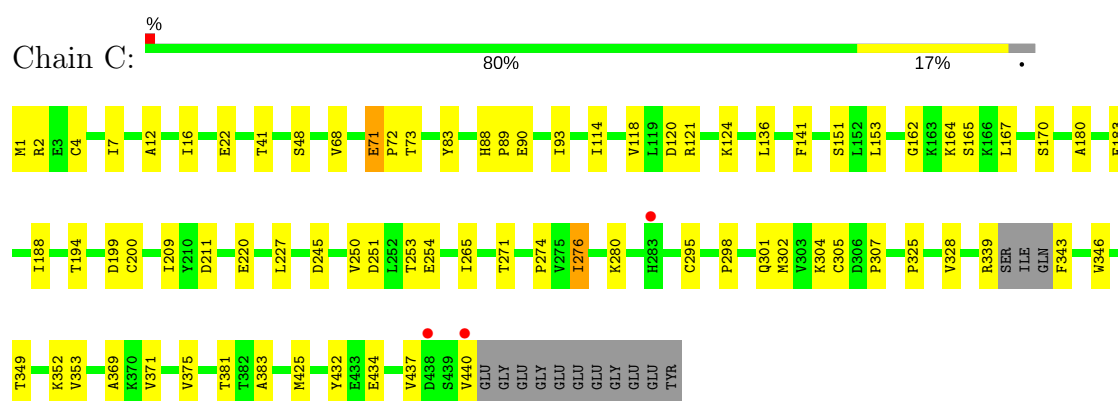
3 Residue-property plots

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.

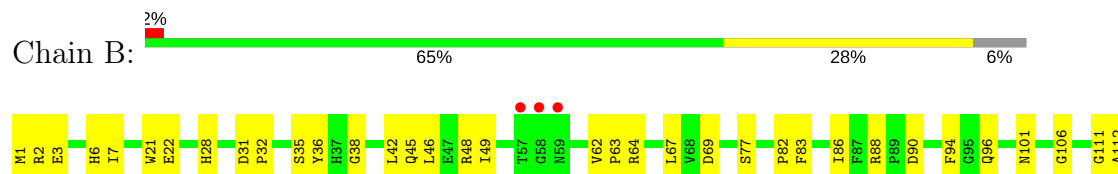
• Molecule 1: Tubulin alpha-1B chain

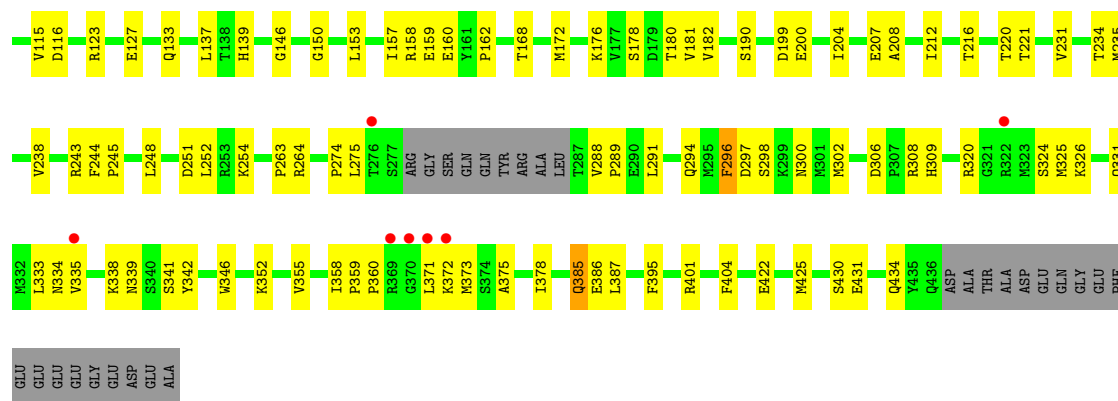


• Molecule 1: Tubulin alpha-1B chain

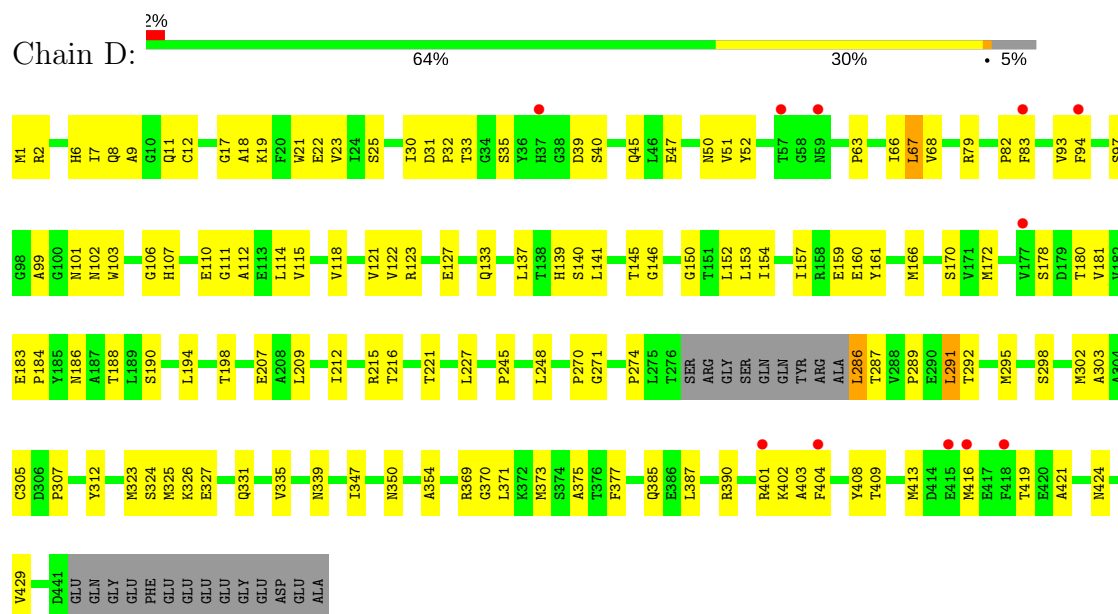


• Molecule 2: Tubulin beta-2B chain

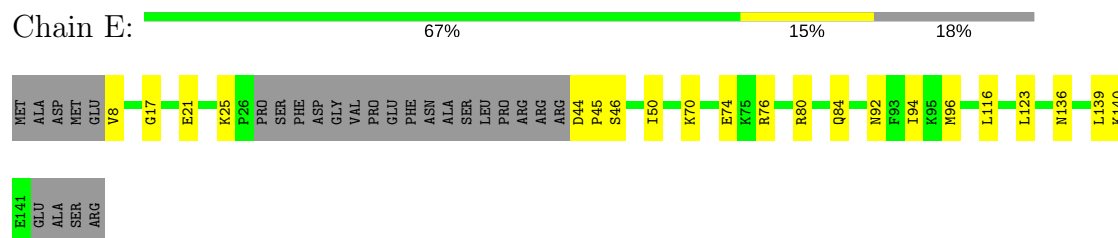




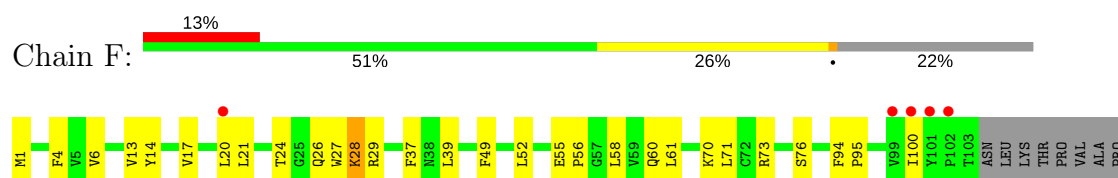
• Molecule 2: Tubulin beta-2B chain

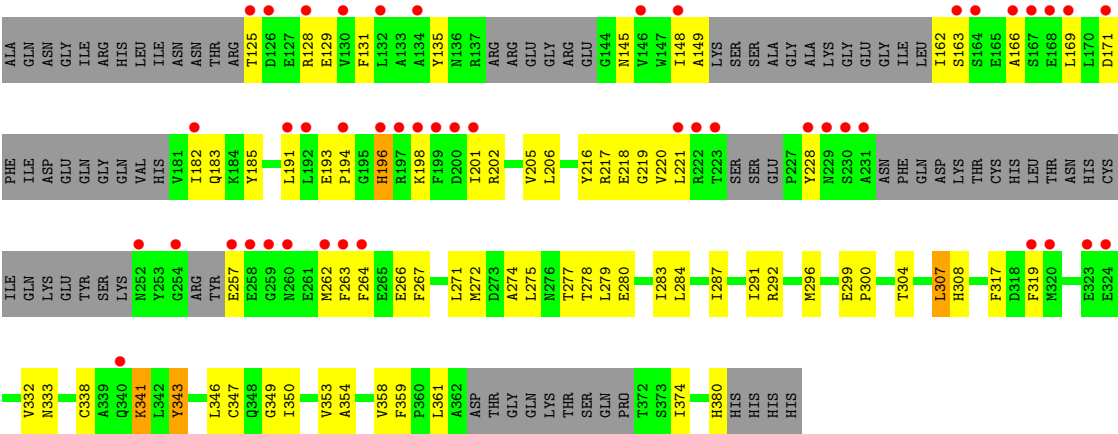


• Molecule 3: Stathmin-4



• 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	103.16Å 154.70Å 180.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.35 – 2.40 77.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (77.35-2.40) 99.8 (77.35-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.188 , 0.241 0.188 , 0.242	Depositor DCC
R_{free} test set	5646 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.5	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	0.96	EDS
Total number of atoms	17322	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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, MG, CA, GTP, ACP, MES, 71E

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	0.27	0/3538	0.42	0/4804
1	C	0.29	0/3540	0.46	0/4807
2	B	0.28	0/3366	0.43	0/4559
2	D	0.25	0/3402	0.42	0/4609
3	E	0.26	0/976	0.36	0/1292
4	F	0.23	0/2527	0.39	0/3413
All	All	0.27	0/17349	0.42	0/23484

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	3442	0	3379	90	0
1	C	3442	0	3369	62	0
2	B	3287	0	3174	100	0
2	D	3323	0	3208	104	0
3	E	970	0	990	21	0
4	F	2460	0	2464	99	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	5	0
9	B	12	13	13	1	0
10	C	47	36	0	2	0
11	F	31	0	14	1	0
12	A	32	0	0	0	0
12	B	30	0	0	1	0
12	C	66	0	0	1	0
12	D	7	0	0	0	0
All	All	17273	49	16659	452	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 13.

All (452) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:LEU:HD21	4:F:58:LEU:HD13	1.43	1.00
2:B:42:LEU:HD23	2:B:358:ILE:HD11	1.44	0.98
4:F:148:ILE:HA	4:F:162:ILE:HG22	1.47	0.97
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.48	0.96
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.50	0.93
1:C:271:THR:HG21	1:C:295[A]:CYS:HA	1.59	0.83
1:C:271:THR:HG21	1:C:295[B]:CYS:HA	1.59	0.82
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.61	0.81
1:A:223:THR:HG22	1:A:225:THR:H	1.46	0.80
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.65	0.79
2:D:1:MET:HG2	2:D:50:ASN:CB	2.12	0.78
2:B:216:THR:HG21	2:B:275:LEU:HD12	1.65	0.78
2:D:1:MET:HG2	2:D:50:ASN:HB2	1.65	0.78
1:A:297:GLU:HG3	1:A:339:ARG:HH12	1.48	0.77
1:C:71:GLU:HG2	1:C:72:PRO:CD	2.14	0.77
2:B:320:ARG:HG2	2:B:359:PRO:HA	1.65	0.77
1:A:175:PRO:HA	1:A:178:SER:HB3	1.66	0.76
1:A:221:ARG:HD2	2:B:325:MET:HB3	1.65	0.76
4:F:28:LYS:HA	4:F:28:LYS:HE3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:THR:HG22	1:C:383:ALA:H	1.47	0.76
4:F:149:ALA:HB2	4:F:182:ILE:HD13	1.67	0.76
4:F:201:ILE:HD13	4:F:221:LEU:HG	1.66	0.75
2:D:11:GLN:HB3	8:D:501:GDP:O2A	1.87	0.74
2:D:93:VAL:HG12	2:D:114:LEU:HD11	1.70	0.73
2:D:8:GLN:HE21	2:D:67:LEU:HG	1.54	0.73
1:A:234:ILE:HD13	1:A:302:MET:SD	2.28	0.72
2:B:360:PRO:HG2	2:B:371:LEU:HD12	1.72	0.71
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.71	0.71
1:A:167:LEU:HD22	1:A:200:CYS:HB3	1.72	0.70
2:D:295:MET:CE	2:D:375:ALA:HB1	2.21	0.70
4:F:349:GLY:O	4:F:353[B]:VAL:HG12	1.90	0.70
1:A:70:LEU:CD1	1:A:110:ILE:HG21	2.22	0.70
2:D:123:ARG:O	2:D:127:GLU:HG2	1.91	0.70
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.73	0.69
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.27	0.69
1:C:12:ALA:O	1:C:16:ILE:HG12	1.92	0.68
1:C:271:THR:CG2	1:C:295[A]:CYS:HA	2.23	0.68
1:C:271:THR:HG21	1:C:295[A]:CYS:CA	2.23	0.68
1:C:271:THR:CG2	1:C:295[B]:CYS:HA	2.23	0.68
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.76	0.68
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.76	0.68
1:C:276:ILE:HD13	1:C:369:ALA:HB3	1.77	0.67
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.30	0.67
5:C:501:GTP:O1G	12:C:601:HOH:O	2.13	0.67
1:C:88:HIS:CD2	1:C:90:GLU:HG2	2.30	0.66
4:F:163:SER:HB2	4:F:169:LEU:HD13	1.78	0.66
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.77	0.66
1:A:276:ILE:HD12	1:A:283:HIS:HD2	1.61	0.66
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.78	0.65
4:F:279:LEU:HG	4:F:284[B]:LEU:HD23	1.77	0.65
2:D:97:SER:HB3	2:D:110:GLU:HG2	1.79	0.65
1:A:175:PRO:HA	1:A:178:SER:CB	2.27	0.65
4:F:262:MET:HE2	4:F:266:GLU:HG2	1.78	0.65
2:B:333:LEU:CD2	4:F:58:LEU:HD13	2.22	0.64
1:C:88:HIS:CD2	1:C:89:PRO:HD2	2.32	0.64
2:B:137:LEU:HB3	2:B:168[B]:THR:HG22	1.78	0.64
1:A:329:ASN:HD21	3:E:8:VAL:CG2	2.11	0.64
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.80	0.64
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.33	0.64
4:F:287:ILE:O	4:F:291:ILE:HG12	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:MET:HE3	2:D:375:ALA:HB1	1.79	0.64
2:D:289:PRO:HA	2:D:331:GLN:HG2	1.80	0.63
2:B:320:ARG:NE	2:B:360:PRO:HD3	2.14	0.63
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.81	0.62
4:F:279:LEU:HG	4:F:284[B]:LEU:CD2	2.30	0.62
4:F:61:LEU:HD22	4:F:358:VAL:HG11	1.82	0.62
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.14	0.62
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.33	0.62
4:F:262:MET:CE	4:F:266:GLU:HG2	2.29	0.62
2:B:360:PRO:CG	2:B:371:LEU:HD12	2.29	0.62
2:D:188:THR:HG22	2:D:421:ALA:HB1	1.82	0.62
2:D:1:MET:HG2	2:D:50:ASN:HB3	1.82	0.62
2:D:409:THR:O	3:E:140:LYS:NZ	2.33	0.61
1:A:2:ARG:CB	1:A:133:GLN:HG2	2.30	0.61
2:D:8:GLN:OE1	2:D:17:GLY:HA3	1.99	0.61
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.36	0.61
2:B:288:VAL:HG12	2:B:331:GLN:HG3	1.82	0.61
4:F:135:TYR:O	4:F:145:ASN:ND2	2.34	0.61
2:B:28:HIS:HB3	2:B:49:ILE:CD1	2.30	0.61
1:C:343:PHE:CD2	1:C:349:THR:HG23	2.36	0.60
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.35	0.60
4:F:20:LEU:O	4:F:24:THR:HG23	2.01	0.60
2:B:238:VAL:HB	2:B:378:ILE:HD11	1.83	0.60
1:A:344:VAL:HG23	1:A:347:CYS:HB2	1.84	0.59
1:C:434:GLU:O	1:C:437:VAL:HG12	2.03	0.59
1:A:147:SER:HB2	1:A:190:THR:HB	1.84	0.59
2:B:325:MET:CE	2:B:355:VAL:HB	2.32	0.59
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.21	0.58
1:A:66[B]:VAL:HG23	1:A:125:LEU:CD1	2.33	0.58
1:A:221:ARG:CD	2:B:325:MET:HB3	2.31	0.58
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.85	0.58
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.85	0.58
2:B:159:GLU:OE1	3:E:76:ARG:NH1	2.34	0.58
2:B:220:THR:HG23	2:B:221:THR:H	1.67	0.58
4:F:1:MET:CE	4:F:28:LYS:HB2	2.33	0.58
1:C:276:ILE:HD11	1:C:371:VAL:CG1	2.34	0.57
1:C:41:THR:OG1	1:C:41:THR:O	2.22	0.57
2:D:207:GLU:HB3	2:D:390:ARG:HH12	1.69	0.57
2:D:323:MET:HB3	2:D:373:MET:HE1	1.85	0.57
2:D:209:LEU:HB3	2:D:227:LEU:HD22	1.85	0.57
2:B:178:SER:HB2	1:C:349:THR:O	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.40	0.57
1:C:180:ALA:O	1:C:183:GLU:HG3	2.05	0.57
1:C:1:MET:O	1:C:2:ARG:HB2	2.04	0.57
2:B:434:GLN:NE2	12:B:602:HOH:O	2.38	0.56
2:B:83:PHE:O	2:B:86:ILE:HG12	2.05	0.56
4:F:148:ILE:HG12	4:F:149:ALA:N	2.20	0.56
4:F:202:ARG:HB3	4:F:220:VAL:CG1	2.34	0.56
4:F:338:CYS:HB3	4:F:343:TYR:CD1	2.40	0.56
1:A:409:VAL:HA	1:A:413:MET:O	2.05	0.56
1:C:220:GLU:HG2	2:D:326:LYS:HD3	1.87	0.56
1:C:271:THR:HG21	1:C:295[B]:CYS:CA	2.23	0.56
2:D:298:SER:OG	2:D:307:PRO:HD2	2.04	0.56
2:D:79:ARG:HH12	2:D:94:PHE:HZ	1.52	0.56
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.88	0.56
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.46	0.56
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.41	0.56
3:E:44:ASP:HB2	3:E:45:PRO:HD2	1.88	0.56
1:C:298:PRO:HA	1:C:301:GLN:OE1	2.06	0.55
3:E:139:LEU:H	3:E:139:LEU:HD22	1.70	0.55
4:F:191:LEU:HD21	4:F:228:TYR:HB3	1.88	0.55
4:F:274:ALA:C	4:F:275:LEU:HD23	2.26	0.55
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.89	0.55
2:B:83:PHE:HB3	2:B:86:ILE:HD13	1.87	0.55
1:C:276:ILE:CD1	1:C:369:ALA:HB3	2.37	0.55
4:F:13:VAL:HG23	4:F:347:CYS:SG	2.47	0.55
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.88	0.55
2:B:306:ASP:OD2	2:B:308:ARG:NH2	2.33	0.55
2:D:118:VAL:O	2:D:121:VAL:HG22	2.07	0.55
1:A:31:GLN:NE2	1:A:35:GLN:HB2	2.21	0.54
2:B:325:MET:HE1	2:B:355:VAL:HB	1.90	0.54
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.89	0.54
4:F:13:VAL:HG13	4:F:14:TYR:CD1	2.42	0.54
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.42	0.54
2:B:248:LEU:HD21	2:B:352:LYS:HB2	1.90	0.54
2:B:42:LEU:HD23	2:B:358:ILE:CD1	2.30	0.54
2:B:234:THR:O	2:B:238:VAL:HG13	2.08	0.54
1:A:336:LYS:HE3	3:E:25:LYS:NZ	2.23	0.54
2:D:160:GLU:HG2	2:D:161:TYR:CE1	2.42	0.54
4:F:283:ILE:O	4:F:287:ILE:HG12	2.08	0.54
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.37	0.54
4:F:95:PRO:HB2	4:F:183:GLN:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:VAL:N	2:B:289:PRO:HD2	2.24	0.53
2:D:106:GLY:O	2:D:111:GLY:HA3	2.09	0.53
4:F:202:ARG:HB3	4:F:220:VAL:HG12	1.90	0.53
2:B:216:THR:HG21	2:B:275:LEU:CD1	2.37	0.53
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.90	0.53
1:A:210:TYR:CE2	1:A:222:PRO:HD2	2.44	0.53
2:D:67:LEU:H	2:D:67:LEU:HD12	1.73	0.53
4:F:299:GLU:N	4:F:300:PRO:HD2	2.24	0.53
2:B:69:ASP:O	2:B:94:PHE:HA	2.08	0.53
1:C:343:PHE:CE2	1:C:349:THR:HG23	2.44	0.53
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.91	0.53
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.91	0.52
4:F:262:MET:CE	4:F:267:PHE:HA	2.39	0.52
1:A:141:PHE:HB3	1:A:187:SER:OG	2.09	0.52
2:B:244:PHE:HB3	2:B:245:PRO:HD2	1.92	0.52
2:D:51:VAL:HG12	2:D:52:TYR:CD2	2.44	0.52
4:F:28:LYS:HA	4:F:28:LYS:CE	2.37	0.52
4:F:292:ARG:O	4:F:296:MET:HB2	2.09	0.52
1:A:66[B]:VAL:HG23	1:A:125:LEU:HD11	1.92	0.52
1:C:251:ASP:OD2	1:C:253:THR:HG22	2.10	0.52
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.44	0.52
2:B:248:LEU:HD21	2:B:352:LYS:CB	2.39	0.52
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.91	0.52
2:B:358:ILE:HD12	2:B:358:ILE:N	2.25	0.52
2:B:264:ARG:NE	2:B:431:GLU:OE2	2.30	0.52
2:B:67:LEU:HD12	2:B:67:LEU:N	2.24	0.52
1:A:406:HIS:ND1	2:B:263:PRO:HD3	2.24	0.52
2:B:28:HIS:HA	2:B:45:GLN:HB3	1.92	0.52
1:A:223:THR:HG22	1:A:224:TYR:N	2.25	0.52
1:A:276:ILE:HD12	1:A:283:HIS:CD2	2.43	0.52
2:B:48:ARG:HB2	2:B:243:ARG:O	2.09	0.51
1:C:22:GLU:HG3	1:C:83:TYR:OH	2.10	0.51
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.93	0.51
2:D:118:VAL:O	2:D:122:VAL:HG23	2.10	0.51
2:D:324:SER:HB3	2:D:327:GLU:HB2	1.93	0.51
4:F:202:ARG:NH2	4:F:333:ASN:HD22	2.08	0.51
2:B:96:GLN:HG3	1:C:1:MET:HG2	1.93	0.51
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.92	0.51
2:D:7:ILE:O	2:D:137:LEU:HD12	2.10	0.51
4:F:26:GLN:HE22	4:F:361:LEU:HA	1.76	0.51
2:B:62:VAL:HG11	2:B:88:ARG:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:262:MET:HE1	4:F:267:PHE:HA	1.93	0.51
4:F:37:PHE:O	4:F:60:GLN:HG2	2.11	0.51
1:A:9:VAL:HG22	1:A:68[B]:VAL:CG1	2.41	0.51
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.24	0.51
4:F:169:LEU:CD2	4:F:182:ILE:HD12	2.41	0.51
2:B:291:LEU:HD13	2:B:373:MET:HG2	1.93	0.50
2:D:291:LEU:HD22	2:D:375:ALA:CB	2.41	0.50
1:A:285:GLN:HG2	1:A:372[B]:GLN:NE2	2.25	0.50
1:C:2:ARG:NH1	1:C:251:ASP:OD1	2.45	0.50
2:D:145:THR:N	8:D:501:GDP:O2B	2.44	0.50
10:C:503:71E:OBA	10:C:503:71E:CD1	2.56	0.50
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.47	0.50
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.46	0.50
4:F:1:MET:HE2	4:F:28:LYS:HB2	1.92	0.50
2:B:153:LEU:O	2:B:157:ILE:HG12	2.10	0.50
4:F:350:ILE:O	4:F:354:ALA:HB3	2.12	0.50
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.48	0.49
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.48	0.49
1:A:7:ILE:HG21	1:A:153:LEU:HD21	1.94	0.49
4:F:263:PHE:CZ	4:F:341:LYS:HG3	2.47	0.49
4:F:148:ILE:HG22	4:F:183:GLN:O	2.12	0.49
2:D:274:PRO:HD2	2:D:371:LEU:HD13	1.95	0.49
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.94	0.49
2:D:12:CYS:CB	2:D:140:SER:HB3	2.42	0.49
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.95	0.49
2:D:82:PRO:O	2:D:83:PHE:HB2	2.12	0.49
2:D:66:ILE:HD13	2:D:122:VAL:HG22	1.95	0.49
11:F:401:ACP:O2A	11:F:401:ACP:O1B	2.31	0.49
1:A:93:ILE:CD1	1:A:118:VAL:HA	2.43	0.48
1:A:253:THR:O	1:A:256:GLN:HG2	2.12	0.48
1:C:68[A]:VAL:HG11	1:C:118:VAL:HG21	1.94	0.48
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.48	0.48
2:D:159:GLU:HG3	3:E:123:LEU:HD13	1.94	0.48
4:F:14:TYR:HA	4:F:17:VAL:HB	1.95	0.48
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.48	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.48	0.48
1:A:401:LYS:HG3	2:B:346:TRP:CD2	2.48	0.48
1:A:33:ASP:HA	1:A:85:GLN:HB2	1.95	0.48
2:D:221:THR:OG1	2:D:221:THR:O	2.32	0.48
2:D:19:LYS:O	2:D:23:VAL:HG23	2.12	0.48
2:B:294:GLN:HG2	2:B:300:ASN:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:VAL:HG11	2:B:404:PHE:CZ	2.49	0.48
2:B:133:GLN:OE1	2:B:252:LEU:HG	2.13	0.48
4:F:267:PHE:CD2	4:F:279:LEU:HD13	2.48	0.48
3:E:70:LYS:O	3:E:74:GLU:HG3	2.12	0.48
2:D:66:ILE:CD1	2:D:122:VAL:HG22	2.44	0.48
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.79	0.48
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.49	0.47
1:A:141:PHE:O	1:A:147:SER:HB3	2.14	0.47
4:F:272:MET:CE	4:F:278:THR:HG22	2.44	0.47
4:F:73:ARG:HB2	4:F:76:SER:HB2	1.94	0.47
2:D:103:TRP:HB2	2:D:186:ASN:OD1	2.14	0.47
1:A:217:LEU:HD21	1:A:368:LEU:CD2	2.40	0.47
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.55	0.47
1:A:79:ARG:HH22	1:A:94:THR:CG2	2.27	0.47
4:F:267:PHE:CZ	4:F:271[B]:LEU:HD11	2.49	0.47
1:A:372[B]:GLN:HE21	1:A:373:ARG:HH12	1.61	0.47
4:F:277[B]:THR:HG22	4:F:278:THR:N	2.30	0.47
1:C:165:SER:HA	1:C:199:ASP:OD2	2.14	0.47
4:F:193:GLU:OE1	4:F:194:PRO:HA	2.15	0.47
1:A:163:LYS:O	1:A:164:LYS:HD3	2.15	0.47
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.96	0.47
2:D:323:MET:HB3	2:D:373:MET:CE	2.44	0.47
1:A:293:ASN:O	1:A:339:ARG:NH2	2.48	0.47
2:B:220:THR:HG23	2:B:221:THR:N	2.29	0.47
1:C:305:CYS:O	1:C:307:PRO:HD3	2.15	0.47
2:D:31:ASP:OD2	2:D:35:SER:HB2	2.15	0.47
3:E:44:ASP:HB2	3:E:45:PRO:CD	2.45	0.47
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.97	0.47
1:A:153:LEU:O	1:A:157:LEU:HG	2.14	0.46
4:F:206:LEU:HD21	4:F:353[B]:VAL:HG13	1.96	0.46
1:A:66[B]:VAL:HG23	1:A:125:LEU:HD12	1.98	0.46
1:C:120[A]:ASP:OD2	1:C:124:LYS:HE3	2.15	0.46
1:C:151:SER:HA	1:C:194[B]:THR:HG22	1.97	0.46
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.97	0.46
3:E:139:LEU:HD22	3:E:139:LEU:N	2.29	0.46
4:F:279:LEU:O	4:F:284[B]:LEU:HD23	2.15	0.46
2:D:25:SER:CB	2:D:30:ILE:HD11	2.44	0.46
2:B:133:GLN:OE1	2:B:251:ASP:HB2	2.15	0.46
2:B:28:HIS:ND1	2:B:49:ILE:HD12	2.30	0.46
1:A:97:GLU:HG3	2:B:2:ARG:CZ	2.45	0.46
2:D:416:MET:HA	2:D:419:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:46:SER:O	3:E:50:ILE:HG13	2.15	0.46
1:A:328:VAL:O	1:A:332:ILE:HG13	2.14	0.46
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.46	0.46
2:D:21:TRP:O	2:D:25:SER:OG	2.20	0.46
2:D:8:GLN:HE21	2:D:67:LEU:CG	2.24	0.46
2:D:18:ALA:O	2:D:22:GLU:HG3	2.16	0.46
4:F:13:VAL:HG13	4:F:14:TYR:HD1	1.81	0.46
4:F:17:VAL:O	4:F:21:LEU:HG	2.16	0.46
4:F:267:PHE:CE2	4:F:271[B]:LEU:HD11	2.50	0.46
4:F:277[A]:THR:HG22	4:F:278:THR:H	1.81	0.46
2:B:106:GLY:O	2:B:111:GLY:HA3	2.16	0.46
2:D:331:GLN:O	2:D:335:VAL:HG13	2.16	0.45
1:A:355:ILE:O	3:E:17:GLY:HA3	2.16	0.45
1:A:71:GLU:OE1	1:A:73:THR:HB	2.15	0.45
2:D:1:MET:CG	2:D:50:ASN:HB2	2.40	0.45
2:D:292:THR:HG22	2:D:335:VAL:HG11	1.99	0.45
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.51	0.45
1:A:136[A]:LEU:HD11	1:A:252:LEU:HD21	1.97	0.45
2:B:82:PRO:O	2:B:83:PHE:HB2	2.17	0.45
2:B:339:ASN:O	2:B:341:SER:N	2.49	0.45
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.97	0.45
4:F:100:ILE:HG21	4:F:128:ARG:HG3	1.99	0.45
4:F:277[B]:THR:HG22	4:F:278:THR:H	1.81	0.45
4:F:4:PHE:CZ	4:F:29:ARG:HB2	2.51	0.45
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.52	0.45
2:D:25:SER:HB3	2:D:30:ILE:CD1	2.47	0.45
1:A:105:ARG:HG2	1:A:110:ILE:HD13	1.99	0.45
2:B:123:ARG:O	2:B:127:GLU:HG3	2.15	0.45
2:B:204:ILE:HG22	2:B:302:MET:HB2	1.99	0.45
2:D:67:LEU:N	2:D:67:LEU:HD12	2.32	0.45
2:B:306:ASP:HB3	2:B:309:HIS:CE1	2.51	0.45
2:D:141:LEU:HD12	2:D:172:MET:SD	2.57	0.45
2:B:101:ASN:OD1	1:C:254:GLU:HG3	2.16	0.45
2:B:112:ALA:O	2:B:115:VAL:HG12	2.17	0.45
2:B:208:ALA:O	2:B:212:ILE:HD13	2.17	0.45
2:B:274:PRO:HA	2:B:294:GLN:OE1	2.17	0.45
4:F:277[A]:THR:HG22	4:F:278:THR:N	2.31	0.45
2:B:137:LEU:HB3	2:B:168[A]:THR:HG22	1.97	0.44
2:D:31:ASP:OD1	2:D:33:THR:OG1	2.28	0.44
2:B:28:HIS:HD1	2:B:49:ILE:HD12	1.82	0.44
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:HD2	9:B:502:MES:H32	1.99	0.44
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.00	0.44
2:B:231:VAL:O	2:B:235:MET:HG3	2.18	0.44
2:D:93:VAL:CG1	2:D:114:LEU:HD11	2.45	0.44
2:D:112:ALA:O	2:D:115:VAL:HG12	2.18	0.44
2:D:141:LEU:HD11	2:D:170:SER:HB3	1.99	0.44
4:F:206:LEU:CD2	4:F:353[B]:VAL:HG13	2.47	0.44
2:B:160:GLU:C	2:B:162:PRO:HD3	2.37	0.44
1:A:252:LEU:O	1:A:255:PHE:HB2	2.17	0.44
4:F:221:LEU:HB2	4:F:262:MET:HB3	1.99	0.44
4:F:358:VAL:HG13	4:F:359:PHE:CD2	2.53	0.44
1:A:298:PRO:HA	1:A:301:GLN:CD	2.38	0.44
2:B:115:VAL:HG13	2:B:116:ASP:N	2.33	0.44
2:B:146:GLY:O	2:B:150:GLY:HA3	2.18	0.44
2:D:150:GLY:O	2:D:154:ILE:HG13	2.18	0.44
2:B:334:ASN:O	2:B:338:LYS:HB2	2.17	0.44
2:B:360:PRO:HG2	2:B:371:LEU:HB2	2.00	0.44
4:F:206:LEU:HD23	4:F:353[B]:VAL:CG1	2.48	0.44
2:B:7:ILE:O	2:B:137:LEU:HD12	2.17	0.43
1:C:71:GLU:HG2	1:C:72:PRO:N	2.32	0.43
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.53	0.43
1:A:83:TYR:HB3	1:A:86:LEU:HD22	1.99	0.43
1:A:3:GLU:O	1:A:133:GLN:HG3	2.18	0.43
2:D:215:ARG:HH11	2:D:215:ARG:HG2	1.83	0.43
2:D:303:ALA:O	2:D:305:CYS:N	2.51	0.43
2:D:403:ALA:HB1	2:D:404:PHE:CD2	2.53	0.43
4:F:71:LEU:O	4:F:332:VAL:HB	2.19	0.43
1:C:48:SER:HB3	1:C:245:ASP:CG	2.38	0.43
2:D:146:GLY:N	8:D:501:GDP:O2B	2.43	0.43
2:D:178:SER:HB2	8:D:501:GDP:O2'	2.18	0.43
4:F:169:LEU:HD21	4:F:182:ILE:HD12	2.01	0.43
2:B:48:ARG:NH1	2:B:245:PRO:HA	2.33	0.43
4:F:191:LEU:HD22	4:F:196:HIS:CE1	2.54	0.43
1:A:7:ILE:HG23	1:A:66[A]:VAL:HG13	2.00	0.43
1:A:161:TYR:HB3	1:A:164:LYS:HG2	2.01	0.43
2:B:28:HIS:HB3	2:B:49:ILE:HD12	1.98	0.43
1:C:276:ILE:HD11	1:C:371:VAL:HG13	2.01	0.43
1:C:276:ILE:HG22	1:C:280:LYS:HD3	2.00	0.43
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.99	0.43
4:F:55:GLU:HA	4:F:56:PRO:HD3	1.90	0.43
1:A:115:ILE:O	1:A:119:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.18	0.43
4:F:347:CYS:HA	4:F:350:ILE:HD12	2.01	0.43
1:A:233:GLN:NE2	1:A:361:THR:O	2.47	0.43
2:D:287:THR:HB	2:D:289:PRO:HD2	2.00	0.43
2:D:387:LEU:C	2:D:387:LEU:HD23	2.39	0.43
1:C:274:PRO:HG2	1:C:371:VAL:HG11	2.00	0.42
2:D:101:ASN:HD22	2:D:180:THR:HG21	1.84	0.42
4:F:94:PHE:HA	4:F:95:PRO:HD3	1.89	0.42
1:A:329:ASN:HD21	3:E:8:VAL:HG21	1.83	0.42
1:A:352:LYS:HE3	3:E:21:GLU:OE1	2.19	0.42
2:B:22:GLU:HG3	2:B:83:PHE:CD1	2.54	0.42
2:B:1:MET:CB	2:B:2:ARG:HA	2.48	0.42
2:D:153:LEU:O	2:D:157:ILE:HG13	2.19	0.42
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.54	0.42
4:F:217:ARG:NH2	4:F:374:ILE:HG22	2.34	0.42
1:A:90:GLU:O	1:A:121:ARG:HD2	2.18	0.42
1:C:265:ILE:HG23	1:C:432:TYR:CE1	2.54	0.42
2:D:295:MET:CG	2:D:377:PHE:HB2	2.49	0.42
4:F:341:LYS:H	4:F:341:LYS:HG2	1.55	0.42
1:A:336:LYS:HE3	3:E:25:LYS:HZ3	1.84	0.42
1:A:406:HIS:CE1	2:B:263:PRO:HD3	2.54	0.42
2:B:31:ASP:OD1	2:B:35:SER:N	2.48	0.42
2:B:371:LEU:C	2:B:373:MET:H	2.23	0.42
1:C:253:THR:HG23	1:C:254:GLU:N	2.34	0.42
2:D:291:LEU:HD22	2:D:375:ALA:HB3	2.02	0.42
1:A:83:TYR:O	1:A:86:LEU:HB2	2.19	0.42
2:D:107:HIS:O	2:D:152:LEU:HD22	2.20	0.42
2:D:271:GLY:N	2:D:377:PHE:O	2.53	0.42
3:E:92:ASN:O	3:E:96:MET:HG3	2.19	0.42
4:F:70:LYS:O	4:F:76:SER:HB3	2.19	0.42
1:A:419:SER:O	1:A:423:GLU:HG3	2.19	0.42
2:B:298:SER:C	2:B:300:ASN:H	2.23	0.42
1:C:295[B]:CYS:SG	1:C:375:VAL:HG13	2.59	0.42
2:D:209:LEU:CB	2:D:227:LEU:HD22	2.49	0.42
2:D:1:MET:HG3	2:D:2:ARG:N	2.35	0.42
2:D:9:ALA:HA	2:D:68:VAL:O	2.19	0.42
4:F:129:GLU:CD	4:F:129:GLU:H	2.22	0.42
1:A:121:ARG:HD3	1:A:121:ARG:HA	1.87	0.42
4:F:191:LEU:HD12	4:F:191:LEU:N	2.34	0.42
4:F:267:PHE:CZ	4:F:271[A]:LEU:HD11	2.55	0.42
2:B:324:SER:C	2:B:326:LYS:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:GLU:HB3	2:B:64:ARG:NH1	2.35	0.41
4:F:296:MET:SD	4:F:380:HIS:HB2	2.60	0.41
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.83	0.41
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.88	0.41
2:D:118:VAL:HG11	2:D:153:LEU:HD11	2.01	0.41
4:F:21:LEU:O	4:F:27:TRP:HB2	2.20	0.41
1:A:217:LEU:HD11	1:A:368:LEU:HD21	2.01	0.41
2:B:297:ASP:OD1	2:B:298:SER:N	2.53	0.41
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.41
2:D:369:ARG:HA	2:D:370:GLY:HA2	1.61	0.41
3:E:136:ASN:O	3:E:140:LYS:HB2	2.20	0.41
2:D:115:VAL:HG21	2:D:152:LEU:HG	2.02	0.41
2:D:335:VAL:O	2:D:339:ASN:HB2	2.19	0.41
2:D:1:MET:CE	2:D:50:ASN:HB2	2.51	0.41
4:F:49:PHE:HA	4:F:52:LEU:HD13	2.01	0.41
1:C:209:ILE:HD11	1:C:302:MET:SD	2.61	0.41
1:C:211:ASP:OD2	1:C:304:LYS:HE3	2.20	0.41
2:D:295:MET:HG3	2:D:377:PHE:HB2	2.01	0.41
4:F:346:LEU:O	4:F:350:ILE:HG13	2.19	0.41
1:A:344:VAL:CG2	1:A:347:CYS:HB2	2.47	0.41
2:B:180:THR:HG22	2:B:182:VAL:H	1.85	0.41
2:B:296:PHE:CD2	2:B:335:VAL:HG11	2.56	0.41
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.38	0.41
4:F:6:VAL:HG22	4:F:29:ARG:NH2	2.35	0.41
2:B:199:ASP:C	2:B:200:GLU:HG3	2.40	0.41
2:D:274:PRO:HB3	2:D:286:LEU:HD11	2.01	0.41
4:F:299:GLU:N	4:F:300:PRO:CD	2.84	0.41
4:F:341:LYS:HE3	4:F:341:LYS:HB3	1.93	0.41
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.56	0.41
2:D:146:GLY:O	2:D:150:GLY:HA3	2.21	0.41
2:D:295:MET:HE2	2:D:375:ALA:HB1	2.02	0.41
3:E:80:ARG:O	3:E:84:GLN:HB2	2.21	0.41
4:F:205:VAL:HG21	4:F:291:ILE:HD12	2.02	0.41
1:A:305:CYS:O	1:A:307:PRO:HD3	2.21	0.41
2:B:385:GLN:HG3	2:B:386:GLU:N	2.35	0.41
1:C:164:LYS:HB2	1:C:164:LYS:HE2	1.94	0.41
4:F:206:LEU:HD23	4:F:353[B]:VAL:HG11	2.02	0.41
2:B:401:ARG:HD3	1:C:346:TRP:CD2	2.56	0.41
1:A:79:ARG:HH22	1:A:94:THR:HG21	1.85	0.40
2:B:1:MET:HB2	2:B:2:ARG:HA	2.03	0.40
1:C:325:PRO:HA	10:C:503:71E:FAQ	2.11	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:VAL:HG13	1:C:254:GLU:OE1	2.21	0.40
2:D:183:GLU:HB2	2:D:184:PRO:HD3	2.03	0.40
2:D:30:ILE:O	2:D:30:ILE:HD12	2.21	0.40
2:D:408:TYR:O	2:D:413:MET:HB2	2.21	0.40
4:F:206:LEU:CD2	4:F:353[B]:VAL:CG1	3.00	0.40
2:B:371:LEU:O	2:B:372:LYS:HB2	2.21	0.40
2:D:194:LEU:HD22	2:D:198:THR:HG21	2.03	0.40
2:D:212:ILE:O	2:D:216:THR:HB	2.21	0.40
2:D:39:ASP:N	2:D:45:GLN:OE1	2.55	0.40
4:F:263:PHE:CE2	4:F:341:LYS:HG3	2.56	0.40
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.57	0.40
1:A:223:THR:CG2	1:A:224:TYR:N	2.84	0.40
1:A:88:HIS:HB2	1:A:89:PRO:HD2	2.03	0.40
1:C:440:VAL:HG12	1:C:440:VAL:O	2.22	0.40
4:F:135:TYR:CE1	4:F:145:ASN:HB3	2.56	0.40
4:F:317:PHE:HB3	4:F:319:PHE:CE2	2.57	0.40
1:A:10:GLY:O	1:A:14:VAL:HG23	2.22	0.40
1:A:217:LEU:CD2	1:A:368:LEU:HD23	2.46	0.40
1:C:328:VAL:HG11	1:C:353:VAL:HG11	2.03	0.40
2:D:99:ALA:O	2:D:102:ASN:HB3	2.22	0.40
4:F:4:PHE:HA	4:F:39:LEU:O	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	441/451 (98%)	422 (96%)	19 (4%)	0	100	100
1	C	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
2	B	415/445 (93%)	398 (96%)	17 (4%)	0	100	100
2	D	420/445 (94%)	399 (95%)	20 (5%)	1 (0%)	51	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	112/143 (78%)	110 (98%)	2 (2%)	0	100	100
4	F	285/384 (74%)	267 (94%)	18 (6%)	0	100	100
All	All	2113/2319 (91%)	2020 (96%)	92 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	401	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/379 (99%)	370 (99%)	4 (1%)	78	90
1	C	375/379 (99%)	372 (99%)	3 (1%)	85	93
2	B	363/383 (95%)	353 (97%)	10 (3%)	49	70
2	D	367/383 (96%)	356 (97%)	11 (3%)	46	67
3	E	105/127 (83%)	104 (99%)	1 (1%)	80	91
4	F	272/342 (80%)	264 (97%)	8 (3%)	48	68
All	All	1856/1993 (93%)	1819 (98%)	37 (2%)	60	79

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	THR
1	A	253	THR
1	A	313	MET
1	A	381	THR
2	B	77	SER
2	B	90	ASP
2	B	139	HIS
2	B	172	MET
2	B	190	SER

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Mol	Chain	Res	Type
2	B	296	PHE
2	B	385	GLN
2	B	387	LEU
2	B	425	MET
2	B	430	SER
1	C	71	GLU
1	C	276	ILE
1	C	339	ARG
2	D	40	SER
2	D	67	LEU
2	D	133	GLN
2	D	139	HIS
2	D	181	VAL
2	D	190	SER
2	D	286	LEU
2	D	291	LEU
2	D	325	MET
2	D	402	LYS
2	D	424	ASN
3	E	116	LEU
4	F	28	LYS
4	F	125	THR
4	F	171	ASP
4	F	196	HIS
4	F	257	GLU
4	F	307	LEU
4	F	341	LYS
4	F	343	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	50	ASN
1	A	329	ASN
2	B	6	HIS
2	B	136	GLN
2	B	433	GLN
1	C	88	HIS
2	D	192	HIS
2	D	197	ASN
2	D	331	GLN

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Mol	Chain	Res	Type
2	D	424	ASN
4	F	26	GLN
4	F	196	HIS
4	F	333	ASN

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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	1.00	1 (3%)	27,54,54	1.81	5 (18%)
8	GDP	B	501	-	25,30,30	1.18	2 (8%)	26,47,47	2.06	6 (23%)
9	MES	B	502	-	12,12,12	2.36	1 (8%)	16,16,16	1.76	5 (31%)
5	GTP	C	501	6	27,34,34	0.97	1 (3%)	27,54,54	1.68	4 (14%)
10	71E	C	503	-	40,53,53	2.88	18 (45%)	52,83,83	1.92	12 (23%)
8	GDP	D	501	-	25,30,30	1.17	2 (8%)	26,47,47	1.93	6 (23%)
11	ACP	F	401	-	27,33,33	1.91	7 (25%)	30,52,52	1.58	3 (10%)

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	GDP	B	501	-	-	0/12/32/32	0/3/3/3
9	MES	B	502	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
10	71E	C	503	-	-	0/30/72/72	0/3/7/7
8	GDP	D	501	-	-	0/12/32/32	0/3/3/3
11	ACP	F	401	-	-	0/15/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	MES	C8-S	-7.46	1.66	1.77
10	C	503	71E	CAE-CAF	-4.67	1.31	1.38
11	F	401	ACP	PB-O2B	-3.24	1.48	1.56
10	C	503	71E	CAK-CAL	-3.11	1.35	1.39
11	F	401	ACP	PG-O2G	-2.78	1.48	1.54
10	C	503	71E	CAI-CAF	2.04	1.55	1.53
10	C	503	71E	CBC-CBH	2.04	1.53	1.49
10	C	503	71E	CAM-CAN	2.05	1.42	1.38
10	C	503	71E	CAI-CBB	2.12	1.56	1.53
10	C	503	71E	OAG-CAE	2.25	1.41	1.37
5	C	501	GTP	C6-N1	2.67	1.37	1.33
10	C	503	71E	CD2-CAD	2.70	1.43	1.38
11	F	401	ACP	PG-O3G	2.80	1.61	1.54
11	F	401	ACP	PB-O3A	2.94	1.61	1.58
8	D	501	GDP	C5-C4	3.06	1.47	1.40
8	B	501	GDP	C5-C4	3.07	1.47	1.40
5	A	501	GTP	C6-N1	3.15	1.38	1.33
11	F	401	ACP	C5-C4	3.17	1.47	1.40
10	C	503	71E	CAP-CAO	3.38	1.43	1.37
10	C	503	71E	CD2-CG	3.59	1.46	1.38
8	B	501	GDP	C6-C5	3.68	1.48	1.41
8	D	501	GDP	C6-C5	3.72	1.48	1.41
11	F	401	ACP	PB-O1B	3.90	1.61	1.51
10	C	503	71E	CAK-NAJ	4.01	1.46	1.39
10	C	503	71E	CAN-CAO	4.81	1.46	1.37
10	C	503	71E	CAD-CAE	4.92	1.49	1.39
10	C	503	71E	CAM-CAK	4.97	1.48	1.39
10	C	503	71E	CBO-N	5.04	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PG-O1G	5.16	1.61	1.50
10	C	503	71E	C-NAV	5.34	1.46	1.34
10	C	503	71E	CAP-CAL	6.38	1.49	1.39
10	C	503	71E	CD1-CAF	6.65	1.49	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	503	71E	CAZ-CAX-NAV	-5.72	103.94	112.38
11	F	401	ACP	N3-C2-N1	-5.70	123.90	128.86
5	A	501	GTP	N3-C2-N1	-5.34	119.67	127.46
10	C	503	71E	CAF-CAI-CBB	-5.28	99.98	112.55
5	C	501	GTP	N3-C2-N1	-5.10	120.02	127.46
8	B	501	GDP	C6-C5-C4	-4.23	116.64	120.84
10	C	503	71E	CG-CB-CA	-4.21	101.63	113.41
8	D	501	GDP	C5-C6-N1	-3.99	117.81	123.48
8	B	501	GDP	C5-C6-N1	-3.86	117.99	123.48
11	F	401	ACP	PA-O3A-PB	-3.65	120.61	132.39
8	B	501	GDP	N3-C2-N1	-3.47	122.39	127.46
8	D	501	GDP	C6-C5-C4	-3.43	117.43	120.84
10	C	503	71E	CAD-CAE-CAF	-3.18	118.74	122.92
8	D	501	GDP	N3-C2-N1	-3.12	122.90	127.46
11	F	401	ACP	C4-C5-N7	-3.11	106.40	109.41
5	C	501	GTP	C5-C6-N1	-3.01	119.20	123.48
8	B	501	GDP	C4-C5-N7	-2.98	106.53	109.41
5	A	501	GTP	C5-C6-N1	-2.72	119.61	123.48
8	D	501	GDP	C4-C5-N7	-2.72	106.78	109.41
9	B	502	MES	C8-C7-N4	-2.67	107.61	112.45
10	C	503	71E	C-CA-N	-2.32	104.82	111.20
10	C	503	71E	O-C-NAV	-2.16	118.83	122.90
10	C	503	71E	CB-CA-N	2.02	115.08	110.80
5	A	501	GTP	N2-C2-N1	2.05	120.52	117.24
9	B	502	MES	C5-N4-C3	2.14	114.19	109.76
10	C	503	71E	CB-CG-CD2	2.19	125.33	120.91
9	B	502	MES	O3S-S-C8	2.24	108.82	106.06
10	C	503	71E	CA-C-NAV	2.37	122.12	116.78
5	A	501	GTP	C6-N1-C2	2.73	119.98	116.06
10	C	503	71E	CBP-CBO-N	2.99	120.57	116.33
9	B	502	MES	O1S-S-C8	3.00	109.36	106.79
10	C	503	71E	OAG-CAE-CAD	3.10	129.80	123.76
5	C	501	GTP	C6-N1-C2	3.15	120.58	116.06
9	B	502	MES	O2S-S-C8	3.18	109.53	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C2-N3-C4	3.73	119.51	115.16
8	D	501	GDP	C6-N1-C2	4.48	122.50	116.06
8	B	501	GDP	C6-N1-C2	4.68	122.79	116.06
8	D	501	GDP	C2-N3-C4	4.75	120.71	115.16
10	C	503	71E	CAF-CAI-CAL	4.77	121.55	114.45
8	B	501	GDP	C2-N3-C4	4.82	120.79	115.16
5	A	501	GTP	C2-N3-C4	4.91	120.89	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	502	MES	1	0
5	C	501	GTP	1	0
10	C	503	71E	2	0
8	D	501	GDP	5	0
11	F	401	ACP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	140:LYS	C	141:GLU	N	3.18

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%)	-0.24	4 (0%) 84 82	49, 74, 118, 168	0
1	C	437/451 (96%)	-0.12	3 (0%) 87 86	43, 60, 93, 140	0
2	B	417/445 (93%)	0.12	10 (2%) 59 56	46, 75, 133, 175	2 (0%)
2	D	422/445 (94%)	-0.07	11 (2%) 56 54	54, 87, 128, 180	6 (1%)
3	E	117/143 (81%)	-0.03	0 100 100	62, 88, 129, 149	0
4	F	298/384 (77%)	0.59	51 (17%) 2 1	72, 104, 165, 195	0
All	All	2128/2319 (91%)	0.02	79 (3%) 42 41	43, 79, 133, 195	8 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	401	ARG	7.1
1	A	282	TYR	5.6
4	F	101	TYR	5.6
4	F	231	ALA	5.3
4	F	169	LEU	5.3
4	F	258	GLU	5.1
4	F	259	GLY	4.8
1	C	440	VAL	4.6
2	D	404	PHE	4.6
4	F	192	LEU	4.3
4	F	323	GLU	4.3
4	F	100	ILE	4.3
4	F	182	ILE	4.0
4	F	128	ARG	3.9
2	B	371	LEU	3.8
4	F	102	PRO	3.6
4	F	130	VAL	3.5
4	F	134	ALA	3.3
4	F	166	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	132	LEU	3.2
4	F	263	PHE	3.2
2	B	276	THR	3.2
4	F	201	ILE	3.2
4	F	196	HIS	3.1
4	F	199	PHE	3.0
4	F	197	ARG	3.0
2	D	94	PHE	2.9
4	F	191	LEU	2.9
2	B	369	ARG	2.9
4	F	252	ASN	2.9
4	F	164	SER	2.9
4	F	320	MET	2.9
2	D	415	GLU	2.8
2	B	59	ASN	2.8
4	F	223	THR	2.7
4	F	148	ILE	2.7
4	F	221	LEU	2.7
2	D	416	MET	2.7
4	F	319	PHE	2.6
4	F	262	MET	2.6
4	F	163	SER	2.6
2	B	58	GLY	2.5
1	C	283	HIS	2.5
2	D	83	PHE	2.5
4	F	167	SER	2.5
4	F	260	ASN	2.5
4	F	264	PHE	2.5
2	B	370	GLY	2.5
4	F	20	LEU	2.5
2	B	322	ARG	2.5
4	F	200	ASP	2.4
2	D	59	ASN	2.4
4	F	125	THR	2.4
4	F	99	VAL	2.4
4	F	254	GLY	2.3
1	A	77	GLU	2.3
2	D	37	HIS	2.3
4	F	126	ASP	2.3
4	F	230	SER	2.3
4	F	146	VAL	2.2
1	C	438	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	177	VAL	2.2
4	F	168	GLU	2.2
4	F	171	ASP	2.2
2	B	57	THR	2.2
2	B	372	LYS	2.2
4	F	228	TYR	2.1
1	A	66[A]	VAL	2.1
4	F	340	GLN	2.1
4	F	257	GLU	2.1
4	F	198	LYS	2.1
4	F	194	PRO	2.1
2	D	418	PHE	2.1
1	A	262	TYR	2.1
2	D	57	THR	2.1
4	F	324	GLU	2.1
2	B	335	VAL	2.1
4	F	229	ASN	2.1
4	F	222	ARG	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
6	MG	B	503	1/1	0.90	0.33	8.22	84,84,84,84	0
5	GTP	C	501	32/32	0.99	0.17	0.98	38,48,59,66	0
6	MG	C	502	1/1	0.99	0.15	0.87	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GTP	A	501	32/32	0.99	0.14	0.18	48,57,70,81	0
8	GDP	B	501	28/28	0.99	0.18	0.16	47,54,64,68	0
8	GDP	D	501	28/28	0.95	0.14	-0.06	72,77,114,144	0
10	71E	C	503	47/47	0.97	0.16	-0.09	36,58,79,91	0
7	CA	A	503	1/1	0.98	0.08	-0.70	102,102,102,102	0
11	ACP	F	401	31/31	0.86	0.17	-1.21	124,139,219,237	0
9	MES	B	502	12/12	0.91	0.13	-1.77	53,83,117,122	0
6	MG	A	502	1/1	0.98	0.12	-	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.