Full wwPDB X-ray Structure Validation Report ⓘ

Dec 9, 2023 – 05:13 pm GMT

PDB ID	:	8CLG
Title	:	Epothilone A and Colchicine bound to tubulin (T2R-TTL) complex
Authors	:	Wranik, M.; Bertrand, Q.; Kepa, M.W.; Weinert, T.; Steinmetz, M.; Standfuss, J.
Deposited on	:	2023-02-16
Resolution	:	2.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

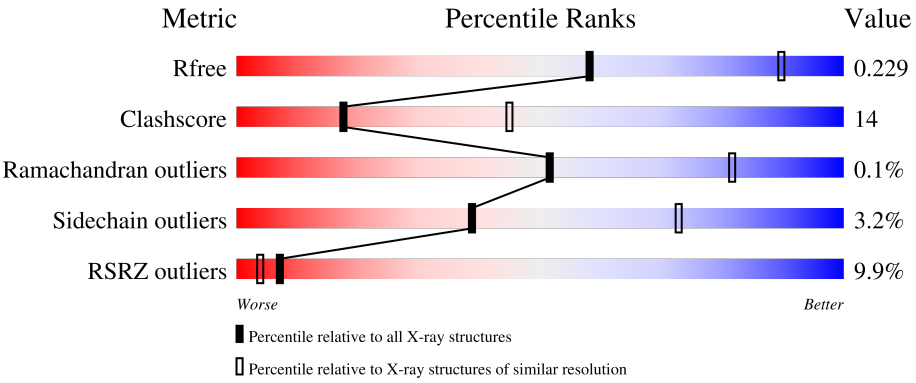
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	440	4% 83% 17%
1	C	440	3% 84% 16%
2	B	431	8% 71% 27%
2	D	431	7% 75% 24%
3	E	123	14% 81% 16%

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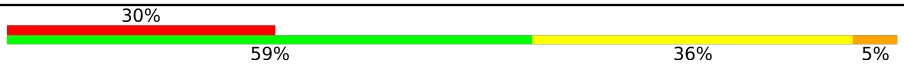
Mol	Chain	Length	Quality of chain
4	F	351	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	EP	B	503	X	-	-	-
8	EP	D	501	X	-	-	-
9	LOC	B	504	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18186 atoms, of which 103 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	12	0
			3480	2211	584	661	24			
1	C	440	Total	C	N	O	S	0	18	0
			3519	2231	588	674	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	7	15	0
			3441	2167	581	664	29			
2	D	431	Total	C	N	O	S	0	6	0
			3411	2143	580	660	28			

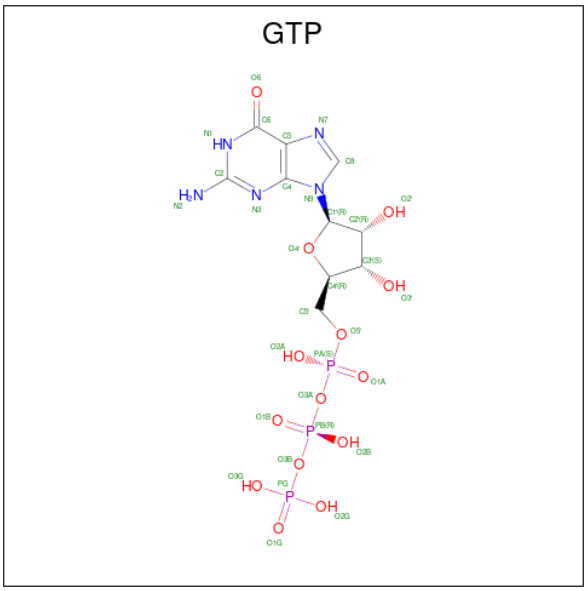
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	5	0
			1042	644	188	204	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	351	Total	C	N	O	S	18	8	0
			2890	1861	488	527	14			

- 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 32 10 5 14 3	0	0
5	C	1	Total C N O P 32 10 5 14 3	0	0

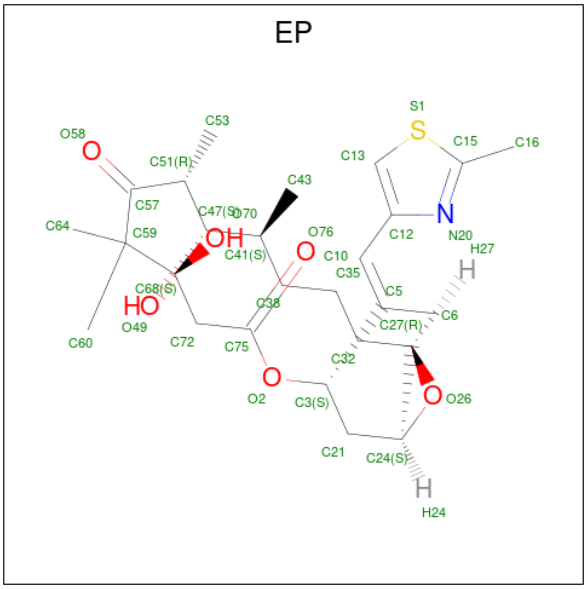
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

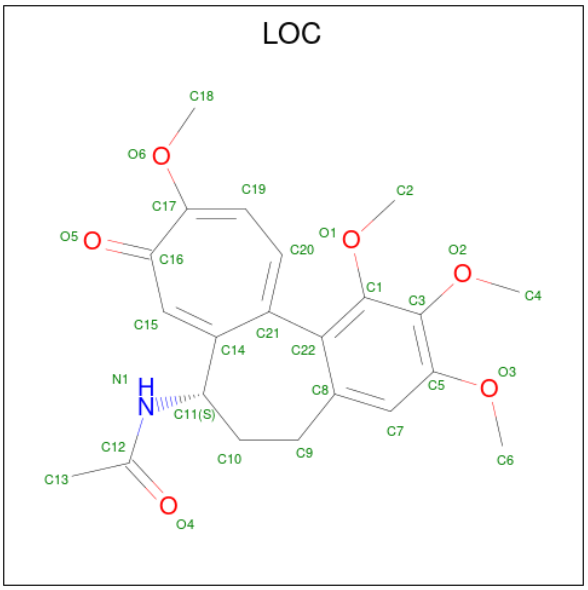
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	2	Total Ca 2 2	2	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is EPOTHILONE A (three-letter code: EP) (formula: $C_{26}H_{39}NO_6S$) (labeled as "Ligand of Interest" by depositor).



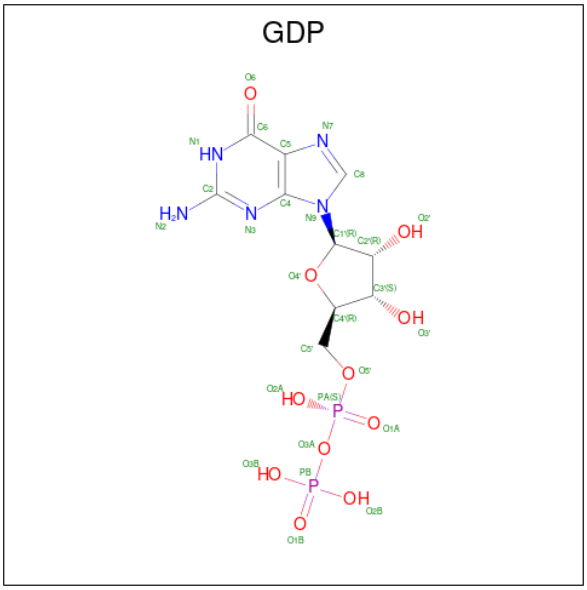
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	S	0	0
			73	26	39	1	6	1		
8	D	1	Total	C	H	N	O	S	0	0
			73	26	39	1	6	1		

- Molecule 9 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]et hanamide (three-letter code: LOC) (formula: $C_{22}H_{25}NO_6$) (labeled as "Ligand of Interest" by depositor).



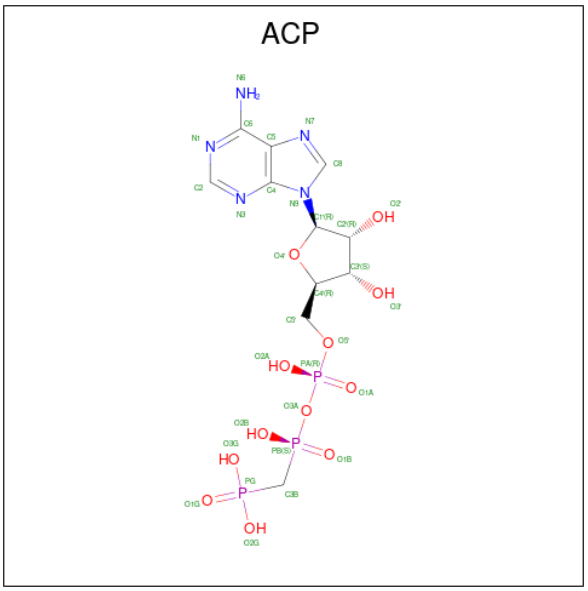
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			54	22	25	1	6		

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



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

- 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	C	N	O	P	0	0
			31	11	5	12	3		

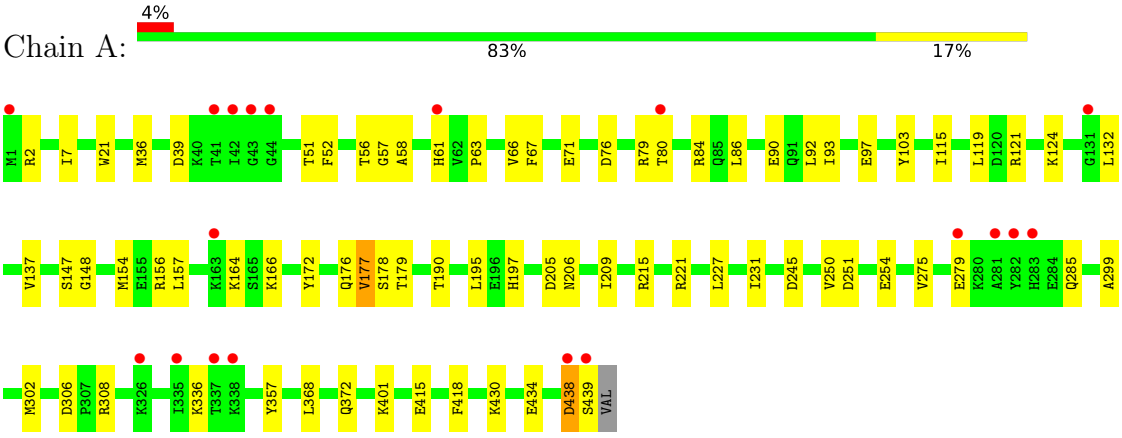
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	8	Total	O	0	0
			8	8		
12	B	9	Total	O	0	0
			9	9		
12	C	21	Total	O	0	0
			21	21		
12	D	4	Total	O	0	0
			4	4		
12	E	1	Total	O	0	0
			1	1		
12	F	1	Total	O	0	0
			1	1		

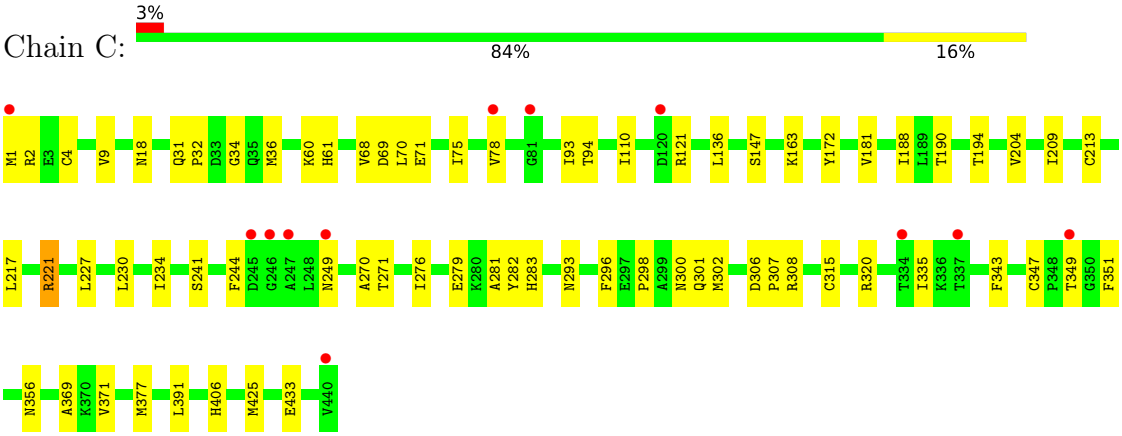
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

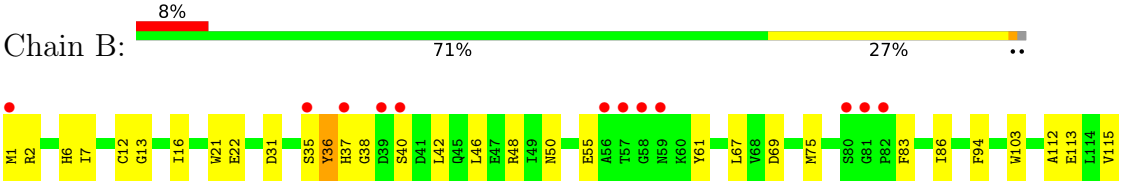
• Molecule 1: Tubulin alpha-1B chain

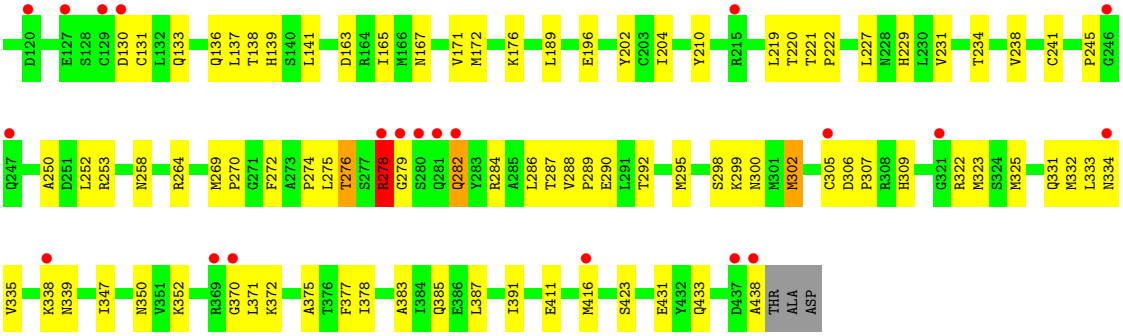


• Molecule 1: Tubulin alpha-1B chain

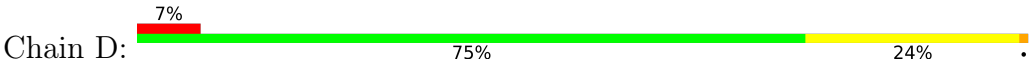


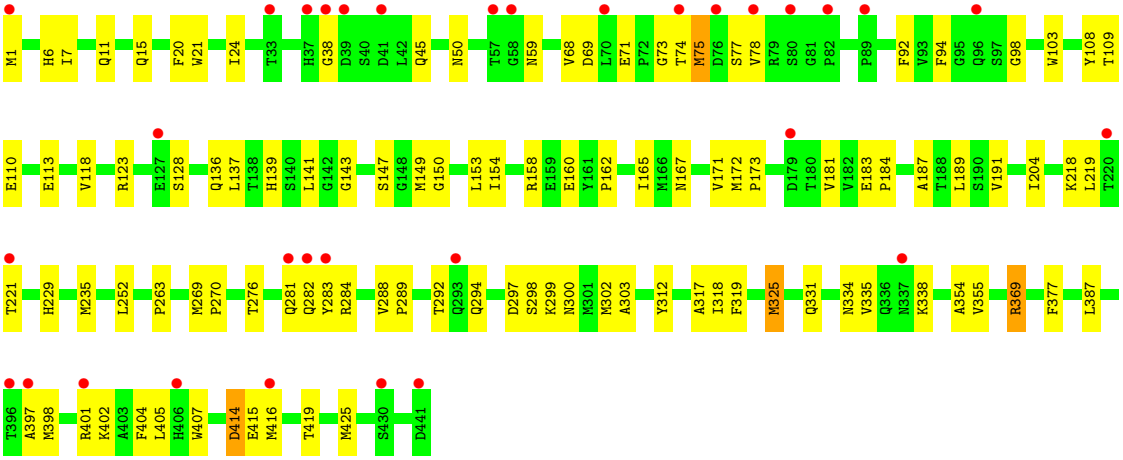
• Molecule 2: Tubulin beta-2B chain



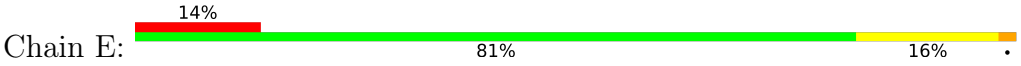


• Molecule 2: Tubulin beta-2B chain

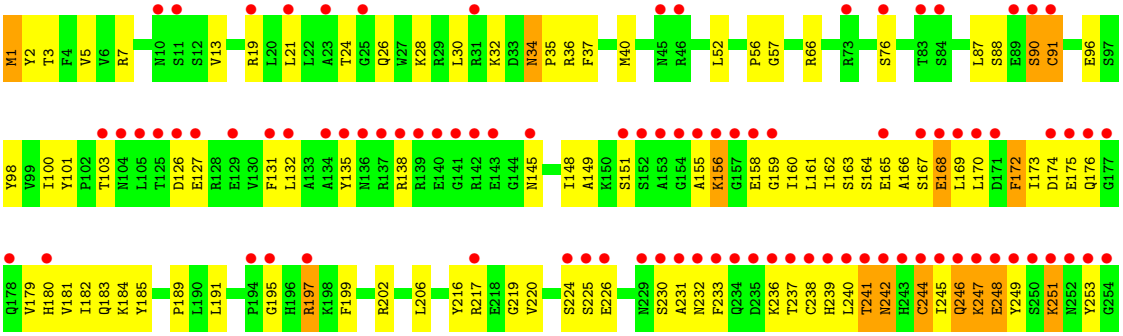


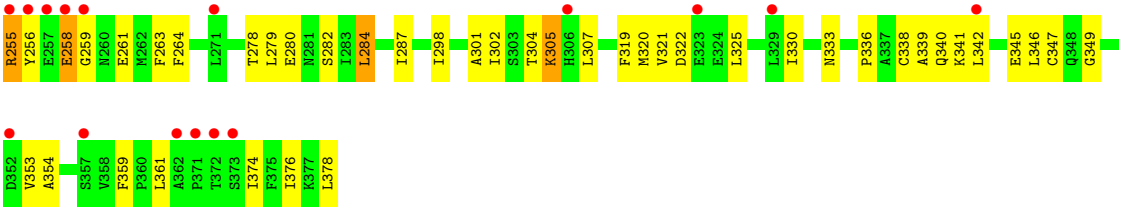


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase




R255
Y256
E257
E258
G259
N260
E261
M262
F263
F264
L271
T278
L279
E280
N281
S282
I283
L284
I287
I298
A301
I302
S303
T304
K305
H306
L307
F319
M320
V321
D322
E323
E324
L325
L329
I330
N333
P336
A337
C338
A339
Q340
K341
L342
E345
L346
C347
Q348
G349
D352
V353
A354
S357
V358
F359
P360
L361
A362
P371
T372
S373
I374
F375
I376
K377
L378

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.76Å 160.76Å 180.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.26 – 2.80 15.26 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.26-2.80) 99.9 (15.26-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20_4487	Depositor
R, R_{free}	0.178 , 0.227 0.183 , 0.229	Depositor DCC
R_{free} test set	2000 reflections (1.86%)	wwPDB-VP
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18186	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, ACP, EP, GDP, LOC, CA

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	0.49	0/3594	0.73	0/4881
1	C	0.55	0/3648	0.73	1/4955 (0.0%)
2	B	0.50	0/3555	0.78	2/4813 (0.0%)
2	D	0.48	0/3504	0.74	1/4748 (0.0%)
3	E	0.54	0/1066	0.81	2/1415 (0.1%)
4	F	0.46	0/2975	0.77	1/4022 (0.0%)
All	All	0.50	0/18342	0.75	7/24834 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
2	D	0	1
4	F	0	1
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	264	ARG	CD-NE-CZ	5.74	131.63	123.60
4	F	181	VAL	CG1-CB-CG2	5.35	119.46	110.90
2	B	264	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	D	158	ARG	CA-CB-CG	5.26	124.97	113.40
1	C	433	GLU	CA-CB-CG	5.13	124.68	113.40
3	E	119	MET	CA-CB-CG	5.10	121.97	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	119	MET	CB-CG-SD	-5.06	97.23	112.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ARG	Sidechain
2	B	278	ARG	Sidechain
2	D	369	ARG	Sidechain
4	F	255	ARG	Sidechain

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	3480	0	3427	68	0
1	C	3519	0	3458	60	2
2	B	3441	0	3356	132	2
2	D	3411	0	3306	84	0
3	E	1042	0	1065	15	0
4	F	2890	0	2894	144	0
5	A	32	0	12	0	0
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	2	0	0	0	0
7	C	1	0	0	0	0
8	B	34	39	37	14	0
8	D	34	39	37	9	0
9	B	29	25	25	9	0
10	B	28	0	12	1	0
10	D	28	0	12	2	0
11	F	31	0	14	4	0
12	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	B	9	0	0	0	0
12	C	21	0	0	0	0
12	D	4	0	0	0	0
12	E	1	0	0	0	0
12	F	1	0	0	1	0
All	All	18083	103	17667	486	2

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 14.

All (486) 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:A:221:ARG:HH21	2:B:325:MET:HE2	1.12	1.07
1:A:176:GLN:HG3	4:F:56:PRO:HB3	1.33	1.06
2:B:274:PRO:HG2	8:B:503:EP:H62	1.39	1.03
2:B:338:LYS:O	2:B:338:LYS:NZ	1.90	1.02
2:D:284:ARG:HH22	2:D:294:GLN:HE22	1.05	0.96
2:D:318:ILE:HD12	2:D:354:ALA:HB3	1.49	0.92
2:B:75:MET:HE1	2:B:94:PHE:HB3	1.51	0.91
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	1.51	0.90
4:F:167:SER:HA	4:F:170:LEU:HG	1.50	0.90
1:C:279:GLU:N	1:C:279:GLU:OE2	2.05	0.90
4:F:155:ALA:H	4:F:158:GLU:HB3	1.36	0.90
1:A:221:ARG:HH21	2:B:325:MET:CE	1.84	0.90
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.06	0.90
1:A:306:ASP:OD1	1:A:308:ARG:HD3	1.74	0.88
4:F:135:TYR:CZ	4:F:166:ALA:HB2	2.08	0.88
1:C:204:VAL:HG22	1:C:302[B]:MET:CE	2.06	0.86
4:F:161:LEU:HD23	4:F:169:LEU:HD23	1.56	0.85
2:D:1:MET:HG3	2:D:50:ASN:HD22	1.41	0.85
2:B:238[B]:VAL:HG22	2:B:378:ILE:HD11	1.60	0.83
4:F:3:THR:HB	4:F:30:LEU:HD11	1.61	0.83
1:C:204:VAL:HG22	1:C:302[B]:MET:HE3	1.61	0.82
4:F:263:PHE:HE1	4:F:341:LYS:HD3	1.44	0.82
8:B:503:EP:O2	8:B:503:EP:O70	1.91	0.81
2:D:317:ALA:O	2:D:318:ILE:HD13	1.79	0.81
2:B:278:ARG:HD2	2:B:279:GLY:HA2	1.63	0.81
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.44	0.81
2:B:331:GLN:HA	2:B:334:ASN:HD21	1.45	0.80
4:F:217:ARG:HD3	4:F:376:ILE:HG13	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:MET:HE2	1:A:154:MET:HA	1.65	0.79
2:D:334:ASN:OD1	2:D:338:LYS:HE3	1.83	0.79
2:B:305:CYS:HB3	2:B:383:ALA:O	1.82	0.79
2:B:331:GLN:HA	2:B:334:ASN:ND2	1.98	0.78
2:B:332:MET:O	2:B:335:VAL:HG12	1.84	0.77
2:B:250:ALA:HB1	9:B:504:LOC:H7	1.65	0.77
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.20	0.77
4:F:3:THR:HB	4:F:30:LEU:CD1	2.14	0.77
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.66	0.76
1:A:209[A]:ILE:HG22	1:A:227:LEU:HD22	1.68	0.76
2:D:1:MET:HG3	2:D:50:ASN:ND2	2.01	0.76
2:B:288:VAL:HG22	2:B:323:MET:HE2	1.67	0.76
2:D:276:THR:OG1	8:D:501:EP:H161	1.85	0.75
2:D:284:ARG:HH22	2:D:294:GLN:NE2	1.82	0.75
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.67	0.74
4:F:3:THR:OG1	4:F:37:PHE:HA	1.87	0.74
2:D:1:MET:CG	2:D:50:ASN:HD22	2.00	0.74
1:A:176:GLN:CG	4:F:56:PRO:HB3	2.14	0.73
4:F:173:ILE:HD13	4:F:180:HIS:HB2	1.69	0.73
4:F:184:LYS:HD2	4:F:185:TYR:N	2.02	0.72
1:A:179:THR:O	2:B:352:LYS:HE2	1.88	0.72
2:B:370:GLY:O	2:B:371:LEU:HD13	1.89	0.72
4:F:32:LYS:HD3	4:F:32:LYS:N	2.04	0.71
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.31	0.71
4:F:167:SER:HA	4:F:170:LEU:CG	2.20	0.71
1:A:56:THR:HG22	1:A:58:ALA:H	1.53	0.71
2:B:75:MET:HE1	2:B:94:PHE:CB	2.19	0.71
2:B:276:THR:OG1	8:B:503:EP:H13	1.90	0.71
4:F:131:PHE:HE1	4:F:182:ILE:HG21	1.52	0.71
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.24	0.70
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.25	0.70
2:B:75:MET:CE	2:B:94:PHE:HB3	2.21	0.70
2:D:1:MET:HG3	2:D:50:ASN:CB	2.22	0.70
2:B:83:PHE:O	2:B:86:ILE:HG22	1.92	0.69
1:A:97:GLU:OE1	2:B:1:MET:HE2	1.92	0.69
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.27	0.69
2:B:75:MET:HE1	2:B:94:PHE:CG	2.28	0.69
2:D:59:ASN:OD1	2:D:59:ASN:O	2.11	0.69
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.74	0.69
2:B:2:ARG:HB2	2:B:2:ARG:CZ	2.22	0.69
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:GLY:O	2:B:282:GLN:HB3	1.92	0.68
4:F:195:GLY:HA3	4:F:197:ARG:HD2	1.74	0.68
2:B:36:TYR:CD2	2:B:46:LEU:HD21	2.28	0.68
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.34	0.68
1:A:215:ARG:NH1	1:A:299:ALA:HB1	2.09	0.68
1:C:18:ASN:ND2	1:C:78:VAL:HG22	2.09	0.67
4:F:34:ASN:HD22	4:F:35:PRO:HD2	1.59	0.67
2:B:295[A]:MET:HE2	2:B:377:PHE:HB2	1.76	0.67
2:B:229:HIS:CG	8:B:503:EP:H433	2.30	0.66
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.31	0.66
1:A:401:LYS:HE2	2:B:438:ALA:HB1	1.77	0.66
1:C:270:ALA:O	1:C:302[B]:MET:HG3	1.95	0.66
2:B:250:ALA:HB3	9:B:504:LOC:H6B	1.76	0.66
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.26	0.66
2:B:287:THR:OG1	2:B:289:PRO:HD2	1.96	0.65
2:B:385:GLN:HE22	2:B:433:GLN:NE2	1.94	0.65
2:B:241[B]:CYS:HB2	9:B:504:LOC:H6B	1.79	0.65
2:D:416:MET:HA	2:D:419:THR:OG1	1.97	0.65
4:F:330:ILE:HG21	11:F:401:ACP:H5'2	1.79	0.65
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.14	0.65
2:D:141:LEU:HD12	2:D:172:MET:SD	2.36	0.65
1:A:166:LYS:HE2	1:A:197:HIS:O	1.97	0.64
4:F:30:LEU:HD22	4:F:34:ASN:OD1	1.98	0.64
3:E:44:ASP:HB3	3:E:45:PRO:HD3	1.79	0.64
2:B:238[B]:VAL:HG22	2:B:378:ILE:CD1	2.26	0.64
1:C:244:PHE:HB2	1:C:356[B]:ASN:HD21	1.61	0.64
2:B:274:PRO:HG2	8:B:503:EP:C6	2.22	0.63
2:D:317:ALA:C	2:D:318:ILE:HD13	2.19	0.63
4:F:132:LEU:HD21	4:F:170:LEU:HD23	1.80	0.63
1:C:276:ILE:CD1	1:C:369:ALA:HB3	2.28	0.63
2:D:276:THR:HB	2:D:281:GLN:HG3	1.79	0.63
1:A:285:GLN:HA	1:A:285:GLN:OE1	1.99	0.63
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.33	0.63
1:A:250:VAL:HG12	1:A:254:GLU:OE1	1.97	0.63
1:A:285:GLN:HG3	1:A:372[B]:GLN:NE2	2.14	0.63
2:B:241[B]:CYS:HB2	9:B:504:LOC:C6	2.29	0.62
4:F:172:PHE:O	4:F:172:PHE:CD1	2.52	0.62
4:F:202:ARG:HB3	4:F:220[B]:VAL:HG12	1.82	0.62
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.81	0.62
4:F:258:GLU:N	4:F:258:GLU:OE1	2.33	0.62
2:B:221:THR:HG22	2:B:221:THR:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1:MET:HE3	4:F:28:LYS:HG2	1.82	0.61
4:F:349:GLY:O	4:F:353[B]:VAL:HG12	1.99	0.61
2:B:136:GLN:HA	2:B:167:ASN:O	2.00	0.61
4:F:172:PHE:O	4:F:172:PHE:HD1	1.84	0.61
1:A:79:ARG:O	1:A:84:ARG:HB2	2.01	0.60
2:B:75:MET:HE1	2:B:94:PHE:CD2	2.37	0.60
1:C:276:ILE:HD12	1:C:276:ILE:O	2.02	0.60
2:B:338:LYS:HG3	2:B:339:ASN:OD1	2.01	0.60
4:F:151:SER:HG	4:F:180:HIS:CE1	2.20	0.60
4:F:172:PHE:O	4:F:175:GLU:HB3	2.02	0.59
4:F:225:SER:H	4:F:246:GLN:HE22	1.50	0.59
1:C:276:ILE:HD13	1:C:281:ALA:HB2	1.83	0.59
2:D:11:GLN:HB3	10:D:502:GDP:O2A	2.02	0.59
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.36	0.59
2:D:294:GLN:HG2	2:D:300:ASN:ND2	2.17	0.59
2:B:141:LEU:HD12	2:B:172:MET:SD	2.42	0.59
2:B:36:TYR:HE1	2:B:38:GLY:HA3	1.68	0.58
1:C:296:PHE:HZ	1:C:351:PHE:HE2	1.50	0.58
2:D:183:GLU:N	2:D:184:PRO:HD2	2.18	0.58
2:B:36:TYR:CE2	2:B:46:LEU:CD1	2.86	0.58
1:A:336:LYS:HD3	1:A:336:LYS:O	2.02	0.58
2:B:2:ARG:NH2	2:B:131:CYS:SG	2.76	0.58
4:F:135:TYR:CE1	4:F:166:ALA:HB2	2.38	0.58
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.38	0.58
2:B:46:LEU:N	2:B:46:LEU:HD12	2.19	0.58
2:B:278:ARG:HE	2:B:282:GLN:HE21	1.50	0.58
2:B:333:LEU:HD13	4:F:57:GLY:HA3	1.85	0.58
4:F:339:ALA:HB3	4:F:342:LEU:HD12	1.85	0.58
2:B:229:HIS:ND1	8:B:503:EP:H433	2.18	0.58
2:D:276:THR:H	8:D:501:EP:H62	1.68	0.58
8:D:501:EP:C75	8:D:501:EP:C6	2.82	0.58
1:C:293[B]:ASN:OD1	1:C:335:ILE:HD11	2.04	0.58
4:F:34:ASN:HD22	4:F:35:PRO:CD	2.16	0.58
4:F:132:LEU:HD21	4:F:170:LEU:CD2	2.34	0.58
2:B:69:ASP:O	2:B:94:PHE:HA	2.04	0.57
2:D:404:PHE:O	2:D:407:TRP:HB2	2.03	0.57
1:A:90:GLU:HG2	1:A:124:LYS:NZ	2.20	0.57
2:D:229:HIS:CB	8:D:501:EP:H433	2.33	0.57
4:F:225:SER:O	4:F:253:TYR:HB3	2.04	0.57
1:C:271:THR:HG23	1:C:300:ASN:O	2.04	0.57
2:B:292:THR:O	2:B:295[A]:MET:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:162:PRO:HB2	3:E:119:MET:HE1	1.86	0.57
2:B:202:TYR:CZ	2:B:238[B]:VAL:HG11	2.40	0.57
1:C:70:LEU:HD13	1:C:110:ILE:CG2	2.35	0.57
4:F:162:ILE:HG13	4:F:236:LYS:HE3	1.87	0.56
1:C:270:ALA:HB3	1:C:302[B]:MET:HG3	1.88	0.56
1:C:315[B]:CYS:SG	1:C:377:MET:SD	3.03	0.56
4:F:96:GLU:OE2	4:F:98:TYR:OH	2.20	0.56
4:F:131:PHE:HE1	4:F:182:ILE:CG2	2.18	0.56
4:F:165:GLU:HB2	4:F:168:GLU:HB3	1.87	0.56
2:D:191:VAL:HG11	2:D:425:MET:HE3	1.88	0.56
8:D:501:EP:C75	8:D:501:EP:H61	2.36	0.56
4:F:161:LEU:HD23	4:F:169:LEU:CD2	2.32	0.56
2:B:288:VAL:HG22	2:B:323:MET:CE	2.35	0.56
1:A:177:VAL:HG21	1:A:206:ASN:HB3	1.86	0.56
2:B:295[B]:MET:SD	2:B:375:ALA:HB1	2.46	0.56
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	1.87	0.56
1:C:301:GLN:NE2	1:C:307:PRO:HG2	2.21	0.56
4:F:5:VAL:HG13	4:F:32:LYS:HA	1.88	0.56
4:F:330:ILE:N	4:F:330:ILE:HD13	2.21	0.56
1:A:176:GLN:HG3	4:F:56:PRO:CB	2.22	0.55
2:B:36:TYR:CE1	2:B:38:GLY:N	2.74	0.55
2:D:123:ARG:NH1	2:D:160:GLU:OE1	2.38	0.55
2:D:171:VAL:HA	2:D:204:ILE:O	2.06	0.55
4:F:131:PHE:O	4:F:135:TYR:HB2	2.05	0.55
1:C:343:PHE:HB2	1:C:349:THR:HG22	1.88	0.55
4:F:345:GLU:O	4:F:347:CYS:N	2.39	0.55
2:B:176:LYS:HD3	2:B:210:TYR:CD2	2.42	0.55
2:B:250:ALA:HB3	9:B:504:LOC:C6	2.37	0.55
2:B:370:GLY:C	2:B:371:LEU:HD22	2.27	0.55
4:F:263:PHE:HE1	4:F:341:LYS:CD	2.18	0.55
4:F:320:MET:HB2	4:F:330:ILE:HD11	1.89	0.55
2:B:227:LEU:O	2:B:231:VAL:HG23	2.05	0.55
2:B:234:THR:O	2:B:238[A]:VAL:HG13	2.07	0.55
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.89	0.55
2:B:288:VAL:CG2	2:B:323:MET:HE2	2.35	0.54
2:D:136:GLN:HA	2:D:167:ASN:O	2.06	0.54
4:F:161:LEU:HB2	4:F:172:PHE:CD2	2.41	0.54
4:F:233:PHE:O	4:F:236:LYS:HG3	2.07	0.54
4:F:191:LEU:HD12	4:F:197:ARG:O	2.06	0.54
4:F:253:TYR:HB2	4:F:256:TYR:CZ	2.43	0.54
1:A:76:ASP:O	1:A:80[A]:THR:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:THR:O	2:D:78:VAL:HG23	2.07	0.54
2:D:276:THR:H	8:D:501:EP:C6	2.20	0.54
2:D:297:ASP:OD2	2:D:299:LYS:HG2	2.08	0.54
4:F:135:TYR:OH	4:F:164:SER:O	2.24	0.54
2:B:219:LEU:HD11	8:B:503:EP:H532	1.89	0.54
2:B:284:ARG:NH2	2:B:290:GLU:OE2	2.40	0.54
2:B:295[B]:MET:CG	2:B:377:PHE:HB2	2.38	0.54
2:B:298:SER:HB2	2:B:307:PRO:HD2	1.88	0.54
2:D:414:ASP:OD2	2:D:414:ASP:N	2.41	0.54
1:A:36:MET:HB3	1:A:61:HIS:NE2	2.23	0.53
1:A:206:ASN:OD1	1:A:209[B]:ILE:HD11	2.08	0.53
1:A:221:ARG:NH2	2:B:325:MET:HE2	1.98	0.53
1:C:1:MET:HG2	1:C:2:ARG:CZ	2.37	0.53
2:B:269:MET:CE	2:B:305:CYS:HB2	2.39	0.53
4:F:131:PHE:CE1	4:F:182:ILE:CG2	2.87	0.53
1:C:209:ILE:HD11	1:C:302[A]:MET:SD	2.48	0.53
4:F:225:SER:H	4:F:246:GLN:NE2	2.06	0.53
1:C:31:GLN:HB3	1:C:32:PRO:HD2	1.90	0.53
1:A:221:ARG:NH2	2:B:325:MET:CE	2.64	0.53
4:F:224:SER:OG	4:F:238:CYS:HA	2.08	0.53
1:C:234:ILE:HG12	1:C:302[B]:MET:SD	2.49	0.53
4:F:138:ARG:C	4:F:145:ASN:HD21	2.11	0.53
1:A:97:GLU:OE1	2:B:1:MET:CE	2.57	0.53
4:F:278:THR:O	4:F:282:SER:OG	2.26	0.53
1:A:154:MET:HE2	1:A:154:MET:CA	2.35	0.52
2:B:278:ARG:NH1	2:B:278:ARG:HG3	2.25	0.52
2:B:1:MET:SD	2:B:133:GLN:HG3	2.49	0.52
4:F:160:ILE:HD12	4:F:160:ILE:N	2.24	0.52
4:F:259:GLY:O	4:F:261:GLU:HG3	2.09	0.52
1:A:209[A]:ILE:HG22	1:A:227:LEU:CD2	2.38	0.52
4:F:191:LEU:HA	4:F:197:ARG:O	2.10	0.52
8:D:501:EP:H61	8:D:501:EP:O76	2.09	0.52
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.92	0.52
4:F:161:LEU:HB2	4:F:172:PHE:CE2	2.45	0.52
2:B:286:LEU:HD11	8:B:503:EP:S1	2.50	0.51
4:F:199:PHE:O	4:F:320:MET:HE3	2.10	0.51
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.93	0.51
2:B:55:GLU:HG2	2:B:61:TYR:CE1	2.45	0.51
1:C:301:GLN:HE22	1:C:307:PRO:HG2	1.75	0.51
2:D:143:GLY:O	2:D:147[B]:SER:OG	2.28	0.51
2:D:181:VAL:HB	2:D:398:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:173:ILE:HD13	4:F:180:HIS:CB	2.40	0.51
1:C:1:MET:HG2	1:C:2:ARG:NH2	2.26	0.51
1:C:75:ILE:HD12	1:C:94:THR:CG2	2.40	0.51
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.91	0.51
4:F:32:LYS:HD3	4:F:32:LYS:H	1.74	0.51
4:F:280:GLU:HG2	4:F:284[B]:LEU:HD12	1.93	0.51
1:A:39:ASP:OD2	1:A:61:HIS:HE1	1.94	0.51
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.93	0.51
4:F:245:ILE:HA	4:F:248:GLU:HB3	1.93	0.51
4:F:21:LEU:O	4:F:24:THR:HG23	2.10	0.51
1:C:343:PHE:CG	1:C:349:THR:HG22	2.46	0.51
2:D:319:PHE:HB2	2:D:355:VAL:HG22	1.93	0.51
2:B:220:THR:O	2:B:222:PRO:HD3	2.11	0.50
4:F:220[B]:VAL:HG23	4:F:263:PHE:CE2	2.46	0.50
9:B:504:LOC:H4A	9:B:504:LOC:O1	2.11	0.50
1:C:9:VAL:HG22	1:C:68[B]:VAL:CG1	2.41	0.50
2:D:191:VAL:CG1	2:D:425:MET:HE3	2.41	0.50
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.92	0.50
3:E:111:ASN:N	3:E:111:ASN:HD22	2.09	0.50
4:F:241:THR:N	11:F:401:ACP:O3'	2.45	0.50
1:A:245:ASP:O	3:E:16:SER:HB2	2.11	0.49
1:A:285:GLN:HG3	1:A:372[B]:GLN:CD	2.32	0.49
2:B:171:VAL:HA	2:B:204:ILE:O	2.12	0.49
1:C:241:SER:HA	1:C:249:ASN:HD21	1.77	0.49
2:D:143:GLY:HA3	10:D:502:GDP:O3A	2.12	0.49
2:D:191:VAL:HG11	2:D:425:MET:CE	2.42	0.49
2:D:284:ARG:NH2	2:D:294:GLN:HE22	1.90	0.49
4:F:244:CYS:O	4:F:246:GLN:N	2.45	0.49
2:B:387:LEU:O	2:B:391:ILE:HD12	2.12	0.49
1:C:351:PHE:CD1	1:C:351:PHE:N	2.81	0.49
2:D:74:THR:O	2:D:75:MET:C	2.50	0.49
2:B:1:MET:HE3	2:B:253:ARG:HH11	1.78	0.49
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.95	0.49
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG23	1.94	0.49
1:A:67:PHE:HB2	1:A:92:LEU:HD23	1.95	0.49
1:C:221:ARG:HG3	2:D:325:MET:HB3	1.94	0.49
4:F:1:MET:CE	4:F:28:LYS:HG2	2.42	0.49
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.48	0.49
2:B:305:CYS:O	2:B:306:ASP:C	2.51	0.48
4:F:189:PRO:O	4:F:191:LEU:HD22	2.13	0.48
2:B:1:MET:CE	2:B:253:ARG:NH1	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TYR:CD1	2:B:37:HIS:N	2.81	0.48
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.48	0.48
4:F:172:PHE:CD1	4:F:172:PHE:C	2.87	0.48
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.94	0.48
2:D:74:THR:HA	2:D:77:SER:OG	2.13	0.48
4:F:172:PHE:HE1	4:F:176:GLN:OE1	1.95	0.48
2:B:250:ALA:HB1	9:B:504:LOC:C7	2.41	0.48
1:C:270:ALA:C	1:C:302[B]:MET:HG3	2.34	0.48
4:F:163:SER:OG	4:F:169:LEU:HG	2.13	0.48
1:C:1:MET:CG	1:C:2:ARG:CZ	2.91	0.48
2:D:11:GLN:O	2:D:15:GLN:HG2	2.13	0.48
2:D:75:MET:HG3	2:D:92:PHE:HD2	1.78	0.48
4:F:216:TYR:CE1	4:F:374:ILE:HD13	2.49	0.48
4:F:226:GLU:HG3	4:F:237:THR:HG21	1.95	0.48
2:B:36:TYR:HE1	2:B:38:GLY:CA	2.27	0.48
4:F:40:MET:SD	4:F:52:LEU:HD21	2.53	0.48
2:B:36:TYR:HD1	2:B:37:HIS:N	2.12	0.48
4:F:3:THR:HB	4:F:30:LEU:HD12	1.94	0.48
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.47
4:F:90:SER:O	4:F:91:CYS:C	2.52	0.47
4:F:162:ILE:HB	4:F:233:PHE:HD2	1.78	0.47
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.95	0.47
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.96	0.47
4:F:226:GLU:HG3	4:F:237:THR:CG2	2.44	0.47
4:F:263:PHE:CE1	4:F:341:LYS:HE3	2.50	0.47
2:D:149:MET:HB3	2:D:149:MET:HE2	1.74	0.47
2:D:402:LYS:CE	2:D:415:GLU:OE2	2.63	0.47
4:F:199:PHE:O	4:F:320:MET:CE	2.62	0.47
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.95	0.47
4:F:34:ASN:HD22	4:F:35:PRO:N	2.12	0.47
2:B:1:MET:HE1	2:B:253:ARG:HH12	1.79	0.47
2:B:322:ARG:HH11	2:B:322:ARG:HB2	1.80	0.47
4:F:126:ASP:OD1	4:F:127:GLU:N	2.47	0.47
1:A:51[B]:THR:HG22	1:A:52:PHE:CD1	2.49	0.47
4:F:32:LYS:H	4:F:32:LYS:CD	2.27	0.47
4:F:148:ILE:HG12	4:F:149:ALA:N	2.29	0.47
4:F:333:ASN:HB3	12:F:501:HOH:O	2.15	0.47
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.50	0.47
1:C:190:THR:O	1:C:194[B]:THR:HG23	2.15	0.47
3:E:138:GLU:O	3:E:139:LEU:HD23	2.15	0.47
4:F:138:ARG:HB2	4:F:145:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:ASP:HB3	2:B:309:HIS:CE1	2.50	0.46
2:B:7:ILE:O	2:B:137:LEU:HA	2.16	0.46
1:C:276:ILE:HD13	1:C:369:ALA:HB3	1.97	0.46
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.97	0.46
1:A:132:LEU:O	1:A:164:LYS:NZ	2.32	0.46
2:B:42:LEU:HD22	2:B:245:PRO:HD2	1.97	0.46
1:C:204:VAL:HG22	1:C:302[B]:MET:HE1	1.91	0.46
2:D:141:LEU:HA	2:D:147[B]:SER:HB3	1.97	0.46
4:F:258:GLU:H	4:F:258:GLU:CD	2.17	0.46
1:A:56:THR:HG22	1:A:57:GLY:N	2.30	0.46
2:B:163:ASP:O	2:B:253:ARG:NH2	2.46	0.46
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.97	0.46
1:A:438:ASP:O	1:A:439:SER:C	2.54	0.46
2:B:302:MET:HE3	2:B:302:MET:HB3	1.86	0.46
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.97	0.46
4:F:100:ILE:HD13	4:F:126:ASP:OD1	2.15	0.46
2:B:275:LEU:HA	8:B:503:EP:O76	2.15	0.46
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.51	0.46
1:C:343:PHE:CB	1:C:349:THR:HG22	2.46	0.46
2:D:276:THR:HG1	8:D:501:EP:H161	1.80	0.46
4:F:237:THR:HG21	4:F:251:LYS:HD3	1.98	0.46
4:F:148:ILE:HG13	4:F:160:ILE:HG23	1.97	0.46
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.51	0.46
2:D:229:HIS:HB3	8:D:501:EP:H433	1.97	0.46
2:B:371:LEU:CD1	8:B:503:EP:H63	2.46	0.45
1:A:156:ARG:HD2	1:A:156:ARG:HA	1.78	0.45
2:B:272:PHE:O	2:B:300:ASN:OD1	2.35	0.45
2:D:404:PHE:O	2:D:405:LEU:C	2.54	0.45
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.99	0.45
2:B:258:ASN:O	9:B:504:LOC:H18A	2.16	0.45
2:D:172:MET:HA	2:D:173:PRO:HD3	1.86	0.45
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.97	0.45
2:B:133:GLN:OE1	2:B:252:LEU:HG	2.16	0.45
2:D:68:VAL:HG12	2:D:149:MET:HE1	1.99	0.45
3:E:81:GLU:O	3:E:84[B]:GLN:HG2	2.16	0.45
4:F:13:VAL:HG21	4:F:336:PRO:O	2.16	0.45
4:F:34:ASN:HD22	4:F:34:ASN:C	2.20	0.45
2:B:269:MET:HE3	2:B:305:CYS:HB2	1.98	0.45
1:C:69:ASP:O	1:C:94:THR:HA	2.17	0.45
2:B:229:HIS:ND1	8:B:503:EP:H382	2.32	0.45
4:F:148:ILE:CG1	4:F:149:ALA:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:284[A]:LEU:HD12	4:F:284[A]:LEU:HA	1.76	0.45
1:C:213:CYS:O	1:C:217:LEU:HB2	2.17	0.45
2:D:69:ASP:O	2:D:94:PHE:HA	2.17	0.45
4:F:103:THR:HG23	4:F:174:ASP:OD2	2.17	0.45
2:D:172:MET:HG3	2:D:387:LEU:HD21	1.99	0.45
4:F:148:ILE:HG22	4:F:183:GLN:O	2.15	0.45
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.52	0.44
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.96	0.44
2:D:123:ARG:NH1	2:D:160:GLU:OE2	2.50	0.44
2:B:2:ARG:HG2	2:B:50[B]:ASN:OD1	2.16	0.44
2:B:276:THR:CB	8:B:503:EP:H13	2.47	0.44
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.35	0.44
2:D:288:VAL:HG12	2:D:331:GLN:HG3	1.98	0.44
4:F:184:LYS:HD2	4:F:184:LYS:C	2.37	0.44
1:A:137:VAL:HG21	1:A:154:MET:CE	2.47	0.44
1:A:308:ARG:HH21	4:F:301:ALA:C	2.21	0.44
2:D:294:GLN:CG	2:D:300:ASN:ND2	2.80	0.44
1:A:115:ILE:O	1:A:119:LEU:HD22	2.17	0.44
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.52	0.44
4:F:159:GLY:C	4:F:160:ILE:HD12	2.37	0.44
4:F:338:CYS:SG	4:F:339:ALA:N	2.90	0.44
1:C:147:SER:HB2	1:C:190:THR:HB	1.99	0.44
4:F:131:PHE:C	4:F:131:PHE:CD2	2.91	0.44
1:A:154:MET:CE	1:A:157:LEU:HD12	2.48	0.44
1:A:415:GLU:O	1:A:418:PHE:HB2	2.17	0.44
2:B:36:TYR:CZ	2:B:46:LEU:CD1	2.99	0.44
1:C:306:ASP:OD1	1:C:308:ARG:HG3	2.18	0.43
4:F:100:ILE:HD13	4:F:100:ILE:HA	1.83	0.43
4:F:101:TYR:HD1	4:F:179:VAL:HG22	1.82	0.43
1:A:430:LYS:HD3	1:A:434:GLU:OE1	2.18	0.43
3:E:75:LYS:HE3	3:E:75:LYS:HB3	1.42	0.43
1:A:115:ILE:HG13	1:A:119:LEU:CD2	2.48	0.43
2:B:295[B]:MET:HG2	2:B:377:PHE:HB2	1.99	0.43
4:F:26:GLN:HB2	4:F:361:LEU:HD12	2.00	0.43
1:A:279:GLU:HA	1:A:279:GLU:OE1	2.18	0.43
4:F:298[B]:ILE:HG12	4:F:298[B]:ILE:O	2.17	0.43
1:A:147:SER:HB2	1:A:190:THR:HB	2.01	0.43
2:B:40:SER:OG	2:B:42:LEU:HB2	2.19	0.43
2:B:141:LEU:CD1	2:B:172:MET:CE	2.97	0.43
2:B:250:ALA:CB	9:B:504:LOC:H7	2.43	0.43
2:D:397:ALA:O	2:D:401:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:HG3	3:E:24:LEU:CD1	2.48	0.43
2:B:75:MET:HE2	2:B:75:MET:HB2	1.81	0.43
2:B:385:GLN:HE22	2:B:433:GLN:HE22	1.65	0.43
1:C:298:PRO:HA	1:C:301:GLN:NE2	2.33	0.43
2:D:294:GLN:CG	2:D:300:ASN:HD22	2.32	0.43
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.99	0.43
4:F:325:LEU:HD23	4:F:325:LEU:HA	1.67	0.43
2:B:31:ASP:OD1	2:B:35:SER:O	2.36	0.43
2:B:1:MET:HE1	2:B:253:ARG:NH1	2.34	0.43
2:D:103:TRP:HD1	2:D:147[A]:SER:OG	2.02	0.43
4:F:226:GLU:CG	4:F:237:THR:HG23	2.49	0.43
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.54	0.43
2:B:141:LEU:HD12	2:B:172:MET:CE	2.49	0.43
4:F:247:LYS:HZ1	4:F:259:GLY:HA2	1.84	0.43
1:C:230:LEU:O	1:C:234:ILE:HD12	2.19	0.42
1:C:209:ILE:HD11	1:C:302[A]:MET:HG3	2.02	0.42
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.19	0.42
4:F:279:LEU:HG	4:F:284[B]:LEU:HG	2.00	0.42
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.00	0.42
2:B:371:LEU:HD11	8:B:503:EP:H63	2.00	0.42
2:D:20:PHE:CD1	2:D:235:MET:HE2	2.54	0.42
4:F:263:PHE:CE1	4:F:341:LYS:HD3	2.36	0.42
2:B:1:MET:HE3	2:B:253:ARG:NH1	2.34	0.42
2:D:7:ILE:O	2:D:137:LEU:HA	2.19	0.42
4:F:184:LYS:HD2	4:F:185:TYR:H	1.79	0.42
1:A:63:PRO:CD	1:A:86:LEU:HG	2.50	0.42
3:E:47:LEU:HD23	3:E:47:LEU:O	2.20	0.42
4:F:239:HIS:O	4:F:240:LEU:C	2.58	0.42
2:B:48:ARG:HH21	2:B:245:PRO:HA	1.84	0.42
2:B:229:HIS:ND1	8:B:503:EP:C38	2.83	0.42
2:D:71:GLU:HG2	2:D:98:GLY:HA2	2.00	0.42
4:F:376:ILE:HG22	4:F:378:LEU:CD1	2.50	0.42
2:D:218:LYS:O	2:D:219:LEU:HD23	2.20	0.42
4:F:5:VAL:HG12	4:F:7:ARG:HG3	2.02	0.42
4:F:304:THR:HG22	4:F:307:LEU:HD12	2.01	0.42
4:F:279:LEU:O	4:F:284[B]:LEU:HG	2.20	0.42
4:F:340:GLN:CD	4:F:340:GLN:H	2.23	0.42
2:B:287:THR:HG22	2:B:290:GLU:OE1	2.20	0.42
1:C:276:ILE:HD11	1:C:371:VAL:CG1	2.49	0.42
2:D:123:ARG:NH1	2:D:160:GLU:CD	2.73	0.42
2:D:282:GLN:HG3	2:D:283:TYR:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HA	1:A:66[B]:VAL:HG23	2.02	0.42
2:B:13:GLY:CA	2:B:138[B]:THR:HG22	2.35	0.42
2:B:270:PRO:HG2	2:B:302:MET:HB2	2.02	0.42
2:B:305:CYS:SG	2:B:387:LEU:HB2	2.60	0.42
4:F:101:TYR:CD1	4:F:179:VAL:HG22	2.54	0.42
2:B:112:ALA:O	2:B:115:VAL:HG12	2.20	0.41
1:A:56:THR:CG2	1:A:57:GLY:N	2.83	0.41
1:A:177:VAL:HG12	1:A:178:SER:N	2.35	0.41
1:A:357:TYR:CD2	3:E:17:GLY:HA2	2.55	0.41
2:D:109:THR:O	2:D:113:GLU:HG3	2.20	0.41
2:D:110:GLU:O	2:D:113:GLU:HB2	2.20	0.41
4:F:195:GLY:C	4:F:197:ARG:HG3	2.40	0.41
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.03	0.41
2:B:2:ARG:HB2	2:B:2:ARG:NH1	2.35	0.41
1:C:302[B]:MET:HE3	1:C:302[B]:MET:HB3	1.94	0.41
3:E:58:GLU:HA	3:E:61:ARG:NH2	2.35	0.41
4:F:298[B]:ILE:HG12	4:F:302:ILE:HG23	2.02	0.41
1:A:51[B]:THR:HG22	1:A:52:PHE:HD1	1.86	0.41
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.79	0.41
1:A:285:GLN:OE1	1:A:285:GLN:CA	2.68	0.41
2:B:12:CYS:HB2	10:B:505:GDP:C8	2.56	0.41
4:F:305:LYS:HD3	4:F:305:LYS:HA	1.72	0.41
4:F:330:ILE:HG21	11:F:401:ACP:C5'	2.47	0.41
2:B:36:TYR:CE1	2:B:38:GLY:CA	3.03	0.41
2:D:108:TYR:O	3:E:134:ARG:HD3	2.20	0.41
2:D:173:PRO:HG2	2:D:187:ALA:HB2	2.02	0.41
2:D:150:GLY:O	2:D:154:ILE:HG13	2.21	0.41
4:F:155:ALA:O	4:F:156:LYS:C	2.59	0.41
4:F:263:PHE:CD1	4:F:341:LYS:HE3	2.55	0.41
1:C:249:ASN:CG	1:C:356[A]:ASN:ND2	2.74	0.41
4:F:88:SER:C	4:F:90:SER:N	2.74	0.41
4:F:231:ALA:O	4:F:233:PHE:HD1	2.04	0.40
2:B:36:TYR:HD1	2:B:37:HIS:H	1.68	0.40
2:B:67:LEU:N	2:B:67:LEU:HD12	2.35	0.40
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.56	0.40
2:D:73:GLY:O	2:D:75:MET:N	2.53	0.40
2:D:118:VAL:HG11	2:D:153:LEU:HD21	2.02	0.40
4:F:321:VAL:HG22	4:F:322:ASP:N	2.35	0.40
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.03	0.40
4:F:34:ASN:ND2	4:F:36:ARG:H	2.20	0.40
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:241:THR:HG23	11:F:401:ACP:O3'	2.21	0.40
4:F:242:ASN:ND2	4:F:245:ILE:HB	2.36	0.40
1:C:270:ALA:HB3	1:C:302[B]:MET:CG	2.50	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:GLU:OE1	1:C:283:HIS:NE2[4_555]	1.57	0.63
2:B:411:GLU:OE1	1:C:282:TYR:OH[4_555]	2.08	0.12

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	449/440 (102%)	432 (96%)	16 (4%)	1 (0%)	47 78
1	C	456/440 (104%)	448 (98%)	8 (2%)	0	100 100
2	B	441/431 (102%)	429 (97%)	12 (3%)	0	100 100
2	D	435/431 (101%)	419 (96%)	16 (4%)	0	100 100
3	E	124/123 (101%)	121 (98%)	3 (2%)	0	100 100
4	F	353/351 (101%)	322 (91%)	29 (8%)	2 (1%)	25 56
All	All	2258/2216 (102%)	2171 (96%)	84 (4%)	3 (0%)	51 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	248	GLU
4	F	346	LEU
1	A	177	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	381/371 (103%)	378 (99%)	3 (1%)	81 94
1	C	389/371 (105%)	384 (99%)	5 (1%)	69 91
2	B	385/372 (104%)	369 (96%)	16 (4%)	30 63
2	D	378/372 (102%)	371 (98%)	7 (2%)	57 85
3	E	115/110 (104%)	107 (93%)	8 (7%)	15 40
4	F	319/313 (102%)	292 (92%)	27 (8%)	10 31
All	All	1967/1909 (103%)	1901 (97%)	66 (3%)	39 71

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	251	ASP
1	A	438	ASP
2	B	36	TYR
2	B	130	ASP
2	B	139	HIS
2	B	196[A]	GLU
2	B	196[B]	GLU
2	B	276	THR
2	B	278	ARG
2	B	282	GLN
2	B	299	LYS
2	B	302	MET
2	B	372	LYS
2	B	416	MET
2	B	423[A]	SER
2	B	423[B]	SER
2	B	431[A]	GLU
2	B	431[B]	GLU
1	C	71	GLU
1	C	163	LYS
1	C	181	VAL

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Mol	Chain	Res	Type
1	C	221	ARG
1	C	347	CYS
2	D	75	MET
2	D	128	SER
2	D	139	HIS
2	D	298	SER
2	D	325	MET
2	D	369	ARG
2	D	414	ASP
3	E	6	MET
3	E	13	LYS
3	E	75	LYS
3	E	77	GLU
3	E	88	GLU
3	E	108[A]	ASN
3	E	108[B]	ASN
3	E	111	ASN
4	F	1	MET
4	F	19	ARG
4	F	34	ASN
4	F	66	ARG
4	F	76[A]	SER
4	F	76[B]	SER
4	F	87	LEU
4	F	90	SER
4	F	91	CYS
4	F	156	LYS
4	F	168	GLU
4	F	172	PHE
4	F	197	ARG
4	F	230	SER
4	F	232	ASN
4	F	241	THR
4	F	242	ASN
4	F	244	CYS
4	F	246	GLN
4	F	247	LYS
4	F	249	TYR
4	F	251	LYS
4	F	255	ARG
4	F	258	GLU
4	F	284[A]	LEU

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Mol	Chain	Res	Type
4	F	284[B]	LEU
4	F	305	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	283	HIS
1	A	329	ASN
1	A	342	GLN
2	B	192	HIS
2	B	282	GLN
2	B	300	ASN
2	B	334	ASN
2	B	424	ASN
2	B	433	GLN
1	C	18	ASN
1	C	256	GLN
1	C	301	GLN
2	D	50	ASN
2	D	59	ASN
2	D	294	GLN
2	D	300	ASN
3	E	92	ASN
3	E	111	ASN
3	E	124	GLN
4	F	34	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
10	GDP	D	502	6	24,30,30	1.04	1 (4%)	30,47,47	1.04	2 (6%)
9	LOC	B	504	-	31,31,31	0.75	0	44,44,44	0.89	1 (2%)
8	EP	D	501	-	32,36,36	0.31	0	39,53,53	0.91	1 (2%)
11	ACP	F	401	-	27,33,33	0.89	1 (3%)	32,52,52	0.85	1 (3%)
5	GTP	A	501	6	26,34,34	1.07	2 (7%)	32,54,54	1.34	6 (18%)
8	EP	B	503	-	32,36,36	0.36	0	39,53,53	0.62	1 (2%)
10	GDP	B	505	6	24,30,30	0.88	0	30,47,47	1.18	4 (13%)
5	GTP	C	501	6	26,34,34	1.04	3 (11%)	32,54,54	0.70	1 (3%)

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
10	GDP	D	502	6	-	8/12/32/32	0/3/3/3
9	LOC	B	504	-	-	4/12/25/25	0/3/3/3
8	EP	D	501	-	4/4/12/12	21/49/55/55	0/2/3/3
11	ACP	F	401	-	-	7/15/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
8	EP	B	503	-	4/4/12/12	25/49/55/55	0/2/3/3
10	GDP	B	505	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	C5-C6	-3.19	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	GDP	C6-N1	-3.12	1.33	1.37
5	C	501	GTP	C5-C6	-2.76	1.41	1.47
11	F	401	ACP	PB-O2B	-2.37	1.50	1.56
5	C	501	GTP	C8-N7	-2.17	1.31	1.35
5	A	501	GTP	C2-N3	2.05	1.38	1.33
5	C	501	GTP	C5-C4	-2.00	1.38	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	504	LOC	C2-O1-C1	-4.13	103.46	114.78
5	A	501	GTP	C8-N7-C5	3.18	109.05	102.99
5	A	501	GTP	C5-C6-N1	2.90	119.07	113.95
10	B	505	GDP	C8-N7-C5	2.65	108.05	102.99
5	A	501	GTP	C2-N1-C6	-2.33	120.80	125.10
5	A	501	GTP	PB-O3B-PG	-2.31	124.89	132.83
8	B	503	EP	O2-C3-C5	2.30	115.77	109.48
11	F	401	ACP	C5-C6-N6	2.28	123.81	120.35
10	B	505	GDP	O6-C6-C5	-2.27	119.94	124.37
10	B	505	GDP	C5-C6-N1	2.23	117.89	113.95
10	B	505	GDP	O3B-PB-O3A	2.22	112.08	104.64
5	A	501	GTP	PA-O3A-PB	-2.20	125.26	132.83
8	D	501	EP	O2-C3-C5	2.20	115.50	109.48
10	D	502	GDP	C8-N7-C5	2.17	107.12	102.99
5	A	501	GTP	O2G-PG-O3B	2.07	111.59	104.64
5	C	501	GTP	O6-C6-C5	2.05	128.38	124.37
10	D	502	GDP	C5-C6-N1	2.02	117.52	113.95

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	503	EP	C41
8	B	503	EP	C24
8	B	503	EP	C3
8	B	503	EP	C27
8	D	501	EP	C41
8	D	501	EP	C24
8	D	501	EP	C3
8	D	501	EP	C27

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	503	EP	C5-C10-C12-N20
8	B	503	EP	C21-C3-C5-C10
8	B	503	EP	C21-C3-C5-C6
8	B	503	EP	C24-C21-C3-C5
8	B	503	EP	C24-C21-C3-O2
8	B	503	EP	C24-C27-C32-C35
8	B	503	EP	O26-C27-C32-C35
8	B	503	EP	C38-C41-C47-O49
8	B	503	EP	C43-C41-C47-O49
8	B	503	EP	C41-C47-C51-C57
8	B	503	EP	O49-C47-C51-C57
8	B	503	EP	C60-C59-C68-O70
8	D	501	EP	C5-C3-O2-C75
8	D	501	EP	C38-C41-C47-O49
8	D	501	EP	C43-C41-C47-O49
8	D	501	EP	O49-C47-C51-C57
8	D	501	EP	C57-C59-C68-O70
8	D	501	EP	C57-C59-C68-C72
8	D	501	EP	C64-C59-C68-O70
8	D	501	EP	C64-C59-C68-C72
8	D	501	EP	C60-C59-C68-O70
8	D	501	EP	C60-C59-C68-C72
8	D	501	EP	C59-C68-C72-C75
8	D	501	EP	O70-C68-C72-C75
8	D	501	EP	C72-C75-O2-C3
8	D	501	EP	O76-C75-O2-C3
9	B	504	LOC	C19-C17-O6-C18
9	B	504	LOC	C16-C17-O6-C18
10	B	505	GDP	C5'-O5'-PA-O1A
10	B	505	GDP	C5'-O5'-PA-O2A
10	D	502	GDP	C5'-O5'-PA-O1A
10	D	502	GDP	C3'-C4'-C5'-O5'
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	C3'-C4'-C5'-O5'
8	B	503	EP	C35-C38-C41-C43
10	D	502	GDP	O4'-C4'-C5'-O5'
8	B	503	EP	C21-C3-O2-C75
8	B	503	EP	O49-C47-C51-C53

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Mol	Chain	Res	Type	Atoms
8	B	503	EP	C41-C47-C51-C53
11	F	401	ACP	O4'-C4'-C5'-O5'
9	B	504	LOC	C3-C5-O3-C6
8	D	501	EP	C41-C47-C51-C57
9	B	504	LOC	C7-C5-O3-C6
8	D	501	EP	C41-C47-C51-C53
8	D	501	EP	O49-C47-C51-C53
8	B	503	EP	C35-C38-C41-C47
8	D	501	EP	C35-C38-C41-C43
10	D	502	GDP	PA-O3A-PB-O1B
8	B	503	EP	C43-C41-C47-C51
8	D	501	EP	C43-C41-C47-C51
11	F	401	ACP	C4'-C5'-O5'-PA
10	D	502	GDP	C5'-O5'-PA-O3A
8	B	503	EP	C68-C72-C75-O2
8	D	501	EP	C27-C32-C35-C38
5	C	501	GTP	C5'-O5'-PA-O2A
10	D	502	GDP	C5'-O5'-PA-O2A
8	B	503	EP	C38-C41-C47-C51
8	D	501	EP	C38-C41-C47-C51
8	B	503	EP	C32-C35-C38-C41
8	B	503	EP	O70-C68-C72-C75
8	B	503	EP	C68-C72-C75-O76
11	F	401	ACP	PG-C3B-PB-O3A
8	B	503	EP	C27-C32-C35-C38
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
8	B	503	EP	C47-C51-C57-C59
10	D	502	GDP	PA-O3A-PB-O2B
10	D	502	GDP	PA-O3A-PB-O3B
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
10	B	505	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O1A

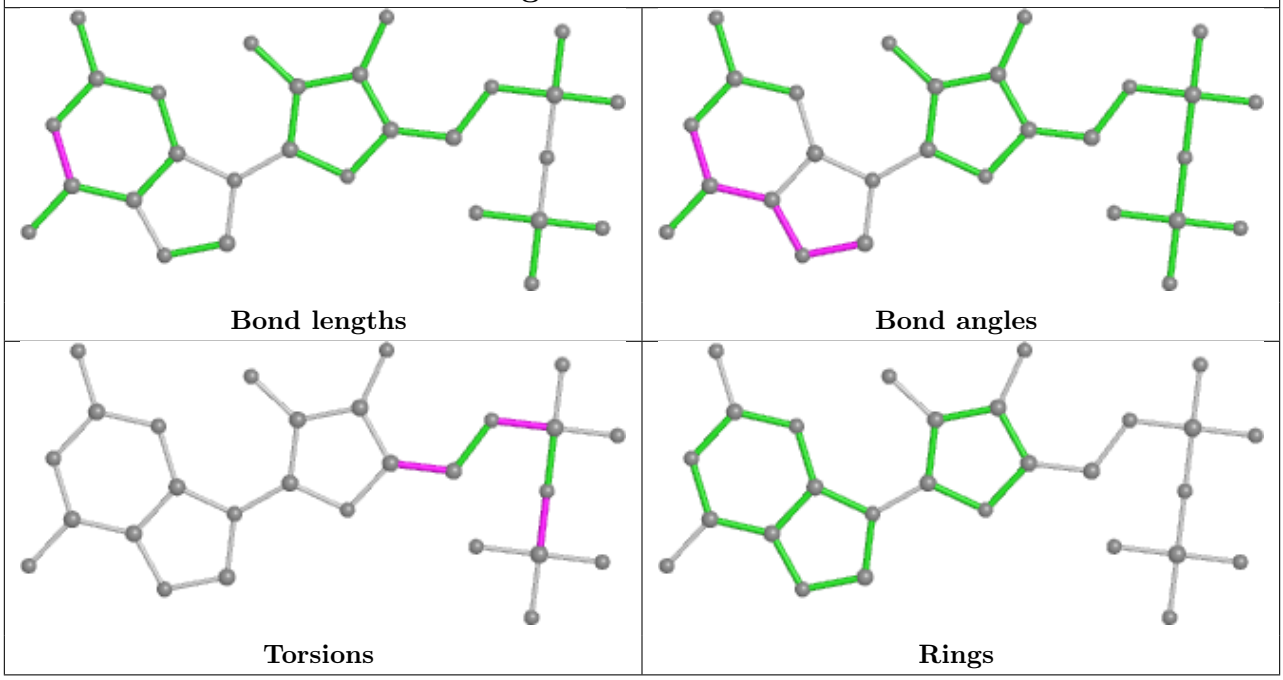
There are no ring outliers.

6 monomers are involved in 39 short contacts:

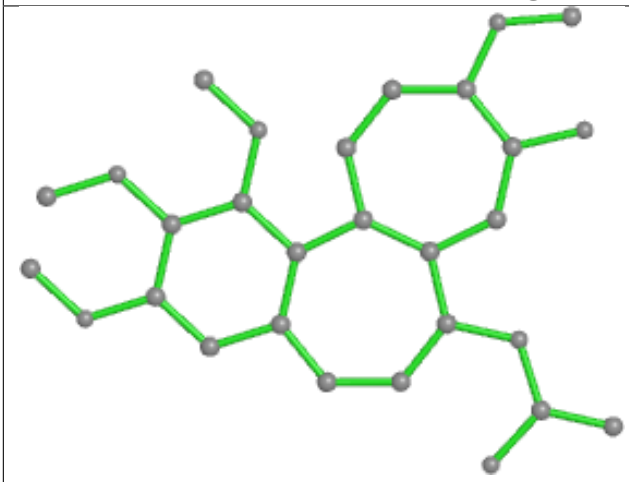
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	502	GDP	2	0
9	B	504	LOC	9	0
8	D	501	EP	9	0
11	F	401	ACP	4	0
8	B	503	EP	14	0
10	B	505	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

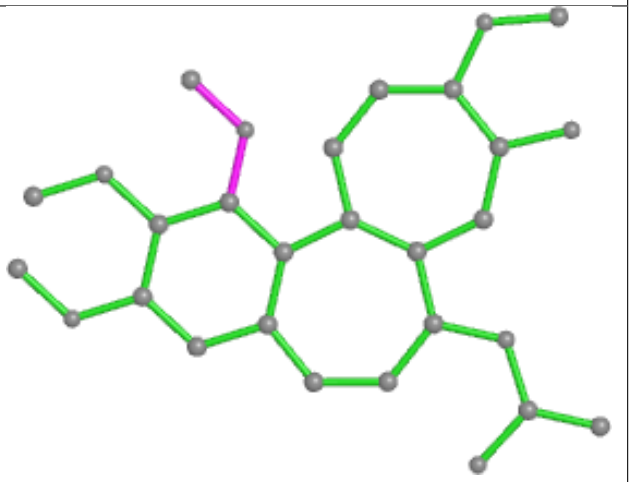
Ligand GDP D 502



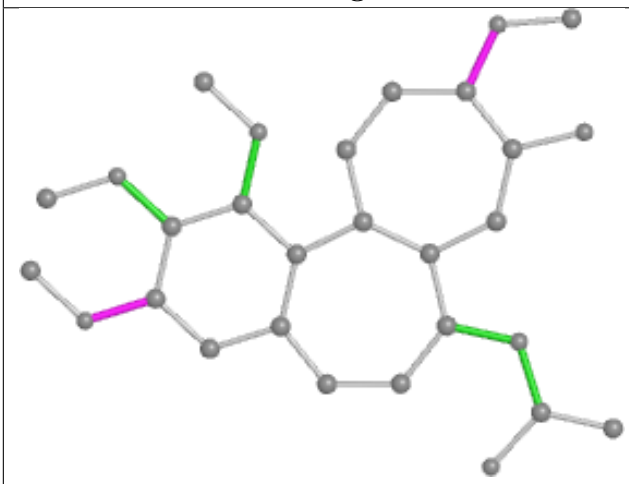
Ligand LOC B 504



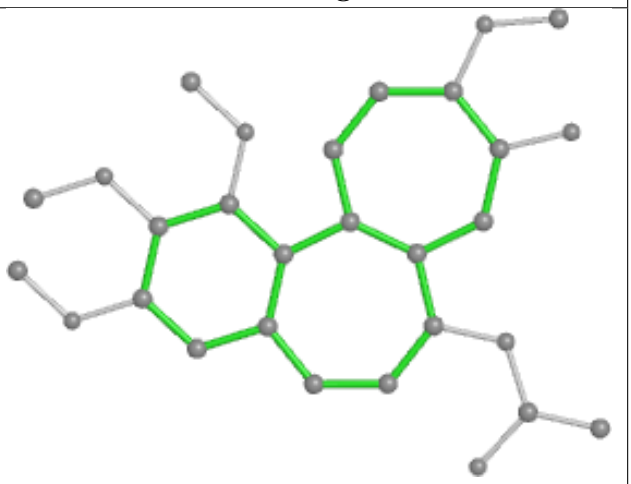
Bond lengths



Bond angles

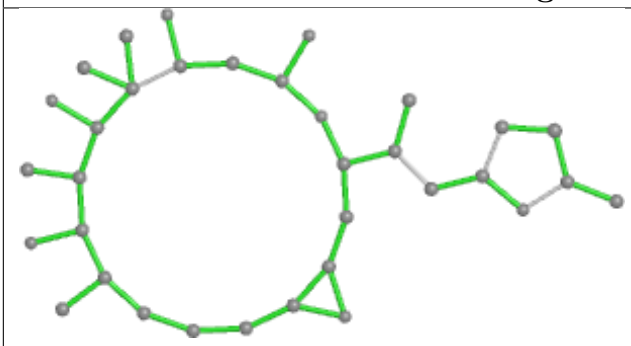


Torsions

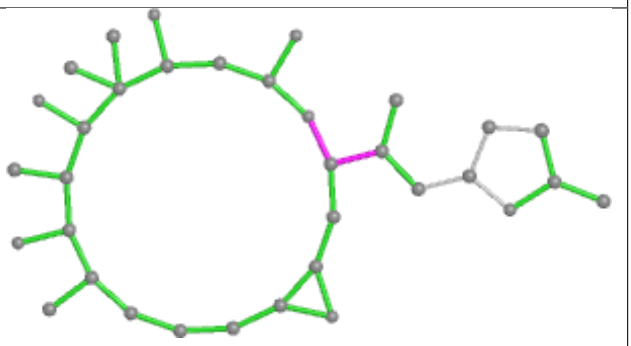


Rings

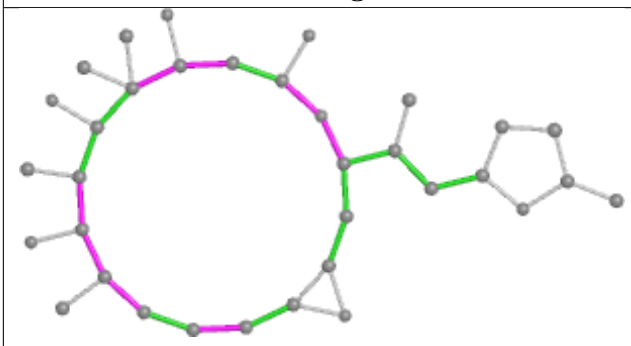
Ligand EP D 501



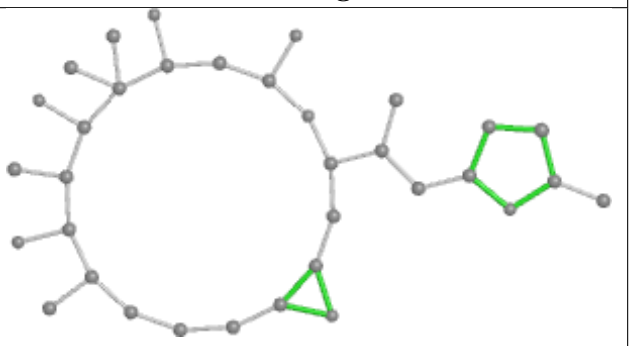
Bond lengths



Bond angles

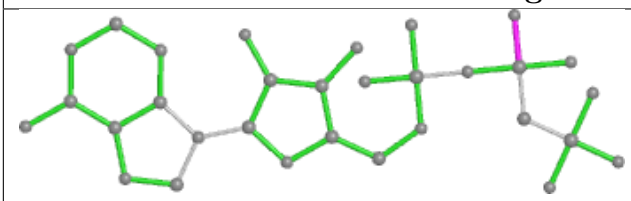


Torsions

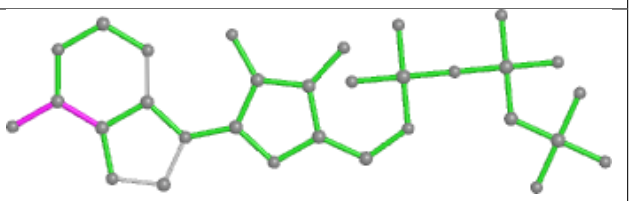


Rings

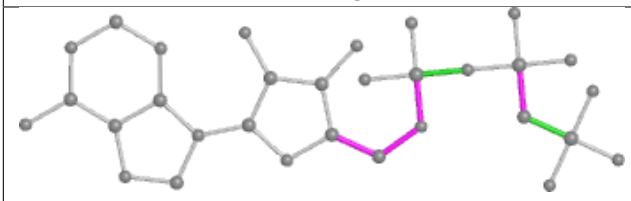
Ligand ACP F 401



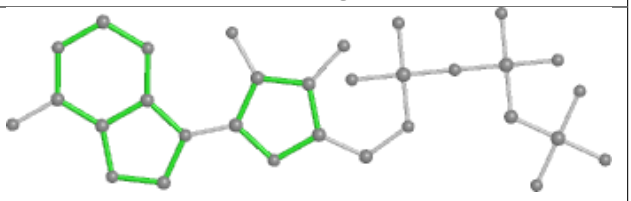
Bond lengths



Bond angles

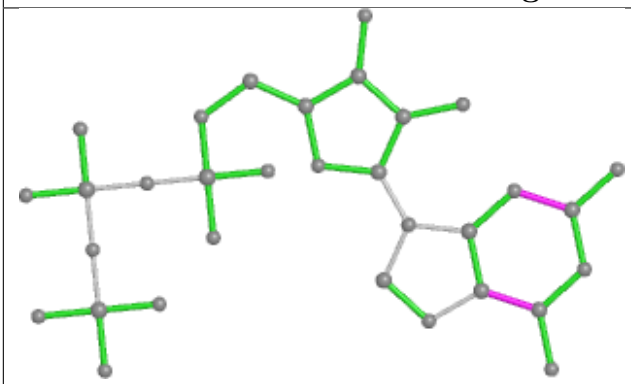


Torsions

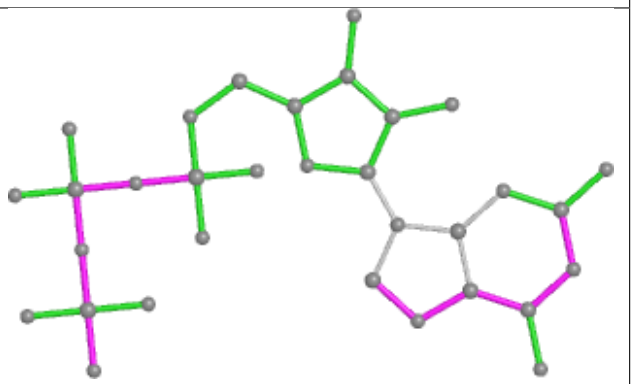


Rings

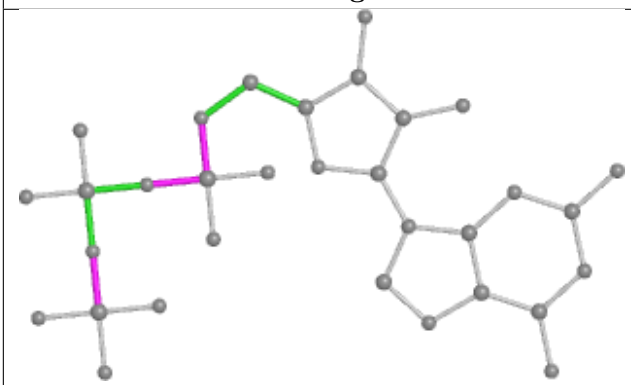
Ligand GTP A 501



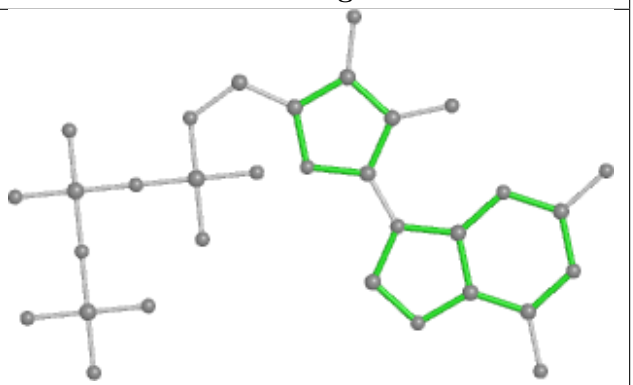
Bond lengths



Bond angles

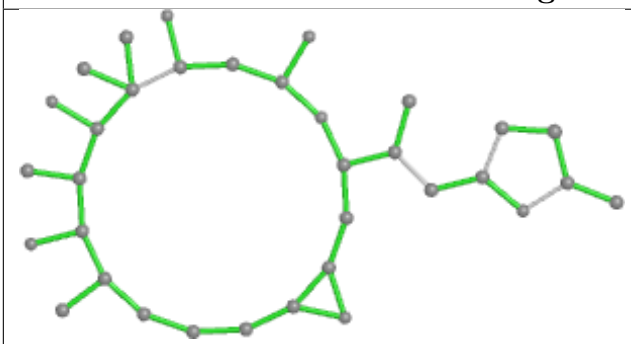


Torsions

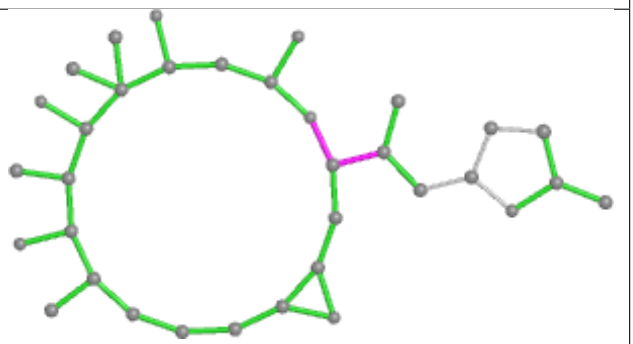


Rings

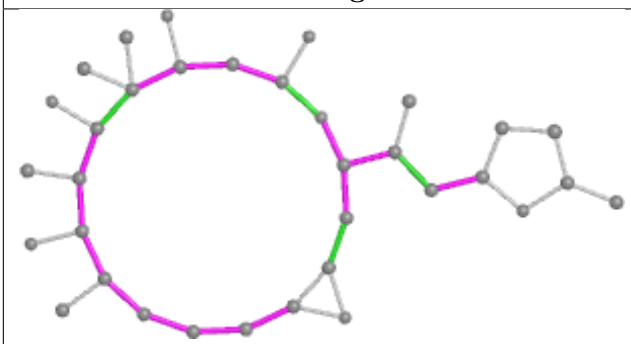
Ligand EP B 503



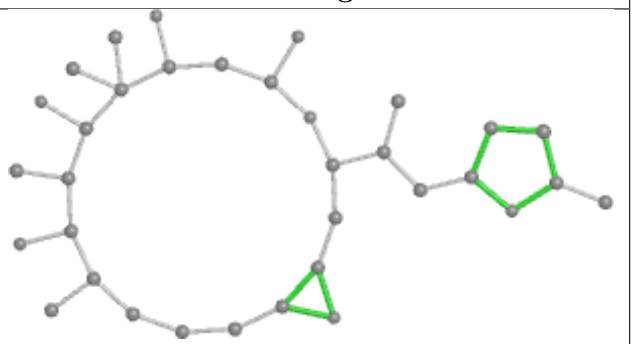
Bond lengths



Bond angles

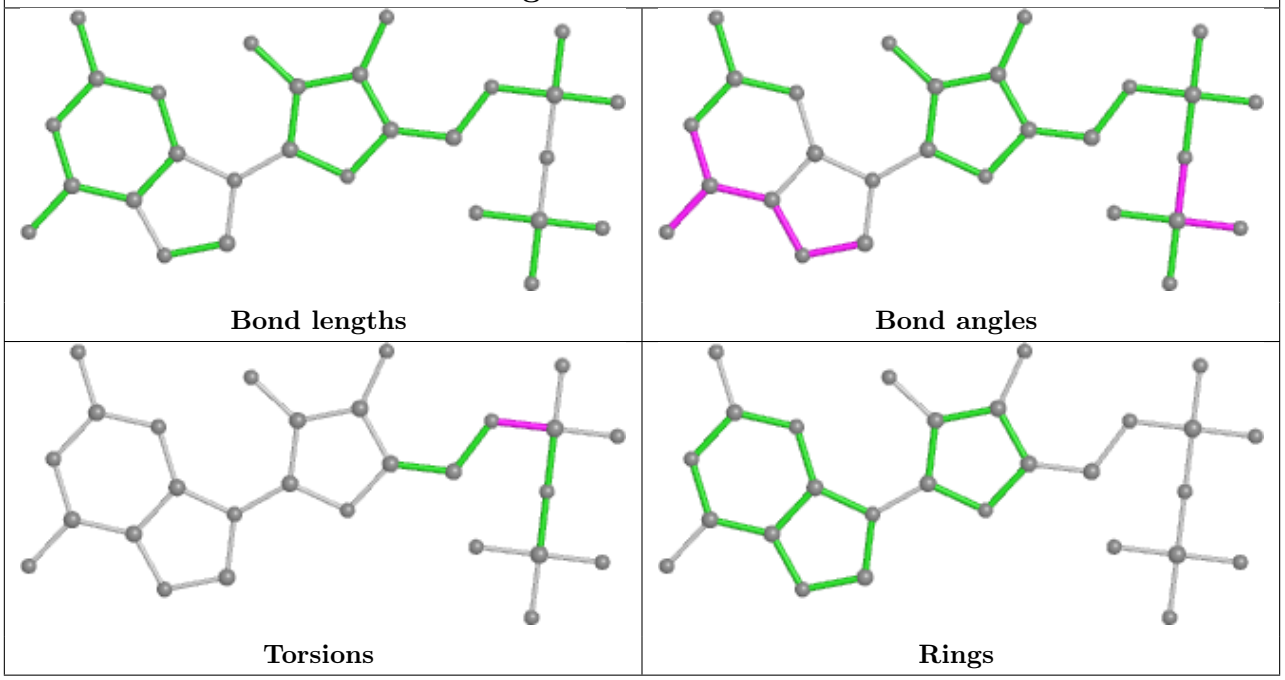


Torsions

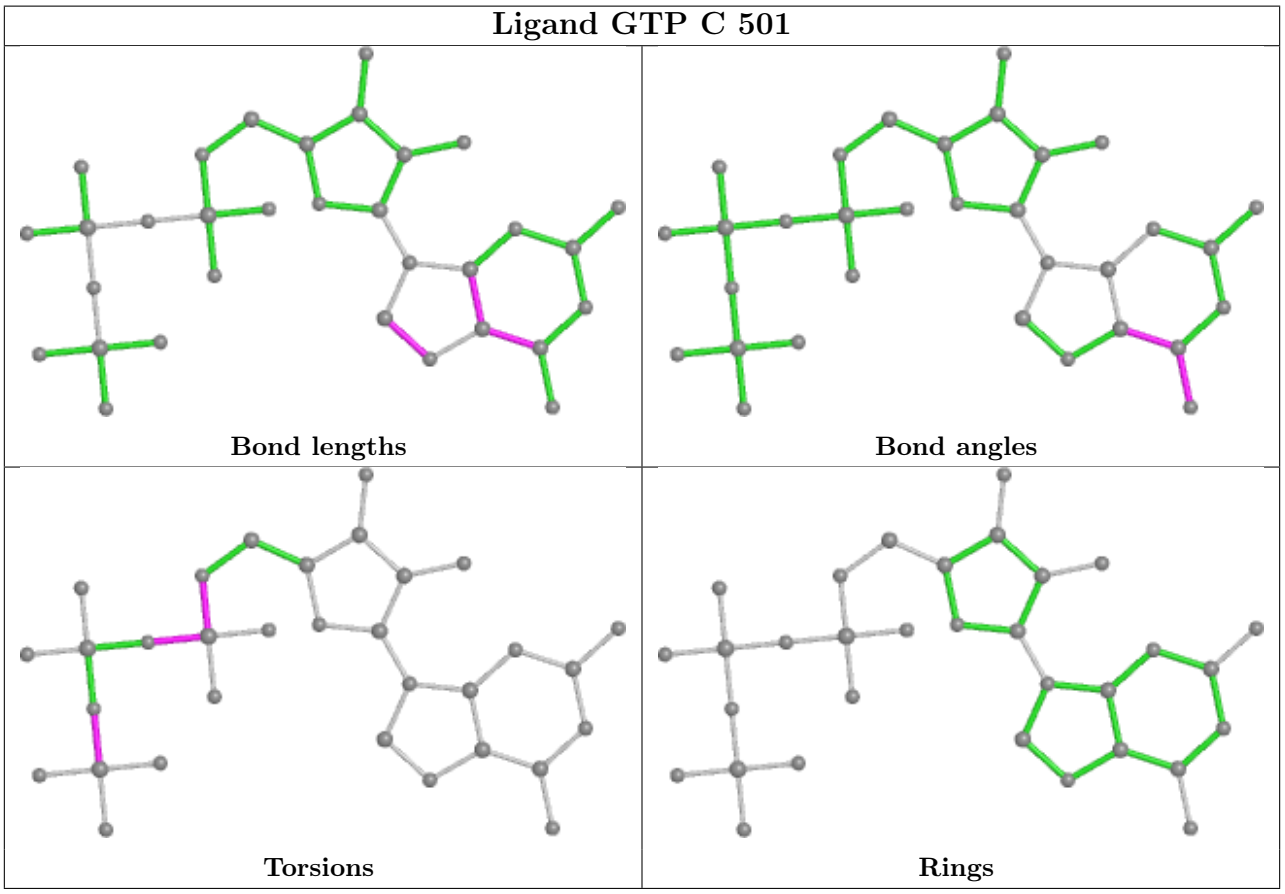


Rings

Ligand GDP B 505



Ligand GTP C 501



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
4	F	2
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	34.14
1	F	362:ALA	C	371:PRO	N	14.08
1	F	105:LEU	C	125:THR	N	12.54

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	439/440 (99%)	0.13	19 (4%) 35 25	35, 55, 98, 179	0
1	C	440/440 (100%)	-0.08	12 (2%) 54 44	26, 44, 79, 115	0
2	B	428/431 (99%)	0.33	33 (7%) 13 7	30, 53, 105, 163	4 (0%)
2	D	431/431 (100%)	0.29	32 (7%) 14 8	38, 64, 108, 170	3 (0%)
3	E	123/123 (100%)	0.68	17 (13%) 2 1	43, 72, 124, 184	0
4	F	351/351 (100%)	1.36	106 (30%) 0 0	48, 88, 184, 219	0
All	All	2212/2216 (99%)	0.39	219 (9%) 7 4	26, 59, 128, 219	7 (0%)

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	371	PRO	12.2
4	F	253	TYR	11.3
3	E	142	GLU	9.0
4	F	137	ARG	8.8
2	D	441	ASP	8.5
4	F	157	GLY	8.3
4	F	372	THR	7.9
4	F	252	ASN	7.8
4	F	254	GLY	7.7
4	F	232	ASN	7.4
4	F	167	SER	7.0
1	A	439	SER	7.0
2	B	279	GLY	6.3
4	F	155	ALA	6.0
4	F	125	THR	6.0
4	F	136	ASN	6.0
4	F	141	GLY	5.9
4	F	255	ARG	5.8
3	E	143	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	438	ASP	5.7
4	F	158	GLU	5.7
4	F	154	GLY	5.6
4	F	171	ASP	5.5
4	F	233	PHE	5.5
4	F	175	GLU	5.5
3	E	141	GLU	5.5
4	F	248	GLU	5.4
4	F	142	ARG	5.4
4	F	138	ARG	5.4
4	F	156	LYS	5.3
2	B	59	ASN	5.3
4	F	251	LYS	5.2
4	F	249	TYR	5.2
2	B	305	CYS	5.2
4	F	139	ARG	5.1
4	F	244	CYS	5.1
4	F	243	HIS	5.0
4	F	250	SER	5.0
4	F	165	GLU	4.8
4	F	178	GLN	4.7
4	F	258	GLU	4.7
2	D	416	MET	4.6
4	F	259	GLY	4.5
4	F	103	THR	4.5
2	D	57	THR	4.5
4	F	238	CYS	4.4
4	F	90	SER	4.4
4	F	126	ASP	4.4
2	D	283	TYR	4.4
4	F	234	GLN	4.3
4	F	241	THR	4.2
1	C	337	THR	4.2
1	A	282	TYR	4.2
2	B	58	GLY	4.2
4	F	91	CYS	4.2
2	B	280	SER	4.1
4	F	104	ASN	4.1
4	F	134	ALA	4.1
4	F	143	GLU	4.0
4	F	194	PRO	4.0
4	F	242	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
4	F	46	ARG	3.9
4	F	237	THR	3.9
2	B	438	ALA	3.9
2	D	80	SER	3.9
4	F	83	THR	3.9
4	F	240	LEU	3.9
2	B	278	ARG	3.8
2	B	80	SER	3.8
4	F	153	ALA	3.8
1	A	337	THR	3.8
2	B	281	GLN	3.8
2	D	179	ASP	3.7
4	F	235	ASP	3.7
4	F	245	ILE	3.7
2	B	321	GLY	3.7
4	F	105	LEU	3.6
4	F	11	SER	3.6
4	F	195	GLY	3.6
4	F	229	ASN	3.6
4	F	225	SER	3.5
2	D	220	THR	3.5
4	F	84	SER	3.5
2	B	1	MET	3.4
4	F	170	LEU	3.4
4	F	159	GLY	3.4
2	B	57	THR	3.4
2	B	369	ARG	3.4
4	F	246	GLN	3.4
2	B	246	GLY	3.3
2	B	370	GLY	3.3
3	E	27	PRO	3.3
2	B	82	PRO	3.2
4	F	129	GLU	3.2
4	F	76[A]	SER	3.2
2	D	76	ASP	3.2
4	F	176	GLN	3.2
2	D	37	HIS	3.2
4	F	89	GLU	3.2
4	F	25	GLY	3.1
2	B	215	ARG	3.1
4	F	168	GLU	3.1
2	D	221[A]	THR	3.1

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Mol	Chain	Res	Type	RSRZ
4	F	132	LEU	3.0
2	B	39	ASP	3.0
4	F	236	LYS	3.0
4	F	256	TYR	3.0
2	D	406	HIS	3.0
2	B	338	LYS	3.0
3	E	44	ASP	3.0
2	B	56	ALA	3.0
1	A	335	ILE	2.9
4	F	174	ASP	2.9
1	A	131	GLY	2.9
1	C	440	VAL	2.9
2	B	129	CYS	2.9
4	F	10	ASN	2.9
4	F	271[A]	LEU	2.9
1	A	80[A]	THR	2.9
1	C	1	MET	2.9
2	D	96	GLN	2.9
2	D	127	GLU	2.9
1	C	334	THR	2.8
4	F	177	GLY	2.8
2	D	89	PRO	2.8
4	F	152	SER	2.8
2	D	82	PRO	2.8
4	F	73	ARG	2.8
4	F	180	HIS	2.8
1	C	247	ALA	2.7
2	D	281	GLN	2.7
4	F	373	SER	2.7
2	B	40	SER	2.7
1	A	44	GLY	2.7
4	F	140	GLU	2.7
2	D	38	GLY	2.7
4	F	21	LEU	2.7
3	E	131	GLU	2.7
4	F	257	GLU	2.7
3	E	6	MET	2.7
1	A	279	GLU	2.7
2	B	247	GLN	2.7
3	E	48	GLU	2.6
3	E	128	LYS	2.6
4	F	224	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	334	ASN	2.6
2	D	337	ASN	2.6
1	A	163	LYS	2.6
4	F	239	HIS	2.6
1	C	249	ASN	2.6
2	D	397	ALA	2.6
3	E	140	LYS	2.6
1	C	349	THR	2.6
1	A	281	ALA	2.6
4	F	135	TYR	2.5
4	F	226	GLU	2.5
2	D	282	GLN	2.5
2	B	437	ASP	2.5
1	A	338	LYS	2.5
4	F	23	ALA	2.4
4	F	323	GLU	2.4
2	B	81	GLY	2.4
1	A	283	HIS	2.4
4	F	231	ALA	2.4
2	B	37	HIS	2.4
4	F	169	LEU	2.4
2	D	39	ASP	2.4
4	F	217	ARG	2.4
4	F	357	SER	2.4
4	F	247	LYS	2.4
3	E	9	ILE	2.4
2	D	58	GLY	2.4
4	F	329	LEU	2.4
2	D	33	THR	2.4
2	B	127	GLU	2.3
3	E	103	GLN	2.3
4	F	342	LEU	2.3
1	C	78	VAL	2.3
1	A	326	LYS	2.3
2	D	293	GLN	2.3
4	F	151	SER	2.3
4	F	197	ARG	2.3
4	F	127	GLU	2.3
4	F	362	ALA	2.3
2	B	35	SER	2.3
3	E	28	SER	2.3
1	A	1	MET	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	106	GLU	2.3
4	F	31	ARG	2.2
1	C	246	GLY	2.2
1	C	120[A]	ASP	2.2
3	E	139	LEU	2.2
4	F	45	ASN	2.2
4	F	306	HIS	2.2
4	F	131	PHE	2.2
1	A	41	THR	2.2
2	D	74	THR	2.2
4	F	230	SER	2.2
2	D	430	SER	2.2
2	D	78	VAL	2.2
3	E	122	ARG	2.2
2	D	401	ARG	2.2
1	A	42	ILE	2.1
4	F	19	ARG	2.1
2	B	416	MET	2.1
2	B	282	GLN	2.1
1	A	61	HIS	2.1
2	B	130	ASP	2.1
4	F	145	ASN	2.1
3	E	138	GLU	2.0
2	D	70	LEU	2.0
1	C	245	ASP	2.0
2	D	41	ASP	2.0
4	F	352	ASP	2.0
1	A	43	GLY	2.0
1	C	81	GLY	2.0
2	B	120	ASP	2.0
2	D	396	THR	2.0
2	D	1	MET	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 monosaccharides in this entry.

6.4 Ligands

LIGAND-RSR INFOmissingINFO

6.5 Other polymers

There are no such residues in this entry.