



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2025 – 07:26 PM JST

PDB ID : 8YEU
Title : Tubulin-RB3_SLD-TTL in complex with compound 2NH2
Authors : Wu, C.Y.; Wang, Y.X.
Deposited on : 2024-02-23
Resolution : 3.05 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

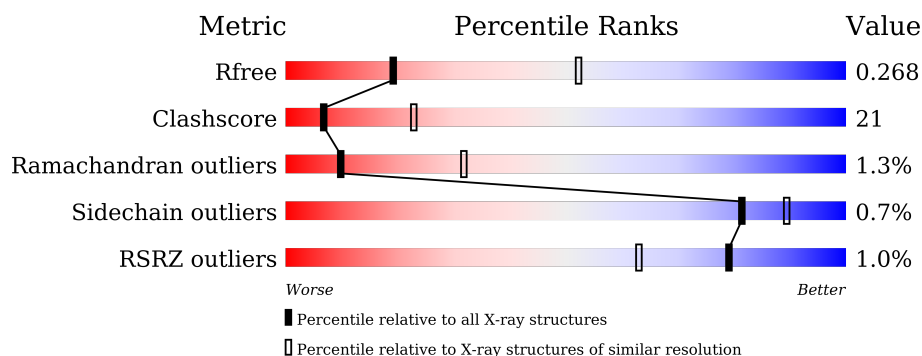
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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}	164625	2258 (3.10-3.02)
Clashscore	180529	2399 (3.10-3.02)
Ramachandran outliers	177936	2269 (3.10-3.02)
Sidechain outliers	177891	2268 (3.10-3.02)
RSRZ outliers	164620	2258 (3.10-3.02)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	440	<div> <div></div> <div>64%35%..</div> </div>
1	C	440	<div> <div></div> <div>72%27%.</div> </div>
2	B	431	<div> <div></div> <div>63%36%.</div> </div>
2	D	431	<div> <div>%</div> <div>49%48%..</div> </div>
3	E	143	<div> <div></div> <div>55%29%.15%</div> </div>
4	F	380	<div> <div>3%</div> <div>50%34%.13%</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17478 atoms, of which 48 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3405	2154	580	649	22			
1	C	440	Total	C	N	O	S	0	0	0
			3433	2172	583	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3351	2104	572	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3300	2076	559	638	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

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

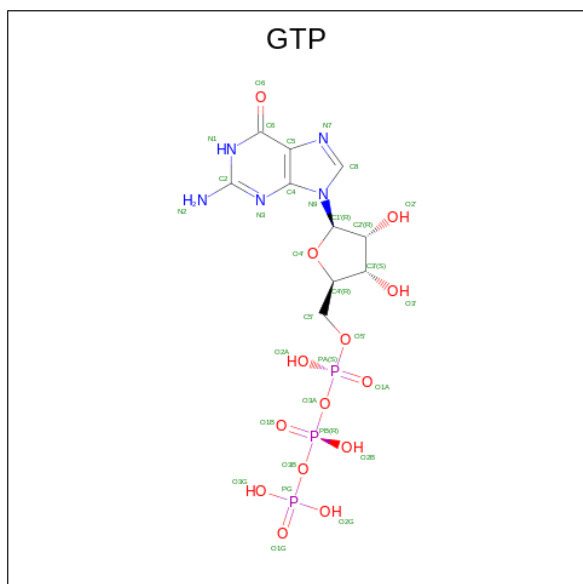
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	0	0
			2713	1740	466	493	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP A0A8C9FGJ1
F	380	HIS	-	expression tag	UNP A0A8C9FGJ1

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

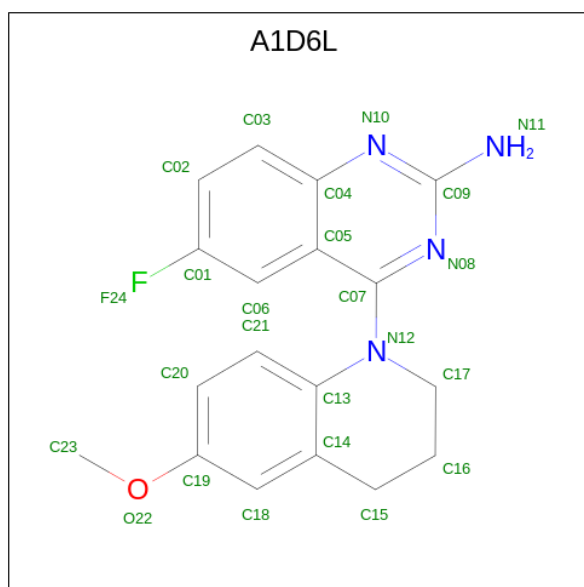
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	1	0
			1	1		
7	B	1	Total	Mg	1	0
			1	1		

Continued on next page...

Continued from previous page...

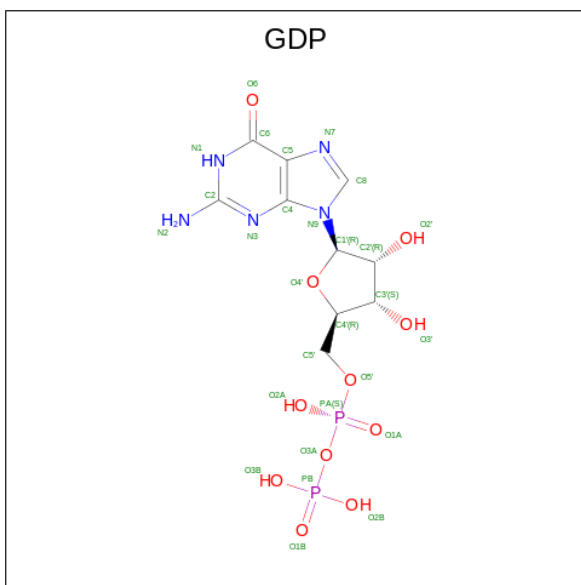
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	1	0
			1	1		

- Molecule 8 is 6-fluoranyl-4-(6-methoxy-3,4-dihydro-2 {H}-quinolin-1-yl)quinazolin-2-amine (three-letter code: A1D6L) (formula: C₁₈H₁₇FN₄O) (labeled as "Ligand of Interest" by depositor).



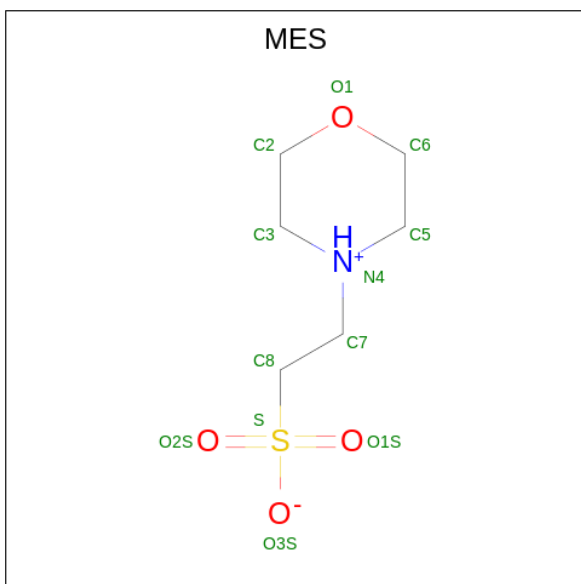
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	F	H	N	O	0	0
			41	18	1	17	4	1		
8	D	1	Total	C	F	H	N	O	0	0
			41	18	1	17	4	1		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



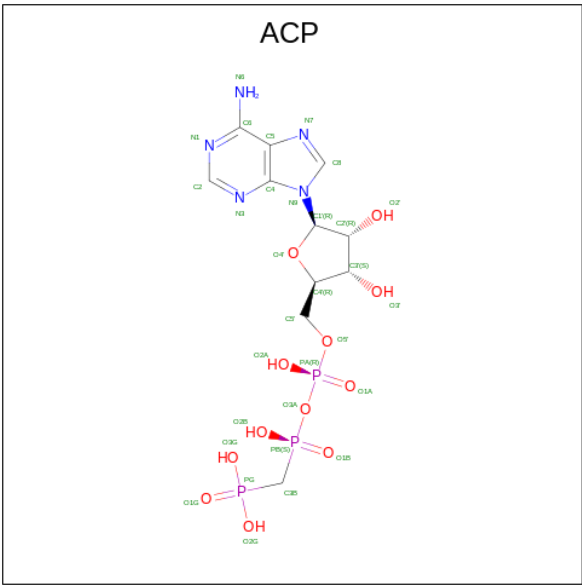
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

Continued on next page...

Continued from previous page...

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

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).

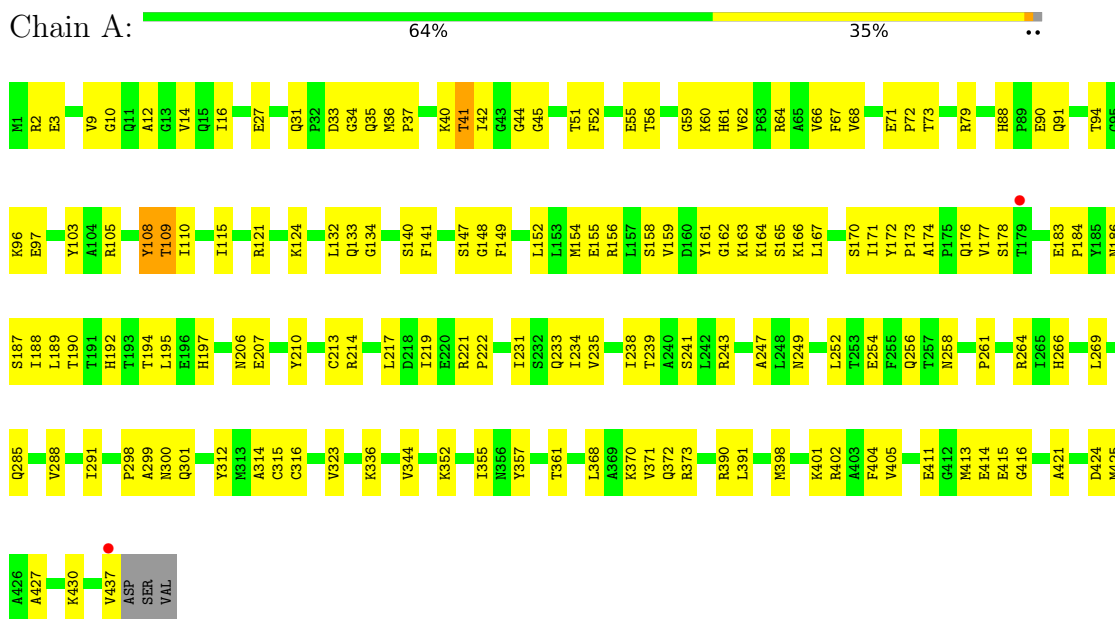


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	45	0
			45	11	14	5	12	3		

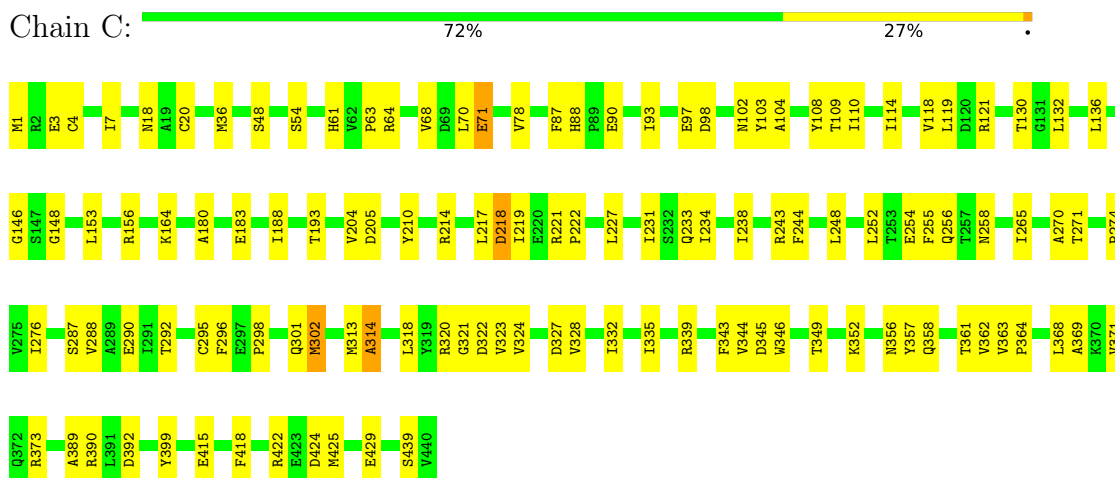
3 Residue-property plots

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: Detyrosinated tubulin alpha-1B chain

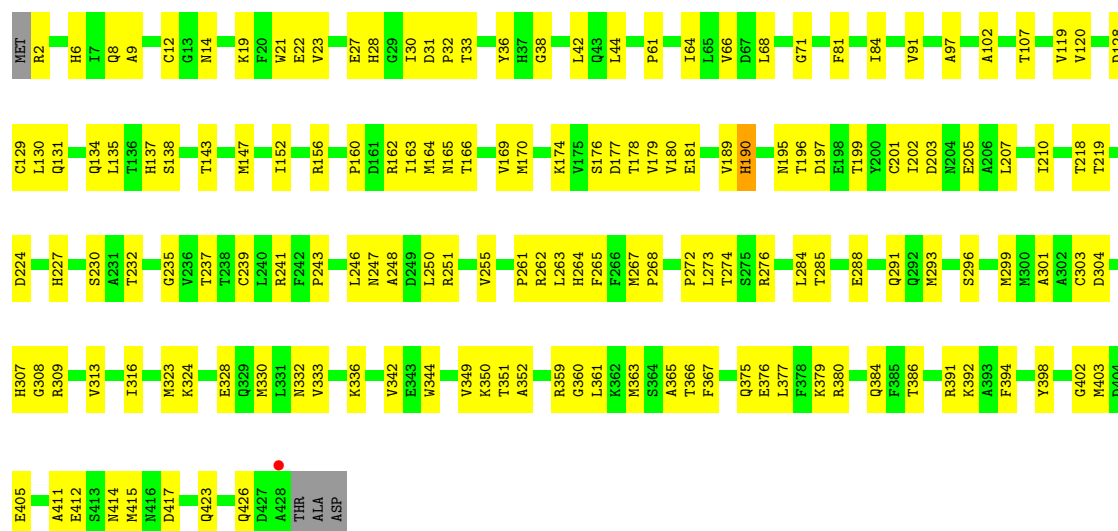


- Molecule 1: Detyrosinated tubulin alpha-1B chain



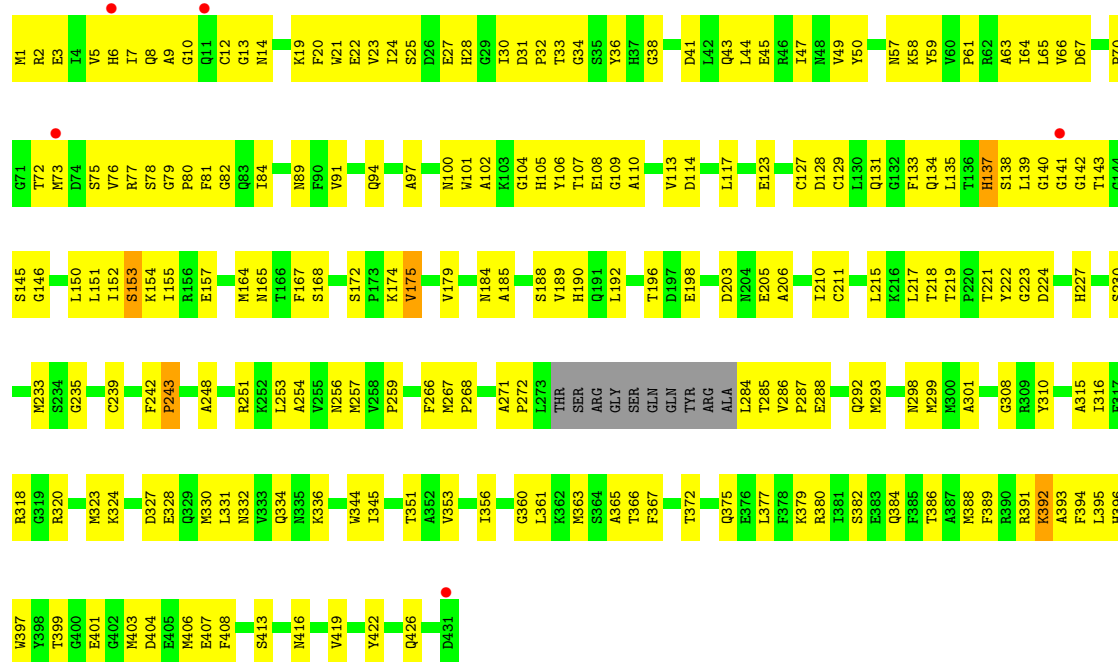
- Molecule 2: Tubulin beta chain

Chain B:  63% 36% .



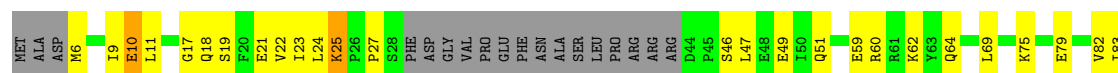
• Molecule 2: Tubulin beta chain

Chain D:  49% 48% ..



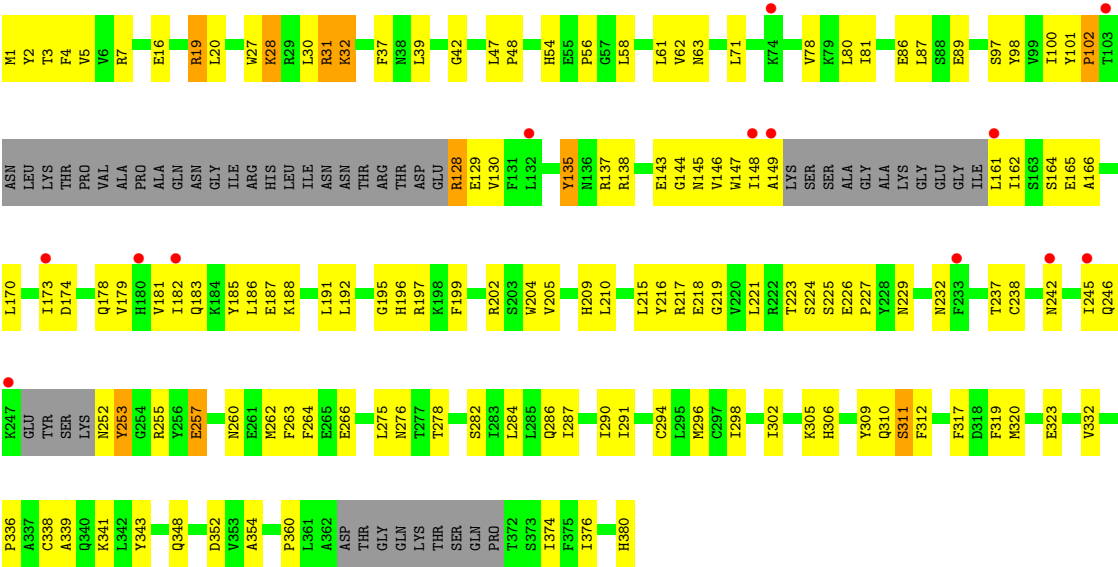
• Molecule 3: Stathmin-4

Chain E:  55% 29% . 15%





● Molecule 4: Tubulin-tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.95Å 156.62Å 181.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.76 – 3.05 62.76 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.76-3.05) 99.9 (62.76-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.210 , 0.268 0.215 , 0.268	Depositor DCC
R_{free} test set	55776 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17478	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: MES, MG, CA, GTP, ACP, A1D6L, GDP

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	0.52	0/3482	0.72	0/4728
1	C	0.56	1/3511 (0.0%)	0.74	2/4768 (0.0%)
2	B	0.51	0/3426	0.69	0/4643
2	D	0.45	0/3373	0.65	0/4570
3	E	0.46	0/1008	0.65	0/1337
4	F	0.42	0/2775	0.64	0/3752
All	All	0.49	1/17575 (0.0%)	0.69	2/23798 (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	C	0	1
4	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	20	CYS	CB-SG	-5.43	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	424	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	C	302	MET	CB-CG-SD	-5.17	96.90	112.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	217	LEU	Peptide
4	F	311	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3405	0	3313	131	0
1	C	3433	0	3337	94	0
2	B	3351	0	3216	141	0
2	D	3300	0	3175	177	0
3	E	1000	0	1018	45	0
4	F	2713	0	2659	154	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	24	17	0	2	0
8	D	24	17	0	2	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	24	0	24	0	0
11	F	31	14	14	0	0
All	All	17430	48	16804	714	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 21.

All (714) 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:308:GLY:HA2	2:B:426:GLN:HE21	1.13	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:149:ALA:HB3	4:F:161:LEU:HD23	1.44	0.98
1:A:88:HIS:N	1:A:91:GLN:OE1	2.00	0.93
1:A:90:GLU:OE1	1:A:124:LYS:NZ	2.04	0.91
1:C:88:HIS:NE2	1:C:90:GLU:HG3	1.87	0.89
2:D:134:GLN:HA	2:D:165:ASN:O	1.72	0.89
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.08	0.88
4:F:100:ILE:HD12	4:F:128:ARG:N	1.89	0.87
2:D:140:GLY:O	2:D:184:ASN:ND2	2.06	0.87
2:B:308:GLY:CA	2:B:426:GLN:HE21	1.87	0.87
2:B:392:LYS:HE3	2:B:405:GLU:OE2	1.75	0.86
2:D:67:ASP:OD2	2:D:72:THR:OG1	1.91	0.86
4:F:16:GLU:O	4:F:20:LEU:HD12	1.76	0.86
1:A:72:PRO:HA	1:A:94:THR:CG2	2.07	0.85
2:D:211:CYS:HA	2:D:215:LEU:HD13	1.59	0.85
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.59	0.84
4:F:138:ARG:NH1	4:F:144:GLY:O	2.09	0.84
2:D:106:TYR:CD1	3:E:133:VAL:HG11	2.13	0.83
2:B:36:TYR:CE1	2:B:38:GLY:HA3	2.13	0.83
4:F:149:ALA:HB3	4:F:161:LEU:CD2	2.08	0.83
4:F:137:ARG:O	4:F:137:ARG:NH1	2.11	0.82
2:D:285:THR:HG22	2:D:288:GLU:HB2	1.61	0.82
2:D:21:TRP:O	2:D:25:SER:OG	1.97	0.82
2:B:324:LYS:O	2:B:328:GLU:HG3	1.80	0.81
2:B:308:GLY:HA2	2:B:426:GLN:NE2	1.95	0.81
2:D:33:THR:OG1	2:D:58:LYS:HE3	1.80	0.81
1:A:72:PRO:HA	1:A:94:THR:HG21	1.62	0.80
2:B:2:ARG:HA	2:B:129:CYS:O	1.81	0.80
2:D:272:PRO:HB3	2:D:284:LEU:HD22	1.64	0.79
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.16	0.79
2:B:81:PHE:O	2:B:84:ILE:HG22	1.83	0.79
2:D:110:ALA:O	2:D:113:VAL:HG12	1.83	0.78
4:F:149:ALA:HB3	4:F:161:LEU:HB3	1.62	0.78
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.83	0.78
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.65	0.78
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.65	0.78
2:D:63:ALA:O	2:D:64:ILE:HD13	1.84	0.78
2:D:267:MET:HE1	2:D:299:MET:HG3	1.65	0.78
2:D:7:ILE:O	2:D:135:LEU:HD12	1.84	0.78
2:D:285:THR:HG23	2:D:288:GLU:H	1.49	0.77
2:D:315:ALA:HB3	2:D:351:THR:HG22	1.65	0.77
4:F:296:MET:HE2	4:F:380:HIS:HB2	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:149:ALA:CB	4:F:161:LEU:HB3	2.13	0.77
2:D:151:LEU:O	2:D:155:ILE:HG13	1.85	0.77
4:F:188:LYS:HD3	4:F:323:GLU:OE1	1.84	0.77
2:D:221:THR:HG23	2:D:224:ASP:H	1.49	0.76
2:D:100:ASN:ND2	2:D:397:TRP:O	2.15	0.76
4:F:199:PHE:CE2	4:F:221:LEU:HD23	2.21	0.76
1:C:287:SER:OG	1:C:290:GLU:HG3	1.85	0.75
2:B:66:VAL:CG1	2:B:147:MET:HE1	2.16	0.75
2:B:309:ARG:NH2	2:B:342:VAL:HA	2.01	0.75
2:D:271:ALA:HB2	2:D:298:ASN:HD22	1.50	0.75
2:D:392:LYS:HG3	2:D:395:LEU:HD12	1.70	0.74
2:D:239:CYS:O	2:D:248:ALA:HB3	1.86	0.74
4:F:135:TYR:OH	4:F:164:SER:O	2.04	0.74
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.23	0.73
2:D:256:ASN:HB3	8:D:501:A1D6L:C23	2.18	0.73
2:B:296:SER:HA	2:B:299:MET:HG2	1.70	0.73
4:F:192:LEU:HD21	4:F:262:MET:CE	2.18	0.73
1:A:176:GLN:NE2	4:F:56:PRO:HB3	2.04	0.73
4:F:226:GLU:OE2	4:F:252:ASN:ND2	2.18	0.72
4:F:100:ILE:HG23	4:F:128:ARG:N	2.05	0.72
2:B:316:ILE:CG2	2:B:366:THR:HB	2.20	0.72
1:A:97:GLU:HG3	2:B:2:ARG:NH1	2.04	0.71
2:B:262:ARG:NH2	2:B:414:ASN:OD1	2.24	0.71
1:C:219:ILE:HG21	1:C:222:PRO:HA	1.70	0.71
2:D:210:ILE:HG22	2:D:215:LEU:CD1	2.20	0.71
2:D:19:LYS:O	2:D:23:VAL:HG23	1.89	0.71
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.25	0.71
4:F:148:ILE:HD13	4:F:162:ILE:HG12	1.70	0.71
2:B:285:THR:O	2:B:288:GLU:N	2.24	0.70
3:E:131:GLU:OE1	3:E:134:ARG:NH2	2.25	0.70
2:D:330:MET:HG3	2:D:351:THR:HG21	1.74	0.70
2:D:324:LYS:O	2:D:328:GLU:HG3	1.91	0.70
2:B:309:ARG:HH21	2:B:342:VAL:HA	1.56	0.70
2:D:401:GLU:HA	3:E:137:LYS:HD2	1.73	0.70
4:F:3:THR:HG22	4:F:28:LYS:HG3	1.74	0.70
4:F:192:LEU:HD21	4:F:262:MET:HE1	1.74	0.70
2:B:375:GLN:HE22	2:B:423:GLN:HG2	1.56	0.69
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.26	0.69
1:C:204:VAL:HG22	1:C:302:MET:HE3	1.74	0.69
2:B:177:ASP:O	1:C:352:LYS:HE2	1.93	0.68
2:B:179:VAL:HG22	1:C:258:ASN:OD1	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:288:GLU:O	2:D:292:GLN:HG3	1.94	0.68
1:A:370:LYS:HD3	1:A:371:VAL:N	2.09	0.67
2:D:285:THR:HG22	2:D:288:GLU:CB	2.24	0.67
2:D:285:THR:HG22	2:D:288:GLU:OE1	1.93	0.67
4:F:98:TYR:O	4:F:181:VAL:HG23	1.93	0.67
2:D:284:LEU:HD21	2:D:292:GLN:OE1	1.94	0.67
4:F:138:ARG:HB3	4:F:145:ASN:HD21	1.58	0.67
2:B:324:LYS:HE3	2:B:328:GLU:OE2	1.94	0.67
4:F:101:TYR:CD1	4:F:179:VAL:HG22	2.29	0.67
1:C:97:GLU:HG3	2:D:2:ARG:NH1	2.09	0.67
3:E:46:SER:HB3	3:E:49:GLU:HG3	1.77	0.67
4:F:3:THR:HB	4:F:30:LEU:HD11	1.77	0.67
2:B:2:ARG:HB3	2:B:131:GLN:CG	2.25	0.67
4:F:149:ALA:CB	4:F:161:LEU:HD23	2.22	0.67
1:A:60:LYS:HD3	1:A:62:VAL:HG22	1.77	0.66
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.31	0.66
2:D:141:GLY:O	2:D:143:THR:N	2.27	0.66
1:A:298:PRO:O	1:A:301:GLN:HG3	1.96	0.66
1:C:214:ARG:O	1:C:218:ASP:HA	1.95	0.66
4:F:148:ILE:HD13	4:F:162:ILE:CG1	2.26	0.66
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.32	0.65
4:F:135:TYR:CD2	4:F:166:ALA:HB2	2.32	0.65
2:D:323:MET:SD	2:D:353:VAL:HG11	2.36	0.65
2:D:332:ASN:OD1	2:D:336:LYS:HE2	1.96	0.65
2:B:307:HIS:O	2:B:426:GLN:NE2	2.29	0.65
1:C:88:HIS:CD2	1:C:90:GLU:H	2.14	0.65
1:A:88:HIS:CD2	1:A:90:GLU:HG3	2.32	0.65
1:C:234:ILE:HD13	1:C:302:MET:SD	2.37	0.65
3:E:6:MET:HG3	3:E:24:LEU:CD2	2.27	0.65
3:E:47:LEU:HD12	3:E:47:LEU:O	1.97	0.65
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.29	0.65
2:B:36:TYR:CD2	2:B:44:LEU:HD11	2.32	0.64
2:B:386:THR:HG22	2:B:412:GLU:OE2	1.97	0.64
2:D:32:PRO:HB3	2:D:81:PHE:HA	1.79	0.64
2:D:210:ILE:HG22	2:D:215:LEU:HD11	1.79	0.64
2:B:66:VAL:HG12	2:B:147:MET:HE1	1.78	0.64
2:B:210:ILE:HG23	2:B:273:LEU:HD13	1.80	0.64
1:A:56:THR:O	1:A:59:GLY:N	2.20	0.64
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.79	0.64
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.27	0.64
2:B:134:GLN:HA	2:B:165:ASN:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ARG:CZ	2:D:323:MET:HB3	2.28	0.64
2:D:267:MET:CE	2:D:299:MET:HG3	2.28	0.64
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.80	0.63
2:D:267:MET:HG2	2:D:301:ALA:HB3	1.80	0.63
2:B:237:THR:HG22	2:B:241:ARG:HG3	1.80	0.63
1:A:31:GLN:HG2	1:A:35:GLN:O	1.97	0.63
2:B:19:LYS:O	2:B:23:VAL:HG23	1.98	0.63
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.34	0.63
2:D:45:GLU:OE1	2:D:243:PRO:HG3	1.97	0.63
1:A:323:VAL:HG12	1:A:355:ILE:HD13	1.81	0.63
4:F:191:LEU:HD22	4:F:196:HIS:CD2	2.35	0.62
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.35	0.62
4:F:138:ARG:CB	4:F:145:ASN:HD21	2.13	0.62
2:B:375:GLN:OE1	2:B:379:LYS:HE3	1.98	0.62
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.35	0.62
2:D:44:LEU:HA	2:D:47:ILE:HB	1.81	0.62
1:A:217:LEU:HB2	1:A:219:ILE:HD12	1.81	0.61
2:D:172:SER:OG	2:D:205:GLU:HB2	1.99	0.61
3:E:96:MET:O	3:E:100:LYS:HD3	2.00	0.61
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.36	0.61
2:B:284:LEU:N	2:B:284:LEU:HD12	2.16	0.61
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.81	0.61
1:A:79:ARG:NH2	1:A:94:THR:OG1	2.34	0.60
1:A:217:LEU:CB	1:A:219:ILE:HD12	2.30	0.60
2:D:221:THR:HG23	2:D:224:ASP:N	2.16	0.60
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.19	0.60
2:D:7:ILE:HG22	2:D:135:LEU:CD1	2.31	0.60
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.32	0.60
2:D:97:ALA:HB2	2:D:143:THR:OG1	2.00	0.60
4:F:138:ARG:HG3	4:F:145:ASN:OD1	2.00	0.60
1:A:72:PRO:CA	1:A:94:THR:HG21	2.31	0.60
4:F:16:GLU:OE2	4:F:19:ARG:HD2	2.02	0.60
1:A:154:MET:HG3	1:A:194:THR:HG23	1.83	0.60
2:D:2:ARG:NH1	2:D:129:CYS:SG	2.74	0.60
2:B:66:VAL:CG1	2:B:147:MET:CE	2.80	0.60
2:D:139:LEU:HA	2:D:145:SER:HB3	1.83	0.60
1:A:234:ILE:O	1:A:238:ILE:HG13	2.02	0.59
3:E:24:LEU:O	3:E:25:LYS:HB2	2.02	0.59
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.37	0.59
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.37	0.59
2:D:36:TYR:CE1	2:D:38:GLY:HA3	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:PRO:HD3	2:D:94:GLN:HA	1.84	0.59
4:F:148:ILE:HD12	4:F:149:ALA:H	1.66	0.59
4:F:191:LEU:N	4:F:191:LEU:HD12	2.17	0.59
1:A:72:PRO:CA	1:A:94:THR:CG2	2.81	0.59
2:D:395:LEU:O	2:D:399:THR:HG22	2.02	0.59
4:F:138:ARG:HD2	4:F:143:GLU:HB2	1.85	0.59
1:A:9:VAL:HG22	1:A:68:VAL:CG1	2.32	0.59
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.85	0.59
3:E:128:LYS:HD2	3:E:128:LYS:O	2.02	0.59
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.32	0.59
3:E:123:LEU:O	3:E:126:LYS:HB2	2.03	0.59
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.38	0.58
2:D:285:THR:HG22	2:D:288:GLU:CG	2.33	0.58
3:E:23:ILE:HG22	3:E:25:LYS:H	1.68	0.58
1:A:402:ARG:NH1	1:A:402:ARG:HG3	2.17	0.58
1:A:414:GLU:O	1:A:416:GLY:N	2.37	0.58
2:D:1:MET:HE3	2:D:128:ASP:HB2	1.86	0.58
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.85	0.58
2:B:251:ARG:O	2:B:255:VAL:HG23	2.04	0.58
2:D:63:ALA:C	2:D:64:ILE:HD13	2.23	0.58
2:D:360:GLY:O	2:D:361:LEU:HD23	2.03	0.58
1:C:68:VAL:HG11	1:C:118:VAL:HG21	1.85	0.57
1:C:219:ILE:CG2	1:C:222:PRO:HA	2.33	0.57
1:C:343:PHE:CG	1:C:349:THR:HG22	2.38	0.57
4:F:226:GLU:HB2	4:F:238:CYS:HB3	1.86	0.57
1:A:41:THR:HG21	1:A:45:GLY:CA	2.34	0.57
1:A:323:VAL:HG12	1:A:355:ILE:CD1	2.34	0.57
1:C:252:LEU:O	1:C:256:GLN:HG3	2.03	0.57
2:D:206:ALA:O	2:D:210:ILE:HG13	2.04	0.57
4:F:195:GLY:HA3	4:F:197:ARG:HD2	1.85	0.57
4:F:217:ARG:HG3	4:F:218:GLU:N	2.18	0.57
1:C:361:THR:HG22	1:C:362:VAL:N	2.18	0.57
4:F:242:ASN:HB2	4:F:245:ILE:HB	1.84	0.57
1:A:187:SER:CB	1:A:391:LEU:HD21	2.34	0.57
4:F:195:GLY:C	4:F:197:ARG:HG3	2.24	0.57
4:F:197:ARG:HH22	4:F:257:GLU:CD	2.07	0.57
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.38	0.57
1:A:214:ARG:HG2	1:A:219:ILE:O	2.04	0.57
2:B:307:HIS:ND1	2:B:376:GLU:OE2	2.29	0.57
2:B:174:LYS:HE3	2:B:205:GLU:CD	2.24	0.57
2:D:157:GLU:CA	3:E:123:LEU:HD13	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:266:PHE:O	2:D:268:PRO:HD3	2.04	0.57
2:D:382:SER:O	2:D:386:THR:HG23	2.05	0.57
2:B:166:THR:OG1	2:B:199:THR:HB	2.05	0.57
1:A:390:ARG:HD2	4:F:54:HIS:CD2	2.39	0.56
4:F:195:GLY:HA3	4:F:197:ARG:CD	2.34	0.56
1:A:88:HIS:NE2	1:A:90:GLU:HG3	2.20	0.56
1:A:288:VAL:HG22	1:A:323:VAL:HG22	1.86	0.56
1:C:361:THR:HG22	1:C:362:VAL:H	1.71	0.56
1:C:363:VAL:HG13	1:C:364:PRO:HD2	1.87	0.56
4:F:135:TYR:HE2	4:F:166:ALA:H	1.53	0.56
4:F:192:LEU:HD21	4:F:262:MET:HE2	1.87	0.56
2:D:139:LEU:HD11	2:D:168:SER:HB3	1.87	0.56
2:B:28:HIS:O	2:B:30:ILE:HD12	2.05	0.56
2:B:164:MET:HG3	2:B:196:THR:HG22	1.88	0.56
2:D:10:GLY:O	2:D:14:ASN:ND2	2.30	0.56
4:F:215:LEU:HD23	4:F:376:ILE:HD12	1.86	0.56
2:D:31:ASP:OD1	2:D:33:THR:HG22	2.06	0.56
2:D:221:THR:HG23	2:D:223:GLY:H	1.71	0.56
4:F:128:ARG:N	4:F:128:ARG:HD2	2.20	0.56
1:A:60:LYS:CD	1:A:62:VAL:HG22	2.35	0.56
1:A:192:HIS:CG	1:A:421:ALA:HA	2.40	0.56
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.35	0.56
2:D:224:ASP:O	2:D:227:HIS:HB3	2.06	0.56
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.41	0.56
1:A:231:ILE:O	1:A:235:VAL:HG23	2.05	0.56
4:F:148:ILE:CD1	4:F:161:LEU:HB2	2.36	0.56
1:A:40:LYS:O	1:A:42:ILE:HG13	2.06	0.56
4:F:146:VAL:HG23	4:F:187:GLU:OE2	2.05	0.56
4:F:229:ASN:ND2	4:F:232:ASN:OD1	2.38	0.56
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.88	0.55
4:F:191:LEU:HA	4:F:197:ARG:O	2.06	0.55
4:F:225:SER:HB2	4:F:252:ASN:HB3	1.88	0.55
1:A:402:ARG:HG3	1:A:402:ARG:HH11	1.71	0.55
2:B:68:LEU:HD12	2:B:97:ALA:HB2	1.89	0.55
2:D:134:GLN:O	2:D:134:GLN:HG3	2.06	0.55
4:F:144:GLY:HA3	4:F:187:GLU:OE1	2.07	0.55
1:C:90:GLU:O	1:C:121:ARG:HD2	2.07	0.55
2:D:7:ILE:HG22	2:D:135:LEU:HD12	1.88	0.55
4:F:3:THR:CB	4:F:30:LEU:HD11	2.35	0.55
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.37	0.55
2:B:380:ARG:O	2:B:384:GLN:HG3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ILE:N	1:C:265:ILE:HD12	2.21	0.55
4:F:147:TRP:O	4:F:162:ILE:HG23	2.07	0.55
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.88	0.55
1:A:96:LYS:HE3	2:B:128:ASP:OD1	2.06	0.55
1:A:147:SER:OG	1:A:186:ASN:HB3	2.07	0.55
2:B:375:GLN:NE2	2:B:423:GLN:HG2	2.22	0.55
2:B:134:GLN:HB2	2:B:165:ASN:HD22	1.72	0.55
1:A:41:THR:HG21	1:A:45:GLY:HA2	1.88	0.55
2:B:304:ASP:HB3	2:B:307:HIS:CG	2.43	0.54
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.43	0.54
1:C:108:TYR:OH	3:E:104:LYS:HD2	2.08	0.54
4:F:47:LEU:C	4:F:47:LEU:HD23	2.28	0.54
1:A:398:MET:CE	1:A:404:PHE:CD2	2.91	0.54
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.43	0.54
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.43	0.54
2:B:156:ARG:NH1	2:B:195:ASN:OD1	2.41	0.54
1:A:88:HIS:CD2	1:A:90:GLU:H	2.25	0.54
4:F:237:THR:O	4:F:246:GLN:NE2	2.41	0.54
2:B:190:HIS:CE1	2:B:414:ASN:HD22	2.26	0.54
3:E:140:LYS:HD3	3:E:141:GLU:OE2	2.08	0.54
2:B:246:LEU:O	2:B:247:ASN:HB3	2.07	0.54
3:E:22:VAL:HG13	3:E:22:VAL:O	2.08	0.54
1:A:40:LYS:O	1:A:42:ILE:N	2.40	0.53
1:A:213:CYS:O	1:A:217:LEU:HB2	2.08	0.53
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.90	0.53
1:A:2:ARG:HB3	1:A:133:GLN:HG3	1.91	0.53
2:B:178:THR:O	2:B:181:GLU:HG3	2.08	0.53
2:D:23:VAL:O	2:D:27:GLU:HG3	2.09	0.53
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.89	0.53
2:B:350:LYS:HG3	8:B:501:A1D6L:O22	2.08	0.53
3:E:130:ALA:O	3:E:133:VAL:HG12	2.09	0.53
1:A:132:LEU:HD23	1:A:164:LYS:HG3	1.89	0.53
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.89	0.53
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.91	0.53
2:D:179:VAL:O	2:D:388:MET:HE1	2.09	0.53
2:D:215:LEU:HD12	2:D:215:LEU:N	2.23	0.53
2:D:218:THR:HG23	2:D:219:THR:H	1.74	0.53
3:E:9:ILE:O	3:E:11:LEU:N	2.42	0.53
4:F:4:PHE:HB3	4:F:27:TRP:CZ3	2.44	0.53
1:A:336:LYS:HG2	3:E:24:LEU:HD13	1.90	0.53
1:A:402:ARG:HG2	1:A:405:VAL:HG21	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:HH11	2:B:323:MET:HB3	1.74	0.53
4:F:102:PRO:HG3	4:F:178:GLN:O	2.09	0.53
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.42	0.53
1:C:3:GLU:O	1:C:132:LEU:HD12	2.08	0.53
4:F:147:TRP:HA	4:F:183:GLN:O	2.09	0.53
2:B:176:SER:HB2	2:B:181:GLU:OE1	2.09	0.53
2:B:189:VAL:HB	2:B:415:MET:HE3	1.91	0.53
1:C:252:LEU:O	1:C:252:LEU:HD12	2.08	0.53
1:C:320:ARG:HA	1:C:356:ASN:O	2.08	0.53
2:D:175:VAL:CG1	2:D:222:TYR:HE1	2.22	0.53
2:D:316:ILE:HD13	2:D:366:THR:HB	1.91	0.52
4:F:148:ILE:O	4:F:182:ILE:HA	2.10	0.52
2:D:80:PRO:O	2:D:81:PHE:HB2	2.09	0.52
2:D:101:TRP:NE1	2:D:146:GLY:HA2	2.23	0.52
1:A:172:TYR:CG	1:A:173:PRO:HD2	2.44	0.52
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.90	0.52
2:D:139:LEU:HD22	2:D:188:SER:HB3	1.92	0.52
4:F:224:SER:OG	4:F:238:CYS:HA	2.10	0.52
1:A:285:GLN:HG3	1:A:372:GLN:NE2	2.25	0.52
1:C:221:ARG:HD2	2:D:327:ASP:OD2	2.10	0.52
2:D:396:HIS:HA	2:D:399:THR:HG22	1.91	0.52
4:F:86:GLU:C	4:F:87:LEU:HD23	2.30	0.52
4:F:138:ARG:HB3	4:F:145:ASN:ND2	2.22	0.52
2:D:106:TYR:OH	2:D:407:GLU:OE2	2.28	0.52
2:B:135:LEU:HD22	2:B:152:ILE:HD11	1.92	0.52
2:D:23:VAL:HG21	2:D:230:SER:HB2	1.90	0.52
2:D:41:ASP:OD1	2:D:41:ASP:N	2.39	0.52
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.92	0.52
2:B:291:GLN:HG3	2:B:291:GLN:O	2.09	0.52
1:A:10:GLY:O	1:A:14:VAL:HG23	2.10	0.52
2:B:156:ARG:O	2:B:160:PRO:HA	2.10	0.52
2:D:393:ALA:HB1	2:D:394:PHE:CD1	2.44	0.52
3:E:100:LYS:O	3:E:103:GLN:HB3	2.10	0.52
2:D:28:HIS:HA	2:D:43:GLN:HB3	1.92	0.51
2:D:251:ARG:HG3	2:D:251:ARG:HH11	1.74	0.51
2:D:388:MET:HG2	2:D:391:ARG:HH21	1.74	0.51
4:F:202:ARG:HD3	4:F:204:TRP:NE1	2.25	0.51
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.91	0.51
2:B:235:GLY:HA3	2:B:366:THR:OG1	2.10	0.51
2:D:102:ALA:HB2	2:D:403:MET:SD	2.50	0.51
2:D:285:THR:HG22	2:D:288:GLU:CD	2.30	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:59:GLU:OE1	3:E:59:GLU:HA	2.09	0.51
1:C:244:PHE:CE1	1:C:358:GLN:HG2	2.45	0.51
4:F:102:PRO:HB2	4:F:174:ASP:HA	1.93	0.51
1:A:298:PRO:O	1:A:300:ASN:N	2.44	0.50
3:E:130:ALA:HA	3:E:133:VAL:HG12	1.93	0.50
2:D:218:THR:HG23	2:D:219:THR:N	2.26	0.50
2:B:197:ASP:O	2:B:264:HIS:HB2	2.11	0.50
4:F:296:MET:HE2	4:F:380:HIS:CB	2.37	0.50
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.41	0.50
1:A:16:ILE:HD13	1:A:171:ILE:HD11	1.94	0.50
1:A:177:VAL:HG21	1:A:206:ASN:HB3	1.94	0.50
2:B:177:ASP:N	2:B:181:GLU:OE2	2.43	0.50
2:D:30:ILE:HD13	2:D:59:TYR:HB2	1.94	0.50
1:A:401:LYS:HG3	2:B:344:TRP:CE3	2.46	0.50
2:B:239:CYS:SG	2:B:316:ILE:HD13	2.51	0.50
2:D:45:GLU:OE1	2:D:243:PRO:CG	2.58	0.50
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.51	0.50
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.41	0.50
1:C:288:VAL:HG22	1:C:323:VAL:HG22	1.92	0.50
2:D:5:VAL:HB	2:D:133:PHE:CD2	2.47	0.50
4:F:262:MET:SD	4:F:266:GLU:HG2	2.51	0.50
4:F:71:LEU:HD12	4:F:80:LEU:HD23	1.92	0.50
2:B:23:VAL:O	2:B:27:GLU:HG3	2.11	0.49
2:D:257:MET:O	2:D:259:PRO:HD3	2.11	0.49
1:A:72:PRO:HA	1:A:94:THR:HG23	1.93	0.49
2:D:75:SER:HA	2:D:78:SER:OG	2.12	0.49
2:D:221:THR:C	2:D:223:GLY:H	2.16	0.49
4:F:296:MET:HE1	4:F:380:HIS:ND1	2.28	0.49
1:A:134:GLY:HA3	1:A:165:SER:O	2.12	0.49
2:D:65:LEU:HD22	2:D:76:VAL:HG11	1.95	0.49
2:D:174:LYS:HE3	2:D:205:GLU:CD	2.33	0.49
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.48	0.49
1:A:357:TYR:CD2	3:E:17:GLY:HA2	2.46	0.49
2:B:360:GLY:O	2:B:361:LEU:HD23	2.12	0.49
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.93	0.49
2:D:242:PHE:CZ	2:D:356:ILE:HG21	2.48	0.49
1:A:183:GLU:N	1:A:184:PRO:CD	2.75	0.49
1:C:70:LEU:HD13	1:C:110:ILE:CG2	2.43	0.49
2:D:72:THR:O	2:D:76:VAL:HG23	2.11	0.49
2:D:285:THR:CG2	2:D:288:GLU:H	2.23	0.49
2:D:380:ARG:O	2:D:384:GLN:HG3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:39:LEU:HD12	4:F:61:LEU:O	2.12	0.49
1:A:109:THR:HG22	1:A:110:ILE:N	2.28	0.49
2:B:293:MET:CE	2:B:365:ALA:HB1	2.43	0.49
2:D:22:GLU:HG2	2:D:81:PHE:CD1	2.47	0.49
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.48	0.49
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.95	0.49
4:F:192:LEU:HD11	4:F:199:PHE:CD1	2.48	0.49
1:A:178:SER:OG	2:B:350:LYS:HE3	2.13	0.49
4:F:138:ARG:CG	4:F:145:ASN:OD1	2.61	0.49
1:A:247:ALA:HB3	3:E:19:SER:OG	2.13	0.48
2:B:190:HIS:CD2	2:B:411:ALA:HA	2.48	0.48
2:D:330:MET:O	2:D:334:GLN:HG3	2.13	0.48
4:F:135:TYR:CE1	4:F:145:ASN:HB3	2.48	0.48
3:E:51:GLN:OE1	3:E:51:GLN:HA	2.11	0.48
1:A:210:TYR:CE2	1:A:222:PRO:HD2	2.48	0.48
2:B:237:THR:HB	2:B:241:ARG:HE	1.77	0.48
2:D:145:SER:HB2	2:D:188:SER:OG	2.13	0.48
3:E:6:MET:HG3	3:E:24:LEU:HD23	1.95	0.48
1:A:312:TYR:O	1:A:344:VAL:HG13	2.14	0.48
2:B:239:CYS:O	2:B:248:ALA:HB3	2.12	0.48
2:D:3:GLU:HB2	2:D:127:CYS:SG	2.53	0.48
2:D:107:THR:O	2:D:110:ALA:HB3	2.14	0.48
2:D:344:TRP:CE3	2:D:345:ILE:HG13	2.48	0.48
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.47	0.48
1:A:90:GLU:O	1:A:121:ARG:HD2	2.13	0.48
1:A:264:ARG:O	1:A:266:HIS:N	2.46	0.48
1:C:88:HIS:CD2	1:C:90:GLU:HG3	2.49	0.48
1:C:119:LEU:HD12	1:C:156:ARG:NH2	2.28	0.48
1:A:424:ASP:O	1:A:427:ALA:HB3	2.13	0.48
2:D:44:LEU:O	2:D:47:ILE:HG22	2.14	0.48
2:D:157:GLU:HA	3:E:123:LEU:HD13	1.96	0.48
4:F:286:GLN:O	4:F:290:ILE:HG13	2.14	0.48
2:B:2:ARG:HB3	2:B:131:GLN:HG2	1.95	0.48
2:B:31:ASP:OD1	2:B:33:THR:CG2	2.62	0.48
1:C:103:TYR:CE2	1:C:148:GLY:HA2	2.49	0.48
2:D:179:VAL:HG11	2:D:394:PHE:CZ	2.48	0.48
4:F:3:THR:HB	4:F:30:LEU:CD1	2.44	0.48
2:B:309:ARG:HE	2:B:342:VAL:HG12	1.79	0.48
2:B:375:GLN:HG3	2:B:376:GLU:N	2.29	0.48
4:F:16:GLU:C	4:F:20:LEU:HD12	2.34	0.48
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.69	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.47	0.47
1:A:27:GLU:HG2	1:A:361:THR:OG1	2.14	0.47
2:D:113:VAL:HG13	2:D:114:ASP:N	2.29	0.47
2:D:372:THR:HA	2:D:422:TYR:CD1	2.48	0.47
2:D:293:MET:CG	2:D:367:PHE:HB2	2.44	0.47
1:A:195:LEU:HD12	1:A:266:HIS:CE1	2.48	0.47
2:B:391:ARG:NH1	1:C:439:SER:OG	2.47	0.47
1:C:109:THR:HG22	1:C:110:ILE:HD13	1.97	0.47
1:A:115:ILE:HD13	1:A:152:LEU:HG	1.96	0.47
1:A:158:SER:OG	1:A:166:LYS:HE2	2.13	0.47
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.95	0.47
4:F:130:VAL:HG12	4:F:130:VAL:O	2.14	0.47
1:A:124:LYS:HE2	1:A:124:LYS:HB3	1.47	0.47
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.49	0.47
2:B:232:THR:HG21	2:B:268:PRO:CB	2.44	0.47
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.49	0.47
1:C:238:ILE:HG22	1:C:252:LEU:HD22	1.97	0.47
1:C:392:ASP:OD2	1:C:429:GLU:OE2	2.33	0.47
2:D:271:ALA:HB2	2:D:298:ASN:ND2	2.23	0.47
1:A:314:ALA:O	1:A:315:CYS:HB2	2.15	0.47
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.96	0.47
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.49	0.47
2:D:49:VAL:HG12	2:D:50:TYR:CD2	2.49	0.47
2:D:167:PHE:CE2	2:D:233:MET:HG2	2.50	0.47
2:D:251:ARG:HG3	2:D:251:ARG:NH1	2.29	0.47
1:A:55:GLU:HA	1:A:60:LYS:O	2.14	0.47
1:A:194:THR:O	1:A:194:THR:HG22	2.15	0.47
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.46	0.47
2:B:359:ARG:HE	2:B:359:ARG:HA	1.79	0.47
2:D:320:ARG:O	2:D:363:MET:HE2	2.15	0.47
4:F:47:LEU:HD23	4:F:48:PRO:N	2.30	0.47
4:F:246:GLN:O	4:F:253:TYR:HD2	1.98	0.47
1:A:2:ARG:CB	1:A:133:GLN:HG3	2.45	0.47
1:A:31:GLN:HG3	1:A:33:ASP:OD1	2.15	0.47
4:F:16:GLU:OE1	4:F:20:LEU:HD11	2.15	0.47
2:D:157:GLU:HA	3:E:123:LEU:CD1	2.45	0.46
2:D:318:ARG:HH21	2:D:356:ILE:HG23	1.80	0.46
4:F:223:THR:O	4:F:260:ASN:HB3	2.14	0.46
1:A:269:LEU:HD11	1:A:301:GLN:HB3	1.97	0.46
2:B:107:THR:HG22	3:E:83:ILE:HG13	1.97	0.46
2:B:263:LEU:N	2:B:263:LEU:HD23	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:LEU:C	2:B:377:LEU:HD23	2.36	0.46
4:F:1:MET:HE1	4:F:28:LYS:HB3	1.96	0.46
4:F:170:LEU:O	4:F:173:ILE:HG12	2.15	0.46
1:A:241:SER:HB2	1:A:249:ASN:O	2.15	0.46
2:B:68:LEU:HD23	2:B:68:LEU:HA	1.77	0.46
2:B:330:MET:O	2:B:333:VAL:HG12	2.16	0.46
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.96	0.46
2:D:5:VAL:O	2:D:133:PHE:HA	2.15	0.46
1:A:167:LEU:HD22	1:A:252:LEU:HD22	1.98	0.46
1:A:174:ALA:HB2	1:A:207:GLU:H	1.80	0.46
2:B:301:ALA:O	2:B:303:CYS:N	2.48	0.46
1:C:254:GLU:HG2	1:C:352:LYS:HE3	1.96	0.46
2:D:164:MET:HG3	2:D:196:THR:HG22	1.97	0.46
2:B:66:VAL:HG11	2:B:147:MET:CE	2.45	0.46
1:C:288:VAL:CG2	1:C:323:VAL:HG22	2.46	0.46
4:F:148:ILE:CD1	4:F:149:ALA:H	2.26	0.46
2:B:91:VAL:CG2	2:B:119:VAL:HG21	2.46	0.46
2:B:304:ASP:OD2	2:B:307:HIS:NE2	2.49	0.46
1:C:265:ILE:HG22	1:C:265:ILE:O	2.16	0.46
2:D:1:MET:HG3	2:D:128:ASP:HB3	1.96	0.46
1:C:363:VAL:CG1	1:C:364:PRO:HD2	2.46	0.46
4:F:89:GLU:OE1	4:F:89:GLU:HA	2.16	0.46
1:A:41:THR:HG22	1:A:44:GLY:O	2.15	0.46
1:A:401:LYS:HG3	2:B:344:TRP:CD2	2.51	0.46
2:B:31:ASP:CG	2:B:33:THR:HG22	2.36	0.46
1:C:324:VAL:HG22	1:C:327:ASP:OD2	2.16	0.46
3:E:139:LEU:O	3:E:139:LEU:HG	2.15	0.46
4:F:148:ILE:HD12	4:F:161:LEU:HB2	1.96	0.46
2:B:23:VAL:HG21	2:B:230:SER:HB2	1.98	0.46
1:C:321:GLY:HA2	1:C:357:TYR:O	2.16	0.46
4:F:4:PHE:HB3	4:F:27:TRP:HZ3	1.80	0.46
1:C:313:MET:O	1:C:314:ALA:HB2	2.16	0.45
2:D:404:ASP:OD2	2:D:406:MET:CE	2.63	0.45
2:B:332:ASN:O	2:B:336:LYS:HG3	2.16	0.45
3:E:130:ALA:C	3:E:133:VAL:HG12	2.36	0.45
4:F:149:ALA:HB2	4:F:161:LEU:HB3	1.96	0.45
4:F:202:ARG:HA	4:F:317:PHE:O	2.16	0.45
4:F:86:GLU:O	4:F:87:LEU:HD23	2.16	0.45
4:F:374:ILE:O	4:F:374:ILE:HG13	2.16	0.45
2:B:267:MET:HG2	2:B:301:ALA:HB3	1.96	0.45
2:D:117:LEU:HD11	2:D:154:LYS:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:327:ASP:O	2:D:331:LEU:HD13	2.15	0.45
1:C:132:LEU:O	1:C:164:LYS:NZ	2.45	0.45
1:C:204:VAL:HG22	1:C:302:MET:CE	2.43	0.45
1:C:296:PHE:CB	1:C:339:ARG:HD2	2.47	0.45
2:D:211:CYS:HB3	2:D:217:LEU:HD12	1.99	0.45
1:A:103:TYR:HD2	1:A:189:LEU:HD13	1.80	0.45
1:C:274:PRO:CG	1:C:371:VAL:HG11	2.47	0.45
3:E:125:GLU:OE1	3:E:125:GLU:HA	2.17	0.45
4:F:138:ARG:CB	4:F:145:ASN:ND2	2.80	0.45
2:D:175:VAL:CG1	2:D:222:TYR:CE1	2.99	0.45
1:A:105:ARG:NH1	1:A:411:GLU:OE2	2.47	0.45
2:B:218:THR:HG23	2:B:219:THR:N	2.32	0.45
4:F:278:THR:O	4:F:282:SER:OG	2.31	0.45
2:B:130:LEU:HD23	2:B:162:ARG:HG3	1.98	0.44
1:A:427:ALA:O	1:A:430:LYS:N	2.48	0.44
2:D:221:THR:C	2:D:223:GLY:N	2.71	0.44
4:F:102:PRO:HA	4:F:174:ASP:OD1	2.16	0.44
4:F:196:HIS:O	4:F:227:PRO:HA	2.17	0.44
1:A:414:GLU:C	1:A:416:GLY:H	2.20	0.44
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.99	0.44
1:C:48:SER:HB3	1:C:243:ARG:O	2.17	0.44
2:D:139:LEU:O	2:D:185:ALA:N	2.50	0.44
3:E:131:GLU:OE1	3:E:131:GLU:HA	2.17	0.44
4:F:31:ARG:HH21	4:F:32:LYS:HG3	1.82	0.44
2:B:189:VAL:HG11	2:B:415:MET:HE2	1.99	0.44
1:C:71:GLU:CG	1:C:98:ASP:HB3	2.44	0.44
2:D:233:MET:HE2	2:D:233:MET:HB3	1.84	0.44
4:F:78:VAL:HG21	4:F:181:VAL:HG21	2.00	0.44
2:B:261:PRO:O	2:B:264:HIS:ND1	2.46	0.44
4:F:7:ARG:HB2	4:F:42:GLY:HA2	1.99	0.44
4:F:186:LEU:CD1	4:F:320:MET:HG2	2.41	0.44
1:A:163:LYS:CB	1:A:164:LYS:NZ	2.81	0.44
1:A:414:GLU:C	1:A:416:GLY:N	2.71	0.44
2:B:2:ARG:NE	2:B:131:GLN:HG2	2.33	0.44
1:C:298:PRO:O	1:C:301:GLN:HG3	2.16	0.44
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.36	0.44
3:E:75:LYS:HE3	3:E:79:GLU:OE2	2.18	0.44
2:D:61:PRO:HD3	2:D:84:ILE:HG12	1.99	0.44
4:F:62:VAL:HG22	4:F:63:ASN:N	2.33	0.44
2:B:64:ILE:HD11	2:B:120:VAL:HA	2.00	0.43
2:B:102:ALA:HB2	2:B:403:MET:SD	2.57	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:ASP:HB3	1:C:422:ARG:NH2	2.33	0.43
2:D:77:ARG:O	2:D:82:GLY:HA3	2.18	0.43
2:D:267:MET:CE	2:D:299:MET:CG	2.96	0.43
2:D:392:LYS:CG	2:D:395:LEU:HD12	2.45	0.43
1:A:34:GLY:O	1:A:61:HIS:N	2.39	0.43
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.48	0.43
2:D:210:ILE:CG2	2:D:215:LEU:HD11	2.48	0.43
4:F:71:LEU:O	4:F:332:VAL:HB	2.18	0.43
1:A:66:VAL:HG23	1:A:91:GLN:O	2.18	0.43
1:C:415:GLU:O	1:C:418:PHE:HB2	2.18	0.43
2:D:8:GLN:HB3	2:D:14:ASN:HA	1.99	0.43
4:F:5:VAL:HG13	4:F:37:PHE:HB3	1.99	0.43
2:B:2:ARG:HB3	2:B:131:GLN:HG3	2.00	0.43
2:B:203:ASP:HB3	2:B:301:ALA:HA	2.00	0.43
2:B:227:HIS:CG	2:B:276:ARG:HG3	2.53	0.43
1:C:328:VAL:O	1:C:332:ILE:HG13	2.19	0.43
2:D:105:HIS:O	2:D:150:LEU:HD22	2.17	0.43
4:F:31:ARG:O	4:F:32:LYS:C	2.56	0.43
4:F:58:LEU:HA	4:F:58:LEU:HD23	1.69	0.43
4:F:192:LEU:HD12	4:F:192:LEU:N	2.33	0.43
4:F:226:GLU:HB2	4:F:238:CYS:CB	2.47	0.43
2:B:246:LEU:HD23	2:B:246:LEU:HA	1.67	0.43
1:C:193:THR:HG22	1:C:193:THR:O	2.18	0.43
1:C:205:ASP:HB3	1:C:302:MET:O	2.19	0.43
1:C:227:LEU:O	1:C:231:ILE:HG13	2.18	0.43
4:F:209:HIS:NE2	4:F:210:LEU:HG	2.33	0.43
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.34	0.43
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.37	0.43
2:D:101:TRP:CD1	2:D:146:GLY:HA2	2.53	0.43
4:F:225:SER:CB	4:F:252:ASN:HB3	2.49	0.43
1:A:68:VAL:HG13	1:A:68:VAL:O	2.19	0.43
2:B:189:VAL:HB	2:B:415:MET:CE	2.49	0.43
2:B:31:ASP:OD1	2:B:33:THR:HG23	2.19	0.43
4:F:296:MET:CE	4:F:380:HIS:ND1	2.82	0.43
4:F:338:CYS:SG	4:F:339:ALA:N	2.91	0.43
2:B:12:CYS:SG	2:B:138:SER:HB3	2.59	0.43
2:B:135:LEU:CD2	2:B:152:ILE:HD11	2.48	0.43
3:E:127:ASP:OD1	3:E:127:ASP:N	2.51	0.43
2:B:313:VAL:HB	2:B:349:VAL:HG22	1.99	0.43
3:E:69:LEU:HD23	3:E:69:LEU:HA	1.67	0.42
4:F:348:GLN:HE21	4:F:352:ASP:CG	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TYR:CZ	2:B:38:GLY:CA	3.00	0.42
2:D:1:MET:CE	2:D:128:ASP:HB2	2.48	0.42
3:E:59:GLU:O	3:E:62:LYS:N	2.53	0.42
4:F:135:TYR:HE1	4:F:145:ASN:HB3	1.83	0.42
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.54	0.42
1:C:322:ASP:OD2	1:C:373:ARG:NH2	2.42	0.42
4:F:97:SER:OG	4:F:183:GLN:HG3	2.19	0.42
4:F:138:ARG:HB3	4:F:145:ASN:OD1	2.19	0.42
4:F:209:HIS:HA	4:F:311:SER:O	2.19	0.42
4:F:338:CYS:HB3	4:F:343:TYR:CZ	2.55	0.42
1:A:141:PHE:CE1	1:A:170:SER:CB	3.02	0.42
2:B:42:LEU:HD22	2:B:243:PRO:HG2	2.00	0.42
2:B:402:GLY:HA3	3:E:82:VAL:HG13	2.01	0.42
1:C:102:ASN:OD1	1:C:104:ALA:N	2.51	0.42
1:C:258:ASN:ND2	1:C:352:LYS:HD2	2.34	0.42
2:D:198:GLU:OE2	2:D:254:ALA:HB2	2.20	0.42
1:A:36:MET:O	1:A:37:PRO:C	2.58	0.42
2:B:66:VAL:HG11	2:B:147:MET:HE3	2.02	0.42
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.01	0.42
1:C:345:ASP:OD1	1:C:345:ASP:C	2.58	0.42
2:D:104:GLY:O	2:D:109:GLY:HA3	2.19	0.42
2:D:320:ARG:O	2:D:363:MET:CE	2.67	0.42
2:D:328:GLU:HG3	2:D:328:GLU:H	1.64	0.42
1:A:234:ILE:HD12	1:A:234:ILE:N	2.35	0.42
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.35	0.42
1:C:4:CYS:HB3	1:C:136:LEU:CD1	2.50	0.42
2:D:64:ILE:HD11	2:D:123:GLU:HG3	2.00	0.42
1:A:34:GLY:HA3	1:A:60:LYS:HG3	2.02	0.42
1:A:178:SER:HB2	1:A:183:GLU:OE2	2.19	0.42
2:B:166:THR:O	2:B:199:THR:HA	2.20	0.42
2:B:316:ILE:HG23	2:B:316:ILE:O	2.20	0.42
1:C:254:GLU:HG2	1:C:352:LYS:CE	2.50	0.42
1:C:389:ALA:O	1:C:390:ARG:C	2.58	0.42
1:A:298:PRO:C	1:A:300:ASN:H	2.22	0.42
2:D:189:VAL:O	2:D:192:LEU:N	2.52	0.42
2:D:327:ASP:O	2:D:331:LEU:CD1	2.68	0.42
4:F:309:TYR:C	4:F:310:GLN:HG2	2.40	0.42
1:A:71:GLU:HG2	1:A:73:THR:H	1.85	0.42
1:A:291:ILE:HD13	1:A:373:ARG:HG3	2.01	0.42
2:B:316:ILE:HG22	2:B:366:THR:O	2.20	0.42
1:C:1:MET:HB3	1:C:130:THR:OG1	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:ALA:O	2:D:13:GLY:HA3	2.20	0.42
2:D:174:LYS:HE3	2:D:205:GLU:OE2	2.20	0.42
4:F:135:TYR:HE2	4:F:166:ALA:N	2.16	0.42
2:B:363:MET:HE2	2:B:363:MET:HB2	1.74	0.41
1:C:54:SER:O	1:C:61:HIS:HA	2.20	0.41
2:D:416:ASN:O	2:D:419:VAL:CG2	2.68	0.41
4:F:138:ARG:CB	4:F:145:ASN:OD1	2.68	0.41
4:F:305:LYS:HE3	4:F:306:HIS:NE2	2.35	0.41
1:A:437:VAL:O	1:A:437:VAL:HG12	2.19	0.41
1:C:54:SER:HB3	1:C:64:ARG:CZ	2.50	0.41
1:C:255:PHE:CD1	1:C:352:LYS:HD3	2.55	0.41
2:D:404:ASP:CG	2:D:406:MET:HG2	2.40	0.41
4:F:31:ARG:NH2	4:F:32:LYS:HG3	2.35	0.41
1:C:399:TYR:CE1	1:C:418:PHE:HB3	2.55	0.41
2:D:253:LEU:HD13	8:D:501:A1D6L:C09	2.49	0.41
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.00	0.41
3:E:60:ARG:O	3:E:64:GLN:HG3	2.21	0.41
4:F:146:VAL:HG12	4:F:185:TYR:CB	2.50	0.41
1:A:161:TYR:O	1:A:163:LYS:N	2.53	0.41
2:B:169:VAL:HA	2:B:202:ILE:O	2.20	0.41
2:B:272:PRO:O	2:B:274:THR:HG23	2.21	0.41
8:B:501:A1D6L:C21	8:B:501:A1D6L:C06	2.99	0.41
2:D:203:ASP:OD2	2:D:377:LEU:HD23	2.20	0.41
3:E:9:ILE:HG13	3:E:10:GLU:HG3	2.02	0.41
4:F:4:PHE:HD2	4:F:27:TRP:HE3	1.68	0.41
2:D:152:ILE:O	2:D:153:SER:C	2.59	0.41
2:D:404:ASP:OD2	2:D:406:MET:HE2	2.21	0.41
1:A:256:GLN:H	1:A:256:GLN:HG3	1.73	0.41
1:C:271:THR:HG21	1:C:295:CYS:O	2.20	0.41
2:D:140:GLY:HA2	2:D:184:ASN:HB2	2.02	0.41
4:F:287:ILE:HG23	4:F:319:PHE:CE1	2.54	0.41
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.56	0.41
1:A:316:CYS:HA	1:A:352:LYS:O	2.19	0.41
2:B:9:ALA:HA	2:B:66:VAL:O	2.21	0.41
2:B:180:VAL:HB	2:B:398:TYR:OH	2.21	0.41
2:B:272:PRO:HD2	2:B:361:LEU:HD13	2.01	0.41
2:D:235:GLY:HA3	2:D:366:THR:OG1	2.20	0.41
2:D:308:GLY:HA2	2:D:426:GLN:CD	2.40	0.41
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.85	0.41
1:A:51:THR:HG22	1:A:52:PHE:CD1	2.55	0.41
2:B:316:ILE:HG21	2:B:366:THR:HB	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:GLU:HG3	2:D:2:ARG:HH12	1.82	0.41
1:C:219:ILE:CG2	1:C:222:PRO:CA	2.98	0.41
1:C:276:ILE:HG23	1:C:369:ALA:HB3	2.03	0.41
2:D:66:VAL:HA	2:D:91:VAL:O	2.20	0.41
2:D:211:CYS:CA	2:D:215:LEU:HD13	2.39	0.41
2:D:316:ILE:O	2:D:365:ALA:HA	2.21	0.41
3:E:6:MET:HG3	3:E:24:LEU:HD22	2.00	0.41
4:F:275:LEU:O	4:F:276:ASN:HB3	2.20	0.41
1:A:68:VAL:HG21	1:A:149:PHE:CE2	2.56	0.41
2:B:351:THR:HG22	2:B:352:ALA:N	2.36	0.41
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.86	0.41
1:C:214:ARG:HG2	1:C:219:ILE:O	2.20	0.41
1:C:302:MET:HE3	1:C:302:MET:HB3	1.91	0.41
2:D:107:THR:OG1	2:D:108:GLU:N	2.54	0.41
2:D:324:LYS:HE2	2:D:328:GLU:OE2	2.21	0.41
2:D:416:ASN:O	2:D:419:VAL:HG23	2.20	0.41
3:E:130:ALA:HA	3:E:133:VAL:CG1	2.50	0.41
4:F:1:MET:HE1	4:F:28:LYS:CB	2.51	0.41
4:F:195:GLY:HA3	4:F:197:ARG:CG	2.50	0.41
4:F:219:GLY:HA3	4:F:264:PHE:CE2	2.56	0.41
4:F:312:PHE:CG	4:F:354:ALA:HB1	2.56	0.41
2:B:414:ASN:O	2:B:417:ASP:HB2	2.21	0.41
2:D:137:HIS:CE1	2:D:139:LEU:HD21	2.56	0.41
2:D:389:PHE:CE1	2:D:408:PHE:HB3	2.55	0.41
4:F:192:LEU:CD2	4:F:262:MET:CE	2.93	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.01	0.40
2:B:324:LYS:HG2	2:B:328:GLU:OE2	2.21	0.40
2:D:89:ASN:ND2	2:D:123:GLU:OE2	2.44	0.40
4:F:202:ARG:HD3	4:F:204:TRP:CE2	2.56	0.40
2:B:219:THR:O	2:B:219:THR:HG22	2.21	0.40
2:B:284:LEU:O	2:B:363:MET:HE1	2.21	0.40
2:B:402:GLY:C	3:E:82:VAL:HG13	2.42	0.40
2:D:2:ARG:HB3	2:D:131:GLN:CG	2.51	0.40
4:F:137:ARG:O	4:F:137:ARG:HD2	2.22	0.40
1:A:217:LEU:HB3	1:A:219:ILE:CD1	2.51	0.40
2:B:203:ASP:O	2:B:207:LEU:HG	2.21	0.40
1:C:318:LEU:HD12	1:C:318:LEU:N	2.35	0.40
2:D:34:GLY:O	2:D:58:LYS:HA	2.21	0.40
2:D:285:THR:CG2	2:D:288:GLU:HB2	2.43	0.40
2:D:375:GLN:O	2:D:379:LYS:HG3	2.21	0.40
4:F:148:ILE:HD13	4:F:162:ILE:HG13	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:148:ILE:HG13	4:F:149:ALA:N	2.36	0.40
1:A:156:ARG:O	1:A:159:VAL:N	2.40	0.40
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.57	0.40
1:C:88:HIS:HD2	1:C:90:GLU:HB2	1.86	0.40
2:D:12:CYS:CB	2:D:138:SER:HB3	2.50	0.40
4:F:232:ASN:OD1	4:F:232:ASN:N	2.50	0.40
1:A:41:THR:O	1:A:55:GLU:OE1	2.40	0.40
2:B:8:GLN:HG3	2:B:14:ASN:OD1	2.21	0.40
2:B:61:PRO:HD3	2:B:84:ILE:HG12	2.04	0.40
2:B:267:MET:HE1	2:B:299:MET:HG3	2.03	0.40
2:B:391:ARG:HA	2:B:391:ARG:HD2	1.87	0.40
1:C:265:ILE:N	1:C:265:ILE:CD1	2.84	0.40
2:D:13:GLY:CA	2:D:137:HIS:HA	2.51	0.40
4:F:2:TYR:OH	4:F:360:PRO:O	2.25	0.40
4:F:61:LEU:HD12	4:F:310:GLN:O	2.22	0.40
4:F:135:TYR:OH	4:F:165:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	435/440 (99%)	396 (91%)	32 (7%)	7 (2%)	8	27
1	C	438/440 (100%)	410 (94%)	25 (6%)	3 (1%)	19	46
2	B	425/431 (99%)	400 (94%)	22 (5%)	3 (1%)	19	46
2	D	417/431 (97%)	379 (91%)	32 (8%)	6 (1%)	9	30
3	E	117/143 (82%)	100 (86%)	14 (12%)	3 (3%)	4	18
4	F	322/380 (85%)	289 (90%)	27 (8%)	6 (2%)	6	23
All	All	2154/2265 (95%)	1974 (92%)	152 (7%)	28 (1%)	10	32

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	109	THR
3	E	10	GLU
4	F	253	TYR
1	C	218	ASP
2	D	79	GLY
2	D	142	GLY
2	D	190	HIS
3	E	27	PRO
4	F	32	LYS
4	F	255	ARG
1	A	299	ALA
2	B	394	PHE
1	C	314	ALA
4	F	129	GLU
1	A	415	GLU
2	B	71	GLY
2	B	143	THR
2	D	57	ASN
3	E	25	LYS
4	F	336	PRO
1	A	108	TYR
1	A	261	PRO
4	F	102	PRO
2	D	243	PRO
1	A	162	GLY
2	D	175	VAL
1	C	146	GLY

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	366/371 (99%)	366 (100%)	0	100	100
1	C	370/371 (100%)	369 (100%)	1 (0%)	91	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	367/372 (99%)	365 (100%)	2 (0%)	86	91
2	D	362/372 (97%)	357 (99%)	5 (1%)	62	79
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	295/338 (87%)	289 (98%)	6 (2%)	50	71
All	All	1869/1951 (96%)	1855 (99%)	14 (1%)	81	89

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	137	HIS
2	B	190	HIS
1	C	71	GLU
2	D	73	MET
2	D	137	HIS
2	D	153	SER
2	D	392	LYS
2	D	413	SER
4	F	19	ARG
4	F	28	LYS
4	F	31	ARG
4	F	128	ARG
4	F	135	TYR
4	F	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
2	B	423	GLN
2	B	426	GLN
1	C	88	HIS
2	D	298	ASN
4	F	246	GLN
4	F	260	ASN
4	F	348	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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
8	A1D6L	B	501	-	27,27,27	2.04	7 (25%)	35,39,39	1.52	7 (20%)
10	MES	B	504	-	12,12,12	2.27	1 (8%)	14,16,16	1.94	6 (42%)
5	GTP	A	501	7	26,34,34	1.12	2 (7%)	32,54,54	1.60	7 (21%)
5	GTP	C	501	7	26,34,34	1.11	2 (7%)	32,54,54	1.58	7 (21%)
11	ACP	F	401	-	27,33,33	0.78	1 (3%)	32,52,52	1.49	2 (6%)
10	MES	B	503	-	12,12,12	2.29	1 (8%)	14,16,16	1.89	4 (28%)
8	A1D6L	D	501	-	27,27,27	1.95	6 (22%)	35,39,39	1.44	7 (20%)
9	GDP	B	502	7	24,30,30	0.94	1 (4%)	30,47,47	1.27	4 (13%)
9	GDP	D	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)

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
8	A1D6L	B	501	-	-	5/6/16/16	0/4/4/4
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
5	GTP	A	501	7	-	9/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	7	-	9/18/38/38	0/3/3/3
11	ACP	F	401	-	-	5/15/38/38	0/3/3/3
10	MES	B	503	-	-	4/6/14/14	0/1/1/1
8	A1D6L	D	501	-	-	6/6/16/16	0/4/4/4
9	GDP	B	502	7	-	4/12/32/32	0/3/3/3
9	GDP	D	502	-	-	3/12/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.66	1.66	1.77
10	B	504	MES	C8-S	-7.62	1.66	1.77
8	B	501	A1D6L	C09-N11	5.78	1.45	1.33
8	D	501	A1D6L	C09-N11	5.75	1.45	1.33
8	B	501	A1D6L	C13-N12	4.70	1.48	1.40
8	D	501	A1D6L	C13-N12	4.48	1.47	1.40
5	A	501	GTP	C5-C6	-3.99	1.39	1.47
5	C	501	GTP	C5-C6	-3.95	1.39	1.47
8	D	501	A1D6L	C05-C04	-3.70	1.36	1.42
8	D	501	A1D6L	C15-C14	3.06	1.56	1.51
8	B	501	A1D6L	C05-C04	-3.02	1.37	1.42
8	D	501	A1D6L	C07-N12	3.00	1.45	1.39
8	B	501	A1D6L	C15-C14	3.00	1.56	1.51
8	B	501	A1D6L	C07-N12	2.97	1.45	1.39
11	F	401	ACP	PB-O3A	2.80	1.61	1.58
8	D	501	A1D6L	C17-N12	-2.71	1.42	1.46
8	B	501	A1D6L	C06-C01	2.49	1.40	1.36
9	D	502	GDP	C6-N1	-2.38	1.34	1.37
8	B	501	A1D6L	C17-N12	-2.35	1.43	1.46
9	B	502	GDP	C6-N1	-2.33	1.34	1.37
5	C	501	GTP	C2-N3	2.21	1.38	1.33
5	A	501	GTP	C2-N3	2.20	1.38	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	PB-O3A-PA	-6.78	111.05	132.56
10	B	504	MES	C5-N4-C3	4.32	118.56	108.83
10	B	503	MES	C5-N4-C3	4.08	118.01	108.83
9	D	502	GDP	PA-O3A-PB	-3.87	119.55	132.83
5	A	501	GTP	PB-O3B-PG	-3.64	120.32	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	PA-O3A-PB	-3.59	120.50	132.83
5	C	501	GTP	PB-O3B-PG	-3.57	120.57	132.83
5	C	501	GTP	PA-O3A-PB	-3.54	120.68	132.83
9	B	502	GDP	PA-O3A-PB	-3.45	121.00	132.83
8	B	501	A1D6L	N08-C07-N12	3.32	119.77	116.26
5	A	501	GTP	C5-C6-N1	3.22	119.63	113.95
5	C	501	GTP	C5-C6-N1	3.13	119.48	113.95
5	C	501	GTP	C8-N7-C5	3.11	108.91	102.99
8	D	501	A1D6L	N10-C09-N08	-3.09	123.10	127.22
5	A	501	GTP	C8-N7-C5	3.06	108.81	102.99
8	B	501	A1D6L	N10-C09-N08	-3.05	123.16	127.22
8	D	501	A1D6L	C01-C06-C05	2.92	121.08	118.80
5	C	501	GTP	C2-N1-C6	-2.85	119.85	125.10
5	A	501	GTP	C2-N1-C6	-2.84	119.87	125.10
8	D	501	A1D6L	C02-C01-C06	-2.84	120.10	123.23
9	D	502	GDP	C3'-C2'-C1'	2.80	105.19	100.98
8	D	501	A1D6L	C05-C04-N10	-2.76	119.88	122.81
8	B	501	A1D6L	N11-C09-N08	2.74	121.51	117.25
10	B	503	MES	O2S-S-C8	2.72	110.19	106.92
5	A	501	GTP	C3'-C2'-C1'	2.71	105.06	100.98
10	B	503	MES	C6-C5-N4	-2.68	106.03	110.10
9	B	502	GDP	C3'-C2'-C1'	2.68	105.02	100.98
8	B	501	A1D6L	C05-C04-N10	-2.64	120.01	122.81
10	B	504	MES	C6-C5-N4	-2.52	106.28	110.10
5	C	501	GTP	C3'-C2'-C1'	2.50	104.75	100.98
8	D	501	A1D6L	N08-C07-N12	2.47	118.87	116.26
11	F	401	ACP	C5-C6-N6	2.35	123.93	120.35
10	B	504	MES	O3S-S-C8	2.35	109.57	105.77
8	B	501	A1D6L	C18-C14-C13	2.34	121.11	118.95
8	D	501	A1D6L	C09-N08-C07	2.33	120.38	113.91
9	D	502	GDP	C8-N7-C5	2.31	107.39	102.99
9	D	502	GDP	C5-C6-N1	2.30	118.02	113.95
9	B	502	GDP	C8-N7-C5	2.30	107.37	102.99
9	B	502	GDP	C5-C6-N1	2.28	117.98	113.95
10	B	504	MES	O1S-S-C8	2.27	109.64	106.92
10	B	503	MES	O3S-S-C8	2.22	109.36	105.77
5	A	501	GTP	O6-C6-C5	-2.18	120.11	124.37
8	B	501	A1D6L	C02-C01-C06	-2.12	120.89	123.23
8	B	501	A1D6L	C09-N08-C07	2.10	119.74	113.91
5	C	501	GTP	O6-C6-C5	-2.10	120.27	124.37
8	D	501	A1D6L	C23-O22-C19	-2.05	113.05	117.51
10	B	504	MES	C7-N4-C3	2.01	116.37	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	O2S-S-C8	2.00	109.33	106.92

There are no chirality outliers.

All (49) 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-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	A1D6L	N08-C07-N12-C13
8	B	501	A1D6L	C05-C07-N12-C17
8	D	501	A1D6L	C05-C07-N12-C13
8	D	501	A1D6L	N08-C07-N12-C13
8	D	501	A1D6L	C05-C07-N12-C17
8	D	501	A1D6L	N08-C07-N12-C17
9	B	502	GDP	C5'-O5'-PA-O1A
9	B	502	GDP	C5'-O5'-PA-O2A
9	D	502	GDP	C5'-O5'-PA-O1A
9	D	502	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
10	B	504	MES	C7-C8-S-O2S
10	B	504	MES	C7-C8-S-O3S
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
8	D	501	A1D6L	C20-C19-O22-C23
8	D	501	A1D6L	C18-C19-O22-C23
8	B	501	A1D6L	C20-C19-O22-C23
8	B	501	A1D6L	C18-C19-O22-C23
5	A	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	C3'-C4'-C5'-O5'
8	B	501	A1D6L	N08-C07-N12-C17
10	B	504	MES	C8-C7-N4-C3
10	B	503	MES	C7-C8-S-O3S
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
9	D	502	GDP	C5'-O5'-PA-O3A
11	F	401	ACP	C4'-C5'-O5'-PA
5	A	501	GTP	C5'-O5'-PA-O1A
10	B	503	MES	C7-C8-S-O1S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	B	503	MES	C7-C8-S-O2S
10	B	504	MES	C7-C8-S-O1S
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O1A
11	F	401	ACP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
9	B	502	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C3'-C4'-C5'-O5'
11	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O2A
9	B	502	GDP	PB-O3A-PA-O2A

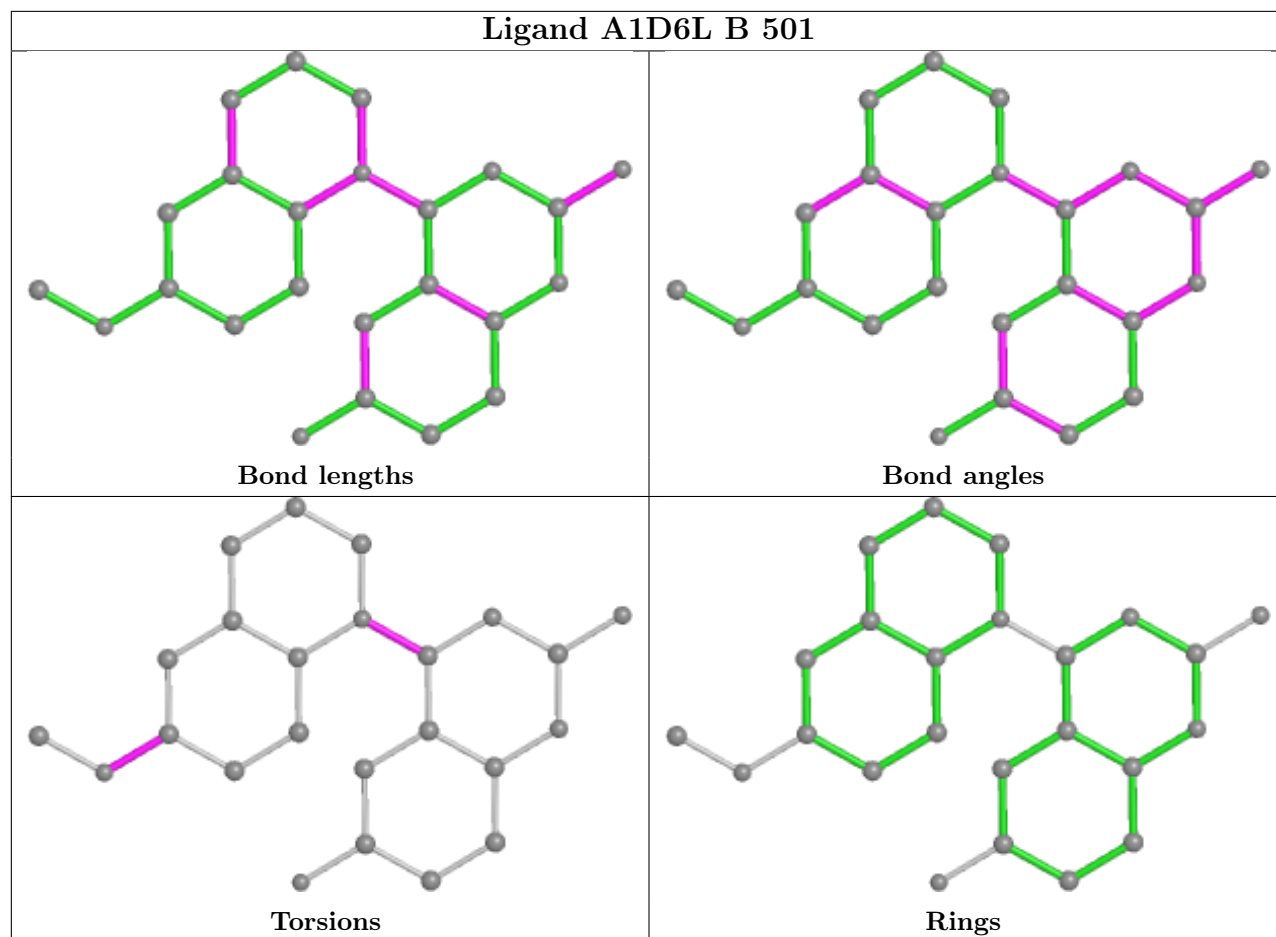
There are no ring outliers.

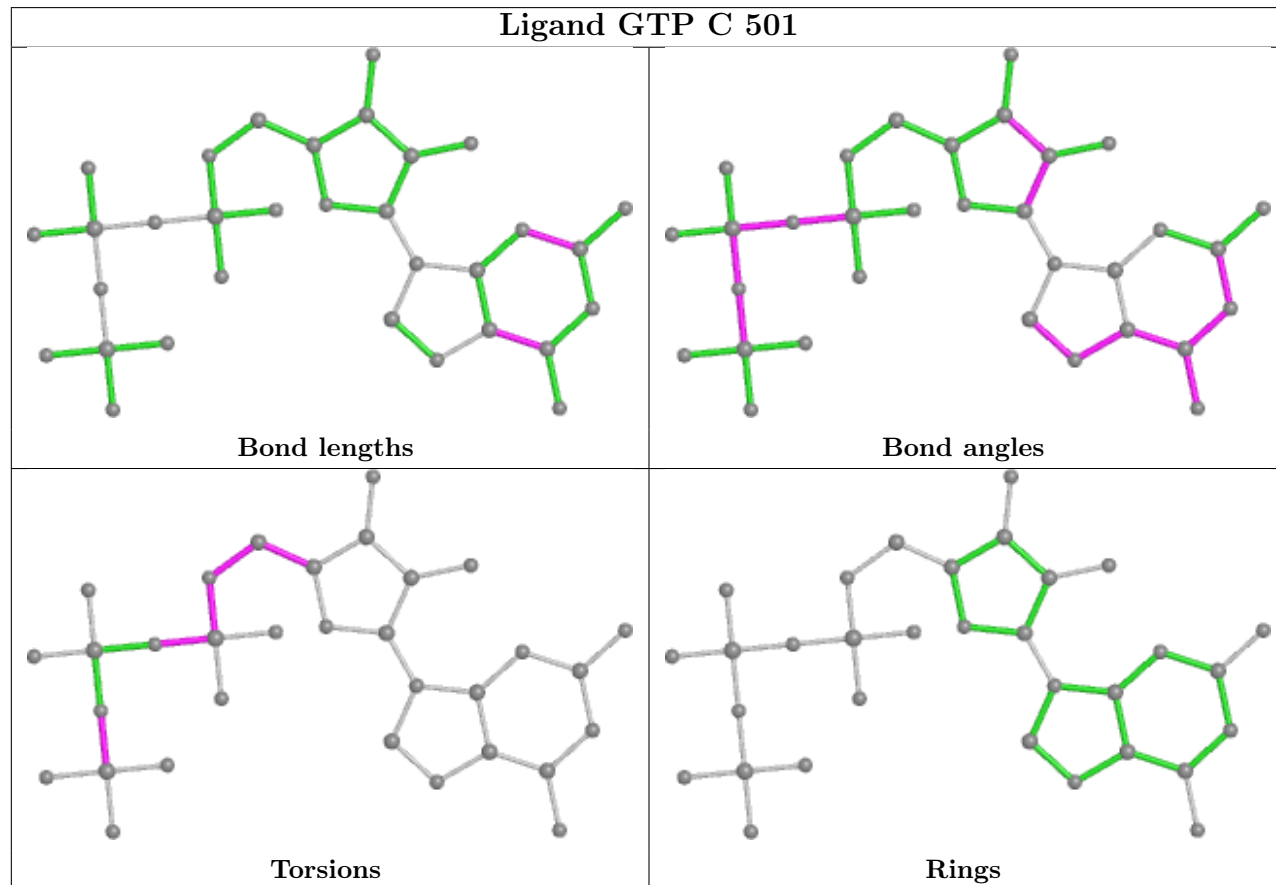
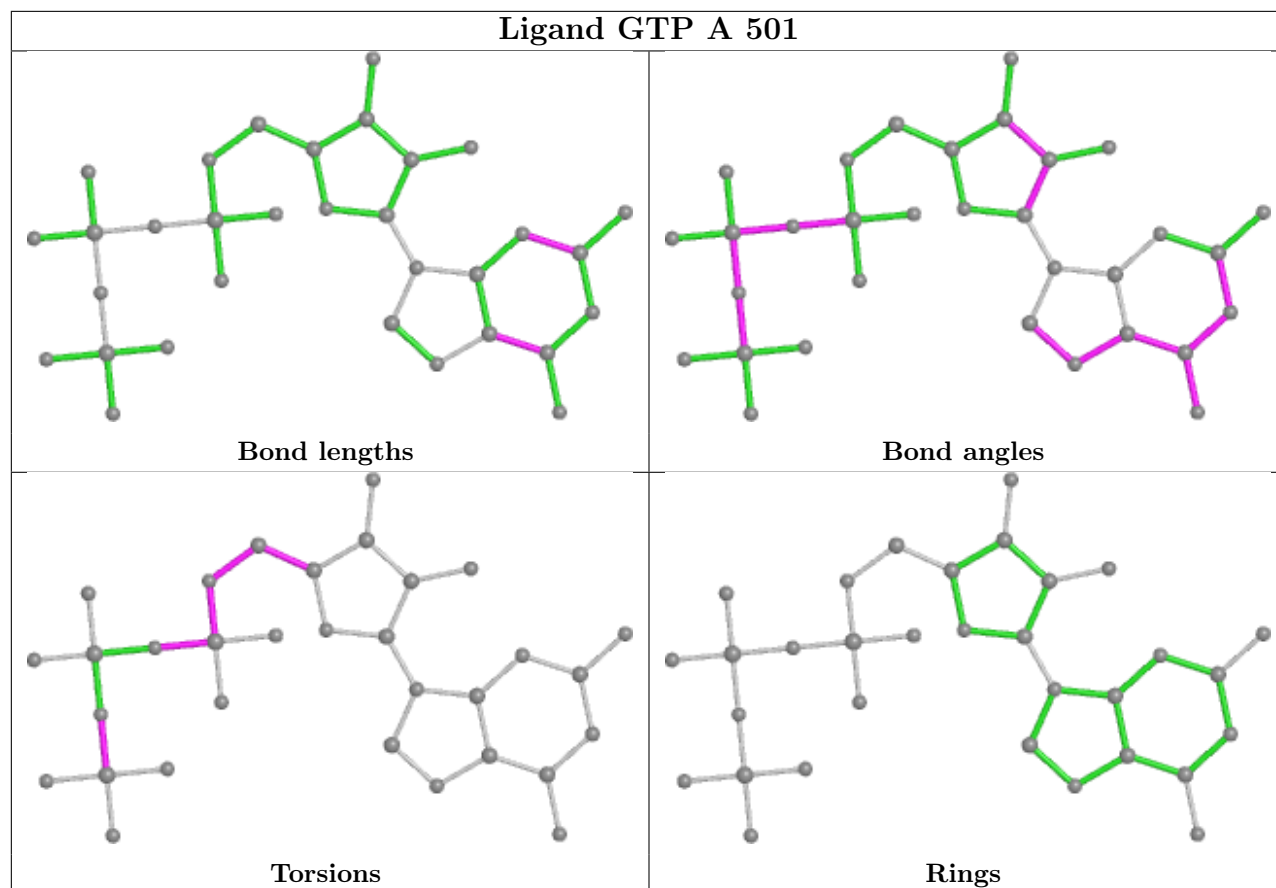
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	A1D6L	2	0
8	D	501	A1D6L	2	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 than 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 A1D6L B 501

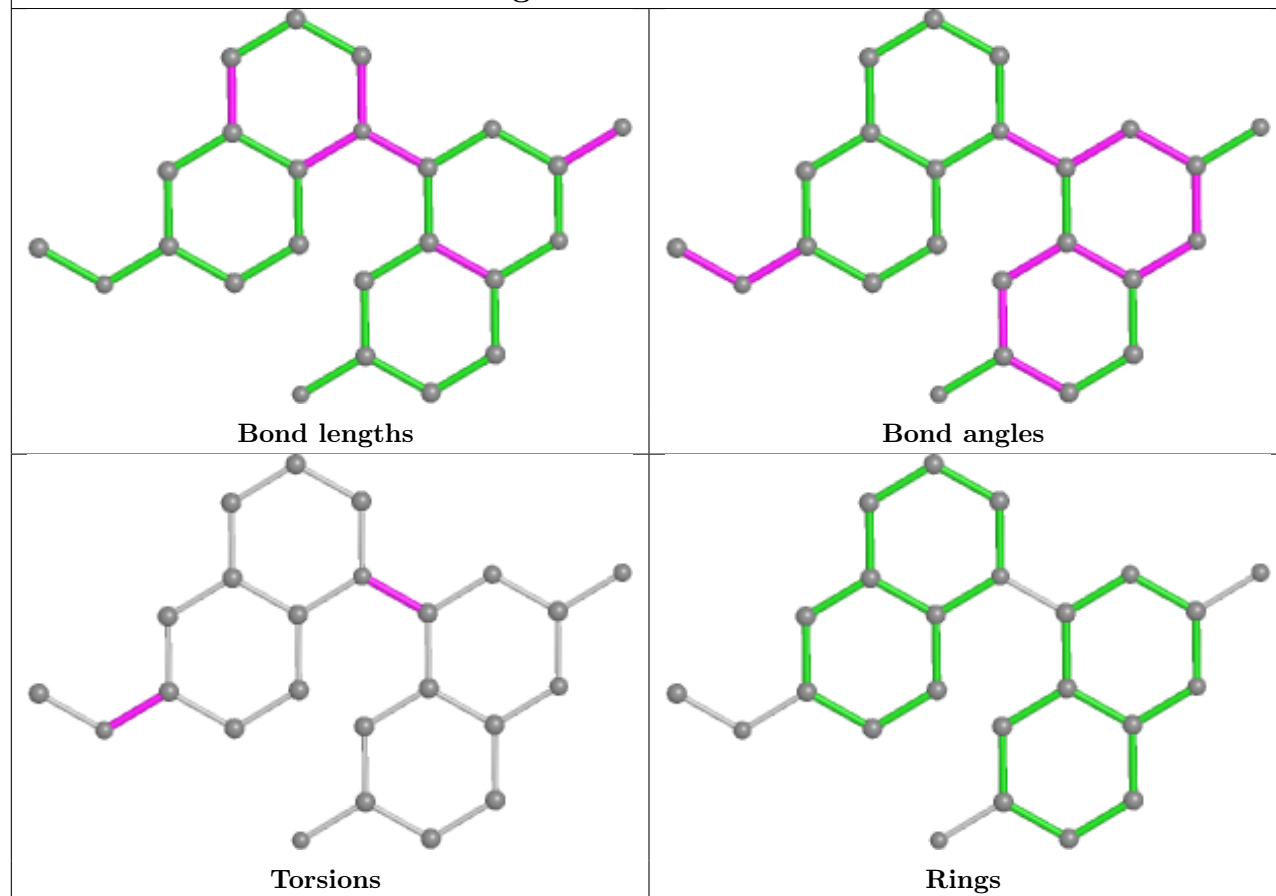


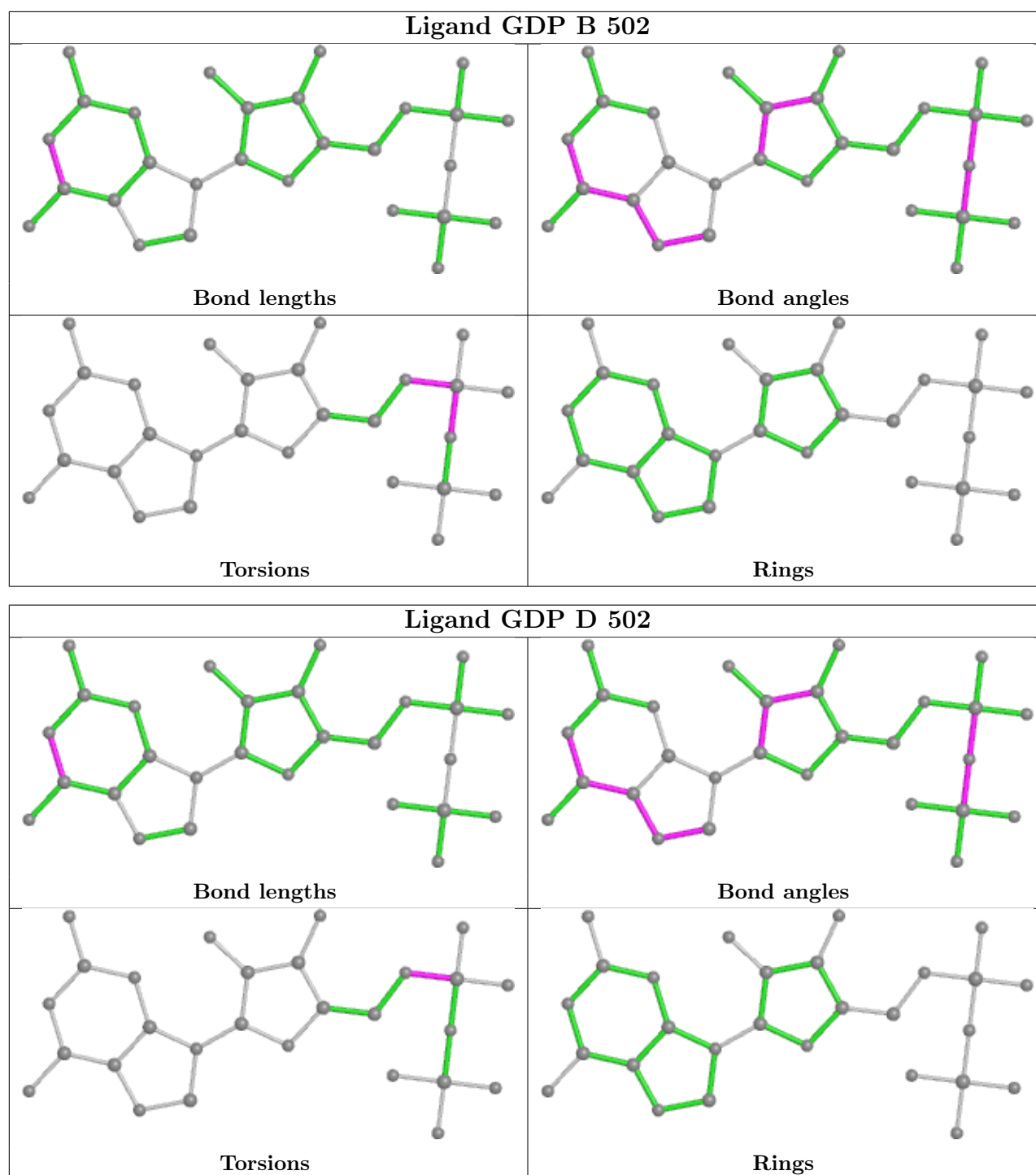


Ligand ACP F 401



Ligand A1D6L D 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/440 (99%)	-0.35	2 (0%) 87 74	33, 52, 75, 116	0
1	C	440/440 (100%)	-0.60	0 100 100	28, 41, 64, 80	0
2	B	427/431 (99%)	-0.45	1 (0%) 92 85	29, 49, 78, 128	0
2	D	421/431 (97%)	0.12	5 (1%) 76 58	34, 73, 109, 127	0
3	E	121/143 (84%)	-0.12	0 100 100	38, 63, 97, 117	0
4	F	332/380 (87%)	0.17	13 (3%) 44 26	46, 77, 145, 159	0
All	All	2178/2265 (96%)	-0.24	21 (0%) 79 63	28, 56, 110, 159	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	141	GLY	4.7
2	D	73	MET	3.6
2	D	431	ASP	3.5
1	A	179	THR	3.3
4	F	173	ILE	3.0
4	F	161	LEU	2.8
4	F	182	ILE	2.8
4	F	132	LEU	2.7
2	D	6	HIS	2.5
2	D	11	GLN	2.5
4	F	103	THR	2.5
1	A	437	VAL	2.4
4	F	242	ASN	2.4
4	F	233	PHE	2.4
4	F	245	ILE	2.3
4	F	247	LYS	2.3
4	F	74	LYS	2.2
4	F	180	HIS	2.2
4	F	149	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	148	ILE	2.1
2	B	428	ALA	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 [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.