



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2024 – 09:57 AM EST

PDB ID : 2HDN  
Title : Trypsin-modified Elongation Factor Tu in complex with tetracycline at 2.8 Angstrom resolution  
Authors : Mui, S.; Heffron, S.E.; Aorora, A.; Abel, K.; Bergmann, E.; Journak, F.  
Deposited on : 2006-06-20  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

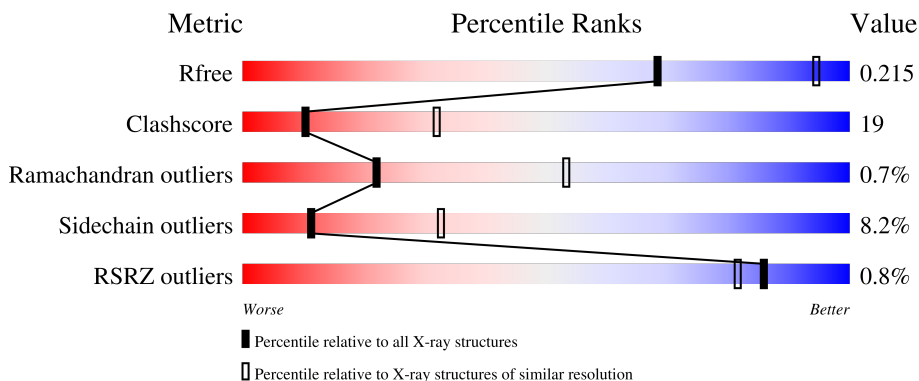
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	37	 3% 68% 19% 11%
1	C	37	 73% 16% 11%
1	E	37	 3% 68% 19% 11%
1	G	37	 78% 11% 11%
1	I	37	 3% 62% 22% 5% 11%

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Mol	Chain	Length	Quality of chain
1	K	37	 76% 14% 11%
2	B	335	 67% 29% .
2	D	335	 64% 32% .
2	F	335	 63% 33% .
2	H	335	 65% 30% .
2	J	335	 70% 27% .
2	L	335	 63% 33% .

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
5	TAC	F	3888	-	-	-	X

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 17608 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Elongation factor EF-Tu.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	33	239	151	43	45	0	0	0
1	C	33	239	151	43	45	0	0	0
1	E	33	239	151	43	45	0	0	0
1	G	33	239	151	43	45	0	0	0
1	I	33	239	151	43	45	0	0	0
1	K	33	239	151	43	45	0	0	0

- Molecule 2 is a protein called Elongation factor EF-Tu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	335	2594	1644	441	496	13	0	0	0
2	D	335	2594	1644	441	496	13	0	0	0
2	F	335	2594	1644	441	496	13	0	0	0
2	H	335	2594	1644	441	496	13	0	0	0
2	J	335	2594	1644	441	496	13	0	0	0
2	L	335	2594	1644	441	496	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	393	GLY	SER	variant	UNP P0A6N1

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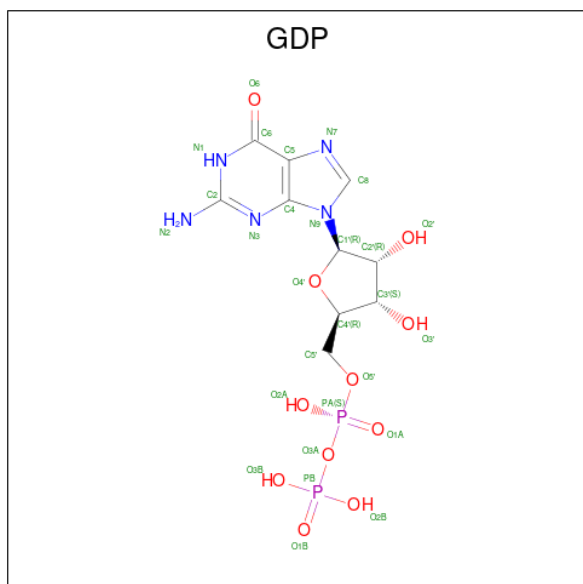
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Chain	Residue	Modelled	Actual	Comment	Reference
D	393	GLY	SER	variant	UNP P0A6N1
F	393	GLY	SER	variant	UNP P0A6N1
H	393	GLY	SER	variant	UNP P0A6N1
J	393	GLY	SER	variant	UNP P0A6N1
L	393	GLY	SER	variant	UNP P0A6N1

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

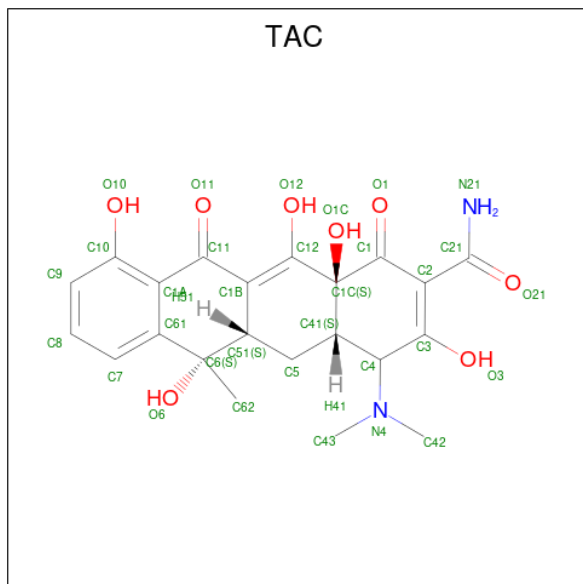
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0
3	K	1	Total Mg 1 1	0	0

- Molecule 4 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
			Total	C	N	O	P		
4	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	D	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	F	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	H	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	J	1	Total 28	C 10	N 5	O 11	P 2	0	0
4	L	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 5 is TETRACYCLINE (three-letter code: TAC) (formula:  $C_{22}H_{24}N_2O_8$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	Total 32	C 22	N 2	O 8	0	0
5	D	1	Total 32	C 22	N 2	O 8	0	0
5	F	1	Total 32	C 22	N 2	O 8	0	0
5	H	1	Total 32	C 22	N 2	O 8	0	0
5	J	1	Total 32	C 22	N 2	O 8	0	0
5	L	1	Total 32	C 22	N 2	O 8	0	0

- Molecule 6 is water.

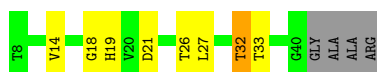
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total O 4 4	0	0
6	B	54	Total O 54 54	0	0
6	C	3	Total O 3 3	0	0
6	D	30	Total O 30 30	0	0
6	E	1	Total O 1 1	0	0
6	F	30	Total O 30 30	0	0
6	G	4	Total O 4 4	0	0
6	H	28	Total O 28 28	0	0
6	I	3	Total O 3 3	0	0
6	J	45	Total O 45 45	0	0
6	K	5	Total O 5 5	0	0
6	L	37	Total O 37 37	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

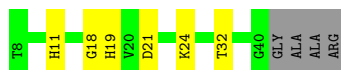
- Molecule 1: Elongation factor EF-Tu

Chain A:  68% 19% 11%



- Molecule 1: Elongation factor EF-Tu

Chain C:  73% 16% 11%




- Molecule 1: Elongation factor EF-Tu

Chain E:  68% 19% 11%



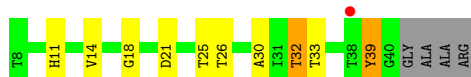
- Molecule 1: Elongation factor EF-Tu

Chain G:  78% 11% 11%



- Molecule 1: Elongation factor EF-Tu

Chain I:  3% 62% 22% 5% 11%



- Molecule 1: Elongation factor EF-Tu

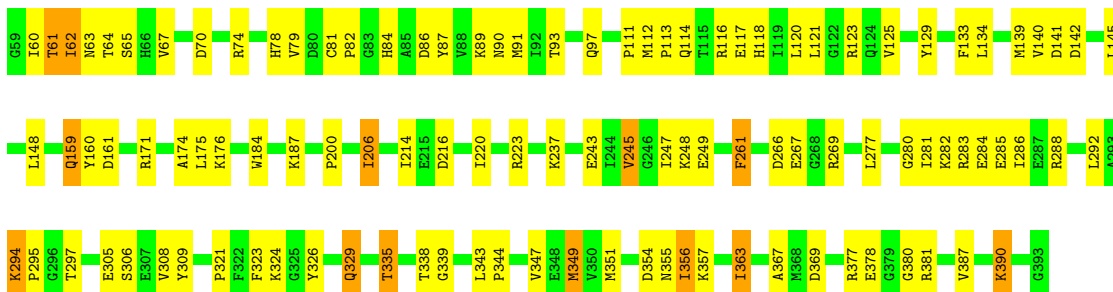
Chain K:  76% 14% 11%





- Molecule 2: Elongation factor EF-Tu

Chain B: 67% 29%



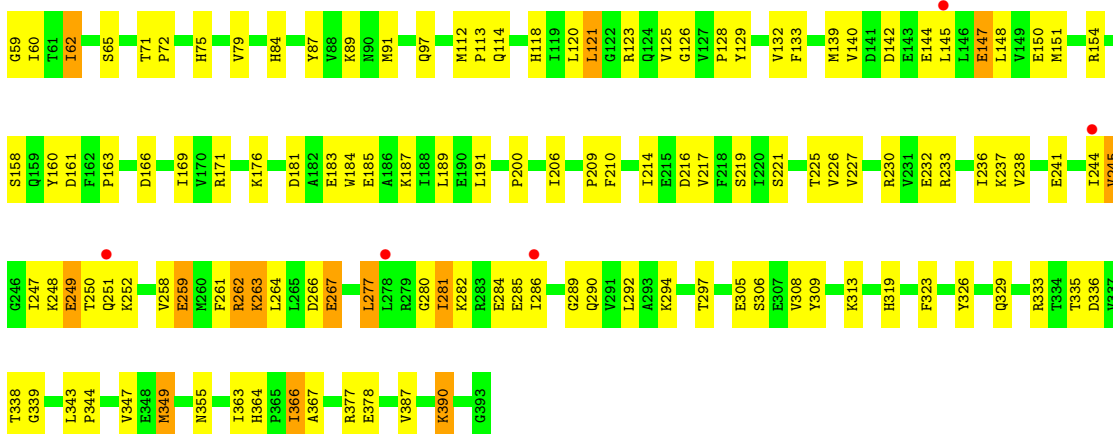
- Molecule 2: Elongation factor EF-Tu

Chain D: 64% 32%



- Molecule 2: Elongation factor EF-Tu

Chain F: 63% 33%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.71Å 156.06Å 134.83Å 90.00° 95.38° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 47.27 – 2.71	Depositor EDS
% Data completeness (in resolution range)	91.6 (40.00-2.80) 86.3 (47.27-2.71)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.73Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.180 , 0.223 0.172 , 0.215	Depositor DCC
$R_{free}$ test set	4781 reflections (7.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtrriage
Anisotropy	0.454	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 62.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, TAC

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	0.74	0/243	0.81	0/332
1	C	0.61	0/243	0.78	0/332
1	E	0.65	0/243	0.83	0/332
1	G	0.66	0/243	0.81	0/332
1	I	0.73	0/243	0.85	0/332
1	K	0.61	0/243	0.77	0/332
2	B	0.74	0/2642	0.90	1/3574 (0.0%)
2	D	0.68	0/2642	0.84	1/3574 (0.0%)
2	F	0.62	0/2642	0.83	1/3574 (0.0%)
2	H	0.61	0/2642	0.82	0/3574
2	J	0.75	0/2642	0.89	2/3574 (0.1%)
2	L	0.68	0/2642	0.85	0/3574
All	All	0.68	0/17310	0.85	5/23436 (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	E	0	1
1	I	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	266	ASP	N-CA-CB	-6.57	98.77	110.60
2	J	363	ILE	CB-CA-C	-5.57	100.46	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	71	THR	N-CA-C	-5.27	96.76	111.00
2	F	71	THR	N-CA-C	-5.26	96.80	111.00
2	D	71	THR	N-CA-C	-5.21	96.93	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	39	TYR	Sidechain
1	I	39	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	239	0	248	12	0
1	C	239	0	247	8	0
1	E	239	0	248	14	0
1	G	239	0	248	7	0
1	I	239	0	247	14	0
1	K	239	0	247	8	0
2	B	2594	0	2605	99	0
2	D	2594	0	2605	103	0
2	F	2594	0	2605	132	0
2	H	2594	0	2605	122	0
2	J	2594	0	2605	107	0
2	L	2594	0	2605	104	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
4	B	28	0	12	1	0
4	D	28	0	12	1	0
4	F	28	0	12	1	0
4	H	28	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	28	0	12	0	0
4	L	28	0	12	0	0
5	B	32	0	22	1	0
5	D	32	0	22	1	0
5	F	32	0	22	0	0
5	H	32	0	22	1	0
5	J	32	0	21	1	0
5	L	32	0	22	1	0
6	A	4	0	0	0	0
6	B	54	0	0	1	0
6	C	3	0	0	0	0
6	D	30	0	0	4	0
6	E	1	0	0	0	0
6	F	30	0	0	4	0
6	G	4	0	0	0	0
6	H	28	0	0	1	0
6	I	3	0	0	0	0
6	J	45	0	0	6	0
6	K	5	0	0	0	0
6	L	37	0	0	3	0
All	All	17608	0	17318	648	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 19.

All (648) 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:J:97:GLN:H	2:J:97:GLN:NE2	1.41	1.19
2:H:60:ILE:HD12	2:H:60:ILE:H	1.17	1.07
2:D:143:GLU:O	2:D:147:GLU:HG2	1.58	1.02
2:L:230:ARG:HH11	2:L:230:ARG:HB2	1.26	1.00
2:H:217:VAL:HG11	2:H:286:ILE:HD12	1.44	0.99
1:C:18:GLY:H	2:D:118:HIS:HD2	1.01	0.99
2:L:84:HIS:HD2	2:L:114:GLN:HG2	1.27	0.98
2:F:214:ILE:HG12	2:F:290:GLN:O	1.63	0.97
1:E:18:GLY:H	2:F:118:HIS:HD2	0.99	0.97
1:A:18:GLY:H	2:B:118:HIS:HD2	0.98	0.96
1:G:18:GLY:H	2:H:118:HIS:HD2	1.00	0.94
2:L:230:ARG:HB2	2:L:230:ARG:NH1	1.81	0.94
2:F:338:THR:HB	2:F:363:ILE:HD12	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:18:GLY:H	2:J:118:HIS:HD2	1.04	0.91
1:K:18:GLY:H	2:L:118:HIS:HD2	1.04	0.91
2:H:288:ARG:HD3	2:H:335:THR:CG2	2.01	0.91
2:F:181:ASP:OD1	2:F:183:GLU:HG2	1.71	0.91
2:J:97:GLN:H	2:J:97:GLN:HE21	1.17	0.90
2:L:84:HIS:CD2	2:L:114:GLN:HG2	2.06	0.89
1:A:18:GLY:H	2:B:118:HIS:CD2	1.90	0.88
2:L:288:ARG:HG2	2:L:335:THR:HG23	1.55	0.88
2:H:288:ARG:HD3	2:H:335:THR:HG23	1.53	0.88
2:D:248:LYS:HE3	2:D:287:GLU:HG2	1.56	0.88
2:H:282:LYS:H	2:H:282:LYS:HZ2	1.17	0.87
2:F:248:LYS:HG3	2:F:249:GLU:H	1.41	0.85
2:J:84:HIS:HD2	2:J:118:HIS:HE1	1.22	0.85
2:F:245:VAL:HG22	2:F:367:ALA:HB2	1.58	0.85
2:H:120:LEU:HD12	2:H:160:TYR:HE2	1.40	0.85
2:B:338:THR:O	2:B:363:ILE:HG22	1.77	0.85
2:J:97:GLN:NE2	2:J:97:GLN:N	2.25	0.84
2:H:60:ILE:H	2:H:60:ILE:CD1	1.89	0.84
2:H:237:LYS:O	2:H:240:GLU:HG3	1.76	0.84
1:E:18:GLY:H	2:F:118:HIS:CD2	1.91	0.84
2:D:279:ARG:NH1	2:D:279:ARG:HB2	1.92	0.84
2:H:217:VAL:CG1	2:H:286:ILE:HD12	2.08	0.83
2:J:279:ARG:HG3	2:J:279:ARG:HH11	1.44	0.83
2:F:262:ARG:HA	2:F:262:ARG:CZ	2.08	0.83
2:H:142:ASP:CG	2:H:145:LEU:HG	1.99	0.83
2:J:245:VAL:HG22	2:J:367:ALA:HB2	1.58	0.83
1:C:18:GLY:H	2:D:118:HIS:CD2	1.93	0.82
1:K:18:GLY:H	2:L:118:HIS:CD2	1.95	0.82
1:I:18:GLY:H	2:J:118:HIS:CD2	1.96	0.82
2:L:248:LYS:HE2	2:L:287:GLU:HG2	1.60	0.82
2:L:248:LYS:HE3	2:L:285:GLU:O	1.79	0.81
2:L:123:ARG:HD2	2:L:160:TYR:O	1.81	0.81
2:B:245:VAL:HG22	2:B:367:ALA:HB2	1.63	0.81
2:F:226:VAL:HG22	2:F:277:LEU:CD2	2.10	0.81
1:G:18:GLY:H	2:H:118:HIS:CD2	1.92	0.81
2:B:377:ARG:HH21	2:B:380:GLY:HA2	1.44	0.80
2:F:338:THR:HB	2:F:363:ILE:CD1	2.12	0.80
2:H:123:ARG:HD2	2:H:160:TYR:O	1.82	0.79
2:H:60:ILE:HD12	2:H:60:ILE:N	1.96	0.79
2:L:97:GLN:CD	2:L:97:GLN:H	1.87	0.78
2:J:84:HIS:HD2	2:J:118:HIS:CE1	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:HIS:HD2	2:D:118:HIS:HE1	1.32	0.78
2:J:288:ARG:HG2	2:J:335:THR:HG23	1.66	0.78
2:F:251:GLN:NE2	2:F:281:ILE:HD11	1.99	0.77
2:D:66:HIS:HB2	6:D:2020:HOH:O	1.82	0.77
2:D:337:VAL:HG21	2:D:366:ILE:HD11	1.66	0.77
2:J:97:GLN:HE21	2:J:97:GLN:N	1.81	0.77
2:H:282:LYS:H	2:H:282:LYS:NZ	1.83	0.77
2:J:123:ARG:HD2	2:J:160:TYR:O	1.85	0.76
1:A:18:GLY:N	2:B:118:HIS:HD2	1.81	0.76
2:D:84:HIS:HD2	2:D:118:HIS:CE1	2.03	0.76
2:L:338:THR:HB	2:L:363:ILE:HD12	1.66	0.76
2:F:259:GLU:HB2	2:F:262:ARG:HH22	1.52	0.75
2:D:248:LYS:HE3	2:D:287:GLU:CG	2.17	0.75
2:F:262:ARG:HA	2:F:262:ARG:NE	2.02	0.74
2:F:248:LYS:CG	2:F:249:GLU:H	1.99	0.74
2:F:123:ARG:HD2	2:F:160:TYR:O	1.87	0.74
2:D:84:HIS:CD2	2:D:118:HIS:HE1	2.06	0.74
1:G:18:GLY:N	2:H:118:HIS:HD2	1.83	0.73
1:E:18:GLY:N	2:F:118:HIS:HD2	1.82	0.73
1:E:39:TYR:OH	2:J:264:LEU:CB	2.35	0.73
2:J:62:ILE:HD12	2:J:90:ASN:ND2	2.04	0.73
2:F:262:ARG:HH11	2:H:283:ARG:HH22	1.36	0.73
2:J:84:HIS:CD2	2:J:118:HIS:HE1	2.07	0.72
2:F:244:ILE:HD13	2:F:292:LEU:CD1	2.19	0.72
1:E:39:TYR:OH	2:J:264:LEU:HB2	1.89	0.72
2:J:281:ILE:CD1	2:J:285:GLU:HB2	2.20	0.72
2:L:84:HIS:HD2	2:L:114:GLN:CG	2.02	0.71
2:L:230:ARG:NH2	2:L:273:ASN:HB2	2.05	0.71
2:B:125:VAL:HG12	2:B:387:VAL:HG11	1.72	0.71
2:D:123:ARG:HD2	2:D:160:TYR:O	1.90	0.71
2:H:301:HIS:HD2	2:H:393:GLY:HA2	1.55	0.71
2:B:123:ARG:HD2	2:B:160:TYR:O	1.91	0.71
2:F:214:ILE:O	2:F:214:ILE:HG13	1.90	0.71
1:K:18:GLY:N	2:L:118:HIS:HD2	1.86	0.71
2:B:356:ILE:HD12	2:B:357:LYS:H	1.56	0.70
2:H:142:ASP:OD2	2:H:145:LEU:HG	1.91	0.70
2:H:245:VAL:HG22	2:H:367:ALA:HB2	1.74	0.70
2:H:121:LEU:O	2:H:125:VAL:HG22	1.92	0.70
2:J:181:ASP:OD1	2:J:183:GLU:HG2	1.90	0.70
2:L:356:ILE:HD12	2:L:357:LYS:H	1.57	0.69
2:H:120:LEU:HD12	2:H:160:TYR:CE2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:ASP:HB2	2:F:145:LEU:HG	1.73	0.69
2:J:241:GLU:OE2	2:J:252:LYS:HE2	1.92	0.69
2:B:329:GLN:NE2	2:B:377:ARG:HB2	2.08	0.69
2:F:84:HIS:CD2	2:F:114:GLN:HG2	2.28	0.68
2:F:258:VAL:O	2:F:264:LEU:HD12	1.93	0.68
2:F:343:LEU:CD1	2:F:347:VAL:HG23	2.24	0.68
2:J:230:ARG:HB2	2:J:230:ARG:HH11	1.58	0.68
2:F:259:GLU:CB	2:F:262:ARG:HH22	2.08	0.67
2:H:244:ILE:HD12	2:H:251:GLN:HB2	1.75	0.67
2:L:288:ARG:HG2	2:L:335:THR:CG2	2.25	0.67
2:L:288:ARG:HH11	2:L:288:ARG:HB2	1.60	0.66
1:C:18:GLY:N	2:D:118:HIS:HD2	1.85	0.66
2:H:143:GLU:O	2:H:147:GLU:HG3	1.96	0.66
2:L:245:VAL:HG22	2:L:367:ALA:HB2	1.78	0.66
2:L:60:ILE:HD12	2:L:93:THR:HG21	1.78	0.66
2:B:323:PHE:CE2	2:B:349:MET:HB2	2.31	0.66
2:F:226:VAL:HG22	2:F:277:LEU:HD21	1.76	0.65
2:H:144:GLU:O	2:H:148:LEU:HG	1.96	0.65
2:H:238:VAL:HG23	2:H:266:ASP:O	1.96	0.65
2:F:147:GLU:O	2:F:151:MET:HG3	1.97	0.65
2:F:262:ARG:HD3	2:H:283:ARG:HH12	1.61	0.65
2:F:60:ILE:HD11	2:F:89:LYS:HB3	1.78	0.65
2:F:323:PHE:CE2	2:F:349:MET:HB3	2.32	0.65
2:H:288:ARG:CD	2:H:335:THR:HG23	2.25	0.65
1:I:32:THR:HG22	1:I:33:THR:N	2.11	0.65
2:J:343:LEU:HB3	2:J:347:VAL:CG2	2.26	0.65
2:L:140:VAL:HG13	2:L:145:LEU:HD23	1.78	0.65
2:H:142:ASP:OD1	2:H:144:GLU:HB3	1.97	0.65
2:B:344:PRO:O	2:B:347:VAL:HG22	1.97	0.64
2:F:171:ARG:O	2:F:187:LYS:HE2	1.97	0.64
2:L:299:LYS:HG3	2:L:301:HIS:HE1	1.61	0.64
2:F:189:LEU:CD1	2:J:266:ASP:HB3	2.28	0.64
2:D:294:LYS:NZ	2:D:294:LYS:HB3	2.13	0.63
2:F:259:GLU:HB2	2:F:262:ARG:NH2	2.13	0.63
1:C:11:HIS:CD2	2:D:75:HIS:HD2	2.16	0.63
1:G:19:HIS:CE1	2:H:114:GLN:HG3	2.33	0.63
2:D:279:ARG:HG3	2:D:279:ARG:O	1.98	0.63
2:F:217:VAL:HG21	2:F:286:ILE:HG21	1.81	0.63
2:F:189:LEU:HD11	2:J:266:ASP:HB3	1.81	0.63
2:L:279:ARG:HG3	2:L:279:ARG:HH11	1.64	0.63
2:B:294:LYS:HB3	2:B:297:THR:HG21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:84:HIS:HD2	2:H:114:GLN:CG	2.13	0.62
2:J:89:LYS:HE2	2:J:309:TYR:CZ	2.34	0.62
2:J:279:ARG:HG3	2:J:279:ARG:NH1	2.11	0.62
2:F:262:ARG:HD2	2:H:283:ARG:NH2	2.15	0.62
2:D:171:ARG:O	2:D:187:LYS:HE2	2.00	0.62
2:D:279:ARG:HB2	2:D:279:ARG:HH11	1.65	0.62
2:B:121:LEU:O	2:B:125:VAL:HG22	1.98	0.62
1:E:39:TYR:CD2	2:F:72:PRO:HG3	2.35	0.62
2:J:338:THR:HB	2:J:363:ILE:CD1	2.30	0.62
2:L:108:THR:HG22	2:L:109:ASP:OD1	2.00	0.62
2:H:237:LYS:HD2	2:H:267:GLU:OE1	2.00	0.61
2:D:230:ARG:HB2	2:D:230:ARG:HH11	1.64	0.61
2:D:288:ARG:HE	2:D:335:THR:CG2	2.13	0.61
2:L:288:ARG:HB2	2:L:288:ARG:NH1	2.15	0.61
2:L:145:LEU:O	2:L:148:LEU:HB3	2.01	0.61
2:F:158:SER:HA	6:F:3064:HOH:O	2.00	0.61
2:D:112:MET:HB3	2:D:113:PRO:CD	2.30	0.61
2:L:264:LEU:C	2:L:265:LEU:HD23	2.21	0.61
2:F:336:ASP:OD1	2:F:377:ARG:HD3	2.01	0.61
2:L:121:LEU:O	2:L:125:VAL:HG22	2.01	0.61
2:B:377:ARG:NH2	2:B:380:GLY:HA2	2.16	0.60
2:B:324:LYS:HZ2	2:B:343:LEU:HB2	1.66	0.60
2:F:262:ARG:HD2	2:H:283:ARG:HH22	1.66	0.60
2:F:329:GLN:HB3	2:F:336:ASP:HB3	1.84	0.60
2:J:281:ILE:HD12	2:J:282:LYS:N	2.17	0.60
2:D:84:HIS:CD2	2:D:118:HIS:CE1	2.85	0.60
2:F:343:LEU:HB3	2:F:347:VAL:CG2	2.32	0.60
2:H:343:LEU:HB3	2:H:347:VAL:CG2	2.31	0.59
2:H:125:VAL:HG12	2:H:387:VAL:HG11	1.83	0.59
2:H:84:HIS:HD2	2:H:114:GLN:HG2	1.68	0.59
1:A:26:THR:HG22	2:B:174:ALA:CB	2.32	0.59
1:A:26:THR:HG22	2:B:174:ALA:HB1	1.84	0.59
2:D:125:VAL:HG12	2:D:387:VAL:HG11	1.84	0.59
2:F:183:GLU:HG3	2:F:184:TRP:N	2.17	0.59
2:H:84:HIS:CD2	2:H:114:GLN:HG2	2.38	0.59
2:B:329:GLN:HE21	2:B:377:ARG:HB2	1.66	0.59
2:B:261:PHE:CG	2:D:288:ARG:HG2	2.37	0.59
2:H:208:LYS:HB3	2:H:233:ARG:HD2	1.84	0.59
2:F:282:LYS:HG3	2:F:284:GLU:HG2	1.85	0.58
2:D:260:MET:CE	2:D:265:LEU:HD11	2.33	0.58
2:F:217:VAL:CG2	2:F:286:ILE:HG21	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:323:PHE:CD2	2:F:349:MET:HB3	2.38	0.58
2:J:305:GLU:CD	2:J:357:LYS:HE3	2.24	0.58
2:J:294:LYS:HD2	6:J:5026:HOH:O	2.02	0.58
2:F:313:LYS:HD2	2:F:319:HIS:HD2	1.69	0.58
1:I:18:GLY:N	2:J:118:HIS:HD2	1.88	0.58
2:H:237:LYS:HG3	2:H:267:GLU:HB3	1.86	0.57
1:A:27:LEU:HD13	2:B:133:PHE:CE2	2.39	0.57
2:F:343:LEU:HD12	2:F:347:VAL:HG23	1.86	0.57
2:J:305:GLU:OE2	2:J:357:LYS:HE3	2.04	0.57
2:D:345:GLU:OE2	2:H:163:PRO:HD3	2.04	0.57
2:F:176:LYS:CB	2:F:184:TRP:CD1	2.87	0.57
2:B:171:ARG:O	2:B:187:LYS:HE2	2.04	0.57
2:H:248:LYS:HZ1	2:H:285:GLU:HA	1.70	0.57
2:L:112:MET:HB3	2:L:113:PRO:CD	2.34	0.57
2:D:74:ARG:HD3	6:D:2059:HOH:O	2.04	0.57
2:J:120:LEU:HD13	2:J:160:TYR:CE1	2.39	0.57
2:B:97:GLN:OE1	2:B:97:GLN:N	2.35	0.57
1:G:19:HIS:HA	2:H:114:GLN:HB2	1.86	0.57
2:D:259:GLU:HG2	2:D:264:LEU:HG	1.86	0.57
2:D:176:LYS:HB3	2:D:184:TRP:CD1	2.40	0.57
2:F:261:PHE:HA	2:H:216:ASP:OD1	2.05	0.57
2:J:323:PHE:CE2	2:J:349:MET:HB3	2.40	0.56
2:L:299:LYS:HG3	2:L:301:HIS:CE1	2.39	0.56
2:B:214:ILE:HD11	2:B:292:LEU:HD13	1.87	0.56
2:J:123:ARG:HG2	6:J:5063:HOH:O	2.04	0.56
2:D:243:GLU:HG2	2:D:252:LYS:HG2	1.87	0.56
2:J:62:ILE:HG22	2:J:62:ILE:O	2.04	0.56
2:J:172:GLY:HA2	2:J:184:TRP:CZ3	2.41	0.56
2:J:264:LEU:HD12	2:J:264:LEU:O	2.05	0.56
2:D:223:ARG:HG3	2:D:223:ARG:HH11	1.70	0.56
2:B:323:PHE:CD2	2:B:349:MET:HB2	2.41	0.56
2:H:301:HIS:CD2	2:H:393:GLY:HA2	2.37	0.56
2:H:308:VAL:O	2:H:355:ASN:HA	2.06	0.56
2:B:288:ARG:HD3	2:B:335:THR:HG23	1.88	0.56
2:L:120:LEU:HD12	2:L:120:LEU:O	2.06	0.55
2:B:140:VAL:HG12	2:B:141:ASP:N	2.21	0.55
2:B:145:LEU:O	2:B:148:LEU:HB3	2.06	0.55
2:B:267:GLU:OE2	2:B:269:ARG:HD3	2.06	0.55
2:J:264:LEU:O	2:J:264:LEU:CD1	2.55	0.55
1:I:26:THR:HG22	2:J:174:ALA:HB1	1.89	0.55
2:L:140:VAL:CG1	2:L:145:LEU:HD23	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:LYS:HG2	2:B:267:GLU:CB	2.37	0.55
2:J:377:ARG:HH21	2:J:380:GLY:HA2	1.72	0.55
1:G:27:LEU:HD13	2:H:133:PHE:CE2	2.41	0.55
2:L:123:ARG:HH11	2:L:161:ASP:HB2	1.71	0.55
2:J:281:ILE:HD12	2:J:281:ILE:C	2.26	0.55
2:L:64:THR:HG22	2:L:81:CYS:SG	2.46	0.55
2:L:97:GLN:CD	2:L:97:GLN:N	2.59	0.55
2:L:142:ASP:OD1	2:L:142:ASP:C	2.45	0.55
2:L:294:LYS:HB3	2:L:297:THR:HG21	1.88	0.55
2:F:123:ARG:HH11	2:F:161:ASP:HB2	1.72	0.55
2:H:142:ASP:OD1	2:H:142:ASP:C	2.45	0.55
2:J:171:ARG:O	2:J:187:LYS:HE2	2.07	0.55
2:B:62:ILE:HD12	2:B:63:ASN:H	1.71	0.55
2:F:112:MET:HB3	2:F:113:PRO:CD	2.37	0.55
2:L:62:ILE:HG21	2:L:90:ASN:ND2	2.22	0.55
2:B:129:TYR:CE2	2:B:200:PRO:HD2	2.42	0.54
2:D:123:ARG:HH11	2:D:161:ASP:HB2	1.71	0.54
2:F:237:LYS:HG3	2:F:267:GLU:HB2	1.89	0.54
2:J:244:ILE:N	2:J:244:ILE:HD12	2.23	0.54
2:H:129:TYR:CE2	2:H:200:PRO:HD2	2.42	0.54
2:D:281:ILE:HG23	2:D:281:ILE:O	2.06	0.54
2:L:329:GLN:HB3	2:L:336:ASP:HB3	1.88	0.54
1:A:27:LEU:HD22	2:B:133:PHE:CD2	2.43	0.54
2:F:89:LYS:HE2	2:F:309:TYR:CZ	2.43	0.54
2:F:121:LEU:O	2:F:125:VAL:HG22	2.08	0.54
2:F:248:LYS:CG	2:F:249:GLU:N	2.69	0.54
2:J:282:LYS:HB2	2:J:285:GLU:HG3	1.89	0.54
2:B:306:SER:HB2	2:B:387:VAL:O	2.08	0.54
2:D:245:VAL:HG22	2:D:367:ALA:HB2	1.90	0.54
2:D:343:LEU:HB3	2:D:347:VAL:CG2	2.38	0.53
2:F:363:ILE:HG22	2:F:364:HIS:CD2	2.42	0.53
2:J:84:HIS:CD2	2:J:118:HIS:CE1	2.88	0.53
2:J:294:LYS:HB3	2:J:297:THR:HG21	1.90	0.53
2:J:349:MET:O	2:J:349:MET:HG3	2.08	0.53
1:E:11:HIS:CD2	2:F:75:HIS:HD2	2.26	0.53
2:J:97:GLN:H	2:J:97:GLN:CD	2.09	0.53
2:J:142:ASP:OD2	2:J:145:LEU:HG	2.09	0.53
2:H:329:GLN:HB3	2:H:336:ASP:HB3	1.90	0.53
2:B:288:ARG:CD	2:B:335:THR:HG23	2.39	0.53
2:F:216:ASP:OD1	2:H:261:PHE:N	2.42	0.53
2:L:343:LEU:HB3	2:L:347:VAL:CG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:HIS:ND1	2:D:114:GLN:HB2	2.23	0.53
2:J:209:PRO:O	2:J:233:ARG:HG3	2.07	0.53
2:J:327:ARG:HG2	2:J:327:ARG:HH11	1.74	0.53
2:D:142:ASP:HB3	2:D:145:LEU:HG	1.90	0.53
2:H:243:GLU:OE1	2:H:295:PRO:HA	2.09	0.53
2:J:172:GLY:HA2	2:J:184:TRP:HZ3	1.74	0.53
2:L:140:VAL:HG12	2:L:142:ASP:H	1.73	0.53
2:F:262:ARG:CD	2:H:283:ARG:HH12	2.22	0.52
2:L:305:GLU:HB3	2:L:390:LYS:HG2	1.91	0.52
2:L:329:GLN:HE22	2:L:379:GLY:H	1.57	0.52
2:B:281:ILE:HD11	2:B:285:GLU:HB2	1.90	0.52
2:B:288:ARG:HD3	2:B:335:THR:CG2	2.39	0.52
2:J:343:LEU:HB3	2:J:347:VAL:HG23	1.90	0.52
2:F:72:PRO:HB3	2:J:223:ARG:NH2	2.24	0.52
2:H:142:ASP:OD1	2:H:144:GLU:N	2.43	0.52
2:D:112:MET:HB3	2:D:113:PRO:HD2	1.92	0.52
2:L:323:PHE:CD2	2:L:349:MET:HB3	2.45	0.52
2:J:230:ARG:HH11	2:J:230:ARG:CB	2.23	0.52
2:B:308:VAL:O	2:B:355:ASN:HA	2.09	0.52
2:F:313:LYS:HD2	2:F:319:HIS:CD2	2.44	0.52
2:B:305:GLU:HB3	2:B:390:LYS:HG2	1.91	0.52
2:L:306:SER:HB2	2:L:387:VAL:O	2.10	0.52
2:D:210:PHE:H	2:D:294:LYS:HG3	1.75	0.52
2:F:259:GLU:OE1	2:F:262:ARG:NH1	2.43	0.52
2:F:344:PRO:O	2:F:347:VAL:HG22	2.10	0.52
2:D:308:VAL:O	2:D:355:ASN:HA	2.10	0.52
2:H:323:PHE:CD2	2:H:349:MET:HB3	2.44	0.52
2:J:338:THR:HB	2:J:363:ILE:HD12	1.92	0.52
2:F:308:VAL:O	2:F:355:ASN:HA	2.10	0.51
2:H:112:MET:HB3	2:H:113:PRO:CD	2.40	0.51
2:J:99:ASP:HA	6:J:5102:HOH:O	2.10	0.51
2:J:344:PRO:O	2:J:347:VAL:HG22	2.11	0.51
2:D:305:GLU:HB3	2:D:390:LYS:HG2	1.92	0.51
2:B:324:LYS:NZ	2:B:343:LEU:HB2	2.25	0.51
2:D:200:PRO:HA	6:D:2108:HOH:O	2.11	0.51
1:I:39:TYR:CG	1:I:39:TYR:O	2.64	0.51
2:L:238:VAL:HG23	2:L:266:ASP:O	2.10	0.51
2:B:294:LYS:HB3	2:B:297:THR:CG2	2.41	0.51
2:F:217:VAL:HG21	2:F:286:ILE:CG2	2.41	0.51
2:L:265:LEU:HD23	2:L:265:LEU:N	2.26	0.51
2:H:87:TYR:O	2:H:91:MET:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:230:ARG:HH11	2:L:230:ARG:CB	2.10	0.51
2:B:89:LYS:HE2	2:B:309:TYR:OH	2.10	0.51
2:B:123:ARG:HH11	2:B:161:ASP:HB2	1.76	0.51
2:H:306:SER:HB2	2:H:387:VAL:O	2.11	0.51
2:B:237:LYS:HG2	2:B:267:GLU:HB3	1.93	0.50
2:D:116:ARG:HD2	6:D:2034:HOH:O	2.11	0.50
2:D:313:LYS:HD2	2:D:319:HIS:CD2	2.46	0.50
2:H:301:HIS:HD2	2:H:393:GLY:CA	2.24	0.50
2:F:214:ILE:HD12	2:H:261:PHE:CE2	2.47	0.50
2:B:64:THR:HG23	2:B:90:ASN:HD21	1.76	0.50
2:H:248:LYS:NZ	2:H:285:GLU:HA	2.25	0.50
2:L:244:ILE:N	2:L:244:ILE:HD12	2.26	0.50
2:H:236:ILE:HG23	2:H:236:ILE:O	2.11	0.50
2:J:171:ARG:HD2	6:J:5043:HOH:O	2.12	0.50
2:B:64:THR:CG2	2:B:90:ASN:HD21	2.24	0.50
2:D:142:ASP:HB3	2:D:145:LEU:CG	2.41	0.50
2:D:155:GLU:O	2:D:159:GLN:HG3	2.10	0.50
2:F:62:ILE:O	2:F:62:ILE:CG2	2.59	0.50
2:D:377:ARG:HH21	2:D:380:GLY:HA2	1.76	0.50
2:J:261:PHE:HZ	2:L:286:ILE:HG22	1.76	0.50
2:D:144:GLU:O	2:D:148:LEU:HD22	2.11	0.50
2:L:64:THR:CG2	2:L:90:ASN:HD21	2.24	0.50
2:B:286:ILE:O	2:D:262:ARG:NH1	2.44	0.50
2:B:356:ILE:HD12	2:B:357:LYS:N	2.24	0.50
2:J:123:ARG:HH11	2:J:161:ASP:HB2	1.77	0.50
2:D:279:ARG:HB2	2:D:279:ARG:CZ	2.41	0.50
2:F:142:ASP:HB2	2:F:145:LEU:CG	2.41	0.50
2:J:306:SER:HB2	2:J:387:VAL:O	2.12	0.50
2:L:308:VAL:O	2:L:355:ASN:HA	2.11	0.50
2:B:74:ARG:HD3	6:B:1059:HOH:O	2.11	0.49
2:D:344:PRO:O	2:D:347:VAL:HG22	2.12	0.49
2:D:147:GLU:O	2:D:151:MET:HG3	2.12	0.49
1:I:11:HIS:CD2	2:J:75:HIS:HD2	2.30	0.49
2:J:281:ILE:HD13	2:J:285:GLU:HB2	1.93	0.49
2:B:159:GLN:HB3	2:B:160:TYR:CD1	2.47	0.49
2:J:308:VAL:O	2:J:355:ASN:HA	2.12	0.49
2:B:243:GLU:HG3	2:B:295:PRO:HA	1.93	0.49
2:F:166:ASP:HB3	6:F:3066:HOH:O	2.11	0.49
2:J:82:PRO:HD3	5:J:5888:TAC:C9	2.42	0.49
2:B:237:LYS:HB2	2:B:237:LYS:NZ	2.28	0.49
2:D:282:LYS:HB2	2:D:285:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:176:LYS:HB3	2:F:184:TRP:CD1	2.48	0.49
2:F:261:PHE:CE2	2:H:288:ARG:HA	2.47	0.49
2:L:171:ARG:O	2:L:187:LYS:HE2	2.12	0.49
2:B:261:PHE:HB3	2:D:288:ARG:HH11	1.78	0.49
1:E:39:TYR:OH	2:J:264:LEU:CA	2.61	0.49
2:H:262:ARG:HH11	2:H:262:ARG:HB2	1.78	0.49
2:F:214:ILE:O	2:F:214:ILE:CG1	2.60	0.49
2:F:305:GLU:HB3	2:F:390:LYS:HG2	1.94	0.49
2:J:261:PHE:HA	2:L:216:ASP:OD1	2.12	0.49
1:G:11:HIS:CD2	2:H:75:HIS:HD2	2.31	0.49
1:A:19:HIS:ND1	2:B:114:GLN:HB2	2.27	0.48
2:B:338:THR:HG22	2:B:339:GLY:N	2.28	0.48
2:D:225:THR:OG1	2:D:281:ILE:O	2.25	0.48
2:D:260:MET:HE2	2:D:265:LEU:HD11	1.93	0.48
2:B:321:PRO:HB2	2:B:349:MET:HG3	1.95	0.48
2:F:262:ARG:HH11	2:H:283:ARG:NH2	2.07	0.48
1:I:25:THR:HG23	6:J:5018:HOH:O	2.13	0.48
1:K:19:HIS:HA	2:L:114:GLN:HB2	1.95	0.48
2:F:214:ILE:HD12	2:H:261:PHE:CZ	2.48	0.48
2:F:238:VAL:HG23	2:F:266:ASP:O	2.13	0.48
2:F:241:GLU:HB3	2:F:252:LYS:HE3	1.95	0.48
2:B:347:VAL:HG23	2:B:347:VAL:O	2.13	0.48
2:F:251:GLN:CD	2:F:281:ILE:HD11	2.34	0.48
2:H:342:GLU:HB2	2:H:359:VAL:HB	1.96	0.48
2:L:243:GLU:HG3	2:L:295:PRO:HA	1.96	0.48
2:B:112:MET:HB3	2:B:113:PRO:CD	2.44	0.48
2:H:343:LEU:HB3	2:H:347:VAL:HG23	1.96	0.48
2:B:329:GLN:NE2	2:B:377:ARG:CB	2.76	0.48
2:F:343:LEU:HD13	2:F:347:VAL:HG23	1.95	0.48
2:H:227:VAL:HG21	2:H:292:LEU:HD22	1.96	0.48
2:B:84:HIS:CD2	2:B:118:HIS:HE1	2.32	0.48
2:F:144:GLU:HA	2:F:144:GLU:OE2	2.12	0.48
2:H:142:ASP:HB3	2:H:145:LEU:HD12	1.96	0.48
1:I:26:THR:HG22	2:J:174:ALA:CB	2.43	0.48
2:L:126:GLY:O	2:L:128:PRO:HD3	2.14	0.48
2:D:140:VAL:HG12	2:D:141:ASP:N	2.29	0.48
2:F:294:LYS:HB3	2:F:297:THR:HG21	1.95	0.48
2:D:238:VAL:HG23	2:D:266:ASP:O	2.14	0.47
2:J:230:ARG:HH12	2:J:273:ASN:HD21	1.62	0.47
2:J:288:ARG:HA	2:L:261:PHE:CZ	2.49	0.47
2:L:133:PHE:CD2	2:L:191:LEU:HD22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:ILE:HD13	2:D:311:LEU:CD2	2.43	0.47
2:L:230:ARG:HH22	2:L:273:ASN:HB2	1.77	0.47
2:D:142:ASP:HB3	2:D:145:LEU:HD12	1.95	0.47
2:F:289:GLY:O	2:F:366:ILE:HD11	2.15	0.47
1:K:11:HIS:CD2	2:L:75:HIS:HD2	2.31	0.47
2:L:327:ARG:HG2	2:L:338:THR:CG2	2.44	0.47
2:D:294:LYS:HB3	2:D:294:LYS:HZ2	1.77	0.47
2:L:344:PRO:O	2:L:347:VAL:HG22	2.14	0.47
2:H:294:LYS:HB3	2:H:297:THR:HG21	1.95	0.47
2:J:64:THR:HG22	2:J:81:CYS:SG	2.55	0.47
2:B:351:MET:HB2	2:B:354:ASP:OD2	2.14	0.47
2:D:132:VAL:HB	2:D:169:ILE:HG12	1.96	0.47
2:F:150:GLU:OE2	2:F:171:ARG:NH2	2.48	0.47
2:F:281:ILE:HD13	2:F:281:ILE:HA	1.77	0.47
2:F:306:SER:HB2	2:F:387:VAL:O	2.15	0.47
2:J:326:TYR:OH	2:J:378:GLU:OE2	2.25	0.47
2:L:267:GLU:OE2	2:L:269:ARG:NH2	2.47	0.47
2:L:377:ARG:HH21	2:L:380:GLY:HA2	1.80	0.47
1:A:32:THR:HG22	1:A:33:THR:N	2.30	0.47
2:F:266:ASP:OD1	2:F:266:ASP:N	2.40	0.47
2:H:97:GLN:C	2:H:97:GLN:CD	2.73	0.47
2:B:220:ILE:HG13	2:B:223:ARG:HB2	1.97	0.47
1:E:37:LYS:NZ	2:F:185:GLU:OE2	2.35	0.47
2:F:262:ARG:HA	2:F:262:ARG:NH1	2.28	0.47
2:H:248:LYS:NZ	2:H:285:GLU:O	2.41	0.47
2:H:323:PHE:HD2	2:H:349:MET:HB3	1.80	0.47
2:J:87:TYR:O	2:J:91:MET:HG3	2.14	0.46
2:J:89:LYS:HE2	2:J:309:TYR:OH	2.14	0.46
2:J:338:THR:HG22	2:J:339:GLY:N	2.31	0.46
2:L:152:GLU:HB3	6:L:6014:HOH:O	2.14	0.46
2:L:259:GLU:HG2	2:L:260:MET:N	2.30	0.46
2:B:61:THR:O	2:B:61:THR:HG22	2.15	0.46
2:F:142:ASP:CB	2:F:145:LEU:HG	2.42	0.46
2:J:62:ILE:HD12	2:J:90:ASN:HD21	1.79	0.46
1:K:19:HIS:ND1	2:L:114:GLN:HB2	2.30	0.46
1:K:37:LYS:NZ	2:L:185:GLU:OE2	2.46	0.46
2:B:142:ASP:HB2	2:B:145:LEU:HD12	1.95	0.46
2:H:281:ILE:HD11	2:H:285:GLU:OE1	2.15	0.46
2:J:129:TYR:CE2	2:J:200:PRO:HD2	2.50	0.46
2:L:237:LYS:HE2	2:L:267:GLU:OE1	2.15	0.46
2:B:84:HIS:CD2	2:B:118:HIS:CE1	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:LEU:HD23	2:B:134:LEU:HA	1.73	0.46
2:B:206:ILE:H	2:B:206:ILE:HG12	1.41	0.46
2:B:343:LEU:HB3	2:B:347:VAL:CG2	2.45	0.46
2:H:214:ILE:HG23	2:H:227:VAL:HB	1.96	0.46
2:F:261:PHE:CA	2:H:216:ASP:OD1	2.64	0.46
2:F:210:PHE:CE1	2:F:236:ILE:HB	2.51	0.46
2:J:220:ILE:HD11	2:L:218:PHE:CE1	2.50	0.46
2:B:283:ARG:HG2	2:B:283:ARG:O	2.14	0.46
2:F:176:LYS:HB3	2:F:184:TRP:HD1	1.80	0.46
2:L:133:PHE:HD2	2:L:191:LEU:HD22	1.81	0.46
2:L:331:TYR:CD1	2:L:377:ARG:NH1	2.83	0.46
2:D:236:ILE:HG23	2:D:236:ILE:O	2.16	0.46
1:E:38:THR:HG22	1:E:39:TYR:CE1	2.51	0.46
2:J:261:PHE:C	2:J:261:PHE:CD1	2.89	0.46
2:J:279:ARG:NH1	2:J:279:ARG:CG	2.78	0.46
2:D:142:ASP:CG	2:D:145:LEU:HG	2.36	0.46
5:H:4888:TAC:O1	5:H:4888:TAC:N21	2.43	0.46
1:I:32:THR:CG2	1:I:33:THR:N	2.76	0.45
2:D:230:ARG:NH1	2:D:273:ASN:HD22	2.13	0.45
2:J:142:ASP:CG	2:J:145:LEU:HG	2.37	0.45
2:J:323:PHE:CD2	2:J:349:MET:HB3	2.52	0.45
2:B:62:ILE:HD11	2:B:90:ASN:ND2	2.30	0.45
2:B:140:VAL:HG12	2:B:142:ASP:H	1.81	0.45
2:D:288:ARG:HE	2:D:335:THR:HG23	1.81	0.45
2:H:62:ILE:O	2:H:62:ILE:CG2	2.65	0.45
2:H:116:ARG:HH21	2:H:159:GLN:HE22	1.65	0.45
2:H:366:ILE:HD13	2:H:366:ILE:HA	1.79	0.45
2:D:344:PRO:HD2	2:D:347:VAL:HG21	1.97	0.45
2:F:126:GLY:O	2:F:128:PRO:HD3	2.15	0.45
2:D:64:THR:HG22	2:D:81:CYS:SG	2.56	0.45
2:L:129:TYR:CE2	2:L:200:PRO:HD2	2.51	0.45
2:D:140:VAL:HG12	2:D:142:ASP:H	1.82	0.45
2:H:282:LYS:O	2:H:284:GLU:N	2.50	0.45
2:D:108:THR:OG1	2:D:109:ASP:OD1	2.35	0.45
2:D:129:TYR:CE2	2:D:200:PRO:HD2	2.52	0.45
2:H:212:LEU:HD12	2:H:230:ARG:O	2.17	0.45
2:H:282:LYS:C	2:H:284:GLU:N	2.69	0.45
2:J:261:PHE:C	2:J:261:PHE:HD1	2.21	0.45
2:J:305:GLU:HB3	2:J:390:LYS:HG2	1.99	0.45
2:L:227:VAL:HG21	2:L:292:LEU:HD22	1.98	0.45
2:F:150:GLU:O	2:F:154:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:294:LYS:HB2	2:F:294:LYS:NZ	2.32	0.45
2:H:150:GLU:O	2:H:154:ARG:HG3	2.16	0.45
2:D:133:PHE:CD2	2:D:191:LEU:HD22	2.52	0.45
1:E:39:TYR:CE2	2:F:72:PRO:HG3	2.51	0.45
2:F:282:LYS:HB3	2:F:285:GLU:HG3	1.99	0.45
2:H:390:LYS:HB2	2:H:390:LYS:NZ	2.32	0.45
2:D:281:ILE:O	2:D:281:ILE:CG2	2.65	0.44
2:H:237:LYS:CD	2:H:267:GLU:HB3	2.47	0.44
2:F:62:ILE:HA	6:F:3048:HOH:O	2.16	0.44
2:F:343:LEU:HB3	2:F:344:PRO:HD2	1.98	0.44
1:I:39:TYR:O	1:I:39:TYR:CD2	2.70	0.44
2:J:61:THR:O	2:J:61:THR:HG22	2.16	0.44
2:J:327:ARG:HG2	2:J:327:ARG:NH1	2.32	0.44
2:L:111:PRO:C	2:L:112:MET:HG2	2.36	0.44
2:L:324:LYS:HG2	2:L:343:LEU:HD12	1.99	0.44
1:E:26:THR:HG23	4:F:3999:GDP:O1A	2.17	0.44
2:H:305:GLU:HB3	2:H:390:LYS:HG2	1.99	0.44
2:H:123:ARG:HH11	2:H:161:ASP:HB2	1.82	0.44
2:H:281:ILE:CD1	2:H:285:GLU:OE1	2.66	0.44
1:A:19:HIS:HA	2:B:114:GLN:HB2	1.99	0.44
2:F:277:LEU:HD22	2:F:277:LEU:HA	1.80	0.44
2:B:62:ILE:HD12	2:B:63:ASN:N	2.33	0.44
2:D:116:ARG:NH2	2:D:156:LEU:HD13	2.33	0.44
2:H:115:THR:O	2:H:119:ILE:HG13	2.18	0.44
2:F:209:PRO:O	2:F:233:ARG:HG3	2.17	0.44
2:H:220:ILE:HD12	2:H:223:ARG:HB2	2.00	0.44
2:D:142:ASP:HB3	2:D:145:LEU:CD1	2.48	0.44
2:H:288:ARG:CG	2:H:335:THR:HG23	2.47	0.44
2:L:356:ILE:HD12	2:L:357:LYS:N	2.30	0.44
2:B:261:PHE:HA	2:D:216:ASP:OD1	2.17	0.43
2:F:132:VAL:HB	2:F:169:ILE:HG12	1.98	0.43
2:H:282:LYS:C	2:H:284:GLU:H	2.20	0.43
2:L:62:ILE:CG2	2:L:90:ASN:ND2	2.81	0.43
2:L:241:GLU:HG3	2:L:253:SER:O	2.17	0.43
2:L:256:THR:CG2	2:L:279:ARG:HB2	2.48	0.43
2:D:149:VAL:O	2:D:153:VAL:HG23	2.18	0.43
2:J:116:ARG:NH2	2:J:159:GLN:OE1	2.51	0.43
2:J:171:ARG:NH1	6:J:5043:HOH:O	2.39	0.43
2:J:323:PHE:CD1	2:J:323:PHE:N	2.85	0.43
2:J:331:TYR:CD1	2:J:377:ARG:NH1	2.84	0.43
2:B:111:PRO:C	2:B:112:MET:HG2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:ASP:O	2:F:145:LEU:N	2.51	0.43
2:F:214:ILE:CG1	2:F:290:GLN:O	2.51	0.43
2:F:282:LYS:C	2:F:284:GLU:N	2.72	0.43
2:L:263:LYS:H	2:L:263:LYS:HG3	1.58	0.43
2:B:89:LYS:HE2	2:B:309:TYR:CZ	2.53	0.43
2:J:121:LEU:O	2:J:125:VAL:HG22	2.19	0.43
2:L:189:LEU:HD23	2:L:189:LEU:HA	1.78	0.43
2:B:82:PRO:HD3	5:B:1888:TAC:C9	2.48	0.43
2:F:125:VAL:HG12	2:F:387:VAL:HG11	2.00	0.43
2:F:326:TYR:OH	2:F:378:GLU:OE2	2.23	0.43
2:H:292:LEU:HD12	2:H:292:LEU:HA	1.86	0.43
2:L:223:ARG:HE	2:L:223:ARG:HB2	1.59	0.43
2:D:176:LYS:HD3	2:D:176:LYS:HA	1.81	0.43
2:D:210:PHE:CE1	2:D:236:ILE:HB	2.54	0.43
2:D:260:MET:HE3	2:D:265:LEU:HD11	1.99	0.43
2:H:132:VAL:HB	2:H:169:ILE:HG12	2.00	0.43
2:J:351:MET:HB2	2:J:354:ASP:OD2	2.19	0.43
2:L:142:ASP:CG	2:L:145:LEU:H	2.21	0.43
2:B:175:LEU:HB2	4:B:1999:GDP:C5	2.54	0.43
2:B:344:PRO:HD2	2:B:347:VAL:HG21	2.00	0.43
2:F:245:VAL:HB	2:F:250:THR:HG22	2.00	0.43
2:F:263:LYS:HB2	2:F:263:LYS:HE3	1.83	0.43
2:L:279:ARG:HG3	2:L:279:ARG:NH1	2.30	0.43
2:B:176:LYS:HB3	2:B:184:TRP:CD1	2.54	0.43
2:F:112:MET:HB3	2:F:113:PRO:HD2	2.00	0.43
2:F:251:GLN:NE2	2:F:252:LYS:O	2.52	0.43
2:F:261:PHE:N	2:H:216:ASP:OD1	2.51	0.43
2:H:97:GLN:NE2	2:H:98:MET:N	2.67	0.43
2:H:288:ARG:HG2	2:H:335:THR:HG23	2.01	0.43
1:I:14:VAL:O	2:J:78:HIS:HA	2.19	0.43
2:D:142:ASP:CB	2:D:145:LEU:HG	2.49	0.43
2:D:210:PHE:HA	2:D:233:ARG:O	2.18	0.43
2:F:133:PHE:CD2	2:F:191:LEU:HD22	2.54	0.43
2:J:132:VAL:HB	2:J:169:ILE:HG12	1.99	0.43
2:J:248:LYS:HE3	2:J:248:LYS:HB2	1.86	0.43
1:A:27:LEU:HD22	2:B:133:PHE:HD2	1.83	0.43
1:C:24:LYS:HB2	1:C:24:LYS:HE2	1.86	0.43
2:D:220:ILE:CG2	2:D:223:ARG:HB3	2.49	0.43
2:F:89:LYS:HE2	2:F:309:TYR:OH	2.18	0.43
2:H:126:GLY:O	2:H:128:PRO:HD3	2.19	0.43
2:L:112:MET:HB3	2:L:113:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:97:GLN:N	2:L:97:GLN:OE1	2.40	0.42
2:B:292:LEU:HA	2:B:292:LEU:HD12	1.85	0.42
2:J:288:ARG:HG2	2:J:335:THR:CG2	2.44	0.42
2:L:312:SER:OG	2:L:315:GLU:HG3	2.19	0.42
2:B:62:ILE:HD12	2:B:62:ILE:HA	1.80	0.42
2:D:126:GLY:O	2:D:128:PRO:HD3	2.19	0.42
2:F:216:ASP:OD1	2:H:261:PHE:HA	2.20	0.42
2:F:248:LYS:HD2	2:F:248:LYS:HA	1.71	0.42
2:H:112:MET:HB3	2:H:113:PRO:HD2	2.00	0.42
2:J:336:ASP:OD1	2:J:377:ARG:HD3	2.18	0.42
2:J:347:VAL:HG23	2:J:347:VAL:O	2.18	0.42
2:L:283:ARG:O	2:L:283:ARG:HG2	2.18	0.42
2:D:66:HIS:HE1	2:D:68:GLU:OE2	2.01	0.42
2:D:87:TYR:O	2:D:91:MET:HG3	2.19	0.42
1:E:19:HIS:CE1	2:F:113:PRO:HD2	2.55	0.42
2:J:210:PHE:HA	2:J:233:ARG:O	2.19	0.42
2:J:338:THR:HB	2:J:363:ILE:HD11	1.99	0.42
1:K:35:LEU:HD23	1:K:35:LEU:HA	1.86	0.42
2:L:220:ILE:HG13	2:L:226:VAL:HG21	2.01	0.42
2:B:60:ILE:HD12	2:B:93:THR:HG21	2.01	0.42
2:D:227:VAL:HG21	2:D:292:LEU:HD22	2.01	0.42
2:F:140:VAL:HG13	2:F:145:LEU:HD12	2.02	0.42
2:J:210:PHE:CE1	2:J:236:ILE:HB	2.55	0.42
2:D:230:ARG:HH12	2:D:273:ASN:HD22	1.67	0.42
2:H:111:PRO:C	2:H:112:MET:HG2	2.40	0.42
2:H:282:LYS:HZ3	2:H:282:LYS:HB2	1.84	0.42
2:L:132:VAL:HB	2:L:169:ILE:HG12	2.02	0.42
2:D:62:ILE:HD11	2:D:90:ASN:ND2	2.34	0.42
2:H:243:GLU:HG3	2:H:295:PRO:HG3	2.01	0.42
2:L:89:LYS:O	2:L:93:THR:HG23	2.20	0.42
2:B:237:LYS:HG2	2:B:267:GLU:HB2	2.02	0.42
2:B:329:GLN:HE21	2:B:377:ARG:CB	2.32	0.42
2:D:331:TYR:CD1	2:D:377:ARG:NH1	2.87	0.42
2:F:129:TYR:CE2	2:F:200:PRO:HD2	2.54	0.42
2:F:227:VAL:HG21	2:F:292:LEU:HD22	2.01	0.42
2:J:112:MET:HB3	2:J:113:PRO:CD	2.50	0.42
2:J:220:ILE:HD11	2:L:218:PHE:CD1	2.55	0.42
2:L:62:ILE:HB	6:L:6048:HOH:O	2.20	0.42
2:D:175:LEU:HB2	4:D:2999:GDP:C5	2.55	0.41
2:F:59:GLY:HA2	6:F:3025:HOH:O	2.19	0.41
2:H:210:PHE:HA	2:H:233:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:336:ASP:OD1	2:H:377:ARG:HD3	2.19	0.41
2:L:66:HIS:HE1	2:L:68:GLU:OE2	2.03	0.41
2:L:363:ILE:HG22	2:L:364:HIS:CG	2.55	0.41
2:D:210:PHE:CZ	2:D:236:ILE:HB	2.55	0.41
1:E:39:TYR:CE2	2:F:72:PRO:CG	3.04	0.41
2:F:261:PHE:CZ	2:H:288:ARG:HA	2.54	0.41
2:L:343:LEU:HB3	2:L:347:VAL:HG23	2.02	0.41
2:B:87:TYR:O	2:B:91:MET:HG3	2.21	0.41
2:B:216:ASP:OD1	2:D:261:PHE:HA	2.21	0.41
2:D:216:ASP:OD2	2:D:218:PHE:CZ	2.73	0.41
2:F:84:HIS:CD2	2:F:118:HIS:CE1	3.07	0.41
2:F:176:LYS:HB2	2:F:184:TRP:CD1	2.55	0.41
2:F:225:THR:OG1	2:F:281:ILE:O	2.30	0.41
2:H:116:ARG:HH21	2:H:159:GLN:NE2	2.18	0.41
2:B:261:PHE:CD2	2:D:288:ARG:HG2	2.55	0.41
2:B:261:PHE:CB	2:D:288:ARG:HH11	2.32	0.41
5:D:2888:TAC:H432	5:D:2888:TAC:O1C	2.19	0.41
2:F:262:ARG:CD	2:H:283:ARG:NH1	2.84	0.41
2:H:116:ARG:NH2	2:H:156:LEU:HD13	2.35	0.41
2:H:171:ARG:O	2:H:187:LYS:HE2	2.20	0.41
2:L:317:GLY:HA3	6:L:6038:HOH:O	2.20	0.41
2:B:288:ARG:HG2	2:B:335:THR:HG23	2.02	0.41
2:D:345:GLU:OE2	2:H:163:PRO:CD	2.67	0.41
2:F:62:ILE:O	2:F:62:ILE:HG22	2.20	0.41
2:F:244:ILE:HD13	2:F:292:LEU:HD11	2.00	0.41
2:H:97:GLN:NE2	2:H:98:MET:C	2.74	0.41
2:H:206:ILE:H	2:H:206:ILE:HG12	1.25	0.41
1:A:14:VAL:O	2:B:78:HIS:HA	2.21	0.41
2:F:87:TYR:O	2:F:91:MET:HG3	2.21	0.41
2:F:347:VAL:HG23	2:F:347:VAL:O	2.20	0.41
2:H:278:LEU:HA	2:H:278:LEU:HD23	1.83	0.41
2:L:178:LEU:HD12	2:L:178:LEU:HA	1.91	0.41
2:B:120:LEU:HD22	2:B:160:TYR:HE2	1.86	0.41
2:D:347:VAL:O	2:D:347:VAL:HG23	2.20	0.41
2:B:140:VAL:HG12	2:B:141:ASP:H	1.84	0.41
2:B:323:PHE:CD1	2:B:323:PHE:N	2.89	0.41
2:D:338:THR:HG22	2:D:339:GLY:N	2.36	0.41
2:F:338:THR:HG22	2:F:339:GLY:N	2.35	0.41
2:H:230:ARG:HG3	2:H:273:ASN:OD1	2.21	0.41
2:H:240:GLU:CD	6:H:4026:HOH:O	2.59	0.41
1:I:30:ALA:HA	2:J:178:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:62:ILE:O	2:J:62:ILE:CG2	2.69	0.41
2:L:151:MET:O	2:L:155:GLU:HG3	2.20	0.41
2:D:209:PRO:O	2:D:233:ARG:HG3	2.21	0.40
2:H:175:LEU:HB2	4:H:4999:GDP:C5	2.57	0.40
2:H:369:ASP:OD1	2:H:369:ASP:N	2.53	0.40
1:I:39:TYR:CD2	1:I:39:TYR:C	2.95	0.40
2:L:301:HIS:HB3	2:L:393:GLY:OXT	2.22	0.40
2:L:363:ILE:HG22	2:L:364:HIS:ND1	2.36	0.40
2:B:82:PRO:HG2	2:B:86:ASP:OD2	2.20	0.40
1:C:19:HIS:CE1	2:D:113:PRO:HD2	2.57	0.40
2:J:288:ARG:CG	2:J:335:THR:HG23	2.43	0.40
2:B:64:THR:HG22	2:B:81:CYS:SG	2.61	0.40
2:H:209:PRO:HB3	2:H:297:THR:HG21	2.03	0.40
2:B:243:GLU:CD	2:B:295:PRO:HA	2.42	0.40
2:B:326:TYR:OH	2:B:378:GLU:OE2	2.23	0.40
2:D:323:PHE:CD1	2:D:323:PHE:N	2.89	0.40
2:L:167:THR:HA	2:L:168:PRO:HD3	1.95	0.40
1:C:19:HIS:HA	2:D:114:GLN:HB2	2.03	0.40
2:H:237:LYS:HD2	2:H:267:GLU:HB3	2.04	0.40
5:L:6888:TAC:H422	5:L:6888:TAC:O1C	2.22	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	31/37 (84%)	29 (94%)	2 (6%)	0	100   100
1	C	31/37 (84%)	29 (94%)	2 (6%)	0	100   100
1	E	31/37 (84%)	30 (97%)	1 (3%)	0	100   100
1	G	31/37 (84%)	30 (97%)	1 (3%)	0	100   100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	31/37 (84%)	29 (94%)	2 (6%)	0	100	100
1	K	31/37 (84%)	29 (94%)	2 (6%)	0	100	100
2	B	333/335 (99%)	316 (95%)	15 (4%)	2 (1%)	25	56
2	D	333/335 (99%)	315 (95%)	16 (5%)	2 (1%)	25	56
2	F	333/335 (99%)	315 (95%)	14 (4%)	4 (1%)	13	39
2	H	333/335 (99%)	312 (94%)	17 (5%)	4 (1%)	13	39
2	J	333/335 (99%)	316 (95%)	16 (5%)	1 (0%)	41	72
2	L	333/335 (99%)	312 (94%)	19 (6%)	2 (1%)	25	56
All	All	2184/2232 (98%)	2062 (94%)	107 (5%)	15 (1%)	22	53

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	283	ARG
2	B	280	GLY
2	F	247	ILE
2	F	333	ARG
2	H	221	SER
2	H	247	ILE
2	H	280	GLY
2	B	247	ILE
2	D	247	ILE
2	J	247	ILE
2	L	247	ILE
2	F	280	GLY
2	D	280	GLY
2	F	163	PRO
2	L	280	GLY

### 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	26/27 (96%)	24 (92%)	2 (8%)	13	35
1	C	26/27 (96%)	24 (92%)	2 (8%)	13	35
1	E	26/27 (96%)	25 (96%)	1 (4%)	33	67
1	G	26/27 (96%)	26 (100%)	0	100	100
1	I	26/27 (96%)	24 (92%)	2 (8%)	13	35
1	K	26/27 (96%)	26 (100%)	0	100	100
2	B	280/280 (100%)	253 (90%)	27 (10%)	8	24
2	D	280/280 (100%)	256 (91%)	24 (9%)	10	30
2	F	280/280 (100%)	254 (91%)	26 (9%)	9	26
2	H	280/280 (100%)	256 (91%)	24 (9%)	10	30
2	J	280/280 (100%)	259 (92%)	21 (8%)	13	37
2	L	280/280 (100%)	259 (92%)	21 (8%)	13	37
All	All	1836/1842 (100%)	1686 (92%)	150 (8%)	11	33

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	32	THR
2	B	61	THR
2	B	62	ILE
2	B	65	SER
2	B	67	VAL
2	B	70	ASP
2	B	79	VAL
2	B	116	ARG
2	B	117	GLU
2	B	139	MET
2	B	159	GLN
2	B	206	ILE
2	B	245	VAL
2	B	248	LYS
2	B	249	GLU
2	B	261	PHE
2	B	277	LEU
2	B	282	LYS
2	B	284	GLU
2	B	294	LYS
2	B	329	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	335	THR
2	B	349	MET
2	B	356	ILE
2	B	363	ILE
2	B	369	ASP
2	B	381	ARG
2	B	390	LYS
1	C	21	ASP
1	C	32	THR
2	D	60	ILE
2	D	62	ILE
2	D	65	SER
2	D	79	VAL
2	D	97	GLN
2	D	148	LEU
2	D	152	GLU
2	D	206	ILE
2	D	221	SER
2	D	230	ARG
2	D	245	VAL
2	D	251	GLN
2	D	261	PHE
2	D	264	LEU
2	D	266	ASP
2	D	269	ARG
2	D	279	ARG
2	D	285	GLU
2	D	327	ARG
2	D	335	THR
2	D	349	MET
2	D	369	ASP
2	D	381	ARG
2	D	390	LYS
1	E	8	THR
2	F	62	ILE
2	F	65	SER
2	F	79	VAL
2	F	97	GLN
2	F	120	LEU
2	F	121	LEU
2	F	139	MET
2	F	147	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	148	LEU
2	F	206	ILE
2	F	219	SER
2	F	221	SER
2	F	230	ARG
2	F	232	GLU
2	F	245	VAL
2	F	249	GLU
2	F	259	GLU
2	F	262	ARG
2	F	263	LYS
2	F	267	GLU
2	F	277	LEU
2	F	281	ILE
2	F	335	THR
2	F	349	MET
2	F	366	ILE
2	F	390	LYS
2	H	60	ILE
2	H	62	ILE
2	H	65	SER
2	H	79	VAL
2	H	121	LEU
2	H	139	MET
2	H	143	GLU
2	H	206	ILE
2	H	208	LYS
2	H	232	GLU
2	H	237	LYS
2	H	245	VAL
2	H	250	THR
2	H	259	GLU
2	H	262	ARG
2	H	264	LEU
2	H	266	ASP
2	H	282	LYS
2	H	287	GLU
2	H	335	THR
2	H	345	GLU
2	H	369	ASP
2	H	381	ARG
2	H	390	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	21	ASP
1	I	32	THR
2	J	61	THR
2	J	62	ILE
2	J	65	SER
2	J	70	ASP
2	J	79	VAL
2	J	97	GLN
2	J	117	GLU
2	J	141	ASP
2	J	148	LEU
2	J	206	ILE
2	J	223	ARG
2	J	230	ARG
2	J	232	GLU
2	J	245	VAL
2	J	259	GLU
2	J	261	PHE
2	J	264	LEU
2	J	277	LEU
2	J	281	ILE
2	J	335	THR
2	J	390	LYS
2	L	60	ILE
2	L	62	ILE
2	L	65	SER
2	L	70	ASP
2	L	79	VAL
2	L	97	GLN
2	L	147	GLU
2	L	206	ILE
2	L	245	VAL
2	L	261	PHE
2	L	264	LEU
2	L	266	ASP
2	L	273	ASN
2	L	277	LEU
2	L	288	ARG
2	L	292	LEU
2	L	299	LYS
2	L	335	THR
2	L	356	ILE

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Mol	Chain	Res	Type
2	L	369	ASP
2	L	390	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
2	B	66	HIS
2	B	84	HIS
2	B	90	ASN
2	B	118	HIS
2	B	319	HIS
2	B	329	GLN
1	C	11	HIS
2	D	66	HIS
2	D	84	HIS
2	D	90	ASN
2	D	118	HIS
2	D	251	GLN
2	D	273	ASN
2	D	319	HIS
1	E	11	HIS
2	F	66	HIS
2	F	84	HIS
2	F	97	GLN
2	F	118	HIS
2	F	319	HIS
2	F	329	GLN
1	G	11	HIS
2	H	84	HIS
2	H	90	ASN
2	H	97	GLN
2	H	118	HIS
2	H	159	GLN
2	H	301	HIS
2	H	319	HIS
1	I	11	HIS
2	J	84	HIS
2	J	97	GLN
2	J	118	HIS
2	J	273	ASN
2	J	301	HIS

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Mol	Chain	Res	Type
2	J	319	HIS
2	J	329	GLN
1	K	11	HIS
2	L	66	HIS
2	L	84	HIS
2	L	90	ASN
2	L	118	HIS
2	L	273	ASN
2	L	301	HIS
2	L	319	HIS
2	L	329	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	TAC	J	5888	3	33,35,35	3.04	14 (42%)	42,58,58	1.85	11 (26%)
4	GDP	H	4999	3	24,30,30	1.12	2 (8%)	30,47,47	1.38	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	TAC	H	4888	3	33,35,35	3.22	16 (48%)	42,58,58	1.42	9 (21%)
5	TAC	B	1888	3	33,35,35	3.21	16 (48%)	42,58,58	1.29	6 (14%)
5	TAC	F	3888	3	33,35,35	3.19	16 (48%)	42,58,58	1.28	5 (11%)
4	GDP	F	3999	3	24,30,30	0.99	2 (8%)	30,47,47	1.41	7 (23%)
5	TAC	L	6888	3	33,35,35	3.17	17 (51%)	42,58,58	1.34	7 (16%)
5	TAC	D	2888	3	33,35,35	3.28	16 (48%)	42,58,58	1.23	4 (9%)
4	GDP	D	2999	3	24,30,30	1.11	2 (8%)	30,47,47	1.42	7 (23%)
4	GDP	L	6999	3	24,30,30	1.07	2 (8%)	30,47,47	1.46	7 (23%)
4	GDP	J	5999	3	24,30,30	1.22	4 (16%)	30,47,47	1.34	5 (16%)
4	GDP	B	1999	3	24,30,30	1.15	4 (16%)	30,47,47	1.33	7 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TAC	J	5888	3	-	3/8/74/74	0/4/4/4
4	GDP	H	4999	3	-	2/12/32/32	0/3/3/3
5	TAC	H	4888	3	-	3/8/74/74	0/4/4/4
5	TAC	B	1888	3	-	1/8/74/74	0/4/4/4
5	TAC	F	3888	3	-	0/8/74/74	0/4/4/4
4	GDP	F	3999	3	-	2/12/32/32	0/3/3/3
5	TAC	L	6888	3	-	2/8/74/74	0/4/4/4
5	TAC	D	2888	3	-	0/8/74/74	0/4/4/4
4	GDP	D	2999	3	-	2/12/32/32	0/3/3/3
4	GDP	L	6999	3	-	2/12/32/32	0/3/3/3
4	GDP	J	5999	3	-	2/12/32/32	0/3/3/3
4	GDP	B	1999	3	-	2/12/32/32	0/3/3/3

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	2888	TAC	C1C-C41	10.10	1.62	1.53
5	H	4888	TAC	C1C-C41	9.45	1.61	1.53
5	B	1888	TAC	C1C-C41	8.80	1.61	1.53
5	L	6888	TAC	C1C-C41	8.68	1.61	1.53
5	F	3888	TAC	C1C-C41	8.27	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	3888	TAC	C1B-C12	7.97	1.46	1.36
5	J	5888	TAC	C1C-C41	7.80	1.60	1.53
5	J	5888	TAC	C1B-C12	7.40	1.45	1.36
5	B	1888	TAC	C1B-C12	7.39	1.45	1.36
5	D	2888	TAC	C1B-C12	7.21	1.45	1.36
5	H	4888	TAC	C1B-C12	7.14	1.45	1.36
5	L	6888	TAC	C1B-C12	7.12	1.45	1.36
5	F	3888	TAC	C6-C61	6.68	1.58	1.53
5	L	6888	TAC	C6-C61	6.35	1.57	1.53
5	D	2888	TAC	C6-C61	6.12	1.57	1.53
5	H	4888	TAC	C1C-C12	5.98	1.57	1.52
5	J	5888	TAC	C6-C61	5.57	1.57	1.53
5	D	2888	TAC	C51-C1B	5.47	1.60	1.52
5	H	4888	TAC	C6-C61	5.41	1.57	1.53
5	B	1888	TAC	C51-C1B	5.21	1.60	1.52
5	B	1888	TAC	C6-C61	4.97	1.56	1.53
5	F	3888	TAC	C51-C1B	4.95	1.59	1.52
5	H	4888	TAC	C51-C1B	4.79	1.59	1.52
5	J	5888	TAC	C51-C1B	4.70	1.59	1.52
5	J	5888	TAC	C1C-C12	4.67	1.56	1.52
5	F	3888	TAC	C1C-C12	4.56	1.56	1.52
5	B	1888	TAC	C1C-C12	4.53	1.56	1.52
5	L	6888	TAC	C51-C1B	4.40	1.59	1.52
5	L	6888	TAC	C1C-C12	4.34	1.55	1.52
5	J	5888	TAC	C4-C3	4.21	1.60	1.51
5	B	1888	TAC	C7-C61	4.20	1.45	1.39
5	D	2888	TAC	C4-N4	4.16	1.56	1.47
5	B	1888	TAC	C4-C3	4.03	1.60	1.51
5	J	5888	TAC	C1A-C61	3.77	1.48	1.41
5	D	2888	TAC	C1C-C12	3.69	1.55	1.52
5	L	6888	TAC	C7-C61	3.68	1.44	1.39
5	F	3888	TAC	C4-N4	3.64	1.55	1.47
5	D	2888	TAC	C7-C61	3.53	1.44	1.39
5	L	6888	TAC	C1C-C1	3.45	1.59	1.55
5	H	4888	TAC	C4-C3	3.44	1.58	1.51
5	H	4888	TAC	C7-C61	3.40	1.43	1.39
5	D	2888	TAC	C1A-C61	3.33	1.47	1.41
5	F	3888	TAC	C4-C3	3.29	1.58	1.51
5	J	5888	TAC	C7-C61	3.27	1.43	1.39
5	B	1888	TAC	C1A-C61	3.26	1.47	1.41
5	B	1888	TAC	C4-N4	3.24	1.54	1.47
5	F	3888	TAC	C7-C61	3.22	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1888	TAC	O11-C11	3.22	1.30	1.23
5	F	3888	TAC	C1A-C61	3.20	1.47	1.41
5	L	6888	TAC	C4-C3	3.15	1.58	1.51
5	L	6888	TAC	C9-C10	3.11	1.45	1.39
5	H	4888	TAC	C1C-C1	3.08	1.59	1.55
4	B	1999	GDP	C5-C6	-3.07	1.41	1.47
5	L	6888	TAC	O1-C1	3.05	1.27	1.22
5	H	4888	TAC	C1A-C61	3.04	1.47	1.41
5	L	6888	TAC	C1A-C61	3.04	1.47	1.41
4	H	4999	GDP	C5-C6	-3.03	1.41	1.47
5	D	2888	TAC	C4-C3	3.02	1.58	1.51
5	B	1888	TAC	C1C-C1	2.97	1.59	1.55
5	B	1888	TAC	C9-C10	2.90	1.44	1.39
5	B	1888	TAC	O1-C1	2.88	1.27	1.22
4	J	5999	GDP	C5-C6	-2.84	1.41	1.47
5	H	4888	TAC	O1-C1	2.83	1.27	1.22
5	D	2888	TAC	O11-C11	2.83	1.29	1.23
4	L	6999	GDP	C5-C6	-2.81	1.41	1.47
5	L	6888	TAC	O3-C3	-2.79	1.24	1.33
5	J	5888	TAC	O1-C1	2.77	1.27	1.22
5	J	5888	TAC	O3-C3	-2.76	1.24	1.33
5	B	1888	TAC	C1A-C10	2.71	1.45	1.41
5	H	4888	TAC	O3-C3	-2.69	1.24	1.33
5	D	2888	TAC	O1-C1	2.69	1.27	1.22
4	J	5999	GDP	C8-N7	-2.68	1.30	1.35
5	D	2888	TAC	O3-C3	-2.68	1.24	1.33
5	L	6888	TAC	C4-N4	2.67	1.53	1.47
5	F	3888	TAC	O3-C3	-2.66	1.24	1.33
5	L	6888	TAC	O11-C11	2.65	1.28	1.23
5	H	4888	TAC	O11-C11	2.60	1.28	1.23
5	B	1888	TAC	O3-C3	-2.60	1.25	1.33
4	H	4999	GDP	C8-N7	-2.54	1.30	1.35
4	D	2999	GDP	C5-C6	-2.53	1.42	1.47
4	D	2999	GDP	C8-N7	-2.49	1.30	1.35
5	H	4888	TAC	C9-C10	2.48	1.43	1.39
5	B	1888	TAC	C2-C3	2.47	1.46	1.40
5	J	5888	TAC	C1A-C10	2.47	1.45	1.41
5	H	4888	TAC	C2-C3	2.46	1.46	1.40
4	B	1999	GDP	C8-N7	-2.44	1.30	1.35
5	L	6888	TAC	C1A-C10	2.44	1.45	1.41
4	F	3999	GDP	C8-N7	-2.43	1.30	1.35
5	F	3888	TAC	O11-C11	2.42	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	5888	TAC	C4-N4	2.41	1.52	1.47
5	F	3888	TAC	C1C-C1	2.40	1.58	1.55
4	L	6999	GDP	C8-N7	-2.39	1.30	1.35
5	F	3888	TAC	C1A-C10	2.36	1.45	1.41
5	F	3888	TAC	C62-C6	2.36	1.55	1.53
5	L	6888	TAC	C62-C6	2.35	1.55	1.53
5	D	2888	TAC	C1A-C10	2.34	1.45	1.41
5	D	2888	TAC	C9-C10	2.33	1.43	1.39
5	F	3888	TAC	O1-C1	2.33	1.26	1.22
4	F	3999	GDP	C5-C6	-2.32	1.42	1.47
5	D	2888	TAC	C2-C3	2.31	1.46	1.40
5	D	2888	TAC	C1C-C1	2.29	1.58	1.55
5	J	5888	TAC	O11-C11	2.28	1.28	1.23
5	J	5888	TAC	C9-C10	2.26	1.43	1.39
4	J	5999	GDP	PB-O3B	-2.23	1.46	1.54
4	J	5999	GDP	C5-C4	-2.22	1.37	1.43
5	L	6888	TAC	C2-C3	2.20	1.45	1.40
5	F	3888	TAC	O6-C6	2.17	1.46	1.43
5	H	4888	TAC	C1A-C10	2.14	1.44	1.41
4	B	1999	GDP	C5-C4	-2.14	1.37	1.43
5	H	4888	TAC	C4-N4	2.13	1.52	1.47
4	B	1999	GDP	PB-O3B	-2.03	1.47	1.54

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	5888	TAC	C43-N4-C4	-5.56	101.03	114.09
5	J	5888	TAC	C1C-C41-C4	4.65	117.99	111.64
5	J	5888	TAC	C11-C1B-C12	3.78	121.79	118.80
5	F	3888	TAC	C1C-C1-C2	3.56	121.40	115.75
5	H	4888	TAC	C42-N4-C4	-3.51	105.86	114.09
5	F	3888	TAC	C11-C1B-C12	3.47	121.55	118.80
5	L	6888	TAC	C1C-C1-C2	3.40	121.14	115.75
5	D	2888	TAC	C1C-C1-C2	3.35	121.07	115.75
5	J	5888	TAC	C43-N4-C42	-3.34	100.53	110.38
5	B	1888	TAC	C1C-C1-C2	3.28	120.96	115.75
5	J	5888	TAC	C1C-C1-C2	3.25	120.92	115.75
5	H	4888	TAC	C1C-C1-C2	3.24	120.91	115.75
4	H	4999	GDP	O3'-C3'-C4'	-3.18	101.86	111.05
5	J	5888	TAC	C41-C1C-C1	3.17	114.69	111.05
5	D	2888	TAC	C11-C1B-C12	3.17	121.31	118.80
5	B	1888	TAC	C43-N4-C4	3.12	121.43	114.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	6999	GDP	O3'-C3'-C4'	-3.07	102.17	111.05
5	L	6888	TAC	C11-C1B-C12	2.98	121.16	118.80
5	L	6888	TAC	C42-N4-C4	2.88	120.85	114.09
5	D	2888	TAC	C41-C1C-C1	2.81	114.27	111.05
4	F	3999	GDP	PA-O3A-PB	-2.81	123.18	132.83
4	L	6999	GDP	PA-O3A-PB	-2.80	123.23	132.83
5	L	6888	TAC	C41-C1C-C1	2.77	114.22	111.05
5	J	5888	TAC	O1C-C1C-C41	-2.76	106.70	110.09
4	D	2999	GDP	PA-O3A-PB	-2.73	123.45	132.83
5	H	4888	TAC	C41-C1C-C1	2.68	114.12	111.05
5	H	4888	TAC	C43-N4-C4	2.66	120.35	114.09
4	D	2999	GDP	O3'-C3'-C4'	-2.64	103.41	111.05
5	B	1888	TAC	C11-C1B-C12	2.63	120.88	118.80
5	H	4888	TAC	O12-C12-C1B	-2.57	120.38	123.90
5	B	1888	TAC	C41-C1C-C1	2.54	113.97	111.05
5	H	4888	TAC	C11-C1B-C12	2.54	120.81	118.80
5	F	3888	TAC	C41-C1C-C1	2.54	113.96	111.05
4	J	5999	GDP	O4'-C1'-C2'	2.54	110.63	106.93
4	J	5999	GDP	O3'-C3'-C4'	-2.49	103.85	111.05
4	B	1999	GDP	PA-O3A-PB	-2.48	124.30	132.83
4	F	3999	GDP	O3'-C3'-C4'	-2.46	103.94	111.05
4	L	6999	GDP	C3'-C2'-C1'	2.46	104.68	100.98
4	J	5999	GDP	O3'-C3'-C2'	-2.46	103.88	111.82
4	H	4999	GDP	PA-O3A-PB	-2.44	124.47	132.83
4	F	3999	GDP	C3'-C2'-C1'	2.44	104.64	100.98
5	J	5888	TAC	O3-C3-C2	-2.38	118.78	122.96
4	H	4999	GDP	C3'-C2'-C1'	2.38	104.56	100.98
4	J	5999	GDP	PA-O3A-PB	-2.38	124.66	132.83
4	L	6999	GDP	O4'-C1'-C2'	2.37	110.39	106.93
4	L	6999	GDP	O3'-C3'-C2'	-2.37	104.16	111.82
4	J	5999	GDP	C3'-C2'-C1'	2.36	104.54	100.98
4	L	6999	GDP	O6-C6-C5	2.36	128.98	124.37
4	D	2999	GDP	C3'-C2'-C1'	2.36	104.53	100.98
4	B	1999	GDP	C3'-C2'-C1'	2.36	104.53	100.98
4	B	1999	GDP	O3'-C3'-C4'	-2.36	104.23	111.05
4	B	1999	GDP	O4'-C1'-C2'	2.35	110.37	106.93
4	F	3999	GDP	O3B-PB-O2B	2.33	116.56	107.64
5	B	1888	TAC	O12-C12-C1B	-2.33	120.71	123.90
4	F	3999	GDP	O6-C6-C5	2.33	128.92	124.37
4	F	3999	GDP	O4'-C1'-C2'	2.33	110.33	106.93
4	D	2999	GDP	O4'-C1'-C2'	2.31	110.30	106.93
5	L	6888	TAC	O1-C1-C2	-2.31	118.70	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	4888	TAC	O1-C1-C2	-2.28	118.75	123.55
4	D	2999	GDP	O6-C6-C5	2.26	128.78	124.37
5	F	3888	TAC	O1-C1-C2	-2.26	118.81	123.55
4	D	2999	GDP	O3'-C3'-C2'	-2.25	104.54	111.82
4	H	4999	GDP	O4'-C1'-C2'	2.25	110.21	106.93
5	J	5888	TAC	O12-C12-C1B	-2.23	120.85	123.90
4	D	2999	GDP	O3B-PB-O2B	2.20	116.06	107.64
5	H	4888	TAC	O1C-C1C-C41	-2.19	107.40	110.09
4	B	1999	GDP	O3'-C3'-C2'	-2.19	104.74	111.82
5	F	3888	TAC	O1C-C1C-C12	-2.18	106.65	110.14
4	B	1999	GDP	O6-C6-C5	2.13	128.54	124.37
5	L	6888	TAC	O1C-C1C-C12	-2.13	106.73	110.14
4	B	1999	GDP	O3B-PB-O2B	2.13	115.77	107.64
5	H	4888	TAC	C21-C2-C1	-2.11	118.47	120.97
4	H	4999	GDP	O6-C6-C5	2.10	128.48	124.37
5	J	5888	TAC	C42-N4-C4	2.10	119.02	114.09
5	B	1888	TAC	O1-C1-C2	-2.08	119.19	123.55
5	J	5888	TAC	O1C-C1C-C12	-2.06	106.84	110.14
5	D	2888	TAC	O1C-C1C-C12	-2.06	106.85	110.14
4	H	4999	GDP	O3'-C3'-C2'	-2.04	105.21	111.82
5	L	6888	TAC	C43-N4-C4	-2.04	109.31	114.09
4	L	6999	GDP	O3B-PB-O2B	2.02	115.34	107.64
4	F	3999	GDP	O3'-C3'-C2'	-2.01	105.31	111.82

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1999	GDP	PA-O3A-PB-O2B
4	D	2999	GDP	PA-O3A-PB-O2B
4	F	3999	GDP	PA-O3A-PB-O2B
4	H	4999	GDP	PA-O3A-PB-O2B
4	J	5999	GDP	PA-O3A-PB-O2B
4	J	5999	GDP	PA-O3A-PB-O3B
4	L	6999	GDP	PA-O3A-PB-O2B
5	H	4888	TAC	C3-C4-N4-C42
5	H	4888	TAC	C3-C4-N4-C43
5	J	5888	TAC	C3-C4-N4-C43
4	B	1999	GDP	PA-O3A-PB-O3B
4	H	4999	GDP	PA-O3A-PB-O3B
4	L	6999	GDP	PA-O3A-PB-O3B
5	B	1888	TAC	C3-C4-N4-C43

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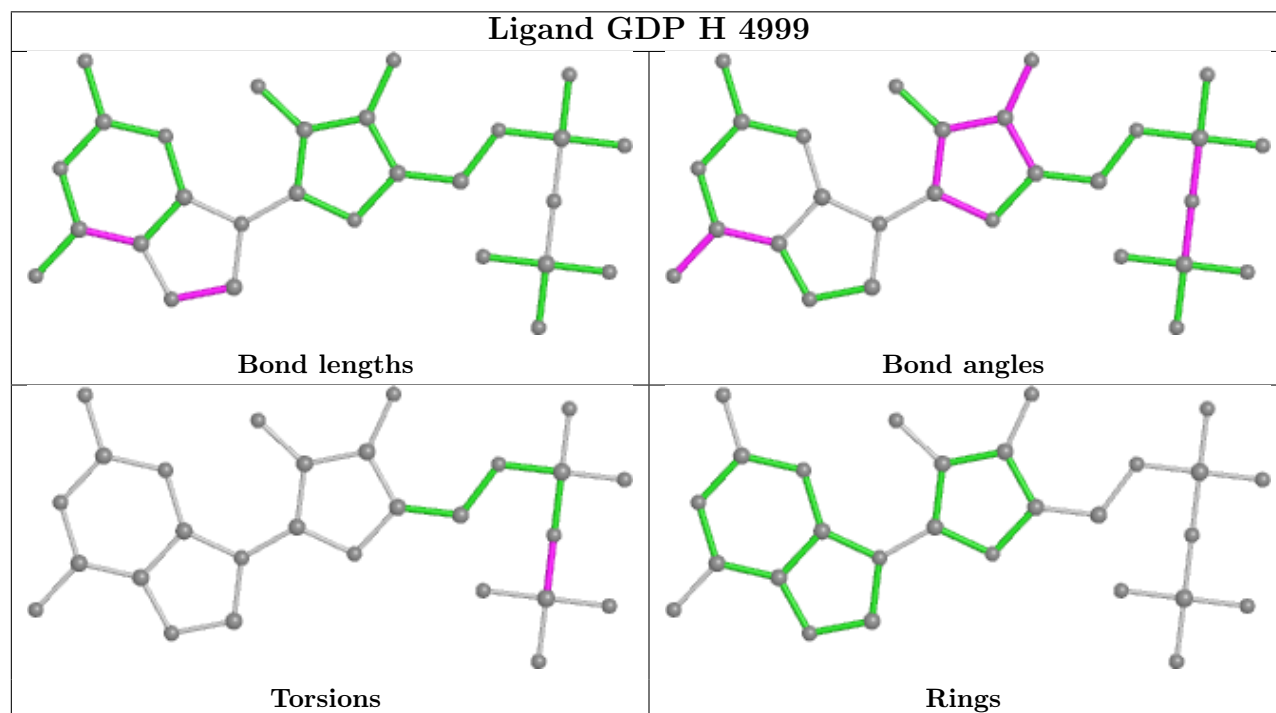
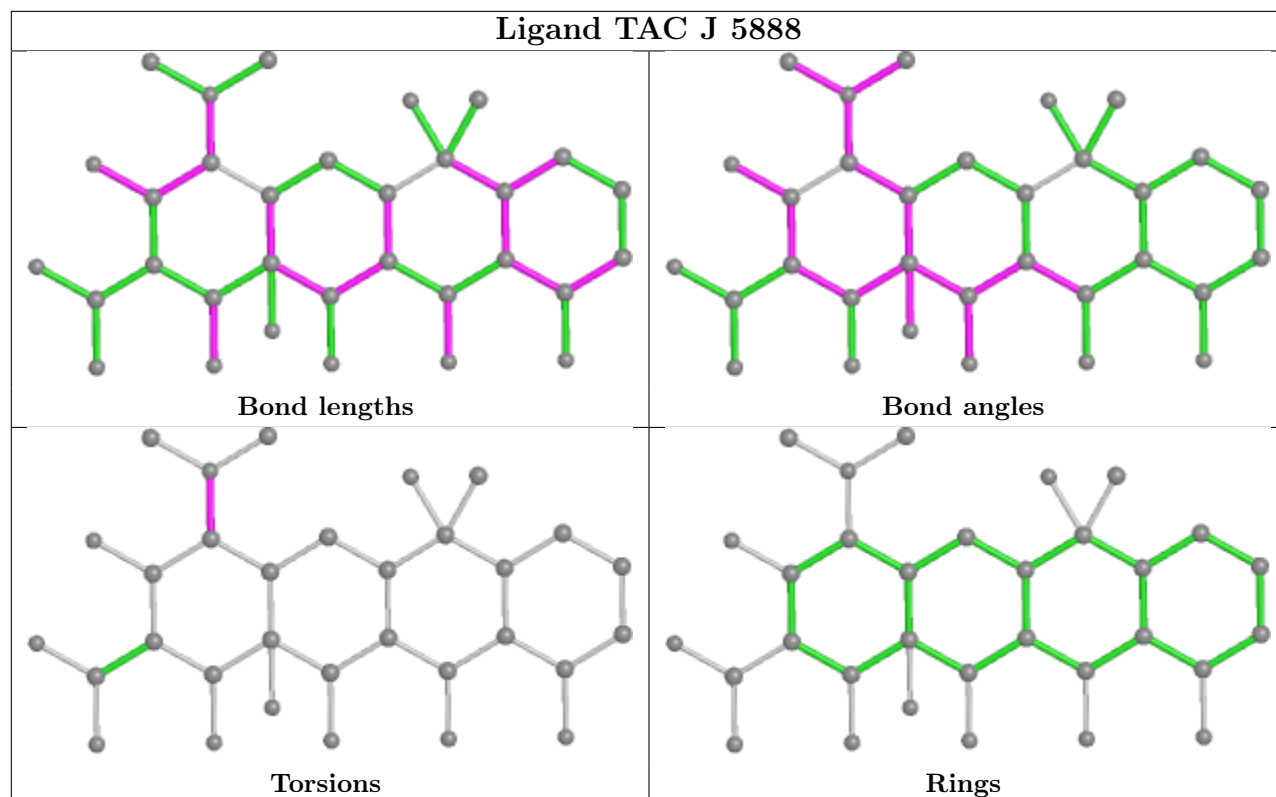
Mol	Chain	Res	Type	Atoms
5	H	4888	TAC	C41-C4-N4-C42
5	J	5888	TAC	C3-C4-N4-C42
5	L	6888	TAC	C3-C4-N4-C43
4	D	2999	GDP	PA-O3A-PB-O3B
4	F	3999	GDP	PA-O3A-PB-O3B
5	J	5888	TAC	C41-C4-N4-C42
5	L	6888	TAC	C41-C4-N4-C42

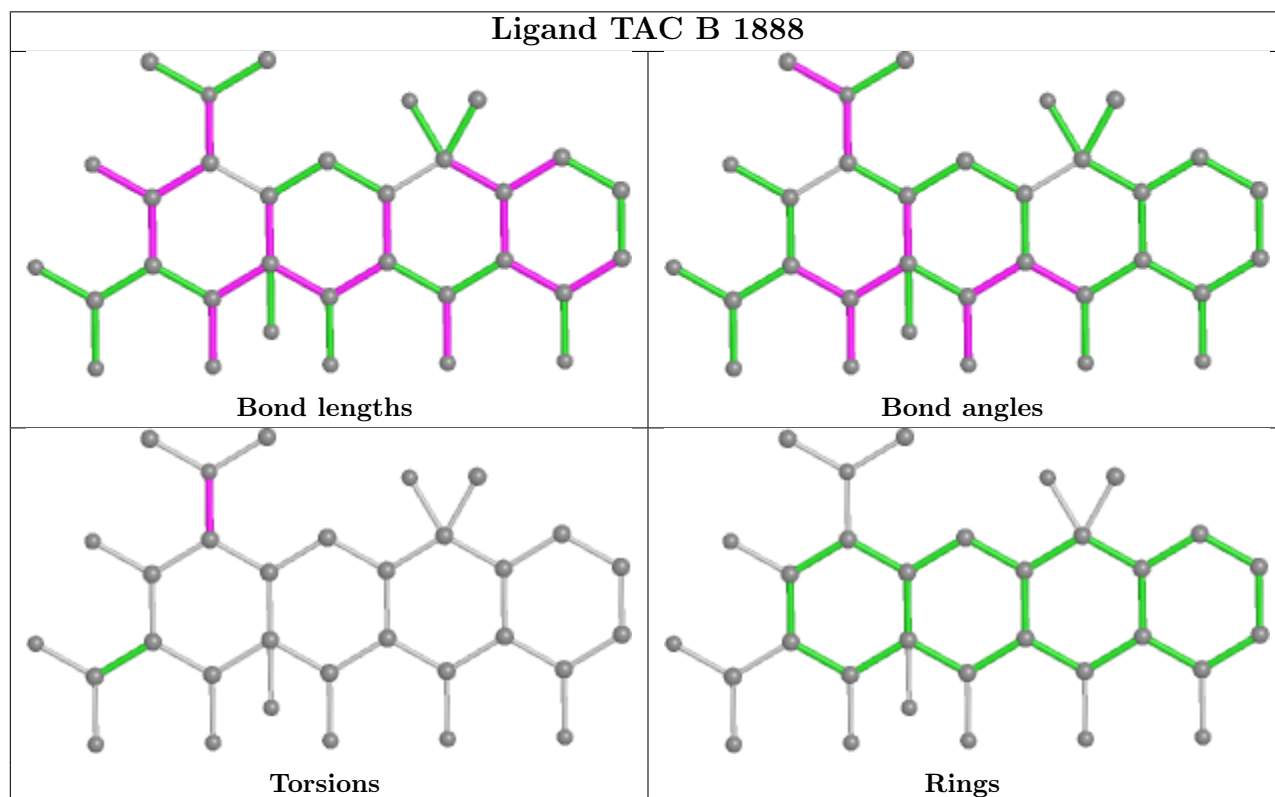
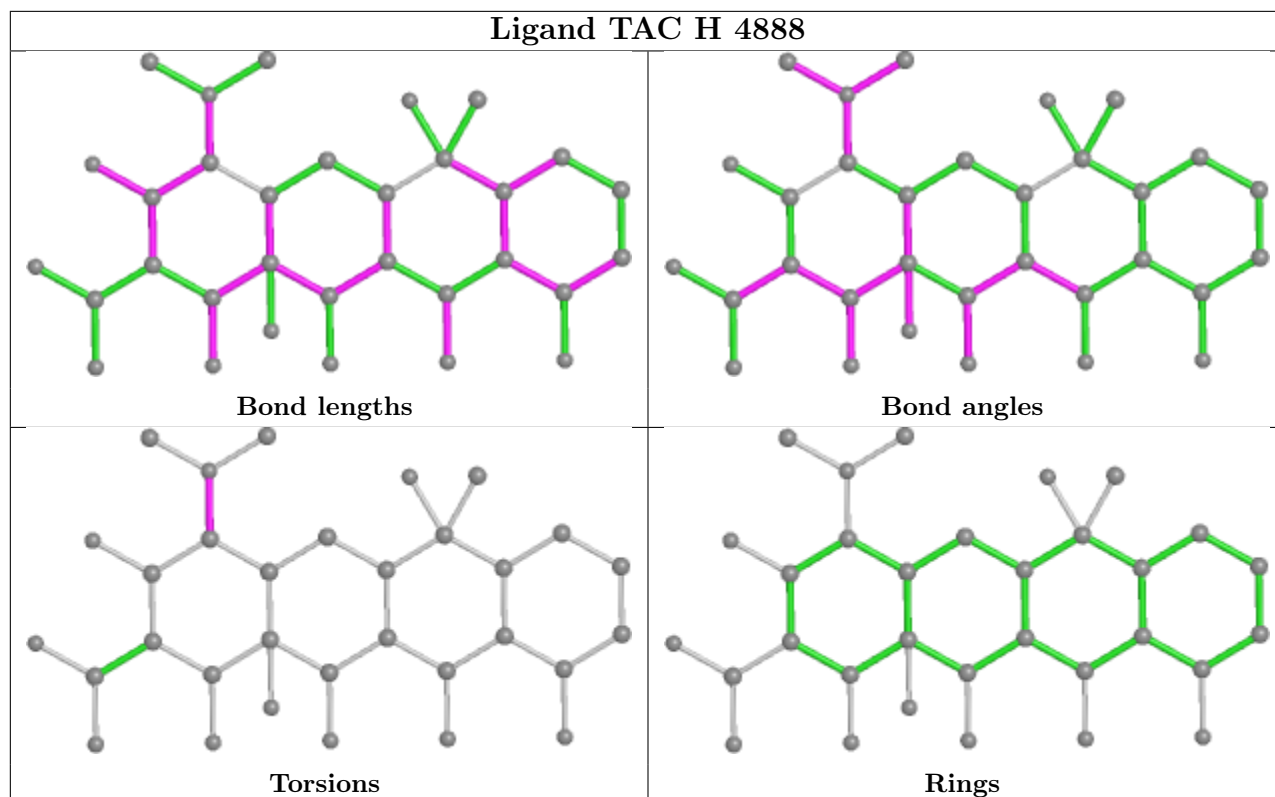
There are no ring outliers.

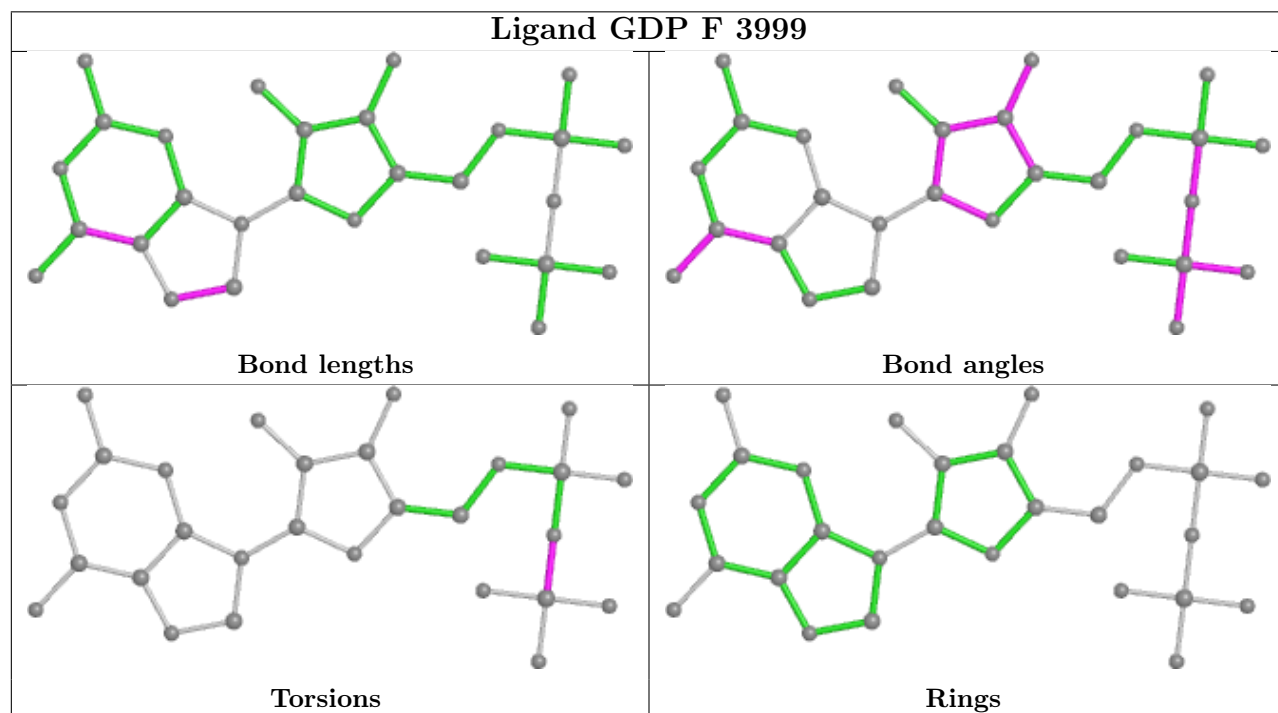
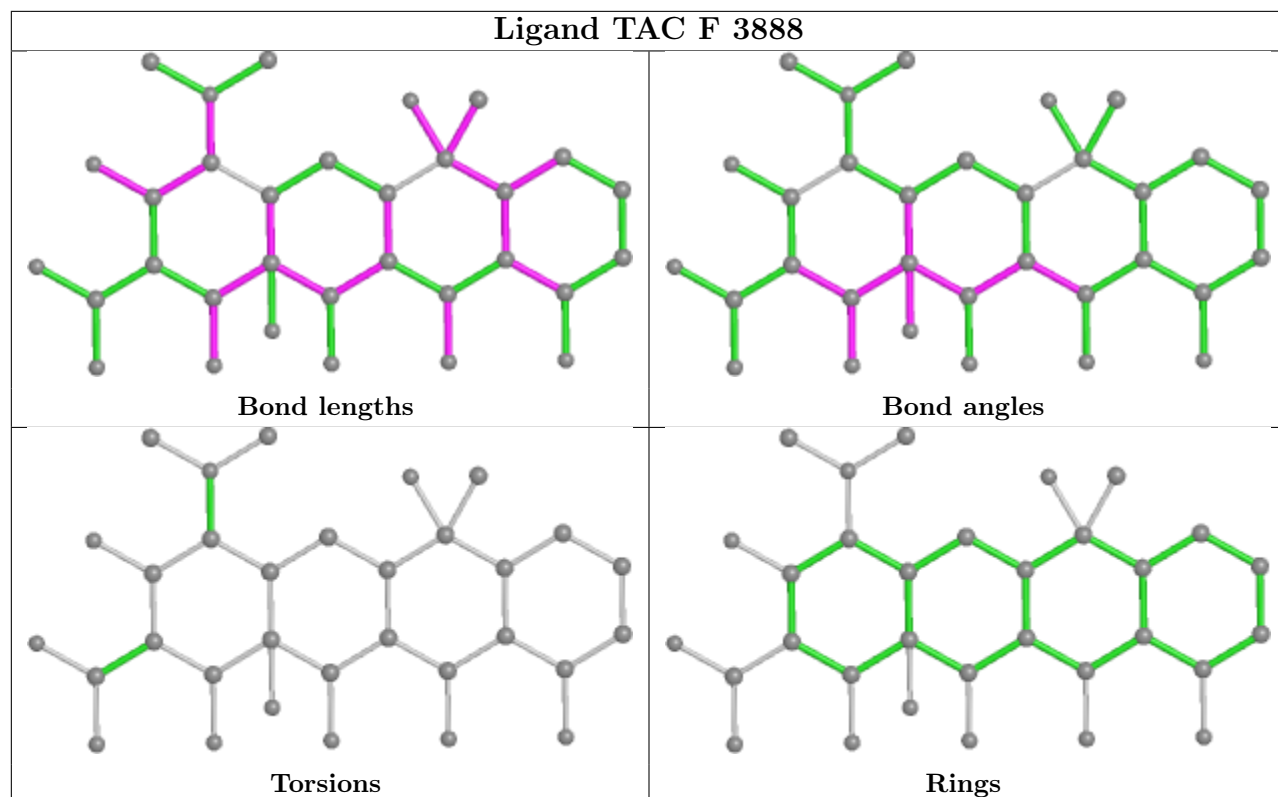
9 monomers are involved in 9 short contacts:

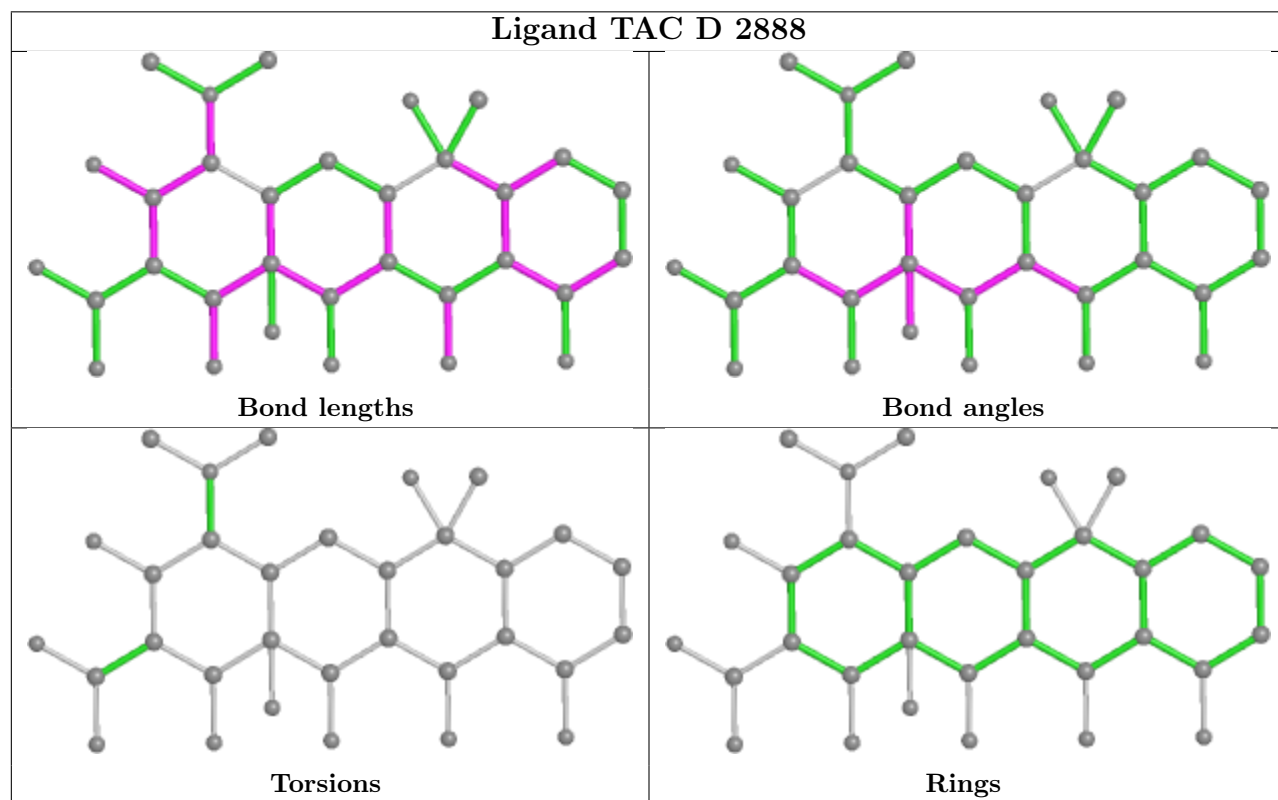
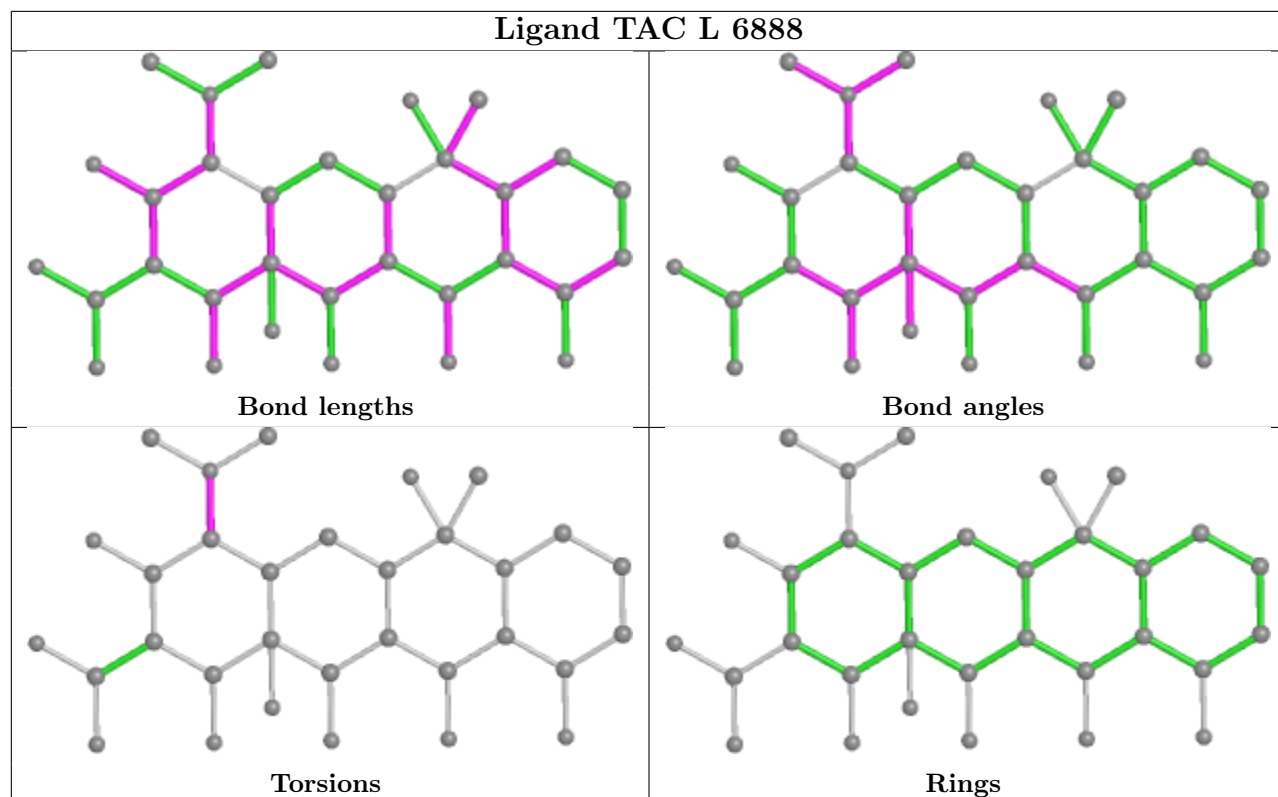
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	5888	TAC	1	0
4	H	4999	GDP	1	0
5	H	4888	TAC	1	0
5	B	1888	TAC	1	0
4	F	3999	GDP	1	0
5	L	6888	TAC	1	0
5	D	2888	TAC	1	0
4	D	2999	GDP	1	0
4	B	1999	GDP	1	0

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

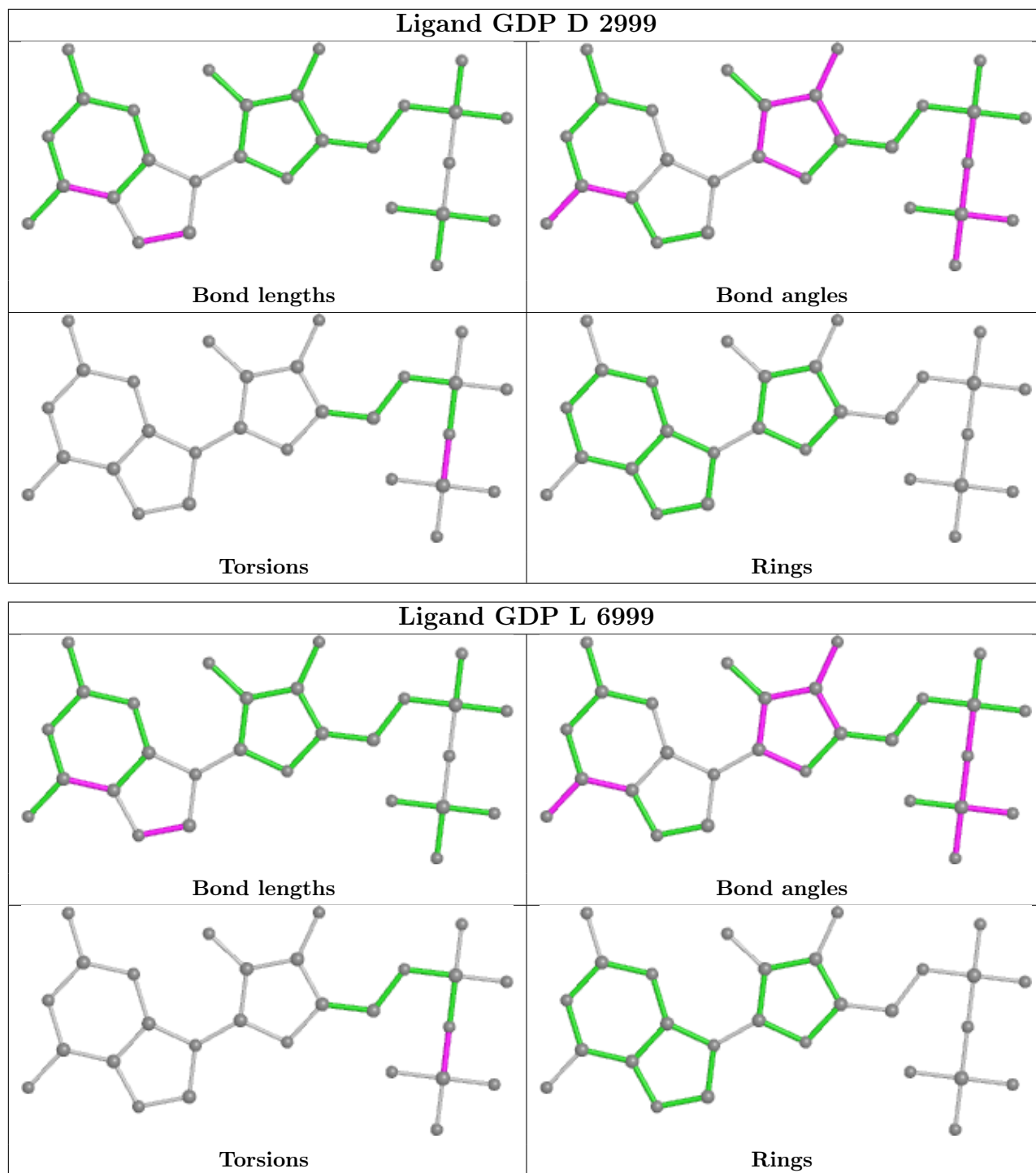


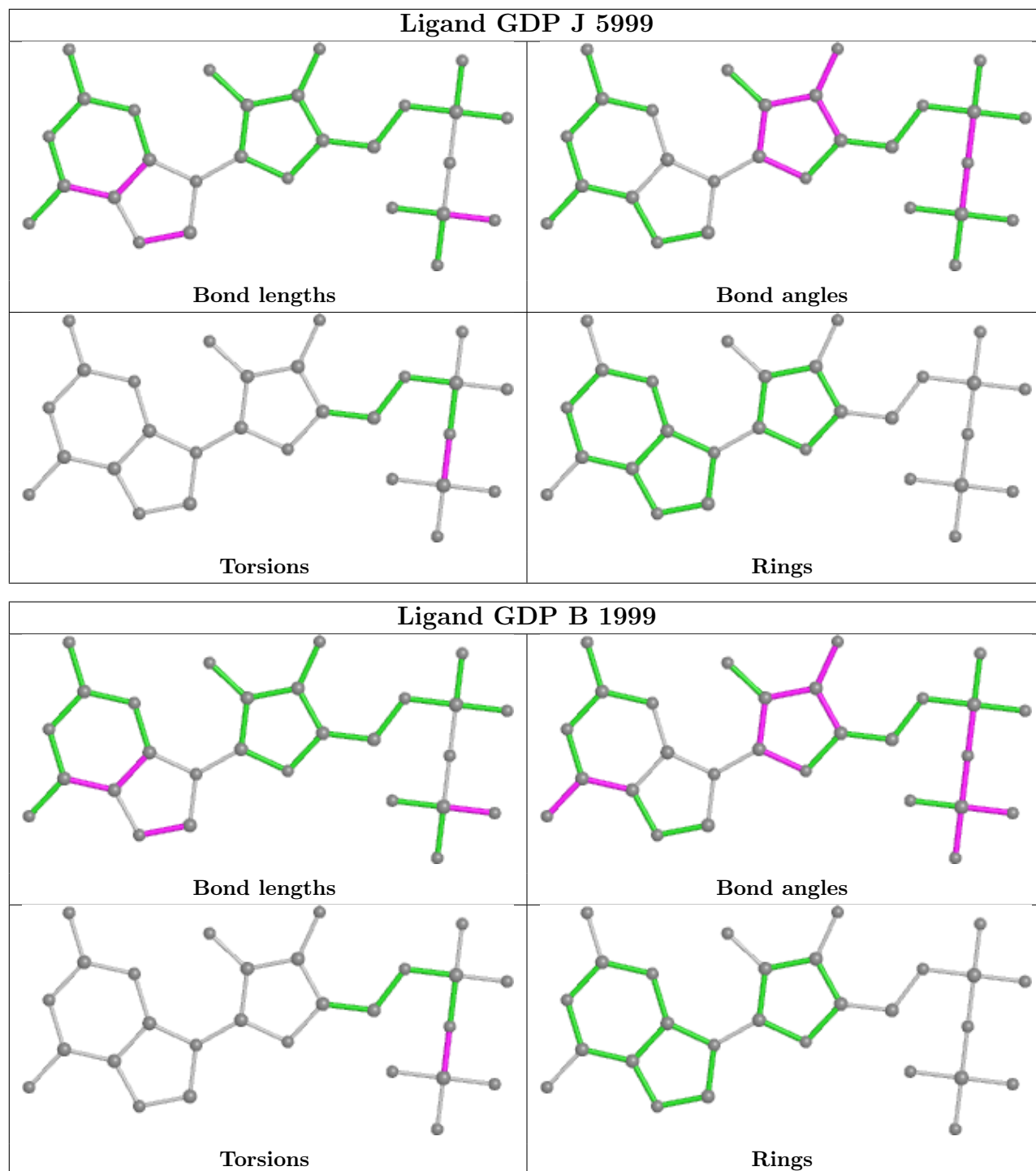












## 5.7 Other polymers [i](#)

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 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	33/37 (89%)	-0.76	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	9, 27, 44, 61	0
1	C	33/37 (89%)	-0.63	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	15, 31, 51, 74	0
1	E	33/37 (89%)	-0.61	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	21, 35, 68, 74	0
1	G	33/37 (89%)	-0.86	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	13, 32, 51, 64	0
1	I	33/37 (89%)	-0.52	1 (3%) <span style="border: 1px solid gray; padding: 2px;">50</span> <span style="border: 1px solid gray; padding: 2px;">40</span>	8, 19, 82, 98	0
1	K	33/37 (89%)	-0.78	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	10, 23, 45, 68	0
2	B	335/335 (100%)	-0.75	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	8, 31, 65, 94	0
2	D	335/335 (100%)	-0.69	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	13, 41, 74, 100	0
2	F	335/335 (100%)	-0.21	5 (1%) <span style="border: 1px solid gray; padding: 2px;">73</span> <span style="border: 1px solid gray; padding: 2px;">68</span>	13, 60, 99, 101	0
2	H	335/335 (100%)	-0.17	10 (2%) <span style="border: 1px solid gray; padding: 2px;">50</span> <span style="border: 1px solid gray; padding: 2px;">40</span>	16, 57, 100, 101	0
2	J	335/335 (100%)	-0.80	1 (0%) <span style="border: 1px solid blue; padding: 2px;">94</span> <span style="border: 1px solid blue; padding: 2px;">93</span>	6, 31, 69, 93	0
2	L	335/335 (100%)	-0.66	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	7, 41, 76, 100	0
All	All	2208/2232 (98%)	-0.56	17 (0%) <span style="border: 1px solid blue; padding: 2px;">86</span> <span style="border: 1px solid blue; padding: 2px;">81</span>	6, 40, 92, 101	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	38	THR	3.5
2	H	222	GLY	2.9
2	F	244	ILE	2.7
2	H	223	ARG	2.7
2	H	221	SER	2.7
2	F	145	LEU	2.5
2	F	278	LEU	2.5
2	H	279	ARG	2.5
2	H	226	VAL	2.4
2	H	266	ASP	2.3
2	J	220	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	219	SER	2.2
2	F	286	ILE	2.2
2	H	281	ILE	2.2
2	H	242	VAL	2.1
2	H	224	GLY	2.1
2	F	251	GLN	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

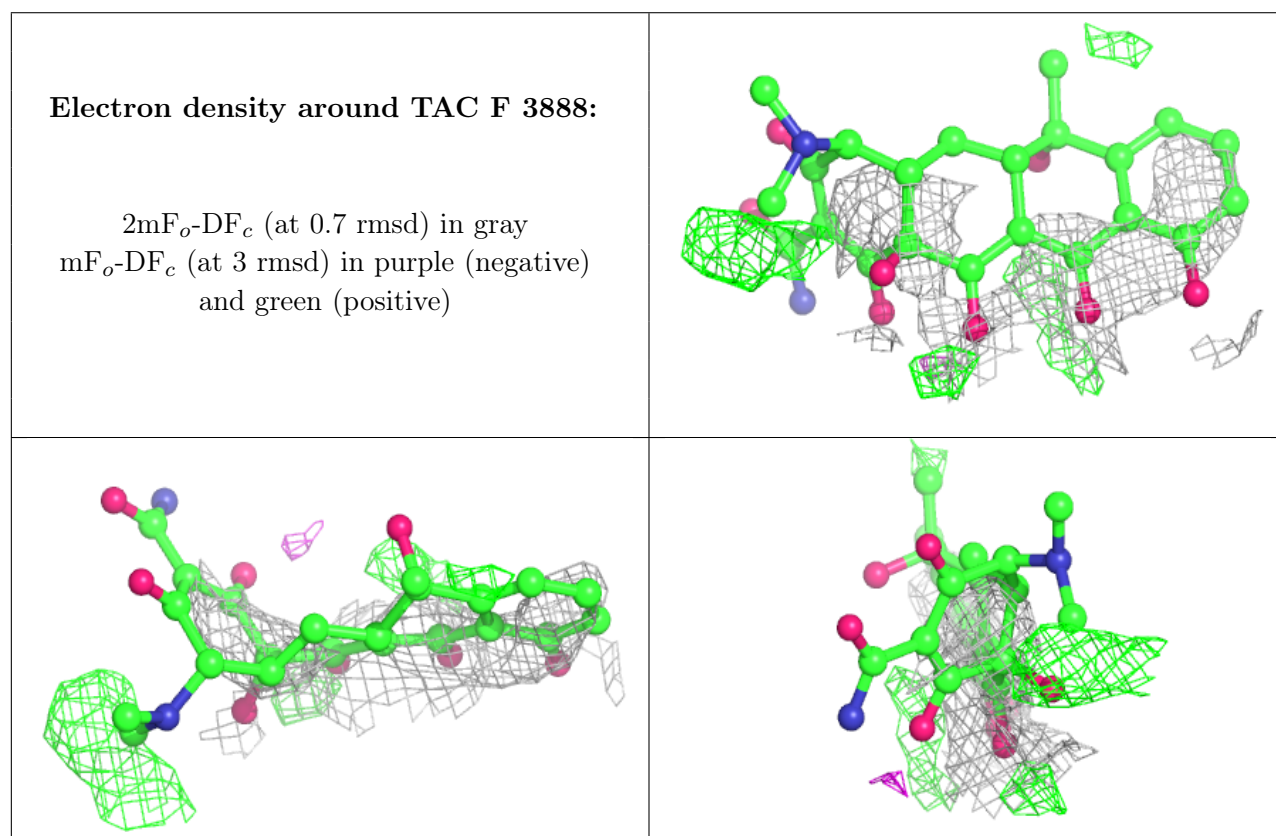
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	TAC	F	3888	32/32	0.78	0.47	32,47,57,60	32
5	TAC	D	2888	32/32	0.81	0.37	37,52,63,64	32
5	TAC	B	1888	32/32	0.85	0.27	34,48,60,64	32
5	TAC	J	5888	32/32	0.86	0.35	33,51,64,67	32
5	TAC	L	6888	32/32	0.90	0.24	35,47,61,64	32
3	MG	A	1998	1/1	0.92	0.18	32,32,32,32	0
5	TAC	H	4888	32/32	0.92	0.21	25,43,55,59	32
3	MG	E	3998	1/1	0.96	0.15	25,25,25,25	0
4	GDP	B	1999	28/28	0.96	0.15	16,43,54,54	0
4	GDP	F	3999	28/28	0.96	0.14	32,42,60,60	0
3	MG	G	4998	1/1	0.97	0.13	43,43,43,43	0
4	GDP	H	4999	28/28	0.97	0.14	19,52,64,66	0
3	MG	C	2998	1/1	0.97	0.19	30,30,30,30	0
4	GDP	D	2999	28/28	0.97	0.16	18,54,77,79	0
4	GDP	J	5999	28/28	0.98	0.13	14,26,33,38	0
4	GDP	L	6999	28/28	0.98	0.12	18,41,58,61	0
3	MG	I	5998	1/1	0.99	0.18	18,18,18,18	0

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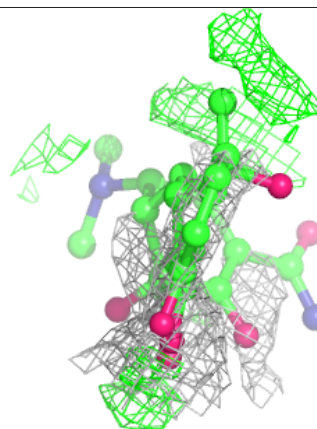
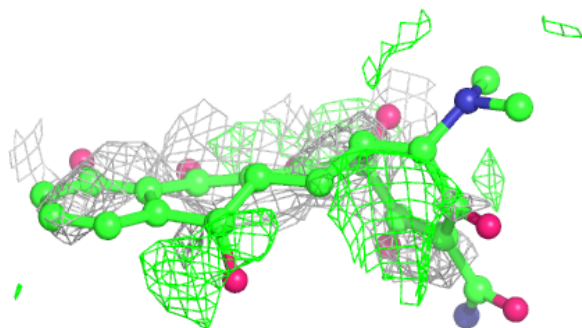
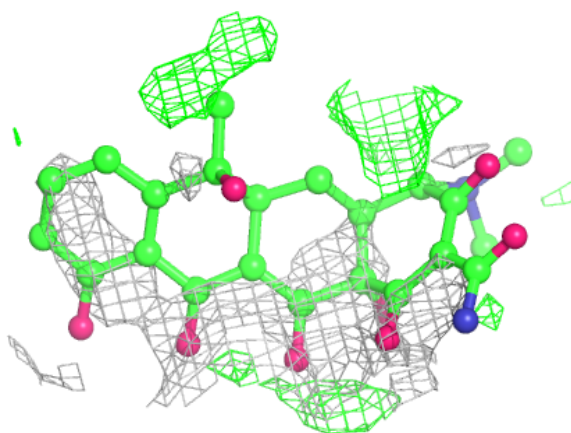
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	K	6998	1/1	0.99	0.12	27,27,27,27	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



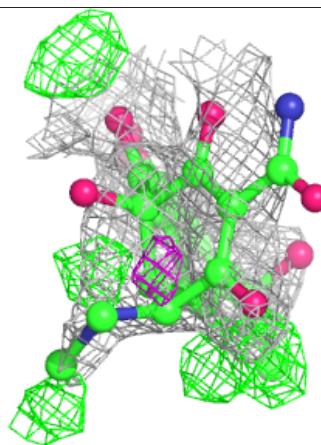
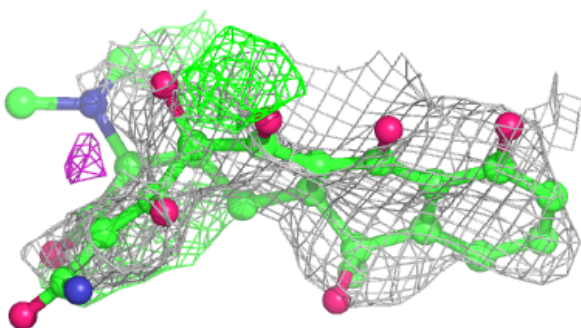
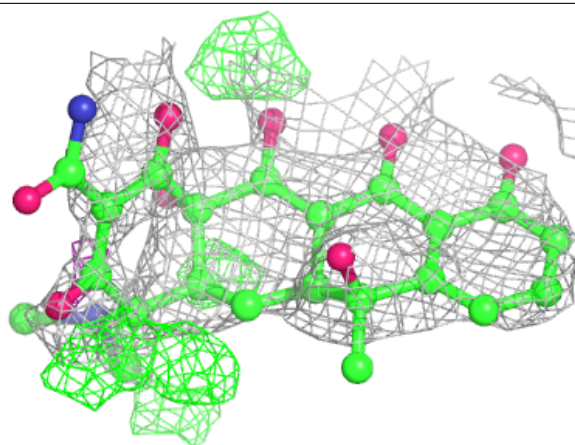
**Electron density around TAC D 2888:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



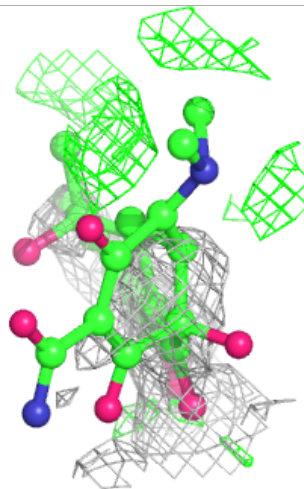
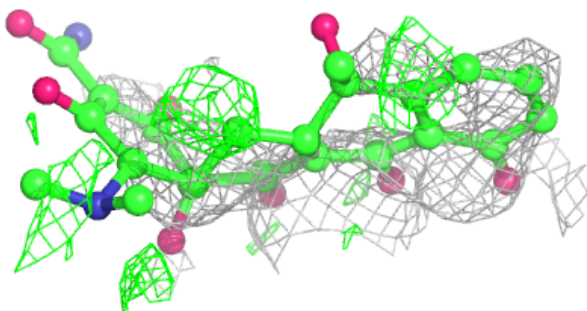
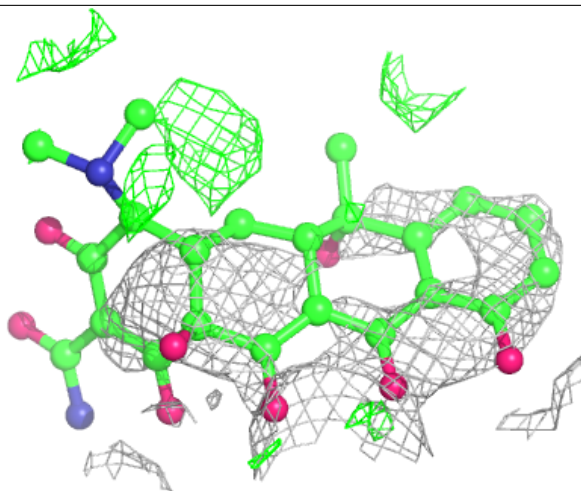
**Electron density around TAC B 1888:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around TAC J 5888:**

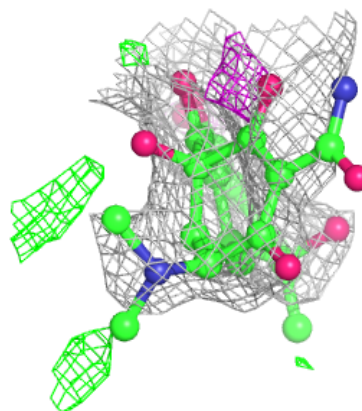
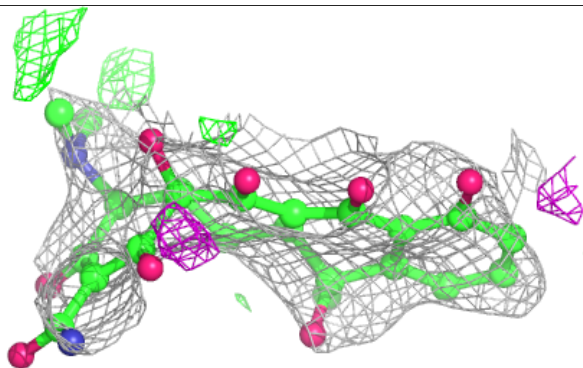
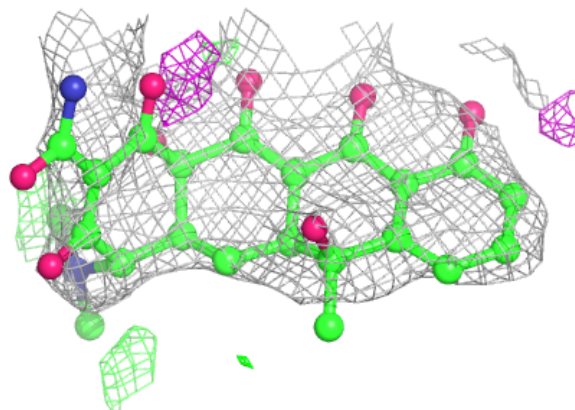
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





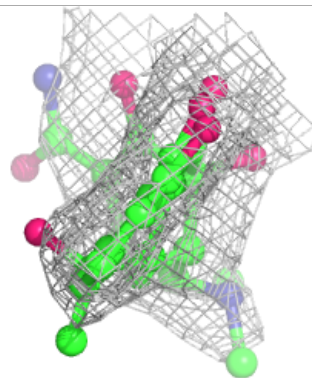
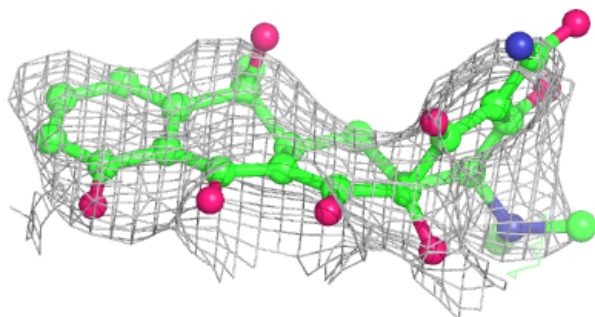
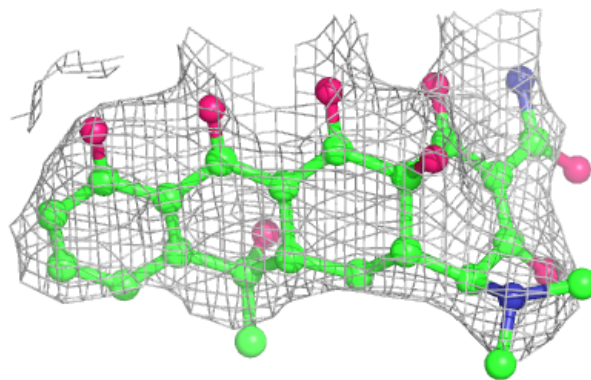
**Electron density around TAC L 6888:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



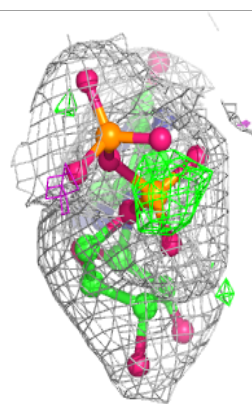
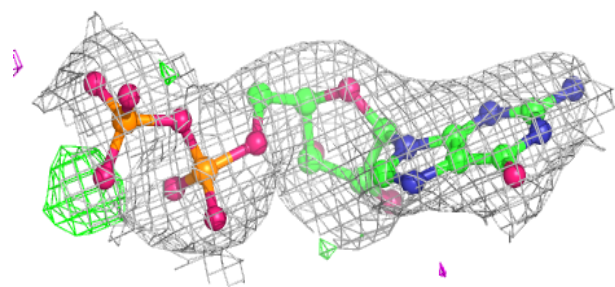
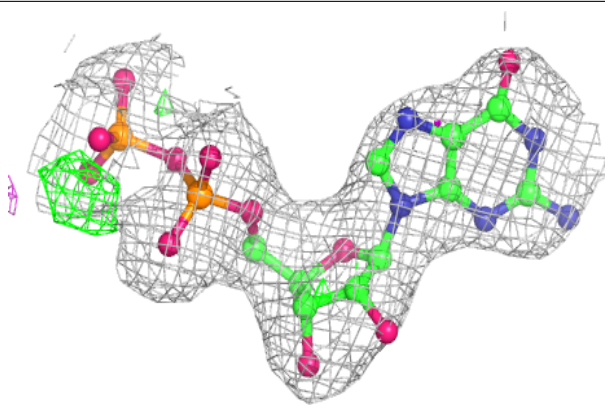
**Electron density around TAC H 4888:**

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and green (positive)

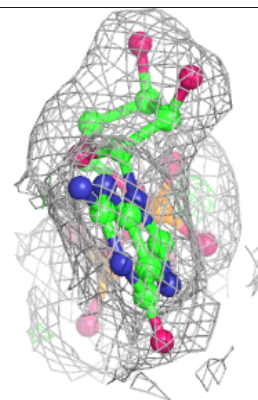
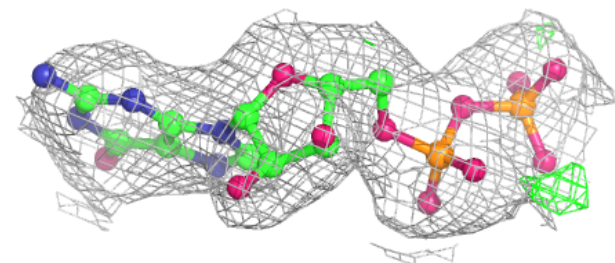
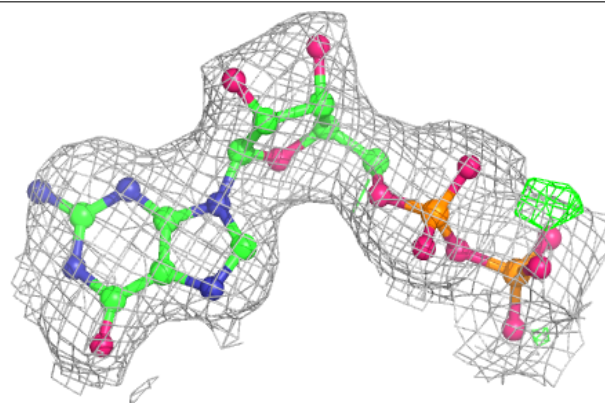


**Electron density around GDP B 1999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

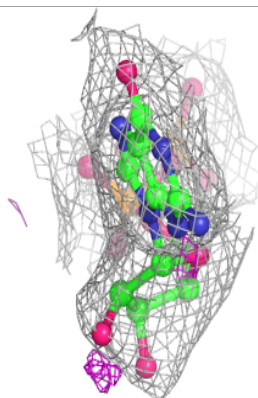
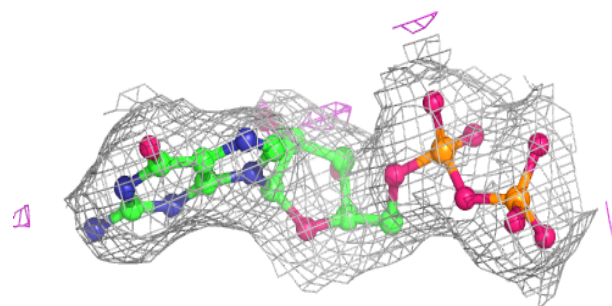
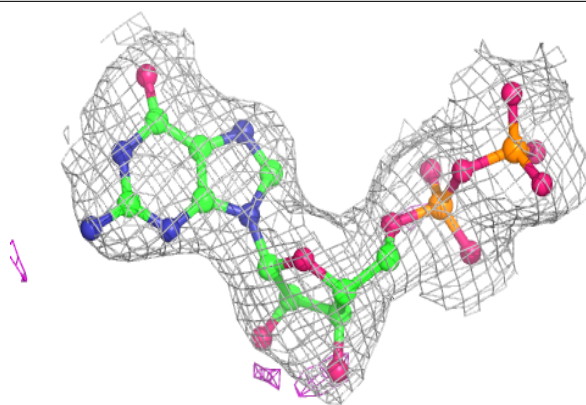
**Electron density around GDP F 3999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

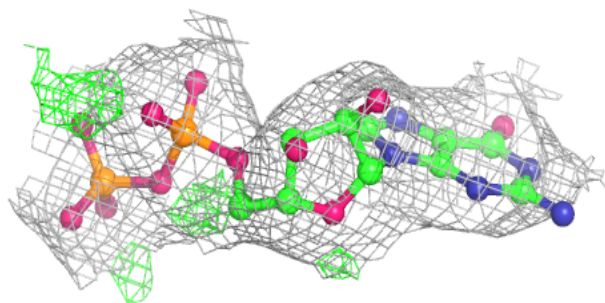
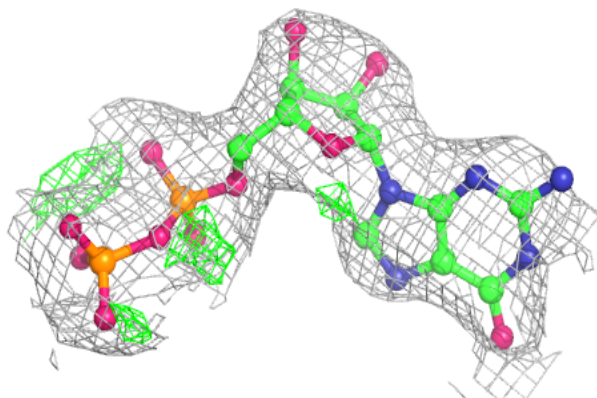


**Electron density around GDP H 4999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

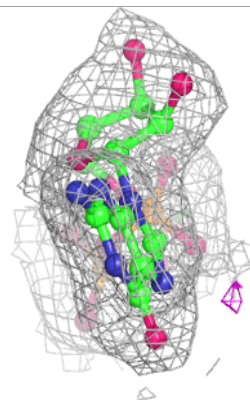
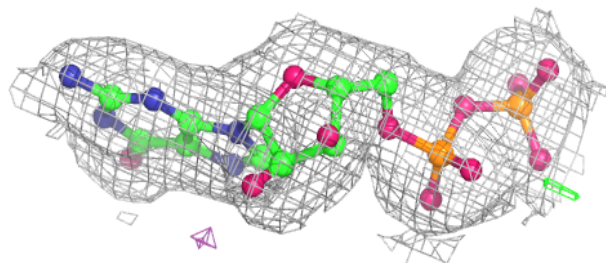
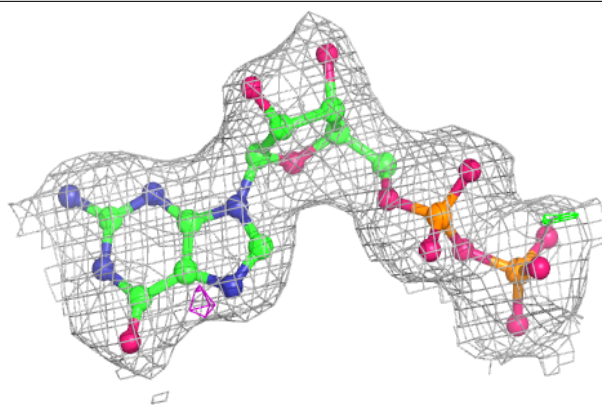
**Electron density around GDP D 2999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

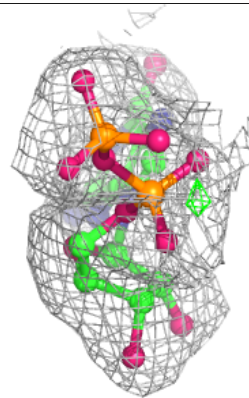
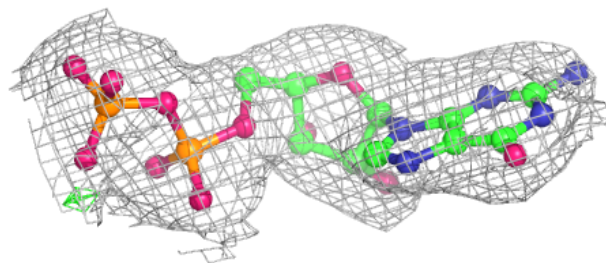
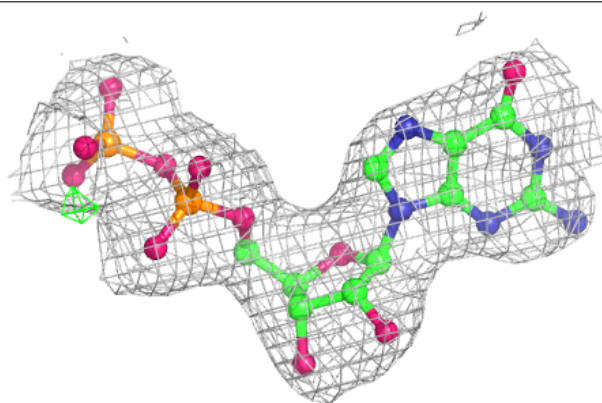


**Electron density around GDP J 5999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around GDP L 6999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.