



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 01:32 PM JST

PDB ID : 8YU9  
Title : Tubulin-RB3-TTL in complex with compound SI10  
Authors : Wu, C.Y.; Wang, Y.X.  
Deposited on : 2024-03-27  
Resolution : 3.25 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](mailto: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>.

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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) : 2.40

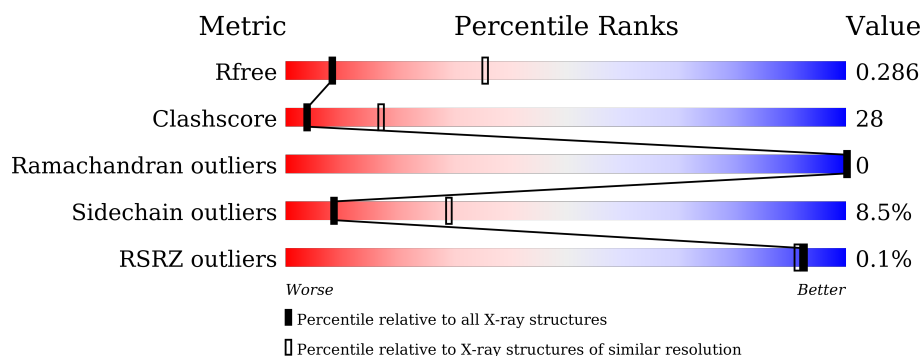
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1482 (3.30-3.22)
Clashscore	180529	1546 (3.30-3.22)
Ramachandran outliers	177936	1536 (3.30-3.22)
Sidechain outliers	177891	1535 (3.30-3.22)
RSRZ outliers	164620	1483 (3.30-3.22)

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  $\geq 3$ , 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>56%</div> <div>41%</div> <div>..</div> </div>
1	C	440	<div> <div>55%</div> <div>41%</div> <div>.</div> </div>
2	B	431	<div> <div>51%</div> <div>46%</div> <div>..</div> </div>
2	D	431	<div> <div>43%</div> <div>48%</div> <div>6%</div> <div>.</div> </div>
3	E	143	<div> <div>48%</div> <div>31%</div> <div>5%</div> <div>16%</div> </div>
4	F	380	<div> <div>35%</div> <div>38%</div> <div>5%</div> <div>22%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	A1D7A	D	501	-	X	-	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17095 atoms, of which 36 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
			3394	2145	579	648	22			
1	C	440	Total	C	N	O	S	0	0	0
			3429	2169	582	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	418	Total	C	N	O	S	0	0	0
			3275	2062	552	634	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			988	611	180	192	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

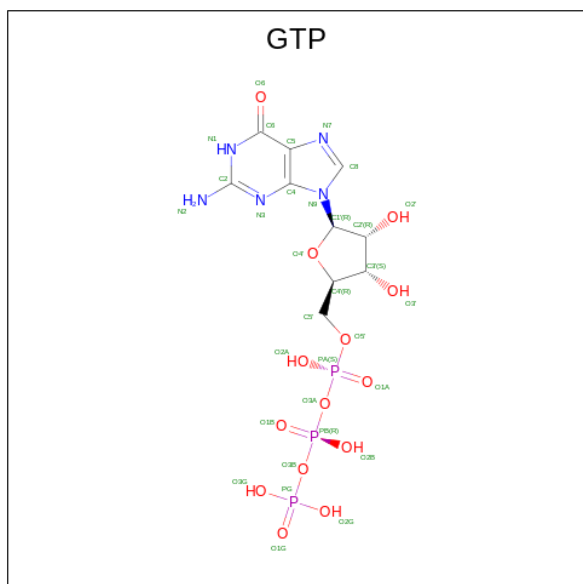
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	298	Total	C	N	O	S	0	0	0
			2396	1547	398	438	13			

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).

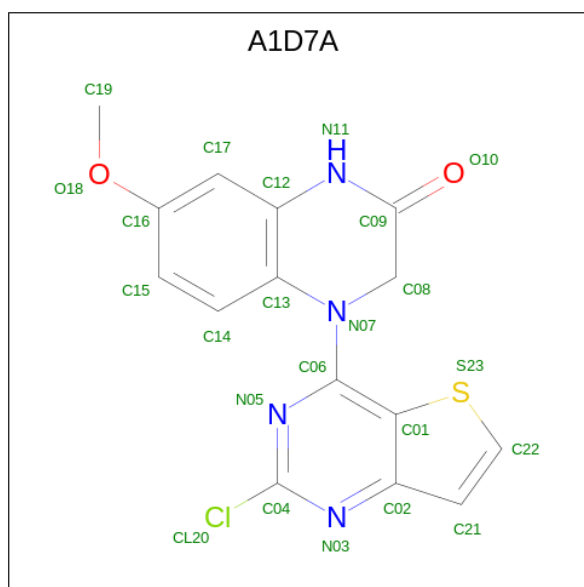
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	1	0
			1	1		
7	B	1	Total	Mg	1	0
			1	1		

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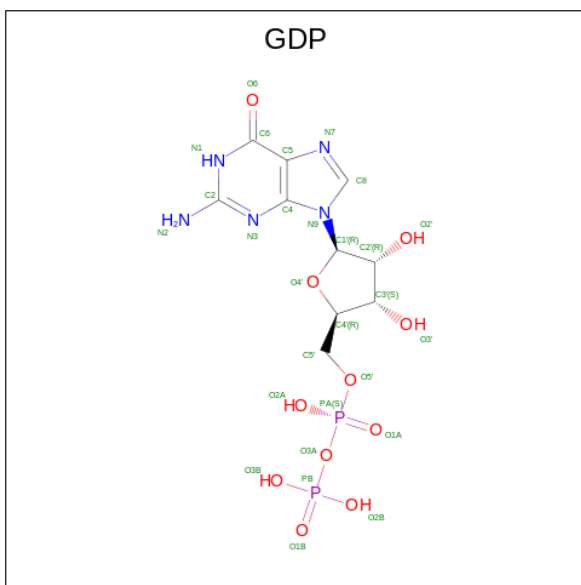
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	1	0
			1	1		

- Molecule 8 is 4-(2-chloranylthieno[3,2-d]pyrimidin-4-yl)-7-methoxy-1,3-dihydroquinoxalin-2-one (three-letter code: A1D7A) (formula: C<sub>15</sub>H<sub>11</sub>ClN<sub>4</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



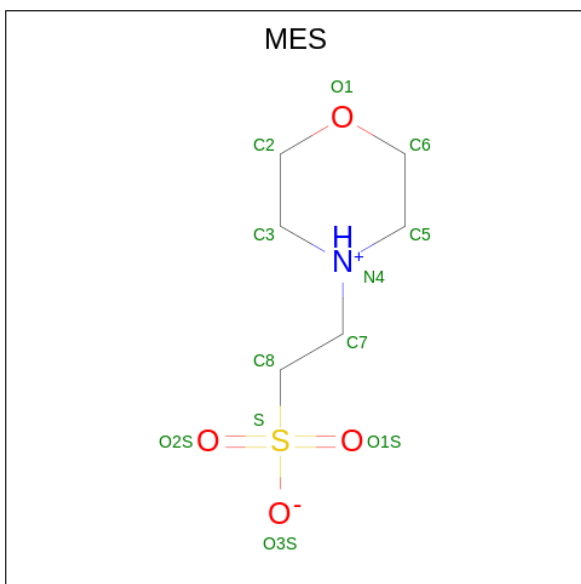
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	B	1	Total	C	Cl	H	N	O	S	0	0
			34	15	1	11	4	2	1		
8	D	1	Total	C	Cl	H	N	O	S	0	0
			34	15	1	11	4	2	1		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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:  $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$ ).



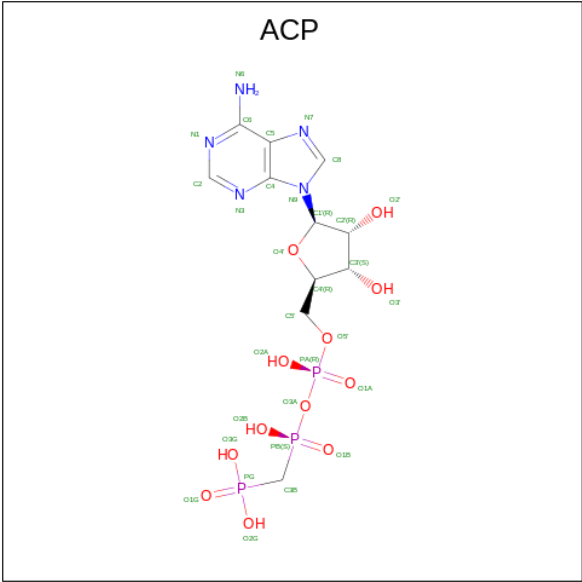
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

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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: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



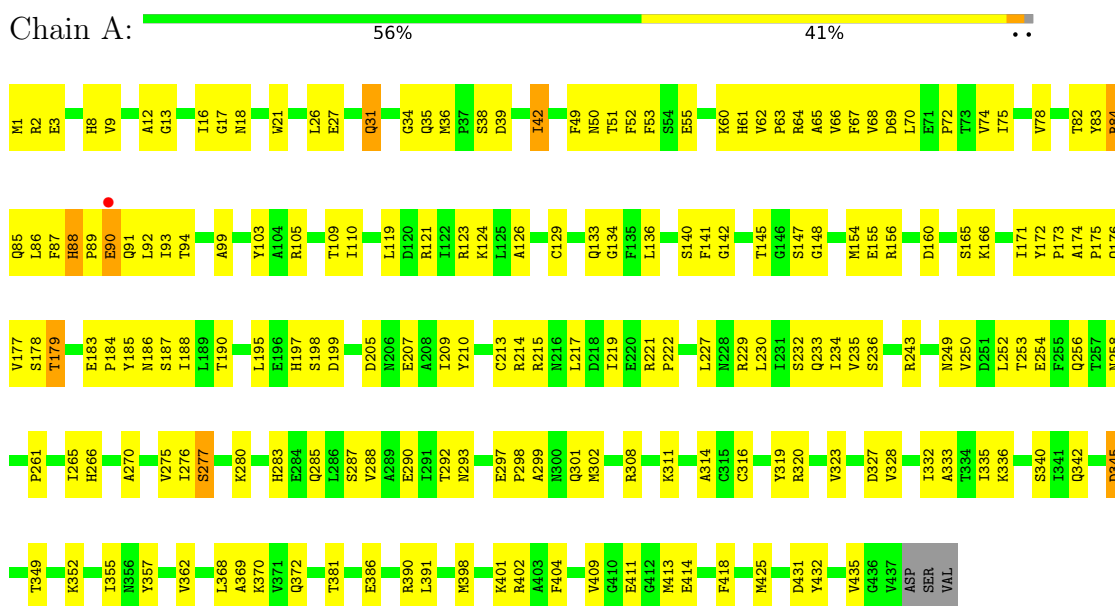
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	45	0
			45	11	14	5	12	3		



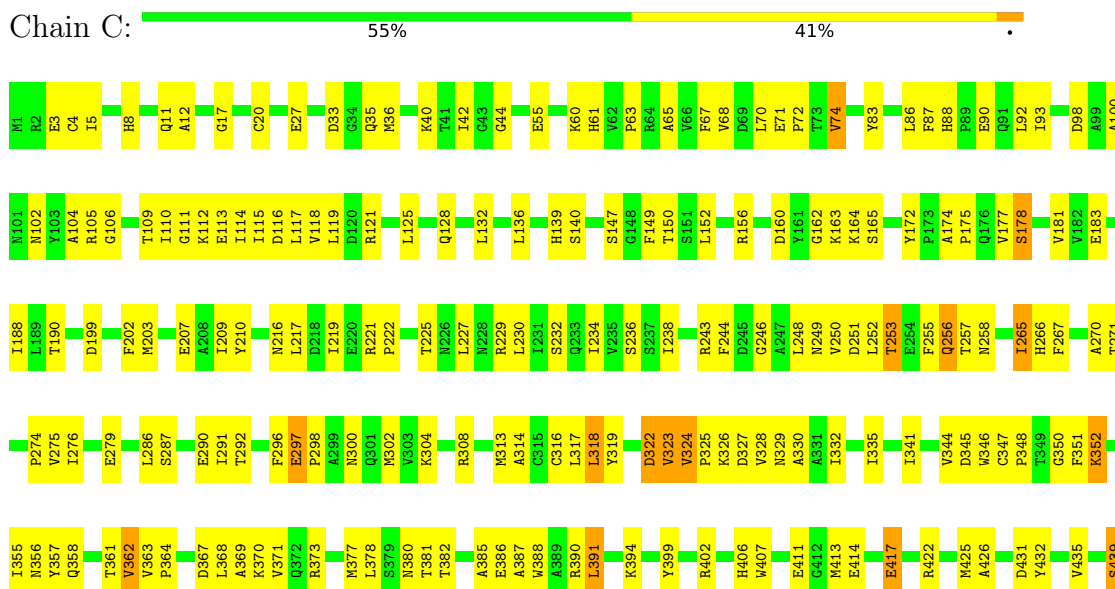
### 3 Residue-property plots

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

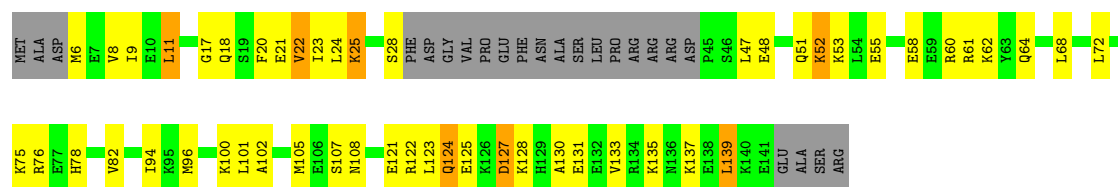


#### • Molecule 1: Detyrosinated tubulin alpha-1B chain

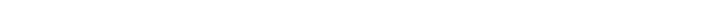


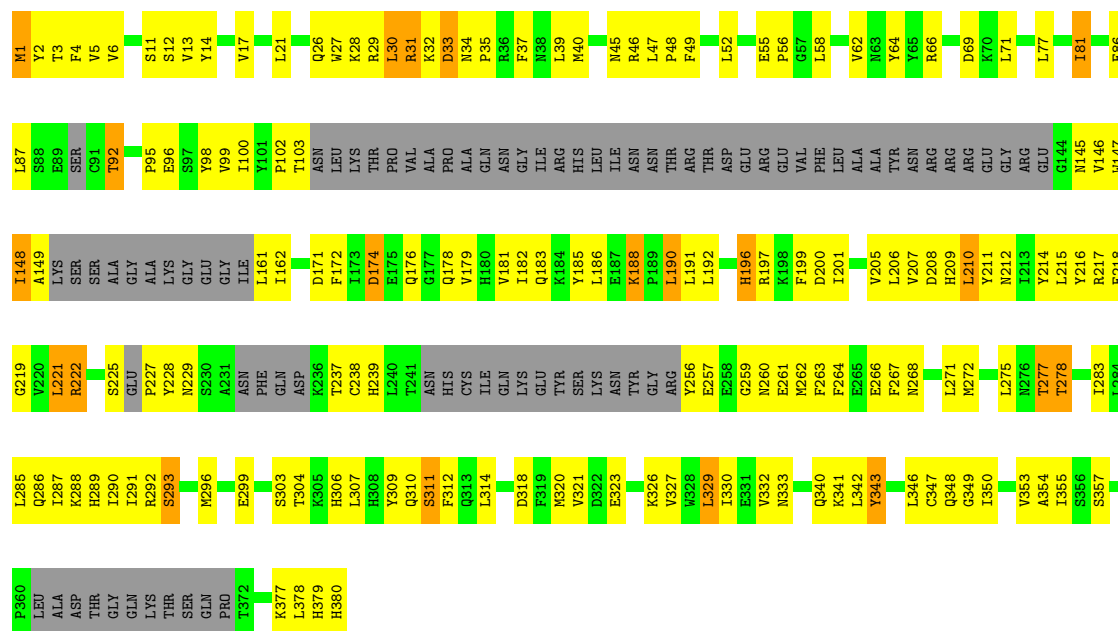


Chain E:  48% 31% 5% 16%



- Molecule 4: Tubulin-tyrosine ligase

Chain F:  35% 38% 5% 22%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.97Å 157.38Å 182.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.33 – 3.25 87.33 – 3.25	Depositor EDS
% Data completeness (in resolution range)	86.9 (87.33-3.25) 86.8 (87.33-3.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 3.26Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, $R_{free}$	0.205 , 0.286 0.205 , 0.286	Depositor DCC
$R_{free}$ test set	46398 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.4	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 74.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	17095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, CA, GDP, A1D7A, MES, ACP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.51	0/3470	0.68	1/4713 (0.0%)
1	C	0.58	1/3507 (0.0%)	0.72	0/4764
2	B	0.54	0/3426	0.70	0/4643
2	D	0.45	0/3347	0.63	0/4536
3	E	0.51	0/996	0.61	0/1320
4	F	0.43	0/2450	0.62	0/3319
All	All	0.51	1/17196 (0.0%)	0.67	1/23295 (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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	20	CYS	CB-SG	-5.42	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	PRO	C-N-CA	-5.61	107.68	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	280	GLN	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	3394	0	3294	174	0
1	C	3429	0	3326	168	0
2	B	3351	0	3214	181	0
2	D	3275	0	3140	255	0
3	E	988	0	1011	54	0
4	F	2396	0	2323	144	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	23	11	0	2	0
8	D	23	11	0	2	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	24	0	26	0	0
11	F	31	14	14	0	0
All	All	17059	36	16396	926	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 28.

All (926) 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:123:ARG:HH22	1:A:160:ASP:HB3	1.16	1.05
4:F:289:HIS:O	4:F:293:SER:OG	1.75	1.03
1:A:336:LYS:HD3	3:E:24:LEU:HD12	1.40	1.01
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.42	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:THR:HA	1:C:256:GLN:HB2	1.43	0.96
2:D:54:ALA:HB3	2:D:58:LYS:HB2	1.47	0.96
1:A:209:ILE:HG22	1:A:227:LEU:HD23	1.49	0.95
2:B:246:LEU:HD12	2:B:352:ALA:HB2	1.49	0.91
2:D:321:MET:HB3	2:D:363:MET:HE1	1.52	0.91
1:C:88:HIS:CD2	1:C:90:GLU:H	1.90	0.90
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.06	0.89
2:D:372:THR:O	2:D:375:GLN:HG2	1.72	0.88
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.54	0.88
2:D:209:ASP:HB3	2:D:213:ARG:NH2	1.88	0.88
2:D:106:TYR:CD1	3:E:133:VAL:HG11	2.09	0.88
4:F:148:ILE:HB	4:F:162:ILE:HG12	1.56	0.88
2:D:121:ARG:NH2	2:D:158:GLU:OE1	2.07	0.87
2:D:179:VAL:HG12	2:D:388:MET:SD	2.13	0.87
1:C:88:HIS:HD2	1:C:90:GLU:H	1.20	0.87
2:B:42:LEU:HD22	2:B:243:PRO:HG2	1.56	0.86
1:C:431:ASP:O	1:C:435:VAL:HG13	1.75	0.86
1:C:40:LYS:O	1:C:42:ILE:HD12	1.75	0.85
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.58	0.85
1:A:323:VAL:HG12	1:A:355:ILE:CD1	2.06	0.85
2:B:70:PRO:HD3	2:B:94:GLN:HA	1.58	0.85
2:B:116:VAL:HG11	2:B:151:LEU:HD11	1.60	0.84
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.59	0.84
4:F:188:LYS:HB3	4:F:323:GLU:HG3	1.59	0.83
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.58	0.83
1:C:175:PRO:HA	1:C:178:SER:OG	1.79	0.83
4:F:191:LEU:HA	4:F:197:ARG:O	1.78	0.83
2:D:89:ASN:ND2	2:D:123:GLU:OE2	2.11	0.83
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.13	0.82
2:D:116:VAL:HG11	2:D:151:LEU:HD21	1.61	0.82
2:B:285:THR:O	2:B:288:GLU:N	2.11	0.82
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.14	0.82
1:A:123:ARG:NH2	1:A:160:ASP:HB3	1.95	0.82
2:D:186:THR:HG23	2:D:415:MET:HE2	1.62	0.82
1:A:90:GLU:OE1	1:A:124:LYS:HD3	1.78	0.81
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.14	0.81
1:C:250:VAL:HG11	1:C:352:LYS:NZ	1.96	0.81
1:A:308:ARG:HG2	1:A:340:SER:HB2	1.63	0.80
2:B:135:LEU:CD2	2:B:152:ILE:HD11	2.12	0.80
1:C:287:SER:OG	1:C:290:GLU:HG3	1.82	0.80
2:D:36:TYR:CZ	2:D:38:GLY:HA3	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:ARG:NH1	2:D:88:ASP:OD2	2.15	0.80
4:F:218:GLU:HB3	4:F:342:LEU:HD13	1.61	0.79
1:C:221:ARG:NH1	2:D:323:MET:HB3	1.97	0.79
1:A:287:SER:OG	1:A:290:GLU:HG3	1.82	0.79
3:E:101:LEU:HD12	3:E:102:ALA:N	1.98	0.79
2:D:330:MET:HG3	2:D:351:THR:HG21	1.64	0.79
1:A:298:PRO:HA	1:A:301:GLN:NE2	1.97	0.79
2:D:209:ASP:HB3	2:D:213:ARG:HH21	1.48	0.78
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.64	0.78
2:B:227:HIS:CG	2:B:276:ARG:HG3	2.18	0.78
2:B:313:VAL:HB	2:B:349:VAL:HG22	1.65	0.78
1:A:123:ARG:HH22	1:A:160:ASP:CB	1.96	0.78
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.18	0.77
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.14	0.77
1:C:221:ARG:CZ	2:D:323:MET:HB3	2.15	0.77
2:B:262:ARG:NH1	2:B:421:GLU:OE1	2.17	0.77
4:F:287:ILE:HG13	4:F:327:VAL:HG11	1.67	0.77
2:B:125:GLU:O	2:B:126:SER:OG	2.02	0.76
2:B:104:GLY:O	2:B:109:GLY:HA3	1.86	0.76
2:D:190:HIS:ND1	2:D:411:ALA:HA	2.00	0.76
2:D:294:PHE:CE2	2:D:333:VAL:HG11	2.20	0.76
1:A:349:THR:HG21	3:E:25:LYS:HE3	1.67	0.76
1:C:250:VAL:HG11	1:C:352:LYS:HZ1	1.49	0.76
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.20	0.76
1:A:323:VAL:HG12	1:A:355:ILE:HD13	1.68	0.75
2:B:31:ASP:OD1	2:B:33:THR:HG23	1.85	0.75
4:F:199:PHE:CE2	4:F:221:LEU:HD23	2.22	0.75
2:B:121:ARG:CZ	2:B:121:ARG:HB2	2.15	0.75
2:D:36:TYR:CE1	2:D:38:GLY:HA3	2.22	0.75
1:A:249:ASN:N	1:A:254:GLU:OE2	2.16	0.74
2:D:67:ASP:OD2	2:D:72:THR:OG1	2.03	0.74
4:F:77:LEU:HD11	4:F:81:ILE:HD12	1.68	0.74
4:F:222:ARG:NH2	4:F:318:ASP:OD2	2.21	0.74
4:F:225:SER:O	4:F:227:PRO:HD3	1.87	0.74
1:C:98:ASP:OD1	1:C:100:ALA:N	2.20	0.74
2:D:19:LYS:O	2:D:23:VAL:HG23	1.88	0.74
4:F:221:LEU:HD22	4:F:262:MET:CE	2.17	0.74
2:D:1:MET:HA	2:D:48:ASN:HD22	1.53	0.74
1:A:179:THR:HA	2:B:350:LYS:HE2	1.70	0.74
4:F:304:THR:HG21	4:F:311:SER:OG	1.87	0.74
4:F:98:TYR:O	4:F:181:VAL:HG23	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293:MET:CG	2:D:367:PHE:HB2	2.18	0.73
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.53	0.73
2:D:286:VAL:HA	2:D:289:LEU:HD12	1.68	0.73
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.22	0.73
1:A:51:THR:HG22	1:A:52:PHE:CD1	2.22	0.73
2:D:175:VAL:HG11	2:D:204:ASN:HD22	1.52	0.73
2:B:215:LEU:HD13	2:B:275:SER:HB3	1.71	0.73
2:D:315:ALA:HB3	2:D:351:THR:HB	1.69	0.73
2:D:285:THR:HG22	2:D:288:GLU:HB2	1.68	0.72
2:D:31:ASP:OD1	2:D:33:THR:HG23	1.88	0.72
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.24	0.72
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.22	0.72
2:B:386:THR:HG22	2:B:412:GLU:OE2	1.88	0.72
1:C:109:THR:HG21	1:C:411:GLU:OE1	1.90	0.72
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.89	0.72
1:C:207:GLU:HG2	1:C:304:LYS:HD2	1.71	0.72
4:F:329:LEU:HD12	4:F:330:ILE:N	2.05	0.72
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.72	0.72
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.71	0.72
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.71	0.71
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.19	0.71
1:A:83:TYR:HD2	1:A:86:LEU:HD22	1.56	0.71
1:A:232:SER:HA	1:A:235:VAL:HB	1.73	0.71
2:B:242:PHE:CD1	2:B:356:ILE:HD12	2.25	0.71
1:C:386:GLU:O	1:C:390:ARG:HG3	1.91	0.71
2:D:294:PHE:CD2	2:D:333:VAL:HG21	2.26	0.71
2:D:375:GLN:HB2	2:D:419:VAL:HG12	1.71	0.71
2:B:36:TYR:CE1	2:B:38:GLY:HA3	2.25	0.71
2:B:135:LEU:HD22	2:B:152:ILE:HD11	1.71	0.70
2:B:246:LEU:HD12	2:B:352:ALA:CB	2.21	0.70
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.26	0.70
2:D:254:ALA:O	2:D:258:VAL:HG23	1.90	0.70
1:A:83:TYR:CD2	1:A:86:LEU:HD22	2.26	0.70
1:C:238:ILE:O	1:C:252:LEU:HD22	1.91	0.70
2:D:102:ALA:HB2	2:D:403:MET:SD	2.31	0.70
4:F:64:TYR:O	4:F:311:SER:HB3	1.92	0.70
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.26	0.70
2:B:246:LEU:CD1	2:B:352:ALA:HB2	2.21	0.70
1:C:296:PHE:CE1	1:C:341:ILE:HD11	2.27	0.70
4:F:209:HIS:CD2	4:F:210:LEU:HG	2.26	0.70
2:D:1:MET:HA	2:D:48:ASN:ND2	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:33:ASP:N	4:F:33:ASP:OD1	2.25	0.70
1:C:345:ASP:OD1	1:C:346:TRP:N	2.25	0.69
2:B:227:HIS:ND1	2:B:276:ARG:HG3	2.07	0.69
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.27	0.69
1:A:179:THR:HA	2:B:350:LYS:CE	2.21	0.69
4:F:219:GLY:HA3	4:F:264:PHE:CE2	2.27	0.69
2:D:134:GLN:HA	2:D:165:ASN:O	1.93	0.69
2:D:110:ALA:O	2:D:113:VAL:HG12	1.93	0.68
2:B:198:GLU:OE2	2:B:253:LEU:HD23	1.94	0.68
1:C:83:TYR:HD2	1:C:86:LEU:HD22	1.57	0.68
1:C:275:VAL:HG12	1:C:275:VAL:O	1.92	0.68
2:D:54:ALA:HB3	2:D:58:LYS:CB	2.21	0.68
2:D:12:CYS:CB	2:D:138:SER:HB3	2.22	0.68
3:E:47:LEU:O	3:E:51:GLN:HG2	1.94	0.68
2:B:235:GLY:HA3	2:B:366:THR:OG1	1.94	0.68
2:B:157:GLU:HG3	3:E:72:LEU:HD12	1.73	0.68
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.58	0.68
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.73	0.68
1:C:68:VAL:HG11	1:C:149:PHE:CE2	2.29	0.68
1:A:345:ASP:N	1:A:345:ASP:OD1	2.25	0.68
1:C:102:ASN:HB3	1:C:105:ARG:HG3	1.74	0.68
1:A:70:LEU:HG	1:A:145:THR:OG1	1.94	0.68
1:A:234:ILE:HD13	1:A:302:MET:SD	2.34	0.68
2:B:42:LEU:HD22	2:B:243:PRO:CG	2.24	0.67
1:C:27:GLU:OE2	1:C:236:SER:OG	2.12	0.67
1:A:293:ASN:HA	1:A:335:ILE:HD11	1.76	0.67
2:B:157:GLU:OE1	3:E:76:ARG:NH1	2.27	0.67
2:B:386:THR:O	2:B:390:ARG:HG2	1.93	0.67
3:E:22:VAL:O	3:E:23:ILE:HD13	1.95	0.67
4:F:190:LEU:HD12	4:F:323:GLU:O	1.94	0.67
1:A:63:PRO:HG2	1:A:87:PHE:CE1	2.30	0.67
2:D:6:HIS:CE1	2:D:8:GLN:HG2	2.30	0.67
2:D:175:VAL:HG11	2:D:204:ASN:ND2	2.10	0.67
2:D:267:MET:HE1	2:D:305:PRO:HG3	1.77	0.67
1:A:253:THR:HA	1:A:256:GLN:OE1	1.94	0.66
1:C:3:GLU:O	1:C:132:LEU:HD12	1.95	0.66
2:D:54:ALA:N	2:D:58:LYS:O	2.28	0.66
2:D:343:GLU:HG3	2:D:430:ALA:HB2	1.77	0.66
1:A:275:VAL:HG12	1:A:275:VAL:O	1.95	0.66
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.31	0.66
4:F:186:LEU:HD13	4:F:320:MET:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:267:PHE:HE2	4:F:283:ILE:HD12	1.60	0.66
1:A:323:VAL:HG12	1:A:355:ILE:HD11	1.77	0.66
2:B:372:THR:O	2:B:375:GLN:HG2	1.96	0.66
1:A:142:GLY:HA3	1:A:183:GLU:OE1	1.96	0.66
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.25	0.65
2:D:104:GLY:O	2:D:109:GLY:HA3	1.96	0.65
1:A:34:GLY:O	1:A:61:HIS:N	2.23	0.65
1:A:72:PRO:HA	1:A:94:THR:HG21	1.77	0.65
2:B:23:VAL:HG21	2:B:230:SER:HB2	1.78	0.65
2:B:179:VAL:HG22	1:C:258:ASN:OD1	1.97	0.65
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.76	0.65
2:D:327:ASP:O	2:D:331:LEU:HD22	1.96	0.65
4:F:55:GLU:OE1	4:F:56:PRO:HD2	1.96	0.65
2:B:68:LEU:CD1	2:B:97:ALA:HB2	2.26	0.65
1:A:221:ARG:NH1	2:B:323:MET:HB3	2.11	0.65
2:B:177:ASP:O	1:C:352:LYS:HE2	1.97	0.65
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.14	0.64
1:C:279:GLU:N	1:C:279:GLU:OE1	2.30	0.64
2:D:221:THR:HG23	2:D:223:GLY:H	1.63	0.64
4:F:191:LEU:HD22	4:F:196:HIS:CD2	2.32	0.64
2:B:42:LEU:CB	2:B:356:ILE:HD11	2.27	0.64
2:D:112:LEU:O	2:D:112:LEU:HG	1.97	0.64
1:C:286:LEU:HA	1:C:290:GLU:OE1	1.98	0.64
2:D:285:THR:HG22	2:D:288:GLU:OE1	1.97	0.64
2:D:99:ASN:O	2:D:99:ASN:ND2	2.23	0.64
2:D:293:MET:HG3	2:D:367:PHE:HB2	1.80	0.64
3:E:121:GLU:HA	3:E:124:GLN:HG2	1.78	0.64
4:F:259:GLY:O	4:F:261:GLU:HG3	1.98	0.64
1:A:109:THR:OG1	1:A:411:GLU:OE1	2.10	0.63
2:D:221:THR:HG23	2:D:223:GLY:N	2.14	0.63
2:D:400:GLY:O	3:E:137:LYS:HD2	1.98	0.63
2:D:6:HIS:HE1	2:D:8:GLN:HG2	1.60	0.63
2:D:212:PHE:O	2:D:216:LYS:HA	1.98	0.63
1:A:232:SER:O	1:A:236:SER:N	2.31	0.63
2:B:324:LYS:O	2:B:328:GLU:HG3	1.99	0.63
2:D:267:MET:CG	2:D:301:ALA:HB3	2.28	0.63
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.33	0.63
1:A:357:TYR:CE1	3:E:17:GLY:HA2	2.33	0.63
2:D:401:GLU:HA	3:E:137:LYS:HD3	1.81	0.63
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.34	0.62
2:B:42:LEU:HB3	2:B:356:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLN:HG3	1:A:372:GLN:OE1	1.99	0.62
1:C:362:VAL:CG2	1:C:370:LYS:HG3	2.30	0.62
2:D:134:GLN:HG3	2:D:167:PHE:HE1	1.64	0.62
2:D:212:PHE:HB3	2:D:213:ARG:HD3	1.81	0.62
1:C:209:ILE:HD11	1:C:302:MET:CE	2.29	0.62
2:D:1:MET:HB2	2:D:3:GLU:OE2	1.99	0.62
2:D:216:LYS:C	2:D:217:LEU:HD23	2.19	0.62
4:F:286:GLN:O	4:F:290:ILE:HG13	1.99	0.62
2:B:229:VAL:O	2:B:233:MET:HG3	2.00	0.62
2:B:324:LYS:HE3	2:B:328:GLU:OE2	2.00	0.62
2:D:373:ALA:O	2:D:376:GLU:N	2.25	0.62
2:D:70:PRO:HG3	2:D:94:GLN:NE2	2.15	0.62
2:D:375:GLN:CB	2:D:419:VAL:HG12	2.29	0.62
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.35	0.61
2:D:267:MET:SD	2:D:303:CYS:HB2	2.40	0.61
2:B:101:TRP:HB2	2:B:184:ASN:OD1	1.99	0.61
2:D:139:LEU:HD12	2:D:170:MET:SD	2.40	0.61
3:E:139:LEU:HD12	3:E:139:LEU:O	2.00	0.61
2:B:68:LEU:HD13	2:B:97:ALA:HB2	1.81	0.61
1:C:422:ARG:NH1	1:C:426:ALA:HB2	2.16	0.61
2:D:318:ARG:NH2	2:D:356:ILE:HD13	2.16	0.61
2:B:103:LYS:O	2:B:108:GLU:N	2.31	0.61
1:A:179:THR:HA	2:B:350:LYS:NZ	2.15	0.61
4:F:329:LEU:HD12	4:F:330:ILE:H	1.65	0.61
1:C:217:LEU:HD13	1:C:367:ASP:HB2	1.83	0.61
1:C:209:ILE:HG22	1:C:227:LEU:CD2	2.31	0.61
2:D:54:ALA:CB	2:D:58:LYS:HB2	2.28	0.60
2:D:117:LEU:HD11	2:D:154:LYS:HB3	1.84	0.60
1:C:172:TYR:CE2	1:C:387:ALA:HB1	2.36	0.60
1:C:255:PHE:HD1	1:C:316:CYS:HG	1.47	0.60
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.16	0.60
1:A:214:ARG:HG2	1:A:219:ILE:O	2.01	0.60
1:C:209:ILE:HG22	1:C:227:LEU:HD23	1.83	0.60
3:E:22:VAL:C	3:E:23:ILE:HD13	2.21	0.60
2:B:172:SER:HB2	2:B:205:GLU:HB2	1.83	0.60
4:F:146:VAL:HG12	4:F:185:TYR:HB3	1.84	0.60
4:F:146:VAL:HG12	4:F:185:TYR:CB	2.32	0.60
1:C:422:ARG:HH12	1:C:426:ALA:HB2	1.66	0.60
1:C:172:TYR:CE2	1:C:391:LEU:HD12	2.37	0.60
4:F:208:ASP:OD2	4:F:212:ASN:HB2	2.01	0.60
1:C:88:HIS:HD2	1:C:90:GLU:N	1.97	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:THR:HG23	2:D:288:GLU:H	1.66	0.60
1:C:250:VAL:HB	1:C:255:PHE:CE2	2.37	0.60
4:F:77:LEU:CD1	4:F:81:ILE:HD12	2.31	0.60
4:F:102:PRO:HB3	4:F:174:ASP:HA	1.82	0.60
4:F:207:VAL:O	4:F:312:PHE:HB2	2.01	0.60
1:A:336:LYS:CD	3:E:24:LEU:HD12	2.23	0.60
1:C:252:LEU:HD12	1:C:252:LEU:O	2.01	0.60
4:F:4:PHE:O	4:F:29:ARG:HA	2.02	0.60
2:B:397:TRP:NE1	1:C:257:THR:HG23	2.16	0.59
2:D:68:LEU:HG	2:D:147:MET:HE2	1.84	0.59
2:D:169:VAL:HA	2:D:202:ILE:O	2.02	0.59
3:E:51:GLN:O	3:E:55:GLU:HG3	2.02	0.59
2:D:44:LEU:HA	2:D:47:ILE:HB	1.84	0.59
4:F:147:TRP:O	4:F:162:ILE:HG23	2.02	0.59
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.37	0.59
1:C:181:VAL:HB	8:D:501:A1D7A:C19	2.32	0.59
3:E:47:LEU:O	3:E:47:LEU:HD23	2.02	0.59
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.38	0.59
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.83	0.59
2:B:273:LEU:HD11	2:B:298:ASN:HA	1.85	0.59
1:C:83:TYR:CD2	1:C:86:LEU:HD22	2.36	0.59
2:D:36:TYR:CD2	2:D:44:LEU:HD11	2.37	0.59
4:F:199:PHE:HA	4:F:222:ARG:O	2.03	0.59
1:A:336:LYS:HD3	3:E:24:LEU:CD1	2.25	0.59
4:F:299:GLU:O	4:F:303:SER:HB2	2.02	0.59
1:C:253:THR:CA	1:C:256:GLN:HB2	2.26	0.59
2:D:130:LEU:HD12	2:D:131:GLN:N	2.18	0.59
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.38	0.59
1:C:115:ILE:HD13	1:C:152:LEU:HG	1.85	0.59
2:D:272:PRO:HB3	2:D:284:LEU:CD2	2.32	0.59
1:A:401:LYS:CE	2:B:428:ALA:HB1	2.33	0.59
2:B:158:GLU:HG2	2:B:159:TYR:CE1	2.38	0.58
2:D:318:ARG:HH21	2:D:356:ILE:HD13	1.67	0.58
2:B:169:VAL:HA	2:B:202:ILE:O	2.02	0.58
1:A:75:ILE:CG2	1:A:92:LEU:HB3	2.34	0.58
1:C:363:VAL:HG13	1:C:364:PRO:HD2	1.85	0.58
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.50	0.58
1:C:246:GLY:HA3	1:C:249:ASN:HB3	1.85	0.58
1:A:70:LEU:HD13	1:A:110:ILE:HG22	1.85	0.58
1:A:133:GLN:HB3	1:A:252:LEU:HD12	1.85	0.58
1:A:293:ASN:CA	1:A:335:ILE:HD11	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:LEU:HB3	2:B:225:LEU:HD22	1.85	0.58
1:C:407:TRP:NE1	2:D:255:VAL:HA	2.19	0.58
4:F:6:VAL:HB	4:F:29:ARG:CZ	2.33	0.58
4:F:215:LEU:HD12	4:F:216:TYR:N	2.18	0.58
2:D:3:GLU:CG	2:D:127:CYS:HB2	2.34	0.58
4:F:292:ARG:O	4:F:296:MET:HG2	2.03	0.58
4:F:221:LEU:HD12	4:F:221:LEU:N	2.19	0.58
1:A:2:ARG:HB2	1:A:133:GLN:NE2	2.18	0.58
1:A:2:ARG:HB3	1:A:133:GLN:HG3	1.85	0.58
2:B:11:GLN:HA	2:B:72:THR:HG21	1.86	0.58
4:F:81:ILE:HG13	4:F:87:LEU:HD13	1.84	0.58
2:B:2:ARG:HA	2:B:129:CYS:O	2.03	0.58
1:C:11:GLN:HG3	1:C:74:VAL:HG11	1.85	0.58
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.34	0.58
1:A:12:ALA:CB	1:A:140:SER:HB3	2.34	0.57
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.84	0.57
2:D:3:GLU:HB2	2:D:127:CYS:SG	2.43	0.57
2:D:68:LEU:HG	2:D:147:MET:CE	2.34	0.57
2:D:209:ASP:O	2:D:213:ARG:NE	2.31	0.57
2:D:205:GLU:HB3	2:D:380:ARG:HH12	1.68	0.57
4:F:185:TYR:OH	4:F:239:HIS:HB3	2.03	0.57
2:B:396:HIS:HA	2:B:399:THR:HG1	1.69	0.57
2:B:396:HIS:HA	2:B:399:THR:OG1	2.04	0.57
3:E:60:ARG:O	3:E:64:GLN:HG3	2.04	0.57
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.86	0.57
2:B:102:ALA:HB2	2:B:403:MET:SD	2.44	0.57
2:B:135:LEU:HD23	2:B:152:ILE:HD11	1.83	0.57
1:C:414:GLU:O	1:C:417:GLU:HG3	2.04	0.57
2:D:30:ILE:HD13	2:D:59:TYR:HB2	1.85	0.57
3:E:127:ASP:OD1	3:E:127:ASP:N	2.36	0.57
1:C:118:VAL:HG21	1:C:149:PHE:CZ	2.40	0.57
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.86	0.57
2:D:158:GLU:HG2	2:D:159:TYR:CE1	2.40	0.57
1:C:165:SER:HA	1:C:199:ASP:OD2	2.05	0.57
3:E:52:LYS:HD2	3:E:53:LYS:N	2.19	0.57
4:F:148:ILE:CB	4:F:162:ILE:HG12	2.32	0.57
1:C:297:GLU:OE1	1:C:298:PRO:HD2	2.05	0.57
2:D:67:ASP:O	2:D:92:PHE:HA	2.05	0.57
4:F:277:THR:HG23	4:F:278:THR:N	2.18	0.57
2:D:246:LEU:HD12	2:D:246:LEU:H	1.69	0.57
1:A:72:PRO:HA	1:A:94:THR:CG2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:TYR:CE1	2:B:220:PRO:HG2	2.40	0.57
4:F:100:ILE:O	4:F:179:VAL:HG23	2.04	0.57
2:D:416:ASN:O	2:D:419:VAL:HG23	2.05	0.56
4:F:21:LEU:O	4:F:27:TRP:HB2	2.04	0.56
1:A:185:TYR:CE2	1:A:398:MET:HE2	2.38	0.56
1:A:386:GLU:O	1:A:390:ARG:HG3	2.04	0.56
1:C:115:ILE:HG23	1:C:116:ASP:N	2.21	0.56
3:E:52:LYS:NZ	3:E:53:LYS:HE3	2.20	0.56
4:F:96:GLU:O	4:F:183:GLN:HA	2.05	0.56
8:B:501:A1D7A:S23	8:B:501:A1D7A:C14	2.93	0.56
1:C:255:PHE:HD1	1:C:316:CYS:SG	2.28	0.56
2:D:12:CYS:SG	2:D:138:SER:HB3	2.46	0.56
2:D:186:THR:CG2	2:D:415:MET:HE2	2.34	0.56
3:E:52:LYS:HZ3	3:E:53:LYS:HE3	1.70	0.56
2:B:91:VAL:CG2	2:B:119:VAL:HG21	2.35	0.56
2:B:359:ARG:HD3	2:B:360:GLY:H	1.71	0.56
2:B:392:LYS:HG2	2:B:395:LEU:HD12	1.86	0.56
2:B:54:ALA:N	2:B:58:LYS:O	2.37	0.56
2:B:284:LEU:HD22	2:B:289:LEU:HD23	1.88	0.56
2:D:350:LYS:HG3	2:D:351:THR:N	2.20	0.56
2:B:23:VAL:O	2:B:27:GLU:HG3	2.06	0.56
2:B:66:VAL:HG22	2:B:116:VAL:CG2	2.36	0.56
2:B:145:SER:O	2:B:149:THR:HG23	2.04	0.56
2:D:73:MET:HG3	2:D:90:PHE:HD2	1.70	0.56
4:F:287:ILE:CG1	4:F:327:VAL:HG11	2.34	0.56
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.70	0.56
1:A:349:THR:CG2	3:E:25:LYS:HE3	2.36	0.56
2:B:66:VAL:HG22	2:B:116:VAL:HG22	1.86	0.56
4:F:314:LEU:HD22	4:F:350:ILE:HD11	1.87	0.56
2:B:166:THR:O	2:B:199:THR:HA	2.06	0.55
2:D:322:SER:HB3	2:D:325:GLU:HB3	1.88	0.55
4:F:186:LEU:HD12	4:F:320:MET:SD	2.46	0.55
4:F:205:VAL:HG21	4:F:291:ILE:HG21	1.87	0.55
3:E:68:LEU:HD12	3:E:68:LEU:O	2.07	0.55
1:A:55:GLU:HA	1:A:60:LYS:O	2.06	0.55
1:C:304:LYS:O	1:C:390:ARG:NH1	2.33	0.55
1:A:221:ARG:HH11	2:B:323:MET:HB3	1.72	0.55
4:F:348:GLN:HA	4:F:348:GLN:NE2	2.21	0.55
2:B:404:ASP:OD1	2:B:405:GLU:N	2.39	0.55
1:C:232:SER:O	1:C:236:SER:N	2.40	0.55
4:F:283:ILE:HG23	4:F:327:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ALA:HA	1:A:129:CYS:SG	2.47	0.55
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.35	0.55
1:C:322:ASP:OD1	1:C:322:ASP:O	2.25	0.55
2:D:217:LEU:HD23	2:D:217:LEU:N	2.22	0.54
3:E:78:HIS:O	3:E:82:VAL:HG23	2.07	0.54
1:C:181:VAL:HG22	1:C:181:VAL:O	2.07	0.54
1:A:288:VAL:HG22	1:A:323:VAL:HG22	1.88	0.54
2:D:171:PRO:HG3	2:D:185:ALA:HB2	1.88	0.54
4:F:186:LEU:CD1	4:F:320:MET:HG2	2.36	0.54
2:D:1:MET:SD	2:D:128:ASP:HB2	2.47	0.54
2:D:310:TYR:HE1	2:D:367:PHE:HZ	1.55	0.54
1:C:316:CYS:O	1:C:377:MET:HG3	2.08	0.54
2:D:247:ASN:HB2	2:D:252:LYS:NZ	2.22	0.54
2:D:372:THR:HB	2:D:422:TYR:O	2.07	0.54
3:E:6:MET:HE2	3:E:24:LEU:HD22	1.89	0.54
1:C:12:ALA:CB	1:C:140:SER:HB3	2.38	0.54
2:B:295:ASP:OD2	2:B:297:LYS:HE2	2.08	0.54
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.90	0.54
2:D:77:ARG:HA	2:D:82:GLY:HA3	1.90	0.54
4:F:227:PRO:HD2	4:F:238:CYS:HB3	1.89	0.54
1:A:69:ASP:O	1:A:94:THR:HA	2.08	0.54
2:B:28:HIS:O	2:B:30:ILE:HD12	2.08	0.54
1:A:401:LYS:HE2	2:B:428:ALA:HB1	1.90	0.54
2:D:272:PRO:HB3	2:D:284:LEU:HD23	1.90	0.53
2:D:375:GLN:HB2	2:D:379:LYS:NZ	2.23	0.53
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.90	0.53
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.90	0.53
2:D:198:GLU:OE1	2:D:253:LEU:HD23	2.08	0.53
1:C:119:LEU:HD11	1:C:156:ARG:CB	2.34	0.53
2:B:130:LEU:HD12	2:B:131:GLN:N	2.23	0.53
2:B:134:GLN:HA	2:B:165:ASN:O	2.08	0.53
2:D:100:ASN:HD22	2:D:397:TRP:HB3	1.74	0.53
1:C:209:ILE:HD11	1:C:302:MET:HE1	1.89	0.53
2:B:70:PRO:HG3	2:B:94:GLN:CD	2.29	0.53
1:C:276:ILE:HG23	1:C:369:ALA:HB3	1.89	0.53
1:C:406:HIS:CG	2:D:261:PRO:HG3	2.44	0.53
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.24	0.53
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.90	0.53
2:D:36:TYR:CE2	2:D:44:LEU:HD11	2.43	0.53
2:D:176:SER:OG	2:D:181:GLU:OE1	2.27	0.53
4:F:3:THR:HB	4:F:30:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:304:THR:O	4:F:310:GLN:NE2	2.41	0.53
1:C:88:HIS:CD2	1:C:90:GLU:HB2	2.44	0.53
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.08	0.53
2:D:179:VAL:O	2:D:388:MET:HE1	2.08	0.53
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.90	0.53
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.27	0.53
1:A:328:VAL:O	1:A:332:ILE:HG13	2.09	0.53
1:C:246:GLY:CA	1:C:249:ASN:HB3	2.37	0.52
1:C:270:ALA:O	1:C:302:MET:HG2	2.09	0.52
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.07	0.52
1:A:166:LYS:N	1:A:199:ASP:OD2	2.36	0.52
2:B:31:ASP:CG	2:B:33:THR:HG23	2.29	0.52
3:E:130:ALA:O	3:E:133:VAL:HG12	2.08	0.52
1:A:9:VAL:HG22	1:A:68:VAL:CG1	2.40	0.52
2:D:63:ALA:C	2:D:64:ILE:HD13	2.30	0.52
4:F:21:LEU:HD21	4:F:355:ILE:HG21	1.89	0.52
1:A:409:VAL:HA	1:A:413:MET:O	2.09	0.52
2:B:172:SER:CB	2:B:205:GLU:HB2	2.39	0.52
2:B:242:PHE:CE1	2:B:356:ILE:HD12	2.44	0.52
2:B:304:ASP:OD1	2:B:307:HIS:ND1	2.42	0.52
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.39	0.52
2:B:73:MET:HE3	2:B:90:PHE:HD2	1.75	0.52
2:B:134:GLN:HG3	2:B:167:PHE:HE1	1.74	0.52
1:A:123:ARG:NH2	1:A:160:ASP:OD2	2.43	0.52
1:A:134:GLY:HA3	1:A:165:SER:O	2.10	0.52
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.45	0.52
2:D:23:VAL:O	2:D:27:GLU:HG3	2.10	0.52
1:C:265:ILE:HG22	1:C:265:ILE:O	2.10	0.52
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.44	0.51
2:B:157:GLU:HG3	3:E:72:LEU:CD1	2.40	0.51
1:C:27:GLU:OE1	1:C:243:ARG:NH1	2.37	0.51
1:C:207:GLU:HG2	1:C:304:LYS:CD	2.38	0.51
2:D:143:THR:HG23	2:D:147:MET:CE	2.40	0.51
2:B:225:LEU:O	2:B:229:VAL:HG23	2.11	0.51
2:D:49:VAL:O	2:D:62:ARG:NH1	2.43	0.51
2:D:91:VAL:CG2	2:D:119:VAL:HG21	2.40	0.51
2:D:285:THR:HG22	2:D:288:GLU:CB	2.36	0.51
4:F:102:PRO:HG3	4:F:178:GLN:O	2.09	0.51
1:A:177:VAL:HG12	1:A:177:VAL:O	2.11	0.51
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.50	0.51
2:B:316:ILE:HG23	2:B:366:THR:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ARG:NH1	2:D:323:MET:CB	2.71	0.51
1:C:271:THR:HG23	1:C:300:ASN:C	2.30	0.51
4:F:13:VAL:HG11	4:F:314:LEU:HD23	1.92	0.51
1:C:413:MET:HA	1:C:417:GLU:OE2	2.09	0.51
4:F:1:MET:HG2	4:F:26:GLN:HA	1.92	0.51
4:F:49:PHE:CD2	4:F:66:ARG:HG3	2.46	0.51
4:F:206:LEU:HD12	4:F:207:VAL:H	1.75	0.51
2:B:274:THR:HG21	2:B:361:LEU:HD21	1.92	0.51
4:F:95:PRO:HB2	4:F:183:GLN:HG2	1.92	0.51
2:B:35:SER:OG	2:B:58:LYS:HE3	2.10	0.51
2:D:12:CYS:HB3	2:D:138:SER:HB3	1.91	0.51
2:D:212:PHE:HD2	2:D:213:ARG:CD	2.24	0.51
4:F:209:HIS:HE2	4:F:210:LEU:CD2	2.23	0.51
1:A:349:THR:O	1:A:349:THR:HG22	2.11	0.51
2:B:29:GLY:O	2:B:36:TYR:HA	2.11	0.51
2:D:150:LEU:O	2:D:154:LYS:HG2	2.10	0.51
1:A:199:ASP:HB3	1:A:256:GLN:HG2	1.94	0.50
2:B:91:VAL:HG21	2:B:119:VAL:HG21	1.92	0.50
2:D:387:ALA:O	2:D:391:ARG:NH1	2.44	0.50
4:F:218:GLU:CB	4:F:342:LEU:HD13	2.36	0.50
2:B:293:MET:CE	2:B:365:ALA:HB1	2.42	0.50
1:C:319:TYR:HB2	1:C:355:ILE:HG12	1.94	0.50
2:D:205:GLU:HB3	2:D:380:ARG:NH1	2.26	0.50
1:A:287:SER:HG	1:A:290:GLU:HG3	1.75	0.50
1:C:250:VAL:HB	1:C:255:PHE:HE2	1.77	0.50
2:D:294:PHE:HE2	2:D:333:VAL:HG11	1.72	0.50
1:A:155:GLU:HG2	1:A:197:HIS:NE2	2.27	0.50
1:A:293:ASN:HA	1:A:335:ILE:CD1	2.41	0.50
2:B:42:LEU:HB2	2:B:356:ILE:HD11	1.93	0.50
2:B:197:ASP:C	2:B:198:GLU:HG3	2.30	0.50
1:C:291:ILE:HD13	1:C:373:ARG:HG3	1.94	0.50
4:F:272:MET:HG2	4:F:277:THR:O	2.11	0.50
1:C:248:LEU:CD1	1:C:325:PRO:HD3	2.42	0.50
1:C:250:VAL:HG11	1:C:352:LYS:HZ2	1.74	0.50
2:D:201:CYS:SG	2:D:265:PHE:HB3	2.52	0.50
1:A:174:ALA:HB1	1:A:207:GLU:HB2	1.94	0.50
1:A:173:PRO:HB3	1:A:183:GLU:OE1	2.11	0.50
2:D:343:GLU:OE2	2:D:430:ALA:N	2.45	0.50
2:B:267:MET:HG2	2:B:301:ALA:HB3	1.94	0.50
1:C:440:VAL:HG23	1:C:440:VAL:O	2.11	0.50
2:D:63:ALA:O	2:D:64:ILE:HD13	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:VAL:HG11	2:D:151:LEU:CD2	2.39	0.50
3:E:8:VAL:CG1	3:E:9:ILE:N	2.75	0.50
1:A:67:PHE:HB2	1:A:92:LEU:HD12	1.93	0.49
4:F:262:MET:HG3	4:F:266:GLU:OE1	2.12	0.49
4:F:346:LEU:O	4:F:346:LEU:HD12	2.12	0.49
1:A:311:LYS:HE3	1:A:342:GLN:OE1	2.12	0.49
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.94	0.49
2:D:143:THR:HG23	2:D:147:MET:HE2	1.94	0.49
2:D:212:PHE:HD2	2:D:213:ARG:HD3	1.78	0.49
4:F:267:PHE:CE2	4:F:283:ILE:HD12	2.45	0.49
1:A:292:THR:HG1	1:A:319:TYR:HH	1.60	0.49
4:F:200:ASP:O	4:F:221:LEU:HA	2.13	0.49
4:F:347:CYS:HA	4:F:350:ILE:HD12	1.94	0.49
1:A:39:ASP:OD2	1:A:49:PHE:HZ	1.95	0.49
1:A:147:SER:HB2	1:A:190:THR:HB	1.95	0.49
2:B:36:TYR:CE2	2:B:44:LEU:HD11	2.47	0.49
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.95	0.49
4:F:296:MET:CE	4:F:380:HIS:HB2	2.43	0.49
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.42	0.49
2:D:150:LEU:CD1	2:D:154:LYS:HE3	2.42	0.49
2:B:68:LEU:HD12	2:B:97:ALA:HB2	1.95	0.49
1:C:102:ASN:HB3	1:C:105:ARG:CG	2.43	0.49
2:D:288:GLU:O	2:D:292:GLN:HG3	2.13	0.49
4:F:1:MET:HE1	4:F:28:LYS:HB3	1.94	0.49
4:F:148:ILE:HG12	4:F:149:ALA:N	2.26	0.49
8:B:501:A1D7A:S23	8:B:501:A1D7A:C13	3.01	0.49
1:C:178:SER:O	2:D:350:LYS:NZ	2.43	0.49
2:D:284:LEU:HD12	2:D:285:THR:H	1.78	0.49
1:C:232:SER:O	1:C:236:SER:HB2	2.13	0.49
1:A:213:CYS:O	1:A:217:LEU:HB2	2.13	0.48
1:C:385:ALA:O	1:C:388:TRP:N	2.46	0.48
4:F:77:LEU:HD11	4:F:81:ILE:CD1	2.39	0.48
4:F:92:THR:O	4:F:92:THR:OG1	2.26	0.48
2:B:12:CYS:SG	2:B:138:SER:HB3	2.53	0.48
1:C:5:ILE:CG2	1:C:125:LEU:HD12	2.42	0.48
2:D:212:PHE:HA	2:D:217:LEU:O	2.13	0.48
4:F:377:LYS:HD3	4:F:379:HIS:NE2	2.28	0.48
1:A:401:LYS:HE3	2:B:428:ALA:HB1	1.95	0.48
2:B:124:SER:O	2:B:127:CYS:HB2	2.13	0.48
2:B:359:ARG:HD3	2:B:360:GLY:N	2.28	0.48
2:D:68:LEU:HD21	2:D:112:LEU:CD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:237:THR:HG22	2:D:240:LEU:HD12	1.96	0.48
1:A:8:HIS:HB3	1:A:13:GLY:C	2.34	0.48
1:A:431:ASP:O	1:A:435:VAL:HG23	2.14	0.48
2:B:6:HIS:CE1	2:B:8:GLN:HG2	2.49	0.48
2:D:382:SER:O	2:D:385:PHE:HB3	2.13	0.48
1:C:8:HIS:CE1	1:C:17:GLY:HA2	2.48	0.48
2:B:139:LEU:HD22	2:B:188:SER:HB3	1.94	0.48
2:B:316:ILE:HD12	2:B:317:PHE:N	2.29	0.48
4:F:3:THR:HG22	4:F:28:LYS:HG2	1.95	0.48
2:B:286:VAL:HB	2:B:287:PRO:HD3	1.96	0.48
1:C:55:GLU:HA	1:C:60:LYS:O	2.13	0.48
2:D:1:MET:CA	2:D:48:ASN:HD22	2.23	0.48
2:D:64:ILE:HD11	2:D:123:GLU:HG3	1.96	0.48
2:D:66:VAL:HA	2:D:91:VAL:O	2.13	0.48
2:D:157:GLU:HA	3:E:123:LEU:HD12	1.96	0.48
2:D:406:MET:O	2:D:410:GLU:HG3	2.14	0.48
1:A:51:THR:HG22	1:A:52:PHE:CE1	2.48	0.48
1:A:75:ILE:HG23	1:A:92:LEU:HB3	1.96	0.47
1:A:99:ALA:HA	1:A:105:ARG:HD3	1.96	0.47
1:C:147:SER:HB2	1:C:190:THR:HB	1.96	0.47
2:D:3:GLU:HG2	2:D:62:ARG:NH2	2.29	0.47
4:F:268:ASN:O	4:F:272:MET:HG3	2.13	0.47
1:A:42:ILE:HD13	1:A:42:ILE:O	2.14	0.47
2:B:103:LYS:HG2	2:B:401:GLU:OE2	2.14	0.47
1:C:4:CYS:HB3	1:C:136:LEU:CD1	2.43	0.47
1:C:246:GLY:HA3	1:C:249:ASN:CB	2.43	0.47
2:D:6:HIS:HE1	2:D:8:GLN:CG	2.26	0.47
2:D:179:VAL:O	2:D:388:MET:CE	2.62	0.47
2:B:36:TYR:CZ	2:B:44:LEU:HD11	2.48	0.47
2:D:211:CYS:SG	2:D:225:LEU:HD23	2.54	0.47
2:D:367:PHE:CD1	2:D:367:PHE:C	2.87	0.47
4:F:307:LEU:HD13	4:F:309:TYR:CE1	2.49	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.48	0.47
2:B:54:ALA:HB3	2:B:58:LYS:O	2.14	0.47
2:B:70:PRO:HG3	2:B:94:GLN:OE1	2.15	0.47
1:C:248:LEU:HD11	1:C:325:PRO:HD3	1.97	0.47
2:D:100:ASN:ND2	2:D:397:TRP:HB3	2.29	0.47
2:D:118:ASP:HA	2:D:121:ARG:HG3	1.97	0.47
1:A:3:GLU:CD	1:A:129:CYS:HB2	2.35	0.47
2:D:6:HIS:CE1	2:D:8:GLN:CG	2.97	0.47
2:D:184:ASN:O	2:D:188:SER:OG	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:221:THR:HG22	2:D:224:ASP:OD1	2.14	0.47
2:B:20:PHE:CE1	2:B:24:ILE:HG21	2.49	0.47
2:B:212:PHE:HA	2:B:217:LEU:O	2.14	0.47
2:D:171:PRO:CG	2:D:185:ALA:HB2	2.44	0.47
3:E:101:LEU:HD12	3:E:102:ALA:CA	2.44	0.47
2:B:186:THR:HA	2:B:415:MET:HE3	1.96	0.47
2:D:68:LEU:HD12	2:D:143:THR:OG1	2.15	0.47
2:D:216:LYS:O	2:D:217:LEU:HD23	2.14	0.47
2:B:341:PHE:CE2	2:B:349:VAL:HG21	2.50	0.47
1:C:317:LEU:HB3	1:C:319:TYR:CE1	2.50	0.47
2:D:45:GLU:HB3	2:D:243:PRO:HG3	1.97	0.47
2:D:423:GLN:NE2	2:D:427:ASP:OD1	2.48	0.47
4:F:47:LEU:HD23	4:F:48:PRO:HD2	1.96	0.47
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.94	0.47
1:A:141:PHE:HB2	1:A:173:PRO:HD3	1.97	0.47
1:C:319:TYR:HB3	1:C:323:VAL:HG21	1.96	0.47
2:D:247:ASN:HB2	2:D:252:LYS:HZ1	1.80	0.47
4:F:191:LEU:CD2	4:F:228:TYR:HB3	2.44	0.47
1:A:277:SER:O	1:A:369:ALA:HB2	2.14	0.46
1:C:358:GLN:CD	1:C:358:GLN:H	2.18	0.46
2:D:134:GLN:HG3	2:D:167:PHE:CE1	2.48	0.46
2:D:385:PHE:CE2	2:D:412:GLU:HB2	2.50	0.46
1:A:60:LYS:HD3	1:A:62:VAL:HG22	1.97	0.46
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.50	0.46
1:A:411:GLU:O	3:E:61:ARG:HD3	2.15	0.46
1:A:2:ARG:CB	1:A:133:GLN:HG3	2.45	0.46
1:A:209:ILE:HD11	1:A:302:MET:SD	2.55	0.46
1:C:106:GLY:O	1:C:111:GLY:HA3	2.16	0.46
1:C:432:TYR:O	1:C:435:VAL:HG22	2.15	0.46
2:D:116:VAL:CG1	2:D:151:LEU:HD21	2.36	0.46
1:A:195:LEU:HD12	1:A:266:HIS:CE1	2.51	0.46
2:B:107:THR:HG21	2:B:401:GLU:OE1	2.16	0.46
2:B:272:PRO:O	2:B:274:THR:HG23	2.15	0.46
2:D:344:TRP:CE3	2:D:345:ILE:HG13	2.51	0.46
4:F:98:TYR:C	4:F:181:VAL:HG23	2.35	0.46
2:B:156:ARG:O	2:B:160:PRO:HA	2.15	0.46
2:B:215:LEU:HD23	2:B:215:LEU:N	2.30	0.46
2:D:130:LEU:HD12	2:D:130:LEU:C	2.35	0.46
2:D:253:LEU:O	2:D:257:MET:HB2	2.15	0.46
1:A:176:GLN:NE2	4:F:56:PRO:HB3	2.31	0.46
2:B:273:LEU:HD23	2:B:273:LEU:HA	1.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:ARG:O	2:D:216:LYS:HG2	2.16	0.46
4:F:188:LYS:HB3	4:F:323:GLU:CG	2.38	0.46
1:A:186:ASN:O	1:A:190:THR:HG22	2.15	0.46
1:C:361:THR:HG22	1:C:362:VAL:N	2.30	0.46
2:D:156:ARG:HD2	2:D:195:ASN:CB	2.46	0.46
4:F:206:LEU:HD12	4:F:207:VAL:N	2.30	0.46
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.45	0.46
2:D:209:ASP:C	2:D:213:ARG:HE	2.17	0.46
4:F:340:GLN:HA	4:F:340:GLN:OE1	2.16	0.46
1:A:349:THR:CB	3:E:25:LYS:HE3	2.46	0.46
2:D:172:SER:CB	2:D:205:GLU:HB2	2.46	0.46
2:D:284:LEU:HD13	2:D:284:LEU:HA	1.86	0.46
2:D:295:ASP:OD1	2:D:297:LYS:HE3	2.16	0.46
4:F:256:TYR:HB2	4:F:257:GLU:OE1	2.15	0.46
1:A:413:MET:HE1	1:A:418:PHE:CE1	2.50	0.45
2:B:324:LYS:HG2	2:B:328:GLU:OE2	2.16	0.45
2:D:210:ILE:HG23	2:D:273:LEU:HD13	1.98	0.45
3:E:11:LEU:HD12	3:E:20:PHE:HB3	1.97	0.45
1:A:66:VAL:HG13	1:A:66:VAL:O	2.16	0.45
2:D:136:THR:O	2:D:137:HIS:HB3	2.17	0.45
3:E:21:GLU:OE2	3:E:23:ILE:HD11	2.16	0.45
1:A:154:MET:CE	1:A:198:SER:HB2	2.47	0.45
1:C:118:VAL:HG21	1:C:149:PHE:HZ	1.79	0.45
2:D:47:ILE:HD11	2:D:51:TYR:CE2	2.51	0.45
4:F:81:ILE:HG13	4:F:87:LEU:CD1	2.45	0.45
1:A:51:THR:HG22	1:A:52:PHE:HD1	1.78	0.45
2:D:29:GLY:O	2:D:36:TYR:HD1	2.00	0.45
2:D:156:ARG:HD2	2:D:195:ASN:HB2	1.97	0.45
2:D:386:THR:HG22	2:D:412:GLU:OE2	2.16	0.45
2:B:295:ASP:OD1	2:B:296:SER:N	2.49	0.45
4:F:201:ILE:HD11	4:F:321:VAL:HG21	1.98	0.45
4:F:218:GLU:HB3	4:F:342:LEU:CD1	2.39	0.45
1:A:221:ARG:NH1	2:B:323:MET:CE	2.80	0.45
1:A:285:GLN:HG3	1:A:372:GLN:CD	2.37	0.45
2:D:285:THR:HG22	2:D:288:GLU:CD	2.36	0.45
1:A:413:MET:CE	1:A:418:PHE:CE1	3.00	0.45
2:B:406:MET:CE	2:B:410:GLU:CG	2.94	0.45
2:D:159:TYR:HB3	2:D:162:ARG:HG2	1.98	0.45
2:D:285:THR:HG22	2:D:288:GLU:CG	2.46	0.45
4:F:45:ASN:O	4:F:46:ARG:HB2	2.16	0.45
1:A:174:ALA:CB	1:A:207:GLU:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:MET:HE3	2:B:365:ALA:HB1	1.99	0.45
4:F:267:PHE:HE2	4:F:283:ILE:CD1	2.27	0.45
4:F:349:GLY:O	4:F:353:VAL:HB	2.17	0.45
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.52	0.45
2:D:257:MET:HE3	2:D:312:THR:OG1	2.17	0.45
2:D:270:PHE:O	2:D:298:ASN:HB3	2.17	0.45
4:F:86:GLU:CD	4:F:86:GLU:H	2.20	0.45
4:F:145:ASN:O	4:F:147:TRP:HD1	2.00	0.45
4:F:272:MET:O	4:F:275:LEU:O	2.35	0.45
4:F:283:ILE:HG23	4:F:327:VAL:CG2	2.46	0.45
1:A:221:ARG:HH11	2:B:323:MET:CB	2.29	0.45
2:D:174:LYS:HE3	2:D:205:GLU:CD	2.38	0.45
2:D:258:VAL:HG12	2:D:260:PHE:O	2.17	0.45
2:D:375:GLN:HB2	2:D:379:LYS:HZ2	1.82	0.45
4:F:257:GLU:O	4:F:257:GLU:HG2	2.17	0.45
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.51	0.45
1:C:65:ALA:O	1:C:125:LEU:HD11	2.16	0.44
1:C:234:ILE:HD12	1:C:234:ILE:H	1.81	0.44
1:C:399:TYR:O	1:C:402:ARG:HD3	2.17	0.44
2:D:303:CYS:HA	2:D:376:GLU:OE1	2.17	0.44
2:D:321:MET:HB3	2:D:363:MET:CE	2.37	0.44
1:A:65:ALA:O	1:A:91:GLN:HG2	2.17	0.44
2:B:397:TRP:CD1	1:C:257:THR:HG23	2.53	0.44
1:C:33:ASP:OD1	1:C:35:GLN:HG2	2.18	0.44
1:C:318:LEU:N	1:C:318:LEU:CD1	2.80	0.44
2:D:224:ASP:OD1	2:D:224:ASP:N	2.50	0.44
4:F:31:ARG:HG3	4:F:32:LYS:N	2.32	0.44
4:F:188:LYS:HD3	4:F:323:GLU:CD	2.38	0.44
2:B:171:PRO:HG3	2:B:185:ALA:HB2	1.99	0.44
2:B:186:THR:HA	2:B:415:MET:CE	2.47	0.44
2:B:207:LEU:CB	2:B:225:LEU:HD22	2.48	0.44
1:C:178:SER:HB2	1:C:183:GLU:OE2	2.17	0.44
2:D:318:ARG:HB2	2:D:364:SER:OG	2.17	0.44
3:E:52:LYS:HZ2	3:E:53:LYS:HG2	1.82	0.44
1:A:183:GLU:N	1:A:184:PRO:CD	2.80	0.44
1:A:280:LYS:HD3	1:A:283:HIS:HB2	2.00	0.44
2:B:215:LEU:HD13	2:B:275:SER:CB	2.45	0.44
2:D:105:HIS:ND1	2:D:150:LEU:HB2	2.33	0.44
2:D:109:GLY:HA3	2:D:147:MET:HG3	1.99	0.44
2:D:401:GLU:HA	3:E:137:LYS:CD	2.46	0.44
4:F:340:GLN:OE1	4:F:340:GLN:CA	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:VAL:HB	2:B:415:MET:CE	2.47	0.44
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.99	0.44
1:A:297:GLU:OE2	4:F:306:HIS:ND1	2.47	0.44
3:E:124:GLN:HG3	3:E:125:GLU:N	2.33	0.44
1:A:276:ILE:HD12	1:A:283:HIS:CE1	2.52	0.44
2:B:227:HIS:CB	2:B:276:ARG:HG3	2.48	0.44
1:C:313:MET:HE2	1:C:382:THR:CG2	2.47	0.44
2:D:3:GLU:HG2	2:D:127:CYS:HB2	1.99	0.44
2:D:272:PRO:HB3	2:D:284:LEU:HD21	1.98	0.44
4:F:71:LEU:O	4:F:332:VAL:HB	2.18	0.44
1:A:333:ALA:HA	3:E:6:MET:HE1	2.00	0.44
2:B:130:LEU:HD12	2:B:130:LEU:C	2.38	0.44
1:C:44:GLY:O	1:C:55:GLU:OE2	2.35	0.44
1:C:181:VAL:O	1:C:181:VAL:CG2	2.65	0.44
1:C:314:ALA:HB3	1:C:380:ASN:H	1.83	0.44
1:C:324:VAL:HG23	1:C:326:LYS:H	1.83	0.44
2:D:216:LYS:HA	2:D:216:LYS:HD3	1.74	0.44
4:F:3:THR:CG2	4:F:30:LEU:HD21	2.48	0.44
1:A:175:PRO:HA	1:A:178:SER:HB3	2.00	0.44
2:B:331:LEU:HD13	4:F:56:PRO:O	2.18	0.44
2:D:393:ALA:HB1	2:D:394:PHE:CD2	2.52	0.44
4:F:146:VAL:HG12	4:F:185:TYR:HB2	2.00	0.44
1:A:31:GLN:HG2	1:A:35:GLN:O	2.18	0.43
1:A:258:ASN:O	1:A:314:ALA:HB1	2.17	0.43
2:B:121:ARG:NE	2:B:158:GLU:OE2	2.41	0.43
2:B:144:GLY:O	2:B:148:GLY:HA3	2.18	0.43
1:C:70:LEU:HD13	1:C:110:ILE:HG22	2.00	0.43
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.53	0.43
1:C:178:SER:CB	1:C:183:GLU:OE2	2.66	0.43
2:D:3:GLU:HB3	2:D:62:ARG:CZ	2.48	0.43
3:E:125:GLU:OE1	3:E:125:GLU:HA	2.18	0.43
4:F:1:MET:CE	4:F:28:LYS:HB3	2.48	0.43
4:F:209:HIS:CD2	4:F:210:LEU:N	2.86	0.43
1:C:102:ASN:OD1	1:C:104:ALA:N	2.51	0.43
1:C:219:ILE:HG21	1:C:222:PRO:HA	1.99	0.43
2:D:47:ILE:O	2:D:51:TYR:HB2	2.18	0.43
2:B:91:VAL:HG21	2:B:119:VAL:CG2	2.48	0.43
1:C:105:ARG:HD3	1:C:411:GLU:OE2	2.18	0.43
2:D:29:GLY:O	2:D:36:TYR:CD1	2.72	0.43
2:D:49:VAL:HG12	2:D:50:TYR:CD2	2.53	0.43
2:D:215:LEU:HD12	2:D:215:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:THR:OG1	1:A:319:TYR:OH	2.34	0.43
2:B:211:CYS:HA	2:B:215:LEU:HB2	2.00	0.43
1:A:63:PRO:HG2	1:A:87:PHE:CD1	2.53	0.43
1:C:362:VAL:HG21	1:C:370:LYS:HG3	2.01	0.43
2:D:179:VAL:O	2:D:388:MET:SD	2.77	0.43
2:D:345:ILE:O	2:D:348:ASN:ND2	2.52	0.43
4:F:13:VAL:HG11	4:F:314:LEU:CD2	2.48	0.43
4:F:172:PHE:O	4:F:176:GLN:HG2	2.18	0.43
1:A:221:ARG:HH11	2:B:323:MET:HE2	1.84	0.43
1:A:323:VAL:O	1:A:355:ILE:HD13	2.17	0.43
2:B:165:ASN:HA	2:B:198:GLU:O	2.18	0.43
2:B:285:THR:O	2:B:288:GLU:HB2	2.19	0.43
1:C:275:VAL:HA	1:C:368:LEU:HD21	2.00	0.43
2:D:380:ARG:O	2:D:384:GLN:HG3	2.19	0.43
3:E:127:ASP:O	3:E:131:GLU:HG2	2.18	0.43
1:A:17:GLY:O	1:A:21:TRP:HD1	2.01	0.43
1:A:398:MET:CE	1:A:404:PHE:CD1	3.01	0.43
2:B:323:MET:HG2	2:B:353:VAL:HG11	2.01	0.43
1:C:270:ALA:HB3	1:C:302:MET:CG	2.48	0.43
2:D:86:ARG:HG2	2:D:89:ASN:CG	2.39	0.43
2:D:373:ALA:C	2:D:375:GLN:N	2.71	0.43
1:A:63:PRO:HD3	1:A:86:LEU:HG	2.00	0.43
2:B:66:VAL:HG21	2:B:116:VAL:HG11	2.01	0.43
2:D:73:MET:HG3	2:D:90:PHE:CD2	2.52	0.43
2:D:267:MET:HG2	2:D:301:ALA:HB3	1.99	0.43
2:D:293:MET:HE3	2:D:293:MET:HB3	1.90	0.43
4:F:191:LEU:HB3	4:F:196:HIS:C	2.39	0.43
1:A:50:ASN:HA	1:A:53:PHE:O	2.18	0.43
1:A:275:VAL:O	1:A:275:VAL:CG1	2.66	0.43
2:B:8:GLN:HB3	2:B:136:THR:OG1	2.18	0.43
2:B:190:HIS:CD2	2:B:411:ALA:HA	2.54	0.43
2:D:156:ARG:CD	2:D:195:ASN:HB3	2.49	0.43
2:D:213:ARG:HG2	2:D:213:ARG:HH11	1.83	0.43
2:D:386:THR:CG2	2:D:412:GLU:OE2	2.67	0.43
4:F:214:TYR:CD2	4:F:353:VAL:HG11	2.54	0.43
2:B:117:LEU:HD11	2:B:154:LYS:HB3	2.00	0.42
2:B:391:ARG:HG3	1:C:346:TRP:HB3	2.01	0.42
1:C:5:ILE:HG23	1:C:125:LEU:HD12	2.01	0.42
2:D:150:LEU:HD11	2:D:154:LYS:HE3	2.00	0.42
1:A:62:VAL:HG11	1:A:88:HIS:CE1	2.54	0.42
2:B:7:ILE:O	2:B:135:LEU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:HIS:CD2	1:C:266:HIS:O	2.73	0.42
2:D:36:TYR:OH	2:D:40:SER:O	2.32	0.42
2:D:166:THR:HG21	2:D:196:THR:HG21	2.01	0.42
4:F:2:TYR:HB2	4:F:27:TRP:CE2	2.54	0.42
1:A:93:ILE:CD1	1:A:121:ARG:HG3	2.45	0.42
1:A:270:ALA:HB3	1:A:302:MET:HG3	2.02	0.42
1:C:71:GLU:HB2	1:C:72:PRO:HD2	2.01	0.42
1:C:115:ILE:CG2	1:C:116:ASP:N	2.82	0.42
1:C:246:GLY:C	1:C:249:ASN:HB3	2.40	0.42
2:D:239:CYS:HB2	8:D:501:A1D7A:CL20	2.56	0.42
4:F:47:LEU:HD23	4:F:47:LEU:C	2.40	0.42
4:F:209:HIS:HE2	4:F:210:LEU:HD23	1.84	0.42
1:A:221:ARG:HH11	2:B:323:MET:CE	2.31	0.42
1:A:270:ALA:O	1:A:302:MET:HG2	2.18	0.42
2:B:176:SER:OG	2:B:181:GLU:OE1	2.27	0.42
1:C:117:LEU:HA	1:C:117:LEU:HD12	1.72	0.42
1:C:328:VAL:O	1:C:332:ILE:HG13	2.19	0.42
2:D:34:GLY:O	2:D:58:LYS:HA	2.18	0.42
2:D:372:THR:HA	2:D:422:TYR:CD1	2.55	0.42
4:F:3:THR:HG21	4:F:30:LEU:HD21	2.02	0.42
4:F:4:PHE:HB2	4:F:39:LEU:HB3	2.00	0.42
2:B:391:ARG:NH1	1:C:439:SER:OG	2.49	0.42
2:D:68:LEU:HD21	2:D:112:LEU:HD22	2.02	0.42
4:F:321:VAL:HA	4:F:326:LYS:O	2.20	0.42
1:A:136:LEU:HD21	1:A:252:LEU:HD21	2.01	0.42
1:A:178:SER:OG	1:A:183:GLU:OE2	2.31	0.42
1:A:398:MET:HE3	1:A:404:PHE:CD1	2.55	0.42
4:F:267:PHE:CE2	4:F:271:LEU:HD11	2.55	0.42
1:A:156:ARG:HD2	1:A:156:ARG:HA	1.69	0.42
2:B:312:THR:HA	2:B:348:ASN:HB2	2.02	0.42
1:C:67:PHE:HB2	1:C:92:LEU:HD22	2.02	0.42
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.54	0.42
2:B:179:VAL:HG21	2:B:394:PHE:CZ	2.55	0.42
3:E:52:LYS:HD2	3:E:53:LYS:HG2	2.00	0.42
4:F:5:VAL:HG13	4:F:30:LEU:HD12	2.02	0.42
1:A:9:VAL:HG22	1:A:68:VAL:HG11	2.02	0.42
1:A:230:LEU:O	1:A:233:GLN:HB2	2.19	0.42
1:A:333:ALA:HA	3:E:6:MET:CE	2.50	0.42
2:B:263:LEU:HD21	2:B:421:GLU:HG2	2.02	0.42
2:B:330:MET:O	2:B:333:VAL:HG12	2.20	0.42
2:D:71:GLY:O	2:D:74:ASP:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:MET:CG	2:D:90:PHE:CD2	3.03	0.42
2:D:236:VAL:HG12	2:D:368:ILE:HG12	2.01	0.42
1:C:156:ARG:HA	1:C:156:ARG:HD2	1.78	0.42
1:C:291:ILE:HD13	1:C:291:ILE:HG21	1.81	0.42
2:D:180:VAL:O	2:D:183:TYR:HB2	2.20	0.42
2:D:182:PRO:HG2	2:D:388:MET:HE3	2.01	0.42
2:D:209:ASP:HB3	2:D:213:ARG:CZ	2.49	0.42
1:A:175:PRO:HA	1:A:178:SER:CB	2.50	0.41
2:B:21:TRP:CH2	2:B:61:PRO:HB3	2.55	0.41
2:B:68:LEU:HD23	2:B:112:LEU:HD23	2.02	0.41
1:C:203:MET:HE2	1:C:267:PHE:CD2	2.55	0.41
2:D:31:ASP:O	2:D:84:ILE:HD12	2.20	0.41
2:D:106:TYR:CG	3:E:133:VAL:HG11	2.53	0.41
1:A:84:ARG:HG3	1:A:85:GLN:N	2.35	0.41
2:B:44:LEU:HD23	2:B:44:LEU:HA	1.72	0.41
2:B:116:VAL:CG1	2:B:151:LEU:HD11	2.41	0.41
2:B:270:PHE:O	2:B:298:ASN:HB3	2.19	0.41
2:B:314:ALA:HB3	2:B:368:ILE:HB	2.02	0.41
1:C:341:ILE:O	1:C:341:ILE:HG22	2.19	0.41
2:D:91:VAL:HG22	2:D:119:VAL:HG21	2.02	0.41
2:D:285:THR:O	2:D:288:GLU:HB2	2.19	0.41
4:F:271:LEU:O	4:F:275:LEU:O	2.39	0.41
2:B:227:HIS:HB2	2:B:276:ARG:HG3	2.02	0.41
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.02	0.41
2:D:217:LEU:HB2	2:D:220:PRO:HB3	2.02	0.41
4:F:1:MET:HE1	4:F:28:LYS:N	2.36	0.41
2:B:263:LEU:HD21	2:B:421:GLU:CG	2.49	0.41
2:B:263:LEU:HD23	2:B:263:LEU:N	2.35	0.41
1:C:216:ASN:HB3	1:C:275:VAL:O	2.19	0.41
2:D:290:THR:HA	2:D:293:MET:HE2	2.03	0.41
4:F:349:GLY:O	4:F:353:VAL:HG23	2.20	0.41
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.87	0.41
2:D:8:GLN:OE1	2:D:65:LEU:HD23	2.20	0.41
2:D:20:PHE:O	2:D:24:ILE:HG12	2.20	0.41
2:D:156:ARG:HD3	2:D:195:ASN:HB3	2.02	0.41
4:F:40:MET:HG2	4:F:62:VAL:HG23	2.02	0.41
4:F:288:LYS:HD2	4:F:378:LEU:HD21	2.02	0.41
1:A:36:MET:HB3	1:A:61:HIS:NE2	2.35	0.41
1:A:174:ALA:HA	1:A:175:PRO:HD3	1.73	0.41
1:A:316:CYS:HA	1:A:352:LYS:O	2.20	0.41
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:LEU:HD21	2:B:421:GLU:CD	2.41	0.41
2:D:20:PHE:CD1	2:D:233:MET:HE2	2.55	0.41
2:D:182:PRO:HB3	2:D:384:GLN:HB2	2.02	0.41
2:D:212:PHE:CD2	2:D:213:ARG:HD3	2.56	0.41
4:F:95:PRO:HB2	4:F:183:GLN:CG	2.50	0.41
2:B:227:HIS:ND1	2:B:276:ARG:CG	2.81	0.41
2:B:293:MET:HE2	2:B:367:PHE:HB2	2.03	0.41
2:D:231:ALA:HB1	2:D:270:PHE:CE2	2.55	0.41
2:D:272:PRO:HD2	2:D:361:LEU:HD13	2.02	0.41
2:D:331:LEU:HD12	2:D:331:LEU:HA	1.86	0.41
2:D:389:PHE:CE1	2:D:408:PHE:CB	3.04	0.41
1:A:1:MET:SD	1:A:1:MET:C	2.99	0.41
1:A:215:ARG:NH2	1:A:299:ALA:HB1	2.36	0.41
2:B:164:MET:HG3	2:B:196:THR:HG22	2.02	0.41
1:C:8:HIS:CE1	1:C:17:GLY:CA	3.04	0.41
1:C:234:ILE:HD13	1:C:302:MET:HE1	2.02	0.41
1:C:368:LEU:HD23	1:C:368:LEU:HA	1.81	0.41
1:A:66:VAL:O	1:A:66:VAL:CG1	2.68	0.41
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.03	0.41
1:A:298:PRO:HA	1:A:301:GLN:HE21	1.82	0.41
2:B:3:GLU:HB3	2:B:62:ARG:CZ	2.51	0.41
2:B:157:GLU:HB2	3:E:72:LEU:HD13	2.02	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.41
1:C:292:THR:HG22	1:C:335:ILE:HD12	2.03	0.41
1:C:350:GLY:C	1:C:351:PHE:HD1	2.24	0.41
2:D:156:ARG:NH1	2:D:156:ARG:HG3	2.35	0.41
2:D:166:THR:CG2	2:D:196:THR:HG21	2.51	0.41
2:D:257:MET:CE	2:D:312:THR:OG1	2.68	0.41
4:F:37:PHE:HZ	4:F:52:LEU:HD23	1.86	0.41
4:F:290:ILE:O	4:F:291:ILE:C	2.58	0.41
2:B:86:ARG:HG3	2:B:87:PRO:HD2	2.03	0.41
1:C:11:GLN:HG3	1:C:74:VAL:CG1	2.51	0.41
1:C:225:THR:O	1:C:229:ARG:HG3	2.21	0.41
3:E:8:VAL:C	3:E:9:ILE:HG23	2.41	0.41
1:A:88:HIS:HB2	1:A:89:PRO:HD2	2.03	0.40
1:C:174:ALA:CB	1:C:207:GLU:H	2.34	0.40
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.37	0.40
2:D:105:HIS:CE1	2:D:150:LEU:HB2	2.56	0.40
2:D:218:THR:HG23	2:D:219:THR:N	2.36	0.40
3:E:8:VAL:O	3:E:9:ILE:CG2	2.70	0.40
4:F:14:TYR:HA	4:F:17:VAL:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:ARG:O	2:D:49:VAL:HG22	2.20	0.40
4:F:209:HIS:CD2	4:F:210:LEU:CG	3.00	0.40
1:A:133:GLN:CB	1:A:252:LEU:HD12	2.50	0.40
2:B:34:GLY:O	2:B:58:LYS:HD3	2.22	0.40
2:B:218:THR:HG23	2:B:219:THR:N	2.36	0.40
2:D:30:ILE:CG2	2:D:84:ILE:HD11	2.51	0.40
2:D:172:SER:HB2	2:D:205:GLU:HB2	2.03	0.40
2:D:330:MET:O	2:D:334:GLN:HG3	2.21	0.40
4:F:3:THR:O	4:F:27:TRP:HZ3	2.04	0.40
1:A:88:HIS:NE2	1:A:91:GLN:HG3	2.36	0.40
1:A:249:ASN:HA	1:A:254:GLU:CD	2.42	0.40
2:B:406:MET:CE	2:B:410:GLU:HG3	2.51	0.40
1:C:202:PHE:HE1	1:C:378:LEU:HD22	1.85	0.40
1:C:329:ASN:O	1:C:330:ALA:C	2.60	0.40
2:B:47:ILE:HD12	2:B:47:ILE:HA	1.99	0.40
1:C:98:ASP:OD1	1:C:100:ALA:CA	2.69	0.40
1:C:230:LEU:O	1:C:234:ILE:HD12	2.21	0.40
2:D:328:GLU:H	2:D:328:GLU:HG2	1.56	0.40
2:D:423:GLN:O	2:D:423:GLN:HG3	2.22	0.40
4:F:191:LEU:HD21	4:F:228:TYR:HB3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/440 (99%)	413 (95%)	22 (5%)	0	100	100
1	C	438/440 (100%)	417 (95%)	21 (5%)	0	100	100
2	B	425/431 (99%)	404 (95%)	21 (5%)	0	100	100
2	D	412/431 (96%)	389 (94%)	23 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	116/143 (81%)	109 (94%)	7 (6%)	0	100	100
4	F	282/380 (74%)	269 (95%)	13 (5%)	0	100	100
All	All	2108/2265 (93%)	2001 (95%)	107 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	364/371 (98%)	344 (94%)	20 (6%)	18	44
1	C	369/371 (100%)	344 (93%)	25 (7%)	13	37
2	B	367/372 (99%)	348 (95%)	19 (5%)	19	46
2	D	359/372 (96%)	324 (90%)	35 (10%)	6	24
3	E	107/127 (84%)	88 (82%)	19 (18%)	1	6
4	F	260/338 (77%)	222 (85%)	38 (15%)	2	11
All	All	1826/1951 (94%)	1670 (92%)	156 (8%)	8	29

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	38	SER
1	A	42	ILE
1	A	74	VAL
1	A	82	THR
1	A	84	ARG
1	A	88	HIS
1	A	90	GLU
1	A	179	THR
1	A	229	ARG
1	A	250	VAL
1	A	277	SER

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Mol	Chain	Res	Type
1	A	320	ARG
1	A	327	ASP
1	A	345	ASP
1	A	362	VAL
1	A	370	LYS
1	A	381	THR
1	A	402	ARG
1	A	414	GLU
2	B	8	GLN
2	B	16	ILE
2	B	33	THR
2	B	52	ASN
2	B	69	GLU
2	B	77	ARG
2	B	86	ARG
2	B	115	SER
2	B	137	HIS
2	B	147	MET
2	B	190	HIS
2	B	198	GLU
2	B	199	THR
2	B	215	LEU
2	B	251	ARG
2	B	316	ILE
2	B	339	SER
2	B	377	LEU
2	B	382	SER
1	C	74	VAL
1	C	128	GLN
1	C	160	ASP
1	C	163	LYS
1	C	164	LYS
1	C	177	VAL
1	C	178	SER
1	C	251	ASP
1	C	253	THR
1	C	256	GLN
1	C	265	ILE
1	C	297	GLU
1	C	318	LEU
1	C	322	ASP
1	C	323	VAL

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Mol	Chain	Res	Type
1	C	324	VAL
1	C	327	ASP
1	C	347	CYS
1	C	352	LYS
1	C	362	VAL
1	C	381	THR
1	C	391	LEU
1	C	394	LYS
1	C	417	GLU
1	C	439	SER
2	D	1	MET
2	D	16	ILE
2	D	30	ILE
2	D	33	THR
2	D	35	SER
2	D	53	GLU
2	D	73	MET
2	D	77	ARG
2	D	86	ARG
2	D	99	ASN
2	D	112	LEU
2	D	115	SER
2	D	121	ARG
2	D	137	HIS
2	D	151	LEU
2	D	174	LYS
2	D	178	THR
2	D	188	SER
2	D	195	ASN
2	D	198	GLU
2	D	213	ARG
2	D	224	ASP
2	D	246	LEU
2	D	284	LEU
2	D	328	GLU
2	D	331	LEU
2	D	339	SER
2	D	350	LYS
2	D	351	THR
2	D	356	ILE
2	D	383	GLU
2	D	391	ARG

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Mol	Chain	Res	Type
2	D	399	THR
2	D	406	MET
2	D	419	VAL
3	E	11	LEU
3	E	18	GLN
3	E	22	VAL
3	E	25	LYS
3	E	48	GLU
3	E	52	LYS
3	E	62	LYS
3	E	75	LYS
3	E	96	MET
3	E	100	LYS
3	E	105	MET
3	E	107	SER
3	E	108	ASN
3	E	122	ARG
3	E	124	GLN
3	E	127	ASP
3	E	128	LYS
3	E	135	LYS
3	E	139	LEU
4	F	1	MET
4	F	11	SER
4	F	12	SER
4	F	30	LEU
4	F	31	ARG
4	F	33	ASP
4	F	58	LEU
4	F	69	ASP
4	F	81	ILE
4	F	92	THR
4	F	99	VAL
4	F	103	THR
4	F	148	ILE
4	F	161	LEU
4	F	171	ASP
4	F	174	ASP
4	F	182	ILE
4	F	188	LYS
4	F	190	LEU
4	F	192	LEU

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Mol	Chain	Res	Type
4	F	196	HIS
4	F	210	LEU
4	F	211	TYR
4	F	217	ARG
4	F	221	LEU
4	F	222	ARG
4	F	229	ASN
4	F	237	THR
4	F	260	ASN
4	F	277	THR
4	F	278	THR
4	F	285	LEU
4	F	293	SER
4	F	311	SER
4	F	329	LEU
4	F	333	ASN
4	F	343	TYR
4	F	357	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	6	HIS
1	C	88	HIS
1	C	301	GLN
2	D	6	HIS
2	D	15	GLN
2	D	48	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

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
11	ACP	F	401	-	27,33,33	2.17	3 (11%)	32,52,52	1.15	3 (9%)
5	GTP	A	501	7	26,34,34	1.10	2 (7%)	32,54,54	1.58	7 (21%)
8	A1D7A	B	501	-	24,26,26	4.07	12 (50%)	25,38,38	3.34	13 (52%)
8	A1D7A	D	501	-	24,26,26	3.35	15 (62%)	25,38,38	4.44	16 (64%)
10	MES	B	503	-	12,12,12	1.14	1 (8%)	14,16,16	0.85	0
9	GDP	B	502	7	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
10	MES	B	504	-	12,12,12	1.12	1 (8%)	14,16,16	0.85	0
9	GDP	D	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
5	GTP	C	501	7	26,34,34	1.11	2 (7%)	32,54,54	1.61	7 (21%)

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
11	ACP	F	401	-	-	2/15/38/38	0/3/3/3
5	GTP	A	501	7	-	9/18/38/38	0/3/3/3
8	A1D7A	B	501	-	-	2/5/18/18	0/4/4/4
8	A1D7A	D	501	-	-	4/5/18/18	0/3/4/4
10	MES	B	503	-	-	0/6/14/14	0/1/1/1
9	GDP	B	502	7	-	3/12/32/32	0/3/3/3
10	MES	B	504	-	-	3/6/14/14	0/1/1/1
9	GDP	D	502	-	-	4/12/32/32	0/3/3/3
5	GTP	C	501	7	-	6/18/38/38	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	A1D7A	C09-N11	12.94	1.49	1.35
11	F	401	ACP	PB-O3A	10.02	1.69	1.58
8	D	501	A1D7A	C09-N11	8.38	1.44	1.35
8	B	501	A1D7A	C04-N03	7.75	1.36	1.30
8	D	501	A1D7A	C04-N03	5.87	1.34	1.30
8	B	501	A1D7A	C17-C12	5.33	1.47	1.39
8	B	501	A1D7A	C12-N11	4.97	1.48	1.39
8	D	501	A1D7A	C13-N07	4.84	1.48	1.40
8	D	501	A1D7A	O18-C16	4.76	1.47	1.37
8	B	501	A1D7A	C13-N07	4.57	1.47	1.40
8	B	501	A1D7A	O18-C16	4.22	1.46	1.37
8	D	501	A1D7A	C17-C12	4.17	1.46	1.39
5	C	501	GTP	C5-C6	-3.94	1.39	1.47
5	A	501	GTP	C5-C6	-3.93	1.39	1.47
8	B	501	A1D7A	C08-C09	3.85	1.56	1.51
8	D	501	A1D7A	C08-C09	3.59	1.55	1.51
8	D	501	A1D7A	C12-N11	3.58	1.46	1.39
8	B	501	A1D7A	C04-CL20	3.56	1.83	1.73
8	D	501	A1D7A	C02-N03	-3.46	1.31	1.37
8	D	501	A1D7A	C12-C13	-3.35	1.36	1.40
8	D	501	A1D7A	C06-N07	3.27	1.46	1.39
8	B	501	A1D7A	C02-N03	-3.27	1.32	1.37
8	B	501	A1D7A	C14-C13	3.06	1.44	1.39
10	B	503	MES	C8-S	3.06	1.81	1.77
10	B	504	MES	C8-S	3.00	1.81	1.77
8	D	501	A1D7A	C04-CL20	2.90	1.81	1.73
8	D	501	A1D7A	C14-C13	2.70	1.44	1.39
8	B	501	A1D7A	C22-S23	2.64	1.83	1.71
9	B	502	GDP	C6-N1	-2.40	1.34	1.37
8	D	501	A1D7A	C14-C15	2.37	1.43	1.38
8	D	501	A1D7A	C22-S23	2.33	1.82	1.71
9	D	502	GDP	C6-N1	-2.32	1.34	1.37
8	D	501	A1D7A	O10-C09	-2.30	1.18	1.23
5	A	501	GTP	C2-N3	2.22	1.38	1.33
5	C	501	GTP	C2-N3	2.22	1.38	1.33
11	F	401	ACP	C8-N7	-2.21	1.30	1.34
11	F	401	ACP	PB-O2B	-2.16	1.51	1.56
8	B	501	A1D7A	C17-C16	2.13	1.42	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	A1D7A	O10-C09-N11	-9.66	112.91	121.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	A1D7A	C19-O18-C16	8.66	136.30	117.51
8	D	501	A1D7A	C21-C02-C01	8.43	116.77	110.62
8	B	501	A1D7A	N03-C04-N05	-7.79	122.78	130.62
8	B	501	A1D7A	C21-C02-C01	7.39	116.01	110.62
8	D	501	A1D7A	N03-C04-N05	-6.92	123.65	130.62
8	D	501	A1D7A	C08-N07-C06	-6.11	105.80	116.39
8	D	501	A1D7A	C14-C13-C12	-5.91	112.29	119.63
8	B	501	A1D7A	C13-C12-N11	-5.19	112.61	119.56
8	B	501	A1D7A	CL20-C04-N03	4.93	119.91	115.70
8	D	501	A1D7A	C15-C16-C17	-4.64	114.15	120.53
8	B	501	A1D7A	C08-N07-C06	-4.46	108.66	116.39
8	D	501	A1D7A	C13-C12-N11	-4.06	114.13	119.56
8	B	501	A1D7A	C14-C13-C12	-4.00	114.66	119.63
5	C	501	GTP	PB-O3B-PG	-3.74	120.01	132.83
5	A	501	GTP	PB-O3B-PG	-3.64	120.34	132.83
8	D	501	A1D7A	C17-C12-C13	3.53	123.40	119.67
5	C	501	GTP	PA-O3A-PB	-3.46	120.94	132.83
9	B	502	GDP	PA-O3A-PB	-3.37	121.25	132.83
5	A	501	GTP	PA-O3A-PB	-3.36	121.29	132.83
9	B	502	GDP	C3'-C2'-C1'	3.32	105.98	100.98
8	B	501	A1D7A	C17-C12-N11	3.31	125.83	119.84
9	D	502	GDP	C3'-C2'-C1'	3.28	105.92	100.98
9	D	502	GDP	PA-O3A-PB	-3.28	121.59	132.83
8	D	501	A1D7A	C04-N05-C06	3.24	120.66	111.04
5	C	501	GTP	C5-C6-N1	3.24	119.67	113.95
11	F	401	ACP	O2B-PB-O1B	3.18	120.69	110.07
5	A	501	GTP	C5-C6-N1	3.17	119.56	113.95
8	D	501	A1D7A	CL20-C04-N03	3.12	118.36	115.70
8	B	501	A1D7A	C15-C16-C17	-3.09	116.28	120.53
8	D	501	A1D7A	O10-C09-C08	3.08	127.36	119.92
5	A	501	GTP	C8-N7-C5	3.03	108.77	102.99
5	C	501	GTP	C8-N7-C5	3.00	108.70	102.99
8	D	501	A1D7A	C12-C17-C16	2.98	123.42	118.01
5	C	501	GTP	C3'-C2'-C1'	2.95	105.41	100.98
8	B	501	A1D7A	C19-O18-C16	-2.93	111.15	117.51
8	D	501	A1D7A	C15-C14-C13	2.91	125.17	119.19
8	D	501	A1D7A	C14-C13-N07	2.91	125.57	121.77
5	C	501	GTP	C2-N1-C6	-2.87	119.81	125.10
5	A	501	GTP	C3'-C2'-C1'	2.87	105.30	100.98
8	B	501	A1D7A	C08-C09-N11	2.84	119.67	116.13
5	A	501	GTP	C2-N1-C6	-2.84	119.87	125.10
11	F	401	ACP	PB-O3A-PA	-2.84	123.56	132.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	A1D7A	C04-N05-C06	2.72	119.12	111.04
8	D	501	A1D7A	C08-C09-N11	2.72	119.52	116.13
8	B	501	A1D7A	C15-C14-C13	2.63	124.59	119.19
11	F	401	ACP	O1G-PG-C3B	-2.39	106.10	111.24
9	B	502	GDP	C8-N7-C5	2.31	107.39	102.99
9	D	502	GDP	C8-N7-C5	2.29	107.36	102.99
9	D	502	GDP	C5-C6-N1	2.27	117.97	113.95
9	B	502	GDP	C5-C6-N1	2.26	117.94	113.95
8	B	501	A1D7A	C09-C08-N07	-2.23	108.51	113.13
5	C	501	GTP	O6-C6-C5	-2.16	120.15	124.37
5	A	501	GTP	O6-C6-C5	-2.13	120.21	124.37

There are no chirality outliers.

All (33) 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
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	A1D7A	C01-C06-N07-C08
8	B	501	A1D7A	N05-C06-N07-C08
8	D	501	A1D7A	C01-C06-N07-C08
8	D	501	A1D7A	N05-C06-N07-C08
9	B	502	GDP	C5'-O5'-PA-O1A
9	B	502	GDP	C5'-O5'-PA-O2A
9	D	502	GDP	PA-O3A-PB-O3B
9	D	502	GDP	C5'-O5'-PA-O3A
8	D	501	A1D7A	C15-C16-O18-C19
8	D	501	A1D7A	C17-C16-O18-C19
5	A	501	GTP	C3'-C4'-C5'-O5'
10	B	504	MES	C7-C8-S-O3S
9	D	502	GDP	PA-O3A-PB-O1B
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C3'-C4'-C5'-O5'
9	D	502	GDP	C5'-O5'-PA-O1A
10	B	504	MES	C7-C8-S-O1S
10	B	504	MES	C7-C8-S-O2S
5	A	501	GTP	O4'-C4'-C5'-O5'
5	C	501	GTP	O4'-C4'-C5'-O5'

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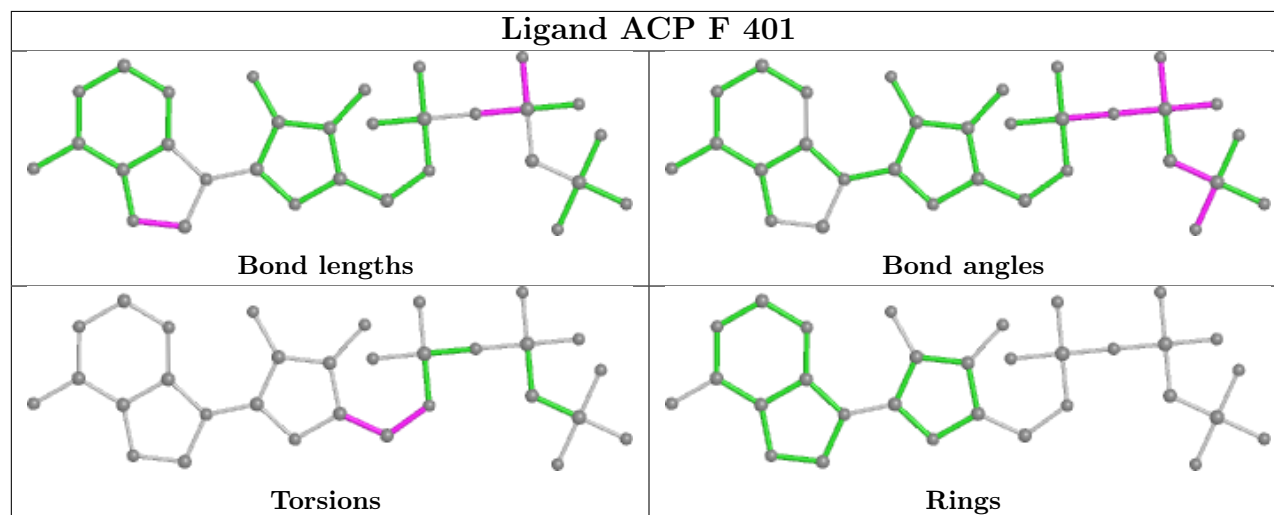
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O3G
9	B	502	GDP	C5'-O5'-PA-O3A
11	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G

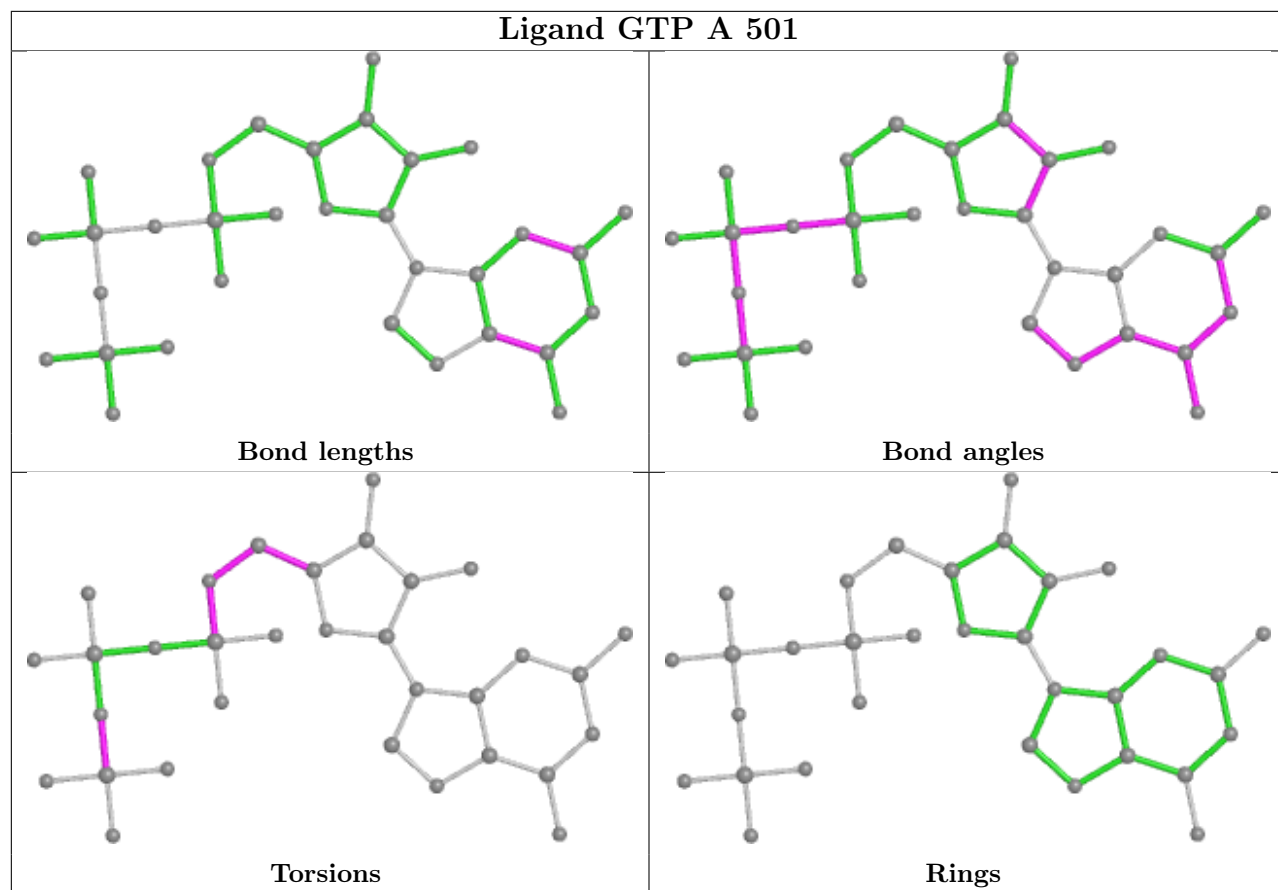
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	A1D7A	2	0
8	D	501	A1D7A	2	0

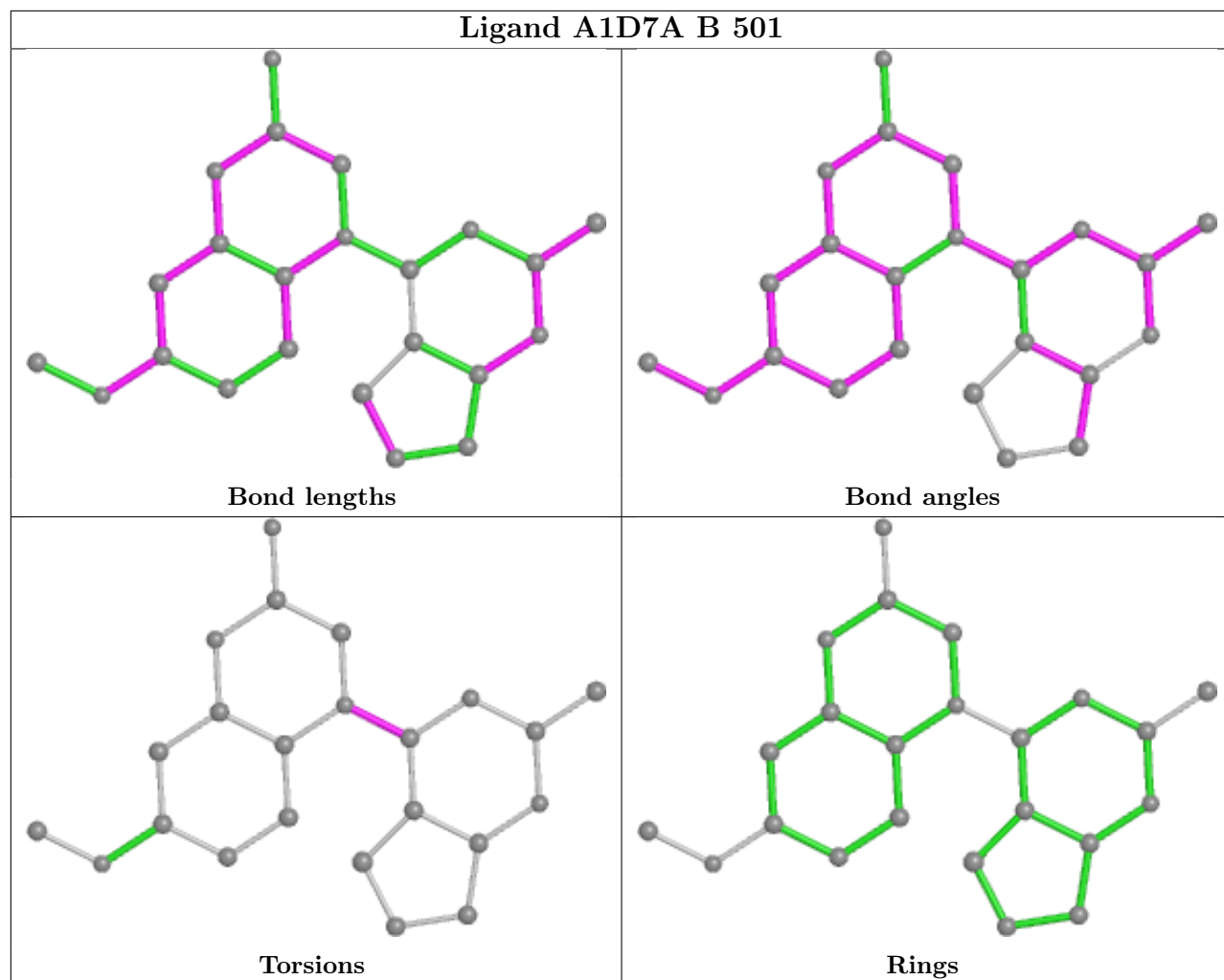
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



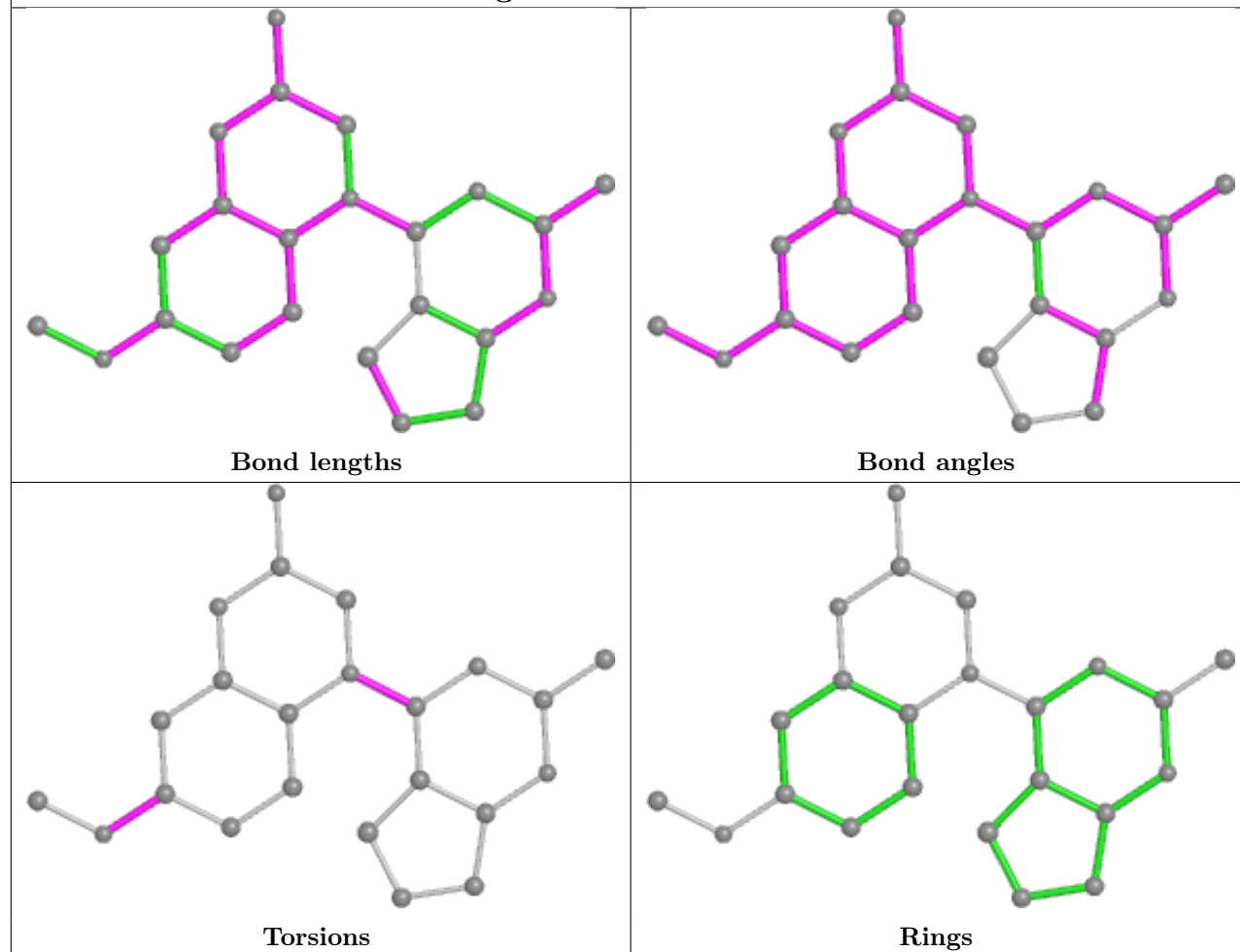




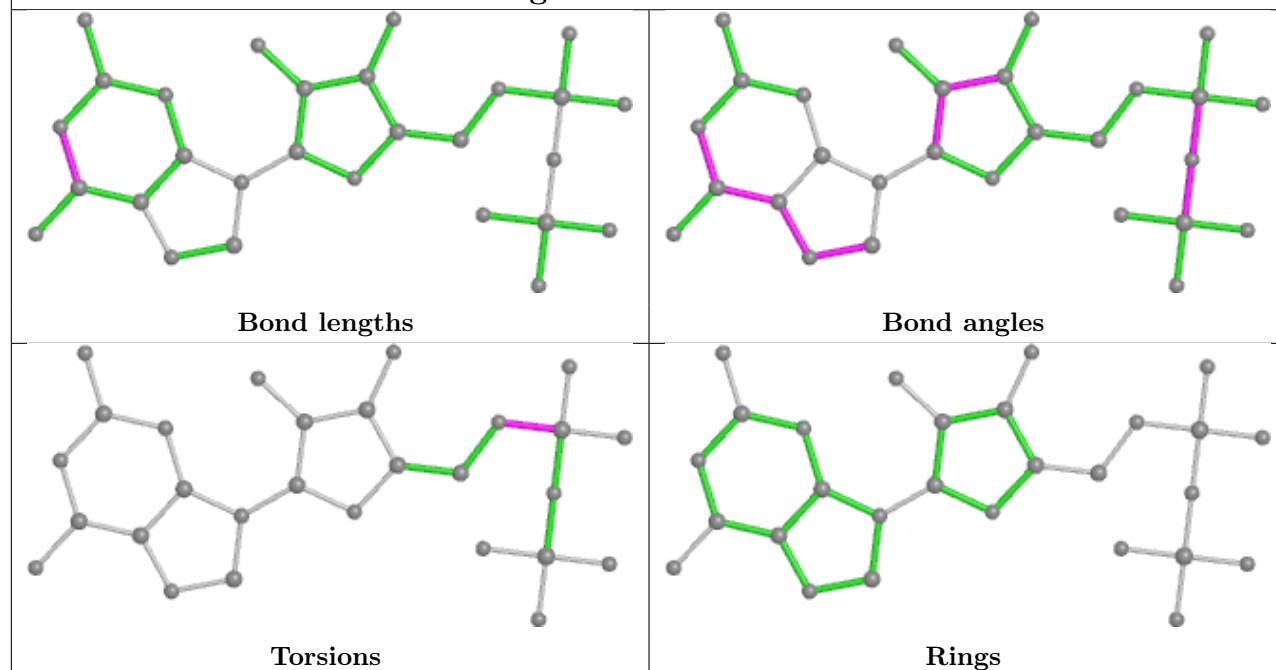
## Ligand A1D7A B 501

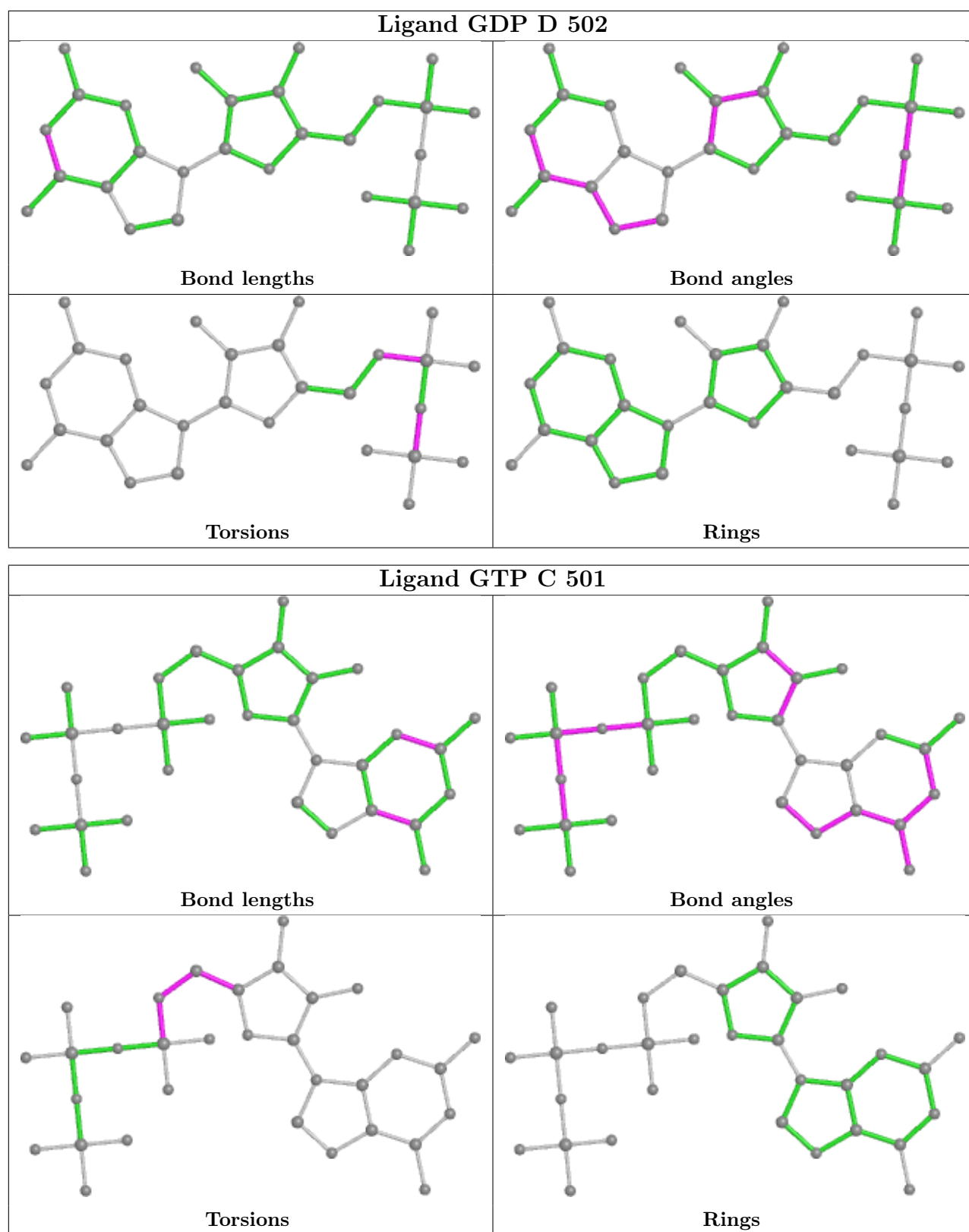


## Ligand A1D7A D 501



## Ligand GDP B 502





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	437/440 (99%)	-0.35	1 (0%) 92 88	48, 73, 103, 150	0
1	C	440/440 (100%)	-0.49	0 100 100	41, 61, 90, 123	0
2	B	427/431 (99%)	-0.38	1 (0%) 92 88	47, 68, 103, 165	0
2	D	418/431 (96%)	-0.13	1 (0%) 92 88	53, 92, 130, 175	0
3	E	120/143 (83%)	-0.16	0 100 100	59, 84, 124, 158	0
4	F	298/380 (78%)	-0.12	0 100 100	63, 96, 155, 234	0
All	All	2140/2265 (94%)	-0.30	3 (0%) 92 91	41, 76, 122, 234	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	GLU	2.3
2	D	73	MET	2.2
2	B	72	THR	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

## 6.5 Other polymers [i](#)

There are no such residues in this entry.