



# Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:38 pm BST

PDB ID : 1F28  
Title : CRYSTAL STRUCTURE OF THYMIDYLATE SYNTHASE FROM PNEUMOCYSTIS CARINII BOUND TO DUMP AND BW1843U89  
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Deposited on : 2000-05-23  
Resolution : 1.90 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.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

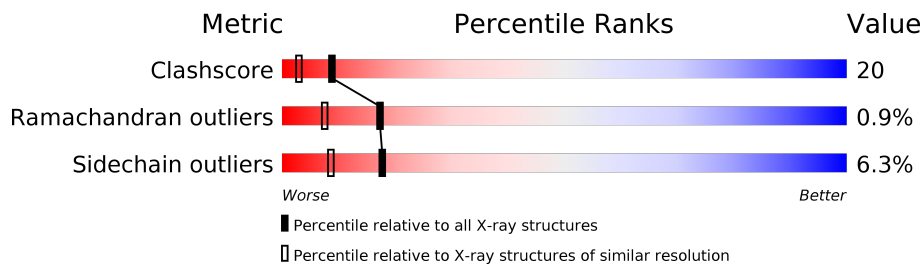
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	297	
1	B	297	
1	C	297	
1	D	297	

## 2 Entry composition [i](#)

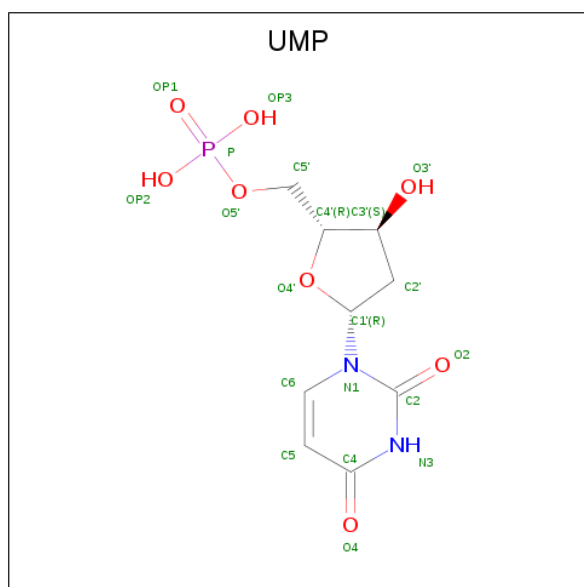
There are 4 unique types of molecules in this entry. The entry contains 10322 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	295	Total 2394	C 1526	N 413	O 440	S 15	0	0	0
1	B	295	Total 2403	C 1530	N 417	O 441	S 15	0	0	0
1	C	295	Total 2394	C 1526	N 413	O 440	S 15	0	0	0
1	D	295	Total 2403	C 1530	N 417	O 441	S 15	0	0	0

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula:  $C_9H_{13}N_2O_8P$ ).



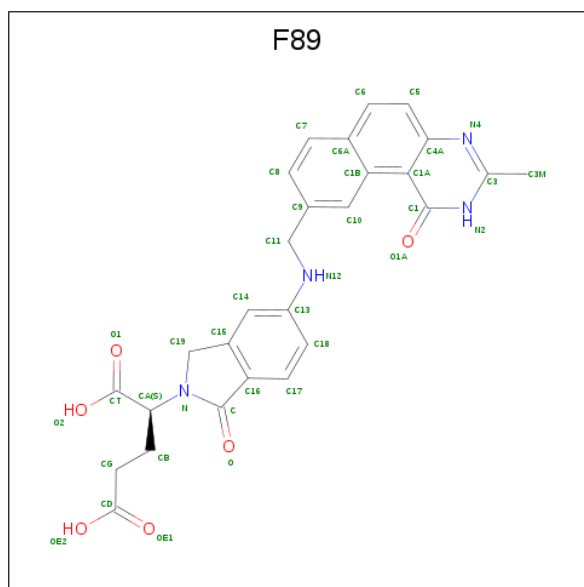
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 20	C 9	N 2	O 8	P 1	0	0
2	B	1	Total 20	C 9	N 2	O 8	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is S)-2-(5(((1,2-DIHYDRO-3-METHYL-1-OXOBENZO(F)QUINAZOLIN-9-YL)METHYL)AMINO)1-OXO-2-ISOINDOLINYL)GLUTARIC ACID (three-letter code: F89) (formula: C<sub>27</sub>H<sub>24</sub>N<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			37	27	4	6		
3	B	1	Total	C	N	O	0	0
			37	27	4	6		
3	C	1	Total	C	N	O	0	0
			37	27	4	6		
3	D	1	Total	C	N	O	0	0
			37	27	4	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total	O	0	0
			121	121		
4	B	125	Total	O	0	0
			125	125		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	C	118	Total 118	O 118	0	0
4	D	136	Total 136	O 136	0	0

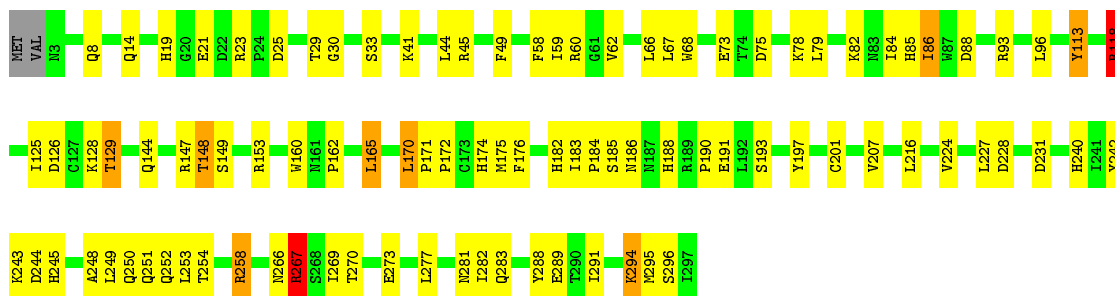
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

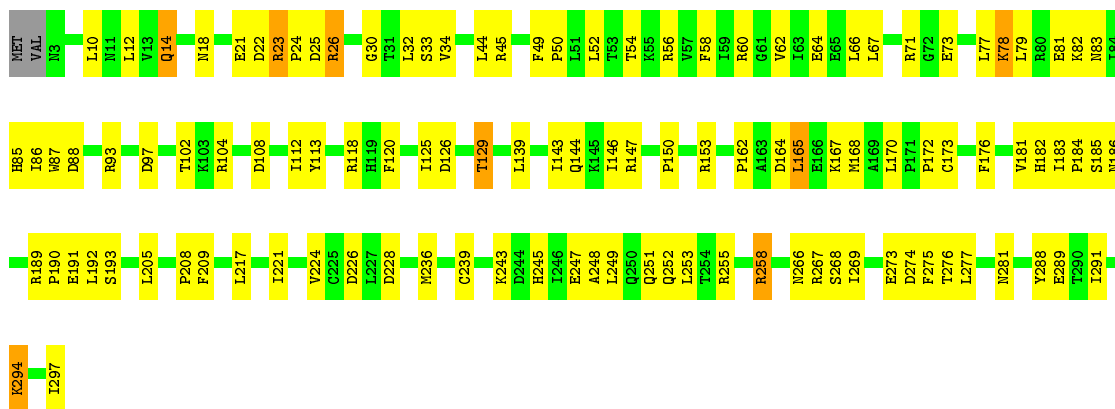
- Molecule 1: THYMIDYLATE SYNTHASE

Chain A: 



- Molecule 1: THYMIDYLATE SYNTHASE

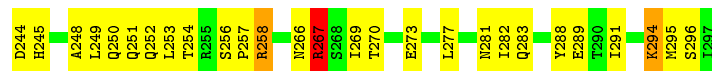
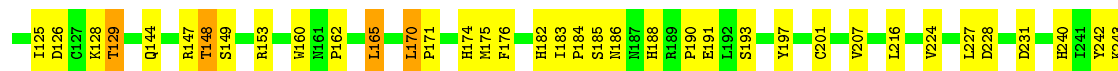
Chain B: 



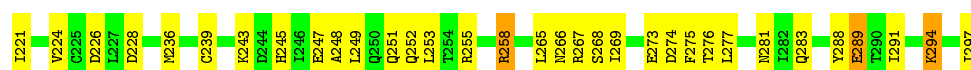
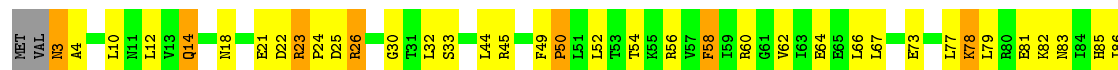
- Molecule 1: THYMIDYLATE SYNTHASE

Chain C: 





• Molecule 1: THYMIDYLATE SYNTHASE



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.44Å 65.90Å 184.94Å 90.00° 90.24° 90.00°	Depositor
Resolution (Å)	22.40 – 1.90	Depositor
% Data completeness (in resolution range)	83.5 (22.40-1.90)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.217 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F89, UMP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.52	0/2456	0.83	4/3331 (0.1%)
1	B	0.51	0/2465	0.76	0/3342
1	C	0.51	0/2456	0.83	4/3331 (0.1%)
1	D	0.51	0/2465	0.75	1/3342 (0.0%)
All	All	0.51	0/9842	0.79	9/13346 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	ARG	NE-CZ-NH2	-13.19	113.70	120.30
1	C	267	ARG	NE-CZ-NH1	12.65	126.63	120.30
1	A	267	ARG	NE-CZ-NH1	-12.50	114.05	120.30
1	A	267	ARG	NE-CZ-NH2	12.35	126.47	120.30
1	C	267	ARG	CD-NE-CZ	6.46	132.64	123.60
1	C	118	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	118	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	267	ARG	CD-NE-CZ	6.33	132.46	123.60
1	D	118	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2394	0	2335	102	0
1	B	2403	0	2351	111	0
1	C	2394	0	2335	105	0
1	D	2403	0	2351	112	0
2	A	20	0	10	0	0
2	B	20	0	11	2	0
2	C	20	0	10	0	0
2	D	20	0	11	2	0
3	A	37	0	22	2	0
3	B	37	0	22	5	0
3	C	37	0	22	4	0
3	D	37	0	22	5	0
4	A	121	0	0	2	0
4	B	125	0	0	9	0
4	C	118	0	0	0	0
4	D	136	0	0	8	0
All	All	10322	0	9502	394	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 20.

All (394) 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:B:150:PRO:HB2	1:B:181:VAL:HG21	1.41	1.01
1:D:150:PRO:HB2	1:D:181:VAL:HG21	1.41	0.99
1:B:146:ILE:HD12	1:B:221:ILE:HD11	1.49	0.94
1:D:146:ILE:HD12	1:D:221:ILE:HD11	1.48	0.93
1:C:58:PHE:CE2	1:C:60:ARG:HB3	2.11	0.85
1:A:58:PHE:CE2	1:A:60:ARG:HB3	2.13	0.83
1:A:184:PRO:HG3	1:A:190:PRO:HG3	1.61	0.81
1:C:184:PRO:HG3	1:C:190:PRO:HG3	1.63	0.79
1:A:176:PHE:CE1	1:B:176:PHE:CE1	2.71	0.79
1:A:176:PHE:HE1	1:B:176:PHE:CE1	2.01	0.78
1:C:58:PHE:HE2	1:C:60:ARG:HB3	1.47	0.77
1:A:8:GLN:HE22	1:A:41:LYS:H	1.33	0.77
1:C:8:GLN:HE22	1:C:41:LYS:H	1.33	0.77
1:C:176:PHE:CE1	1:D:176:PHE:CE1	2.72	0.77
1:B:60:ARG:NH2	1:B:82:LYS:O	2.18	0.76
1:C:176:PHE:HE1	1:D:176:PHE:CE1	2.03	0.76
1:A:58:PHE:HE2	1:A:60:ARG:HB3	1.49	0.76
1:A:147:ARG:HH21	1:A:224:VAL:HG12	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ARG:HH22	1:D:276:THR:HG23	1.50	0.74
1:B:267:ARG:HH22	1:B:276:THR:HG23	1.50	0.74
1:C:147:ARG:HH21	1:C:224:VAL:HG12	1.52	0.74
1:D:60:ARG:NH2	1:D:82:LYS:O	2.21	0.74
1:A:147:ARG:NH2	1:A:224:VAL:HG12	2.04	0.72
1:C:125:ILE:HB	1:C:129:THR:HG21	1.71	0.71
1:C:147:ARG:NH2	1:C:224:VAL:HG12	2.05	0.71
1:A:125:ILE:HB	1:A:129:THR:HG21	1.72	0.70
1:D:146:ILE:CD1	1:D:221:ILE:HD11	2.21	0.70
1:B:86:ILE:HG22	3:B:402:F89:HG2	1.74	0.70
1:B:146:ILE:CD1	1:B:221:ILE:HD11	2.21	0.70
1:B:126:ASP:OD1	1:B:129:THR:HG22	1.94	0.67
1:A:58:PHE:HD1	3:A:401:F89:O	1.77	0.67
1:D:245:HIS:O	1:D:249:LEU:HD23	1.96	0.66
1:D:236:MET:HE3	1:D:239:CYS:SG	2.34	0.66
1:D:173:CYS:SG	2:D:304:UMP:C6	2.89	0.65
1:A:289:GLU:CD	1:A:289:GLU:H	1.99	0.65
1:D:247:GLU:CD	1:D:248:ALA:H	2.00	0.65
1:A:118:ARG:HH22	1:A:273:GLU:CG	2.10	0.64
1:C:289:GLU:CD	1:C:289:GLU:H	2.00	0.64
1:C:118:ARG:HH22	1:C:273:GLU:CG	2.10	0.64
1:B:245:HIS:O	1:B:249:LEU:HD23	1.98	0.64
1:D:126:ASP:OD1	1:D:129:THR:HG22	1.98	0.64
1:B:173:CYS:SG	2:B:302:UMP:C6	2.91	0.64
1:D:125:ILE:HB	1:D:129:THR:HG21	1.80	0.64
1:B:58:PHE:CZ	1:B:60:ARG:NH1	2.67	0.63
1:B:184:PRO:HG3	1:B:190:PRO:HG3	1.80	0.63
1:C:118:ARG:HH22	1:C:273:GLU:CD	2.02	0.63
1:C:84:ILE:HG22	1:C:86:ILE:HD11	1.81	0.63
1:B:247:GLU:CD	1:B:248:ALA:H	2.02	0.63
1:B:125:ILE:HB	1:B:129:THR:HG21	1.81	0.62
1:D:58:PHE:CZ	1:D:60:ARG:NH1	2.68	0.62
1:A:118:ARG:HH22	1:A:273:GLU:CD	2.03	0.62
1:C:170:LEU:HD23	1:C:171:PRO:HD2	1.82	0.62
1:A:170:LEU:HD23	1:A:171:PRO:HD2	1.82	0.62
1:B:267:ARG:NH2	1:B:274:ASP:O	2.33	0.61
1:D:217:LEU:O	1:D:221:ILE:HG22	2.01	0.61
1:D:267:ARG:NH2	1:D:274:ASP:O	2.34	0.61
1:A:84:ILE:HG22	1:A:86:ILE:HD11	1.83	0.61
1:D:267:ARG:NH2	1:D:276:THR:HG23	2.16	0.61
1:A:58:PHE:CD1	3:A:401:F89:O	2.52	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:GLY:HA3	1:D:243:LYS:HD2	1.82	0.61
1:D:86:ILE:HG22	3:D:404:F89:HG2	1.82	0.60
1:B:267:ARG:NH2	1:B:276:THR:HG23	2.17	0.60
1:B:30:GLY:HA3	1:B:243:LYS:HD2	1.82	0.60
1:B:150:PRO:O	1:B:181:VAL:HG22	2.01	0.60
1:D:184:PRO:HG3	1:D:190:PRO:HG3	1.83	0.60
1:B:236:MET:HE3	1:B:239:CYS:SG	2.41	0.60
1:C:14:GLN:NE2	1:C:253:LEU:HD13	2.15	0.60
1:A:85:HIS:HD2	1:A:88:ASP:OD1	1.85	0.60
1:D:145:LYS:HD2	4:D:994:HOH:O	2.01	0.60
1:D:187:ASN:HA	4:D:705:HOH:O	2.01	0.59
1:A:162:PRO:HA	1:A:165:LEU:HD22	1.85	0.59
1:D:12:LEU:HD21	1:D:236:MET:HE3	1.84	0.59
1:A:14:GLN:NE2	1:A:253:LEU:HD13	2.17	0.59
1:C:162:PRO:HA	1:C:165:LEU:HD22	1.85	0.59
1:B:45:ARG:HD2	4:B:504:HOH:O	2.02	0.58
1:B:12:LEU:CD2	1:B:236:MET:HE1	2.34	0.58
1:B:217:LEU:O	1:B:221:ILE:HG22	2.04	0.58
1:D:150:PRO:O	1:D:181:VAL:HG22	2.03	0.58
1:D:86:ILE:HG21	3:D:404:F89:C15	2.34	0.58
1:C:59:ILE:HG12	1:C:282:ILE:HD12	1.86	0.57
1:A:21:GLU:OE2	1:B:182:HIS:HD2	1.86	0.57
1:C:170:LEU:HD23	1:C:171:PRO:CD	2.34	0.57
1:C:85:HIS:HD2	1:C:88:ASP:OD1	1.87	0.57
1:B:266:ASN:CG	1:B:267:ARG:H	2.08	0.57
1:D:266:ASN:CG	1:D:267:ARG:H	2.08	0.57
1:A:59:ILE:HG12	1:A:282:ILE:HD12	1.86	0.57
1:B:247:GLU:CG	1:B:248:ALA:N	2.68	0.57
1:B:267:ARG:HE	1:B:269:ILE:HD11	1.69	0.57
1:D:247:GLU:CG	1:D:248:ALA:N	2.67	0.57
1:B:52:LEU:HD22	1:B:208:PRO:HB3	1.87	0.56
1:D:267:ARG:HE	1:D:269:ILE:HD11	1.70	0.56
1:C:176:PHE:CE1	1:D:176:PHE:CD1	2.93	0.56
1:A:176:PHE:CE1	1:B:176:PHE:CD1	2.93	0.56
1:A:201:CYS:HB3	1:A:207:VAL:CG2	2.35	0.56
1:A:23:ARG:HD3	4:A:790:HOH:O	2.04	0.56
1:C:281:ASN:OD1	1:C:283:GLN:HG3	2.06	0.56
1:C:118:ARG:NH2	1:C:273:GLU:HG2	2.21	0.56
1:A:118:ARG:NH2	1:A:273:GLU:HG2	2.21	0.56
1:C:258:ARG:NE	1:C:288:TYR:CE1	2.74	0.55
1:A:281:ASN:OD1	1:A:283:GLN:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD23	1:A:171:PRO:CD	2.36	0.55
1:D:12:LEU:HD21	1:D:236:MET:CE	2.37	0.55
1:B:86:ILE:HG21	3:B:402:F89:C15	2.37	0.55
1:B:183:ILE:HG12	1:B:184:PRO:HD2	1.89	0.55
1:B:247:GLU:HG2	1:B:248:ALA:N	2.21	0.55
1:B:12:LEU:HD21	1:B:236:MET:CE	2.37	0.55
1:C:21:GLU:OE2	1:D:182:HIS:HD2	1.89	0.55
1:A:258:ARG:NE	1:A:288:TYR:CE1	2.75	0.55
1:A:294:LYS:H	1:A:294:LYS:CD	2.20	0.54
1:D:183:ILE:HG12	1:D:184:PRO:HD2	1.89	0.54
1:A:75:ASP:HB3	1:A:78:LYS:HD3	1.89	0.54
1:C:186:ASN:HB2	1:C:188:HIS:CE1	2.43	0.54
1:A:294:LYS:N	1:A:294:LYS:HD2	2.23	0.54
1:C:201:CYS:HB3	1:C:207:VAL:CG2	2.38	0.54
1:C:294:LYS:H	1:C:294:LYS:CD	2.20	0.54
1:C:84:ILE:CG2	1:C:86:ILE:HD11	2.38	0.54
1:B:14:GLN:HG2	1:B:253:LEU:HD13	1.90	0.54
1:C:58:PHE:HD1	3:C:403:F89:O	1.91	0.54
1:C:224:VAL:HG13	1:C:270:THR:O	2.07	0.53
1:A:186:ASN:HB2	1:A:188:HIS:CE1	2.43	0.53
1:A:251:GLN:O	1:A:254:THR:N	2.27	0.53
1:A:176:PHE:CZ	1:B:176:PHE:CE1	2.95	0.53
1:D:247:GLU:HG2	1:D:248:ALA:N	2.22	0.53
1:C:58:PHE:CD1	3:C:403:F89:O	2.61	0.53
1:B:77:LEU:O	1:B:81:GLU:HG3	2.08	0.53
1:C:197:TYR:CE2	1:D:176:PHE:HZ	2.26	0.53
1:A:254:THR:HG22	1:C:19:HIS:CD2	2.43	0.53
1:D:14:GLN:HG2	1:D:253:LEU:HD13	1.91	0.53
1:B:162:PRO:HA	1:B:165:LEU:HD22	1.91	0.53
1:C:294:LYS:N	1:C:294:LYS:HD2	2.24	0.53
1:A:84:ILE:CG2	1:A:86:ILE:HD11	2.39	0.53
1:B:236:MET:HE2	4:B:858:HOH:O	2.09	0.53
1:C:266:ASN:O	1:C:267:ARG:CB	2.56	0.53
1:B:266:ASN:CG	1:B:267:ARG:N	2.62	0.53
1:C:251:GLN:O	1:C:254:THR:N	2.27	0.53
1:A:118:ARG:HH22	1:A:273:GLU:HG2	1.74	0.52
1:B:45:ARG:NE	1:B:191:GLU:OE2	2.42	0.52
1:C:118:ARG:HH22	1:C:273:GLU:HG2	1.74	0.52
1:A:266:ASN:O	1:A:267:ARG:CB	2.57	0.52
1:B:86:ILE:HB	4:B:596:HOH:O	2.09	0.52
1:A:224:VAL:HG13	1:A:270:THR:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:ARG:NE	1:D:191:GLU:OE2	2.43	0.52
1:C:176:PHE:CZ	1:D:176:PHE:CE1	2.97	0.52
1:D:86:ILE:HG22	3:D:404:F89:CG	2.39	0.52
1:D:283:GLN:HG3	4:D:1005:HOH:O	2.10	0.52
1:A:294:LYS:HD2	1:A:294:LYS:H	1.74	0.52
1:D:267:ARG:HB3	1:D:269:ILE:CD1	2.39	0.52
1:C:75:ASP:HB3	1:C:78:LYS:HD3	1.92	0.51
1:A:245:HIS:O	1:A:249:LEU:HD23	2.10	0.51
1:D:266:ASN:CG	1:D:267:ARG:N	2.63	0.51
1:B:297:ILE:O	1:B:297:ILE:HG22	2.11	0.51
1:C:144:GLN:HE21	1:C:144:GLN:HA	1.76	0.51
1:C:294:LYS:HD2	1:C:294:LYS:H	1.75	0.51
1:A:243:LYS:C	1:A:245:HIS:H	2.14	0.51
1:A:59:ILE:HD12	1:A:62:VAL:HB	1.92	0.51
1:D:297:ILE:O	1:D:297:ILE:HG22	2.11	0.51
1:B:267:ARG:HB3	1:B:269:ILE:CD1	2.40	0.51
1:B:267:ARG:NE	1:B:269:ILE:HD11	2.25	0.51
1:B:294:LYS:H	1:B:294:LYS:CE	2.24	0.51
1:A:197:TYR:CE2	1:B:176:PHE:HZ	2.28	0.50
1:A:277:LEU:O	1:A:277:LEU:HD23	2.10	0.50
1:A:144:GLN:HE21	1:A:144:GLN:HA	1.77	0.50
1:C:153:ARG:NH1	1:D:25:ASP:OD2	2.44	0.50
1:C:277:LEU:O	1:C:277:LEU:HD23	2.10	0.50
1:D:162:PRO:HA	1:D:165:LEU:HD22	1.93	0.50
1:A:58:PHE:HZ	1:A:60:ARG:HH11	1.59	0.50
1:C:176:PHE:HE1	1:D:176:PHE:CD1	2.28	0.50
1:D:267:ARG:NE	1:D:269:ILE:HD11	2.25	0.50
1:A:59:ILE:HG12	1:A:282:ILE:CD1	2.41	0.50
1:D:265:LEU:HD23	4:D:963:HOH:O	2.10	0.50
1:D:294:LYS:CE	1:D:294:LYS:H	2.25	0.50
1:C:45:ARG:NH2	1:C:231:ASP:OD1	2.44	0.50
1:A:186:ASN:HB2	1:A:188:HIS:ND1	2.27	0.50
1:A:176:PHE:HE1	1:B:176:PHE:CD1	2.28	0.49
1:C:258:ARG:HG2	1:C:258:ARG:HH11	1.76	0.49
1:C:59:ILE:HG12	1:C:282:ILE:CD1	2.41	0.49
1:B:86:ILE:HG21	3:B:402:F89:C16	2.42	0.49
1:C:182:HIS:HE1	1:C:193:SER:OG	1.95	0.49
1:C:186:ASN:HB2	1:C:188:HIS:ND1	2.27	0.49
1:C:250:GLN:HA	1:C:253:LEU:HD12	1.95	0.49
1:D:182:HIS:HE1	1:D:193:SER:OG	1.95	0.49
1:B:45:ARG:NH1	4:B:504:HOH:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:HIS:O	1:C:249:LEU:HD23	2.12	0.49
1:D:85:HIS:HD2	1:D:88:ASP:OD1	1.96	0.49
1:A:250:GLN:HA	1:A:253:LEU:HD12	1.95	0.49
1:C:59:ILE:HD12	1:C:62:VAL:HB	1.94	0.49
1:D:248:ALA:HB1	1:D:291:ILE:CG2	2.42	0.49
1:B:126:ASP:OD1	1:B:129:THR:CG2	2.60	0.49
1:B:269:ILE:HG21	1:B:275:PHE:CE1	2.47	0.49
1:D:86:ILE:HG21	3:D:404:F89:C16	2.43	0.49
1:A:190:PRO:HB2	1:A:227:LEU:HD22	1.95	0.49
1:A:183:ILE:HD11	1:B:23:ARG:HB3	1.94	0.49
1:A:294:LYS:H	1:A:294:LYS:CE	2.26	0.48
1:B:248:ALA:HB1	1:B:291:ILE:CG2	2.43	0.48
1:C:190:PRO:HB2	1:C:227:LEU:HD22	1.95	0.48
1:B:14:GLN:NE2	1:B:18:ASN:ND2	2.61	0.48
1:D:77:LEU:O	1:D:81:GLU:HG3	2.13	0.48
1:A:85:HIS:CD2	1:A:88:ASP:OD1	2.66	0.48
1:C:294:LYS:H	1:C:294:LYS:CE	2.26	0.48
1:D:73:GLU:OE2	1:D:78:LYS:HG2	2.14	0.48
1:B:164:ASP:HA	1:B:167:LYS:HE2	1.95	0.48
1:C:295:MET:HG2	1:C:296:SER:N	2.29	0.48
1:A:128:LYS:NZ	1:A:128:LYS:HB2	2.29	0.48
1:B:26:ARG:HD3	2:B:302:UMP:OP1	2.13	0.48
1:C:128:LYS:HB2	1:C:128:LYS:NZ	2.29	0.48
1:A:254:THR:HG22	1:C:19:HIS:HD2	1.77	0.48
1:A:295:MET:HG2	1:A:296:SER:N	2.29	0.48
1:B:182:HIS:HE1	1:B:193:SER:OG	1.96	0.48
1:B:73:GLU:OE2	1:B:78:LYS:HG2	2.14	0.48
1:C:243:LYS:C	1:C:245:HIS:H	2.16	0.48
1:A:182:HIS:HE1	1:A:193:SER:OG	1.97	0.48
1:D:52:LEU:HD22	1:D:208:PRO:HB3	1.96	0.48
1:B:294:LYS:H	1:B:294:LYS:HE3	1.79	0.48
1:C:58:PHE:HZ	1:C:60:ARG:HH11	1.62	0.48
1:D:64:GLU:CG	1:D:82:LYS:HD2	2.43	0.47
1:C:224:VAL:O	1:C:224:VAL:HG12	2.14	0.47
1:A:266:ASN:O	1:A:267:ARG:HB3	2.13	0.47
1:D:126:ASP:OD1	1:D:129:THR:CG2	2.62	0.47
1:B:147:ARG:HH21	1:B:224:VAL:HG12	1.79	0.47
1:A:176:PHE:CZ	1:B:176:PHE:HE1	2.32	0.47
1:B:64:GLU:HG2	1:B:82:LYS:HD2	1.97	0.47
1:D:269:ILE:HG21	1:D:275:PHE:CE1	2.50	0.47
1:D:45:ARG:NH1	4:D:573:HOH:O	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLN:O	1:A:148:THR:HB	2.14	0.47
1:B:12:LEU:HD21	1:B:236:MET:HE1	1.96	0.47
1:C:197:TYR:CD2	1:D:176:PHE:HZ	2.33	0.46
1:D:294:LYS:HE3	1:D:294:LYS:H	1.80	0.46
1:A:172:PRO:HG3	4:A:822:HOH:O	2.15	0.46
1:A:224:VAL:HG12	1:A:224:VAL:O	2.15	0.46
1:A:153:ARG:NH1	1:B:25:ASP:OD2	2.48	0.46
1:C:258:ARG:HG2	1:C:258:ARG:NH1	2.30	0.46
1:D:147:ARG:HH21	1:D:224:VAL:HG12	1.80	0.46
1:D:62:VAL:CG2	1:D:209:PHE:HD2	2.29	0.46
1:D:64:GLU:HG2	1:D:82:LYS:HD2	1.98	0.46
1:A:185:SER:O	1:A:186:ASN:HB2	2.15	0.46
1:B:62:VAL:CG2	1:B:209:PHE:HD2	2.29	0.46
1:B:266:ASN:O	1:B:267:ARG:HB3	2.16	0.46
1:B:289:GLU:OE2	1:B:289:GLU:N	2.35	0.46
1:D:14:GLN:NE2	1:D:18:ASN:ND2	2.64	0.46
1:D:168:MET:SD	1:D:172:PRO:HD3	2.56	0.46
1:B:192:LEU:CD2	1:B:221:ILE:HG23	2.46	0.46
1:B:64:GLU:CG	1:B:82:LYS:HD2	2.45	0.46
1:B:85:HIS:HD2	1:B:88:ASP:OD1	1.99	0.46
1:C:144:GLN:O	1:C:148:THR:HB	2.15	0.46
1:C:176:PHE:CZ	1:D:176:PHE:HE1	2.33	0.46
1:A:19:HIS:CD2	1:C:254:THR:HG22	2.51	0.46
1:C:85:HIS:CD2	1:C:88:ASP:OD1	2.69	0.46
1:A:126:ASP:OD1	1:A:129:THR:HG22	2.16	0.46
1:A:160:TRP:CD2	1:A:175:MET:HE3	2.51	0.46
1:A:258:ARG:HH11	1:A:258:ARG:HG2	1.80	0.46
1:B:168:MET:SD	1:B:172:PRO:HD3	2.56	0.46
1:B:258:ARG:HG2	1:B:258:ARG:HH11	1.81	0.46
1:C:183:ILE:HG23	1:C:184:PRO:HD2	1.98	0.46
1:A:197:TYR:CD2	1:B:176:PHE:HZ	2.35	0.45
1:B:258:ARG:NE	1:B:288:TYR:CE1	2.84	0.45
1:C:183:ILE:HD11	1:D:23:ARG:HB3	1.97	0.45
1:D:267:ARG:HH22	1:D:276:THR:CG2	2.26	0.45
1:B:23:ARG:HD3	1:B:33:SER:HB3	1.98	0.45
1:B:23:ARG:HA	1:B:24:PRO:HD3	1.84	0.45
1:C:183:ILE:HD12	1:D:21:GLU:HB3	1.98	0.45
1:B:248:ALA:O	1:B:251:GLN:HG2	2.17	0.45
1:D:258:ARG:NE	1:D:288:TYR:CE1	2.85	0.45
1:D:45:ARG:HD2	4:D:573:HOH:O	2.17	0.45
1:A:126:ASP:OD1	1:A:129:THR:CG2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ILE:CD1	1:B:22:ASP:O	2.64	0.45
1:A:277:LEU:C	1:A:277:LEU:HD23	2.37	0.45
1:D:192:LEU:CD2	1:D:221:ILE:HG23	2.47	0.45
1:B:255:ARG:HD3	1:B:288:TYR:CG	2.52	0.45
1:C:84:ILE:HG22	1:C:86:ILE:CD1	2.46	0.45
1:D:258:ARG:HG2	1:D:258:ARG:HH11	1.82	0.45
1:A:183:ILE:HG23	1:A:184:PRO:HD2	1.99	0.44
1:D:23:ARG:HA	1:D:24:PRO:HD3	1.85	0.44
1:D:255:ARG:HD3	1:D:288:TYR:CG	2.53	0.44
1:B:258:ARG:HG2	1:B:258:ARG:NH1	2.31	0.44
1:C:185:SER:O	1:C:186:ASN:HB2	2.17	0.44
1:C:269:ILE:HD12	1:C:269:ILE:N	2.31	0.44
1:D:247:GLU:CG	1:D:248:ALA:H	2.29	0.44
1:A:269:ILE:N	1:A:269:ILE:HD12	2.31	0.44
1:B:97:ASP:OD1	1:B:102:THR:HA	2.18	0.44
1:D:289:GLU:N	1:D:289:GLU:OE2	2.37	0.44
1:D:49:PHE:HA	1:D:50:PRO:HD3	1.71	0.44
1:B:281:ASN:HB2	4:B:896:HOH:O	2.17	0.44
1:D:147:ARG:NH2	1:D:224:VAL:HG12	2.32	0.44
1:D:147:ARG:NH2	1:D:224:VAL:CG1	2.80	0.44
1:D:258:ARG:HG2	1:D:258:ARG:NH1	2.32	0.44
1:A:19:HIS:HD2	1:C:254:THR:HG22	1.83	0.44
1:B:71:ARG:NH2	4:B:864:HOH:O	2.49	0.44
1:D:118:ARG:HH22	1:D:273:GLU:CG	2.30	0.44
1:A:45:ARG:NH2	1:A:231:ASP:OD1	2.50	0.44
1:B:267:ARG:HH22	1:B:276:THR:CG2	2.27	0.44
1:B:267:ARG:O	1:B:268:SER:OG	2.28	0.44
1:B:34:VAL:HG13	4:B:839:HOH:O	2.18	0.44
1:D:97:ASP:OD1	1:D:102:THR:HA	2.18	0.44
1:A:251:GLN:O	1:A:252:GLN:C	2.57	0.44
1:A:258:ARG:NH1	1:A:258:ARG:HG2	2.33	0.44
1:A:267:ARG:HB3	1:A:269:ILE:CD1	2.48	0.44
1:C:45:ARG:HD3	1:C:191:GLU:OE2	2.18	0.44
1:C:251:GLN:O	1:C:252:GLN:C	2.57	0.44
1:C:160:TRP:CD2	1:C:175:MET:HE3	2.52	0.43
1:C:267:ARG:HB3	1:C:269:ILE:CD1	2.47	0.43
1:D:164:ASP:HA	1:D:167:LYS:HE2	2.00	0.43
1:D:266:ASN:O	1:D:267:ARG:HB3	2.19	0.43
1:C:86:ILE:HG12	3:C:403:F89:C16	2.47	0.43
1:A:84:ILE:HG22	1:A:86:ILE:CD1	2.47	0.43
1:B:12:LEU:HD21	1:B:236:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ASN:O	1:C:267:ARG:HB3	2.17	0.43
1:D:86:ILE:HD12	3:D:404:F89:C8	2.49	0.43
1:C:197:TYR:CE2	1:D:176:PHE:CZ	3.06	0.43
1:B:118:ARG:HH22	1:B:273:GLU:CG	2.30	0.43
1:B:147:ARG:NH2	1:B:224:VAL:CG1	2.81	0.43
1:D:23:ARG:HD3	1:D:33:SER:HB3	2.00	0.43
1:D:26:ARG:HD3	2:D:304:UMP:OP1	2.18	0.43
1:B:147:ARG:NH2	1:B:224:VAL:HG12	2.33	0.43
1:C:144:GLN:NE2	1:C:144:GLN:HA	2.34	0.43
1:C:256:SER:HA	1:C:257:PRO:HD3	1.90	0.43
1:D:10:LEU:HD11	1:D:54:THR:HG21	2.01	0.43
1:C:183:ILE:CD1	1:D:22:ASP:O	2.66	0.43
1:B:10:LEU:HD11	1:B:54:THR:HG21	2.01	0.43
1:B:32:LEU:HD23	1:B:32:LEU:HA	1.91	0.43
1:B:49:PHE:HA	1:B:50:PRO:HD3	1.72	0.43
1:B:189:ARG:HB3	1:B:228:ASP:OD2	2.19	0.43
1:C:148:THR:HG22	1:C:149:SER:N	2.33	0.43
1:D:267:ARG:O	1:D:268:SER:OG	2.29	0.43
1:C:191:GLU:HA	1:C:228:ASP:O	2.19	0.42
1:A:144:GLN:NE2	1:A:144:GLN:HA	2.34	0.42
1:A:294:LYS:N	1:A:294:LYS:CD	2.81	0.42
1:D:12:LEU:CD2	1:D:236:MET:HE1	2.49	0.42
1:B:113:TYR:CE1	1:B:172:PRO:HB3	2.54	0.42
1:B:247:GLU:CG	1:B:248:ALA:H	2.31	0.42
1:D:113:TYR:CE1	1:D:172:PRO:HB3	2.54	0.42
1:A:183:ILE:HD12	1:B:21:GLU:HB3	2.00	0.42
1:D:32:LEU:HD23	1:D:32:LEU:HA	1.92	0.42
1:B:183:ILE:HG12	1:B:184:PRO:CD	2.50	0.42
1:D:236:MET:CE	4:D:960:HOH:O	2.67	0.42
1:D:248:ALA:O	1:D:251:GLN:HG2	2.19	0.42
1:C:294:LYS:N	1:C:294:LYS:CD	2.81	0.42
1:C:29:THR:HG22	1:C:30:GLY:N	2.33	0.42
1:C:60:ARG:NH2	1:C:82:LYS:O	2.40	0.42
1:B:139:LEU:O	1:B:143:ILE:HG12	2.20	0.42
1:A:191:GLU:HA	1:A:228:ASP:O	2.20	0.42
1:C:126:ASP:OD1	1:C:129:THR:HG22	2.20	0.42
1:A:201:CYS:HB3	1:A:207:VAL:HG22	2.01	0.42
1:A:25:ASP:OD2	1:B:153:ARG:NH1	2.53	0.42
1:C:120:PHE:CZ	1:D:162:PRO:HD2	2.55	0.42
1:D:183:ILE:HG12	1:D:184:PRO:CD	2.50	0.42
1:A:148:THR:HG22	1:A:149:SER:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ALA:HB1	1:A:291:ILE:CG2	2.50	0.42
1:C:197:TYR:CD2	1:D:176:PHE:CZ	3.08	0.42
1:B:191:GLU:HG3	4:B:616:HOH:O	2.19	0.41
1:C:242:TYR:O	1:C:245:HIS:HB2	2.21	0.41
1:C:277:LEU:C	1:C:277:LEU:HD23	2.40	0.41
1:C:294:LYS:HE3	1:C:294:LYS:H	1.85	0.41
1:D:248:ALA:HB1	1:D:291:ILE:HG21	2.02	0.41
1:A:294:LYS:HE3	1:A:294:LYS:H	1.85	0.41
1:A:49:PHE:CZ	1:A:216:LEU:HG	2.55	0.41
1:D:145:LYS:HE2	4:D:631:HOH:O	2.20	0.41
1:A:242:TYR:O	1:A:245:HIS:HB2	2.21	0.41
1:B:185:SER:O	1:B:186:ASN:HB2	2.20	0.41
1:B:87:TRP:CE2	3:B:402:F89:H7	2.55	0.41
1:C:201:CYS:HB3	1:C:207:VAL:HG22	2.01	0.41
1:D:185:SER:O	1:D:186:ASN:HB2	2.20	0.41
1:D:3:ASN:HB3	1:D:4:ALA:H	1.63	0.41
1:C:68:TRP:CD1	1:C:73:GLU:HB2	2.56	0.41
1:D:189:ARG:HB3	1:D:228:ASP:OD2	2.21	0.41
1:A:68:TRP:CD1	1:A:73:GLU:HB2	2.56	0.41
1:B:86:ILE:HD12	3:B:402:F89:C8	2.51	0.41
1:C:113:TYR:CE1	1:C:174:HIS:CE1	3.09	0.41
1:A:251:GLN:HA	1:A:254:THR:HG23	2.03	0.41
1:B:144:GLN:NE2	4:B:885:HOH:O	2.53	0.41
1:C:87:TRP:CE2	3:C:403:F89:H7	2.56	0.41
1:B:248:ALA:HB1	1:B:291:ILE:HG21	2.03	0.41
1:A:45:ARG:HD3	1:A:191:GLU:OE2	2.21	0.41
1:A:60:ARG:NH2	1:A:82:LYS:O	2.41	0.41
1:D:265:LEU:HA	1:D:265:LEU:HD13	1.96	0.41
1:D:294:LYS:CD	1:D:294:LYS:H	2.33	0.41
1:A:113:TYR:CE1	1:A:174:HIS:CE1	3.09	0.41
1:B:252:GLN:HB2	1:B:291:ILE:HD12	2.01	0.41
1:D:252:GLN:HB2	1:D:291:ILE:HD12	2.01	0.41
1:C:248:ALA:HB1	1:C:291:ILE:CG2	2.51	0.41
1:A:248:ALA:HB1	1:A:291:ILE:HG21	2.03	0.41
1:B:181:VAL:HG23	1:B:181:VAL:O	2.20	0.41
1:A:162:PRO:HD2	1:B:120:PHE:CE1	2.56	0.40
1:A:33:SER:HB2	1:A:240:HIS:HB3	2.03	0.40
1:A:29:THR:HG22	1:A:30:GLY:N	2.35	0.40
1:B:104:ARG:HD2	1:B:108:ASP:HB3	2.03	0.40
1:C:49:PHE:CZ	1:C:216:LEU:HG	2.56	0.40
1:C:33:SER:HB2	1:C:240:HIS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:HIS:CD2	1:D:88:ASP:OD1	2.75	0.40
1:B:294:LYS:H	1:B:294:LYS:CD	2.34	0.40
1:C:147:ARG:NH2	1:C:224:VAL:CG1	2.81	0.40
1:C:197:TYR:CZ	1:D:176:PHE:HZ	2.39	0.40
1:D:281:ASN:HD21	1:D:283:GLN:HE21	1.69	0.40
1:C:126:ASP:OD1	1:C:129:THR:CG2	2.70	0.40
1:C:64:GLU:HB3	1:C:84:ILE:HD13	2.03	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	293/297 (99%)	277 (94%)	13 (4%)	3 (1%)	15	6
1	B	293/297 (99%)	277 (94%)	15 (5%)	1 (0%)	41	31
1	C	293/297 (99%)	278 (95%)	12 (4%)	3 (1%)	15	6
1	D	293/297 (99%)	275 (94%)	14 (5%)	4 (1%)	11	3
All	All	1172/1188 (99%)	1107 (94%)	54 (5%)	11 (1%)	17	7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	TYR
1	A	267	ARG
1	C	113	TYR
1	C	267	ARG
1	A	244	ASP
1	D	113	TYR
1	C	244	ASP
1	D	58	PHE

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Mol	Chain	Res	Type
1	D	289	GLU
1	D	50	PRO
1	B	112	ILE

### 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	264/268 (98%)	250 (95%)	14 (5%)	22	13
1	B	266/268 (99%)	247 (93%)	19 (7%)	14	6
1	C	264/268 (98%)	250 (95%)	14 (5%)	22	13
1	D	266/268 (99%)	246 (92%)	20 (8%)	13	5
All	All	1060/1072 (99%)	993 (94%)	67 (6%)	18	8

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	66	LEU
1	A	67	LEU
1	A	79	LEU
1	A	86	ILE
1	A	93	ARG
1	A	96	LEU
1	A	118	ARG
1	A	129	THR
1	A	148	THR
1	A	165	LEU
1	A	170	LEU
1	A	258	ARG
1	A	294	LYS
1	B	14	GLN
1	B	23	ARG
1	B	26	ARG
1	B	44	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	56	ARG
1	B	66	LEU
1	B	67	LEU
1	B	78	LYS
1	B	79	LEU
1	B	83	ASN
1	B	93	ARG
1	B	129	THR
1	B	165	LEU
1	B	170	LEU
1	B	205	LEU
1	B	226	ASP
1	B	258	ARG
1	B	277	LEU
1	B	294	LYS
1	C	44	LEU
1	C	66	LEU
1	C	67	LEU
1	C	79	LEU
1	C	86	ILE
1	C	93	ARG
1	C	96	LEU
1	C	118	ARG
1	C	129	THR
1	C	148	THR
1	C	165	LEU
1	C	170	LEU
1	C	258	ARG
1	C	294	LYS
1	D	3	ASN
1	D	14	GLN
1	D	23	ARG
1	D	26	ARG
1	D	44	LEU
1	D	56	ARG
1	D	66	LEU
1	D	67	LEU
1	D	78	LYS
1	D	79	LEU
1	D	83	ASN
1	D	93	ARG
1	D	129	THR

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Mol	Chain	Res	Type
1	D	165	LEU
1	D	170	LEU
1	D	205	LEU
1	D	226	ASP
1	D	258	ARG
1	D	277	LEU
1	D	294	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	8	GLN
1	A	14	GLN
1	A	19	HIS
1	A	85	HIS
1	A	144	GLN
1	A	182	HIS
1	A	252	GLN
1	B	7	GLN
1	B	14	GLN
1	B	18	ASN
1	B	85	HIS
1	B	144	GLN
1	B	182	HIS
1	B	252	GLN
1	B	283	GLN
1	C	8	GLN
1	C	14	GLN
1	C	19	HIS
1	C	85	HIS
1	C	144	GLN
1	C	182	HIS
1	C	252	GLN
1	D	7	GLN
1	D	14	GLN
1	D	18	ASN
1	D	19	HIS
1	D	85	HIS
1	D	144	GLN
1	D	182	HIS
1	D	252	GLN

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Mol	Chain	Res	Type
1	D	283	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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
3	F89	D	404	-	34,41,41	3.25	22 (64%)	45,60,60	3.52	10 (22%)
3	F89	A	401	-	34,41,41	3.37	23 (67%)	45,60,60	3.21	9 (20%)
2	UMP	C	303	1	18,21,21	3.97	6 (33%)	21,31,31	1.45	5 (23%)
2	UMP	B	302	-	18,21,21	1.95	5 (27%)	21,31,31	1.55	4 (19%)
2	UMP	A	301	1	18,21,21	3.79	7 (38%)	21,31,31	1.80	5 (23%)
3	F89	C	403	-	34,41,41	3.37	23 (67%)	45,60,60	3.22	10 (22%)
3	F89	B	402	-	34,41,41	3.27	23 (67%)	45,60,60	3.46	10 (22%)
2	UMP	D	304	-	18,21,21	1.92	6 (33%)	21,31,31	1.59	5 (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
3	F89	D	404	-	-	4/12/30/30	0/5/5/5
3	F89	A	401	-	-	4/12/30/30	0/5/5/5
2	UMP	C	303	1	-	2/7/22/22	0/2/2/2
2	UMP	B	302	-	-	2/7/22/22	0/2/2/2
2	UMP	A	301	1	-	1/7/22/22	0/2/2/2
3	F89	C	403	-	-	4/12/30/30	0/5/5/5
3	F89	B	402	-	-	4/12/30/30	0/5/5/5
2	UMP	D	304	-	-	1/7/22/22	0/2/2/2

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	303	UMP	C6-N1	13.14	1.52	1.35
2	A	301	UMP	C6-N1	12.10	1.50	1.35
2	C	303	UMP	C6-C5	7.72	1.55	1.38
2	A	301	UMP	C6-C5	7.64	1.54	1.38
3	D	404	F89	C1B-C6A	6.08	1.54	1.42
3	A	401	F89	C14-C13	6.04	1.49	1.39
3	C	403	F89	C14-C13	5.92	1.49	1.39
3	B	402	F89	C1B-C6A	5.78	1.53	1.42
3	A	401	F89	C1B-C6A	5.65	1.53	1.42
3	C	403	F89	C1B-C6A	5.57	1.53	1.42
3	C	403	F89	C17-C16	5.24	1.48	1.39
3	A	401	F89	C17-C16	5.19	1.48	1.39
3	D	404	F89	C17-C16	5.07	1.48	1.39
3	B	402	F89	C17-C16	4.95	1.47	1.39
3	D	404	F89	C18-C13	4.87	1.47	1.39
3	C	403	F89	C18-C17	4.86	1.47	1.38
3	B	402	F89	C18-C13	4.85	1.47	1.39
3	A	401	F89	C18-C17	4.76	1.47	1.38
3	B	402	F89	C14-C13	4.76	1.47	1.39
2	D	304	UMP	C4-N3	4.73	1.41	1.33
3	B	402	F89	C18-C17	4.72	1.47	1.38
3	C	403	F89	C1A-C4A	4.70	1.50	1.42
3	B	402	F89	CA-N	4.69	1.53	1.47
3	D	404	F89	CA-N	4.64	1.53	1.47
3	D	404	F89	C8-C9	4.61	1.48	1.38
3	A	401	F89	C18-C13	4.59	1.47	1.39
3	D	404	F89	C14-C13	4.58	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	F89	C1A-C4A	4.56	1.50	1.42
3	D	404	F89	C18-C17	4.56	1.47	1.38
2	B	302	UMP	C4-N3	4.52	1.40	1.33
3	C	403	F89	C18-C13	4.51	1.46	1.39
3	A	401	F89	C1B-C1A	4.43	1.50	1.41
2	A	301	UMP	O4'-C1'	4.42	1.52	1.42
3	A	401	F89	CA-N	4.41	1.53	1.47
2	B	302	UMP	O4'-C1'	4.38	1.52	1.42
3	C	403	F89	C1B-C1A	4.35	1.50	1.41
2	C	303	UMP	O4'-C1'	4.28	1.51	1.42
3	B	402	F89	C8-C9	4.22	1.47	1.38
3	C	403	F89	CA-N	4.21	1.53	1.47
3	C	403	F89	CB-CA	4.17	1.58	1.53
3	B	402	F89	C10-C1B	4.16	1.48	1.41
3	C	403	F89	C7-C8	4.15	1.45	1.36
3	A	401	F89	C8-C9	4.12	1.47	1.38
3	A	401	F89	C7-C8	4.11	1.45	1.36
3	C	403	F89	C8-C9	4.08	1.47	1.38
3	A	401	F89	CB-CA	4.05	1.58	1.53
3	C	403	F89	C10-C1B	4.04	1.48	1.41
3	B	402	F89	C1A-C4A	4.04	1.49	1.42
3	D	404	F89	C1B-C1A	4.03	1.49	1.41
3	D	404	F89	C10-C1B	3.98	1.48	1.41
3	A	401	F89	C10-C1B	3.97	1.48	1.41
3	D	404	F89	C19-C15	-3.91	1.45	1.50
3	B	402	F89	C1B-C1A	3.91	1.49	1.41
3	B	402	F89	C1-N2	3.90	1.39	1.33
3	B	402	F89	C7-C8	3.87	1.44	1.36
3	C	403	F89	C1-N2	3.87	1.39	1.33
3	B	402	F89	C19-C15	-3.84	1.45	1.50
3	A	401	F89	C6-C5	3.83	1.45	1.35
3	D	404	F89	C6-C5	3.81	1.45	1.35
3	B	402	F89	C6-C5	3.78	1.45	1.35
3	A	401	F89	C1-N2	3.77	1.39	1.33
3	D	404	F89	C1-N2	3.76	1.39	1.33
3	D	404	F89	C-N	3.72	1.39	1.36
3	C	403	F89	C14-C15	3.71	1.45	1.39
3	D	404	F89	C7-C8	3.69	1.44	1.36
3	D	404	F89	C1A-C4A	3.69	1.49	1.42
3	C	403	F89	C6-C5	3.66	1.45	1.35
3	D	404	F89	CB-CA	3.66	1.57	1.53
3	C	403	F89	C10-C9	3.65	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	F89	C10-C9	3.65	1.46	1.37
3	A	401	F89	C10-C9	3.61	1.45	1.37
3	A	401	F89	C14-C15	3.58	1.45	1.39
2	A	301	UMP	C4-N3	3.55	1.39	1.33
2	C	303	UMP	C4-N3	3.47	1.39	1.33
3	B	402	F89	C-N	3.43	1.39	1.36
3	A	401	F89	C13-N12	3.34	1.48	1.38
3	D	404	F89	C10-C9	3.32	1.45	1.37
3	B	402	F89	CB-CA	3.32	1.57	1.53
3	C	403	F89	C13-N12	3.25	1.48	1.38
3	C	403	F89	C16-C15	3.23	1.44	1.39
2	D	304	UMP	C6-N1	3.22	1.39	1.35
2	D	304	UMP	O4'-C1'	3.10	1.49	1.42
3	A	401	F89	C16-C15	3.05	1.43	1.39
3	D	404	F89	C16-C15	2.92	1.43	1.39
2	D	304	UMP	O4'-C4'	2.91	1.51	1.45
3	B	402	F89	C5-C4A	2.86	1.46	1.41
3	C	403	F89	C5-C4A	2.85	1.46	1.41
3	B	402	F89	C13-N12	2.82	1.46	1.38
3	B	402	F89	C16-C15	2.80	1.43	1.39
3	B	402	F89	C3-N4	2.76	1.38	1.34
3	A	401	F89	C5-C4A	2.70	1.46	1.41
3	D	404	F89	C5-C4A	2.69	1.46	1.41
3	D	404	F89	C13-N12	2.67	1.46	1.38
3	C	403	F89	C19-C15	-2.61	1.46	1.50
3	A	401	F89	C3-N4	2.52	1.38	1.34
3	A	401	F89	C-N	2.52	1.38	1.36
3	B	402	F89	C3-N2	2.51	1.38	1.34
3	A	401	F89	C19-C15	-2.50	1.46	1.50
2	C	303	UMP	O4'-C4'	2.50	1.50	1.45
2	A	301	UMP	O4'-C4'	2.46	1.50	1.45
3	C	403	F89	C3-N4	2.46	1.38	1.34
2	A	301	UMP	P-OP3	-2.45	1.45	1.54
2	B	302	UMP	O4'-C4'	2.44	1.50	1.45
3	B	402	F89	C14-C15	2.40	1.43	1.39
3	A	401	F89	C3-N2	2.34	1.38	1.34
2	C	303	UMP	P-OP3	-2.31	1.45	1.54
3	D	404	F89	C3-N4	2.28	1.38	1.34
2	D	304	UMP	P-OP3	-2.25	1.46	1.54
2	A	301	UMP	P-OP2	-2.25	1.46	1.54
2	D	304	UMP	C2-N3	2.21	1.42	1.38
3	C	403	F89	C-N	2.19	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	UMP	P-OP3	-2.18	1.46	1.54
3	C	403	F89	C3-N2	2.17	1.37	1.34
3	D	404	F89	C14-C15	2.15	1.43	1.39
2	B	302	UMP	P-OP1	-2.07	1.43	1.50

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	404	F89	C19-N-CA	-15.64	109.06	123.71
3	B	402	F89	C19-N-CA	-15.52	109.17	123.71
3	A	401	F89	C19-N-CA	-14.35	110.27	123.71
3	C	403	F89	C19-N-CA	-14.09	110.52	123.71
3	D	404	F89	C3-N4-C4A	10.88	123.92	116.54
3	B	402	F89	C3-N4-C4A	9.96	123.29	116.54
3	C	403	F89	C3-N4-C4A	9.94	123.28	116.54
3	B	402	F89	CA-N-C	9.86	137.12	121.82
3	D	404	F89	CA-N-C	9.69	136.84	121.82
3	A	401	F89	C3-N4-C4A	9.61	123.05	116.54
3	C	403	F89	CA-N-C	8.57	135.11	121.82
3	A	401	F89	CA-N-C	8.52	135.03	121.82
3	C	403	F89	C1A-C1-N2	-4.67	119.94	124.09
2	A	301	UMP	C5-C6-N1	-4.60	110.40	120.68
3	D	404	F89	C1A-C1-N2	-4.53	120.07	124.09
3	A	401	F89	C1A-C1-N2	-4.52	120.08	124.09
3	B	402	F89	C1A-C1-N2	-4.45	120.14	124.09
3	A	401	F89	N4-C3-N2	-4.07	118.23	125.72
3	D	404	F89	N4-C3-N2	-4.06	118.25	125.72
3	B	402	F89	N4-C3-N2	-4.05	118.26	125.72
3	C	403	F89	N4-C3-N2	-4.00	118.36	125.72
2	A	301	UMP	OP3-P-O5'	3.80	116.83	106.73
2	B	302	UMP	C5-C4-N3	-3.59	115.42	123.31
3	D	404	F89	C16-C-N	-3.38	104.45	106.44
2	A	301	UMP	C6-N1-C2	3.28	126.40	121.20
2	C	303	UMP	C5-C6-N1	-3.25	113.44	120.68
2	D	304	UMP	C5-C4-N3	-3.21	116.24	123.31
3	B	402	F89	C3M-C3-N2	3.03	121.88	117.15
2	C	303	UMP	C6-N1-C2	3.03	126.00	121.20
3	D	404	F89	C3M-C3-N2	2.91	121.69	117.15
3	B	402	F89	C16-C-N	-2.88	104.75	106.44
2	D	304	UMP	O4'-C1'-C2'	-2.68	101.18	106.25
2	D	304	UMP	P-O5'-C5'	2.64	125.55	118.30
2	D	304	UMP	O4'-C4'-C3'	-2.62	99.55	105.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	F89	C3M-C3-N2	2.57	121.16	117.15
3	A	401	F89	C3M-C3-N2	2.56	121.15	117.15
2	B	302	UMP	O4'-C1'-C2'	-2.50	101.53	106.25
2	C	303	UMP	O4'-C1'-C2'	-2.40	101.71	106.25
3	B	402	F89	C15-C19-N	2.36	102.96	102.18
2	B	302	UMP	O4'-C4'-C3'	-2.35	100.18	105.67
3	B	402	F89	CB-CA-N	2.32	115.30	112.65
2	D	304	UMP	C4'-O4'-C1'	2.32	115.06	109.45
2	A	301	UMP	O4'-C1'-C2'	-2.31	101.89	106.25
2	C	303	UMP	OP3-P-O5'	2.31	112.87	106.73
2	B	302	UMP	O5'-P-OP1	-2.29	100.06	106.47
3	C	403	F89	O-C-C16	-2.24	124.31	128.68
3	A	401	F89	C3M-C3-N4	2.23	120.62	117.16
3	D	404	F89	C19-N-C	2.20	114.03	113.12
3	C	403	F89	C7-C6A-C6	-2.15	118.16	123.19
3	C	403	F89	C3M-C3-N4	2.13	120.47	117.16
3	C	403	F89	C16-C-N	-2.12	105.20	106.44
3	B	402	F89	C7-C6A-C6	-2.11	118.26	123.19
3	A	401	F89	O-C-C16	-2.10	124.58	128.68
3	A	401	F89	C7-C6A-C6	-2.10	118.28	123.19
3	D	404	F89	C7-C6A-C6	-2.07	118.35	123.19
2	A	301	UMP	O4'-C4'-C3'	-2.04	100.92	105.67
2	C	303	UMP	O4'-C4'-C3'	-2.02	100.96	105.67
3	D	404	F89	O-C-C16	-2.01	124.77	128.68

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	404	F89	CT-CA-N-C19
3	D	404	F89	CB-CA-N-C19
3	D	404	F89	CB-CA-N-C
3	D	404	F89	CA-CB-CG-CD
3	B	402	F89	CB-CA-N-C
3	B	402	F89	CA-CB-CG-CD
3	B	402	F89	CB-CA-N-C19
3	A	401	F89	CT-CA-N-C19
3	C	403	F89	CT-CA-N-C19
3	B	402	F89	CT-CA-N-C19
3	A	401	F89	CB-CA-N-C
3	A	401	F89	CA-CB-CG-CD
2	C	303	UMP	C5'-O5'-P-OP1

*Continued on next page...*

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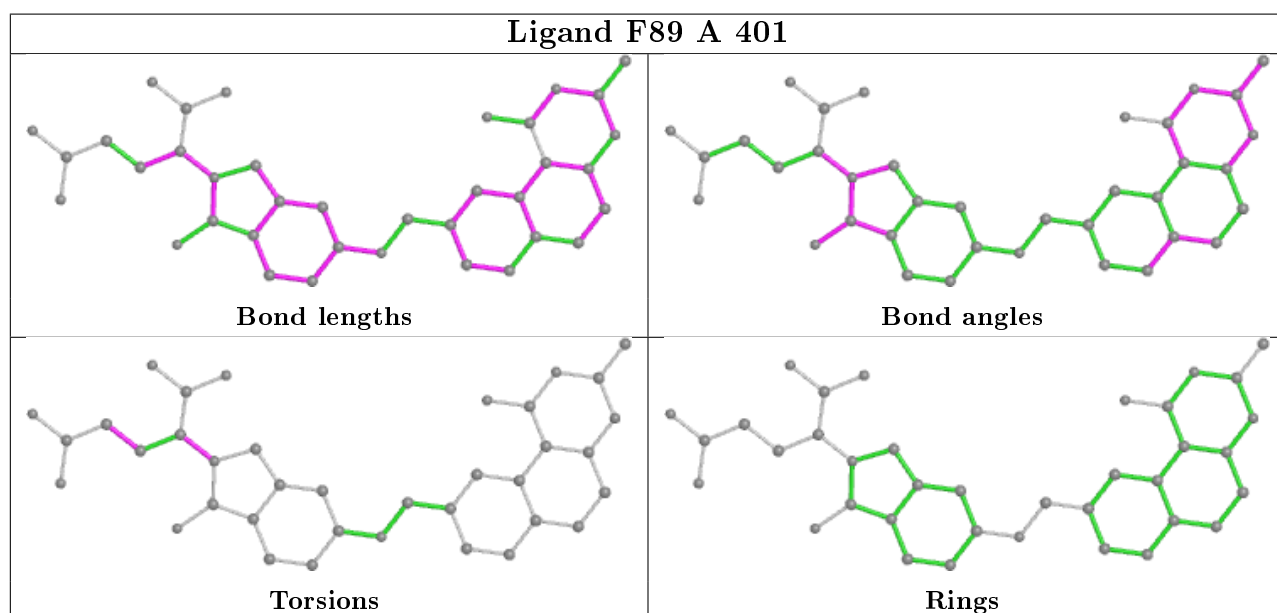
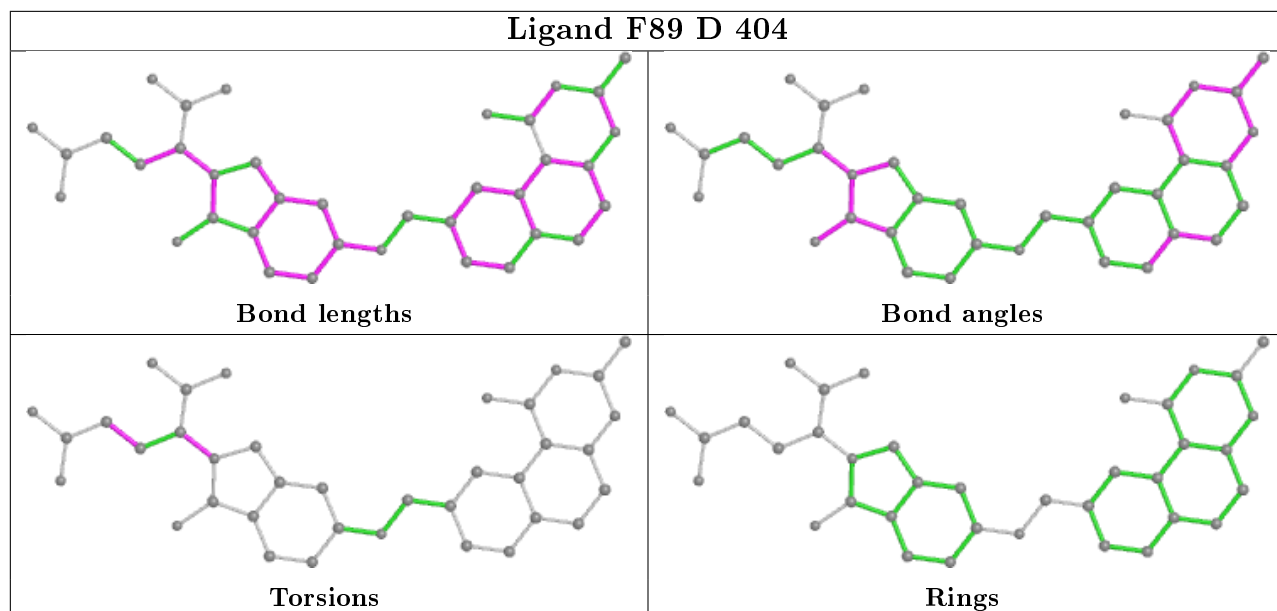
Mol	Chain	Res	Type	Atoms
3	C	403	F89	CB-CA-N-C
3	A	401	F89	CB-CA-N-C19
3	C	403	F89	CB-CA-N-C19
3	C	403	F89	CA-CB-CG-CD
2	C	303	UMP	O4'-C4'-C5'-O5'
2	B	302	UMP	C3'-C4'-C5'-O5'
2	A	301	UMP	O4'-C4'-C5'-O5'
2	D	304	UMP	O4'-C4'-C5'-O5'
2	B	302	UMP	O4'-C4'-C5'-O5'

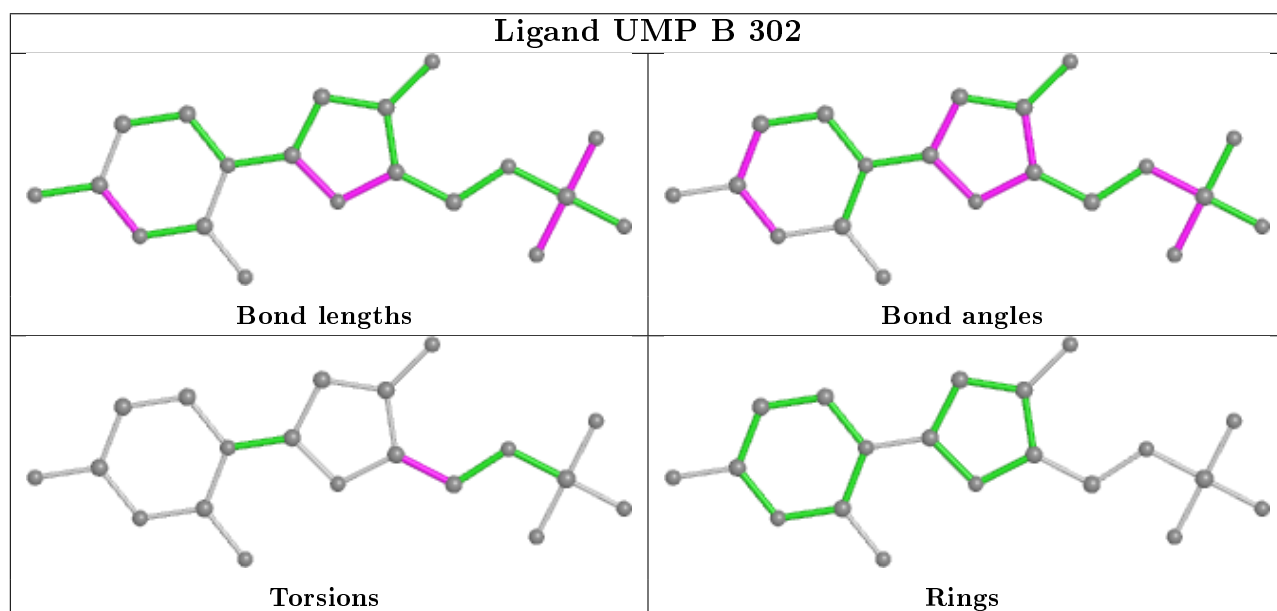
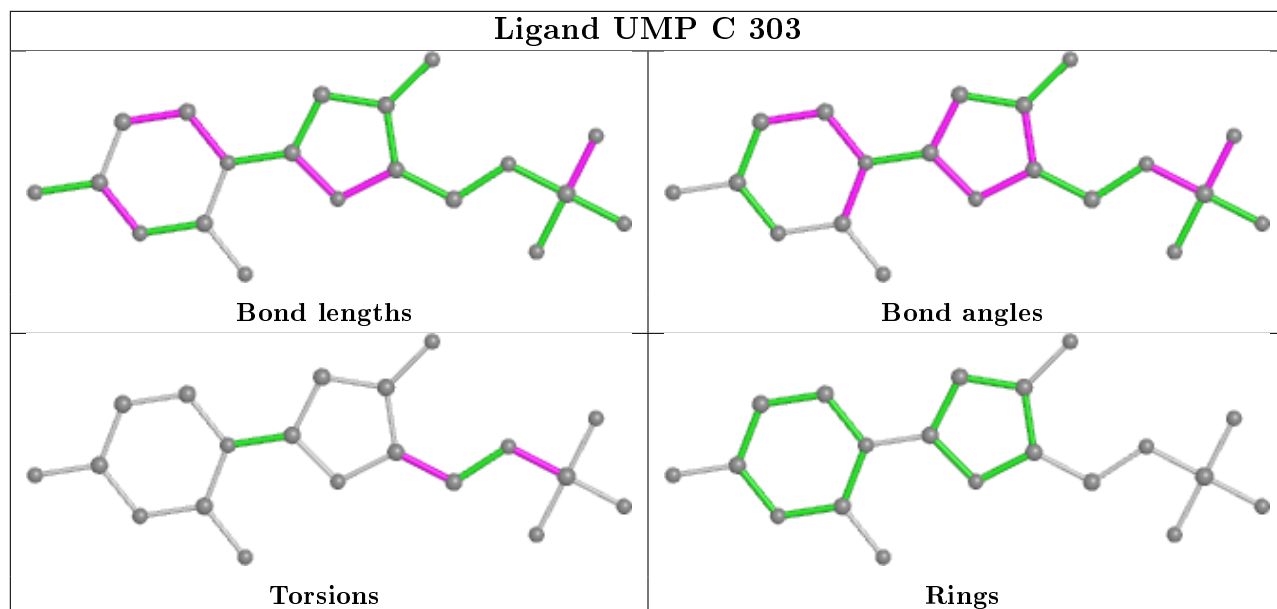
There are no ring outliers.

6 monomers are involved in 20 short contacts:

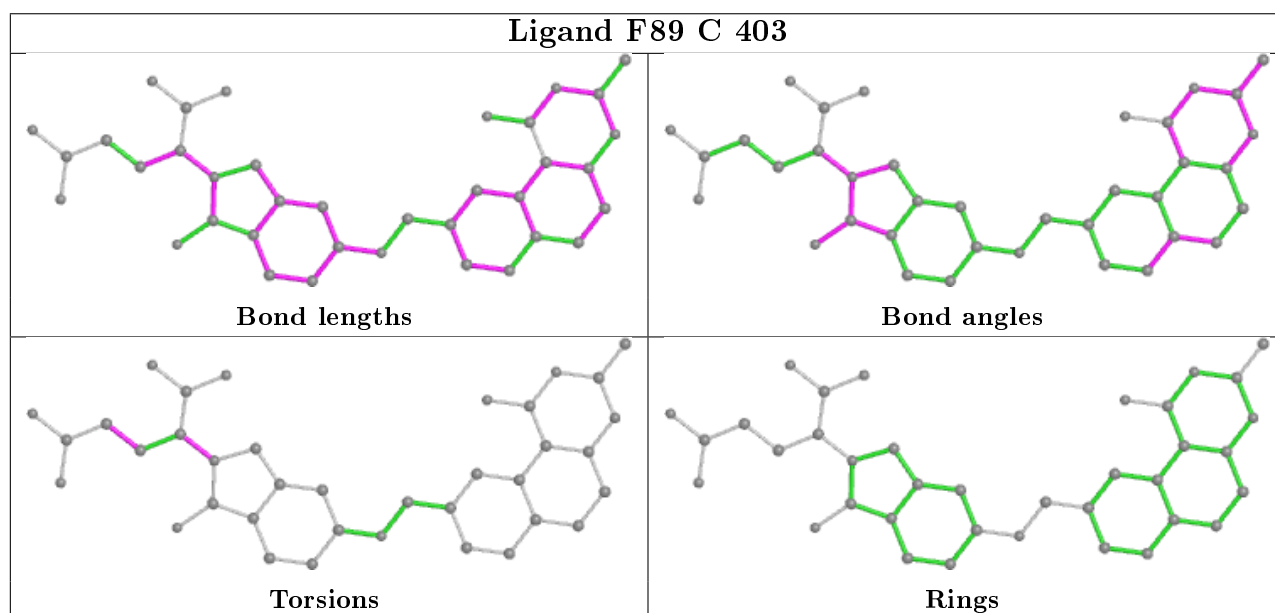
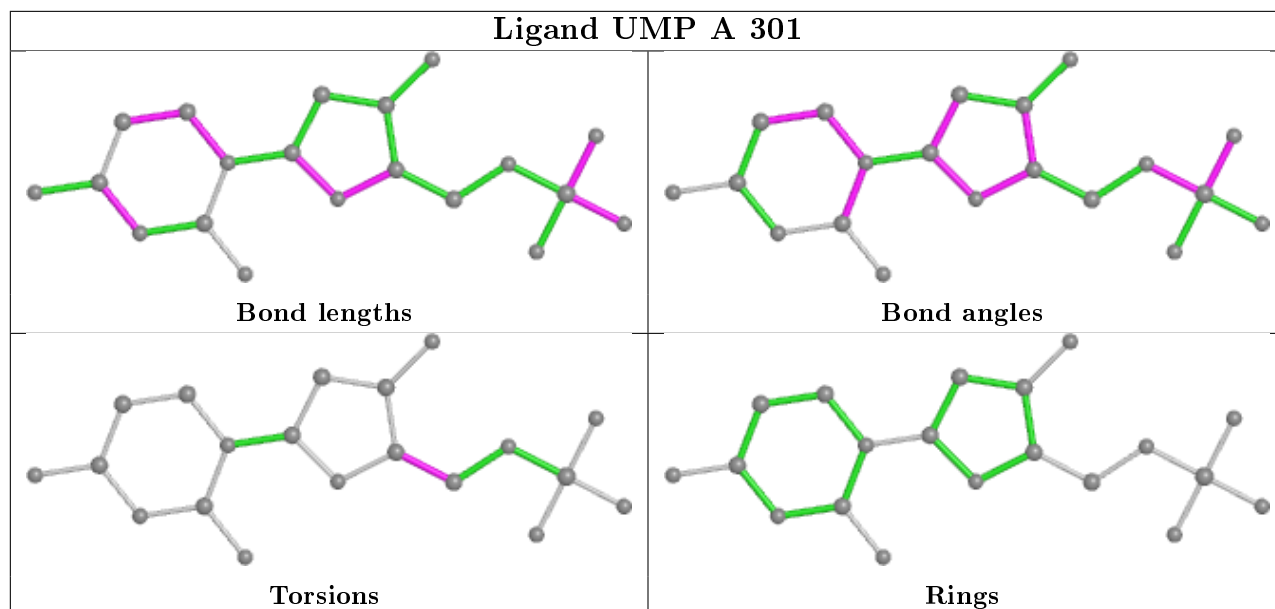
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	404	F89	5	0
3	A	401	F89	2	0
2	B	302	UMP	2	0
3	C	403	F89	4	0
3	B	402	F89	5	0
2	D	304	UMP	2	0

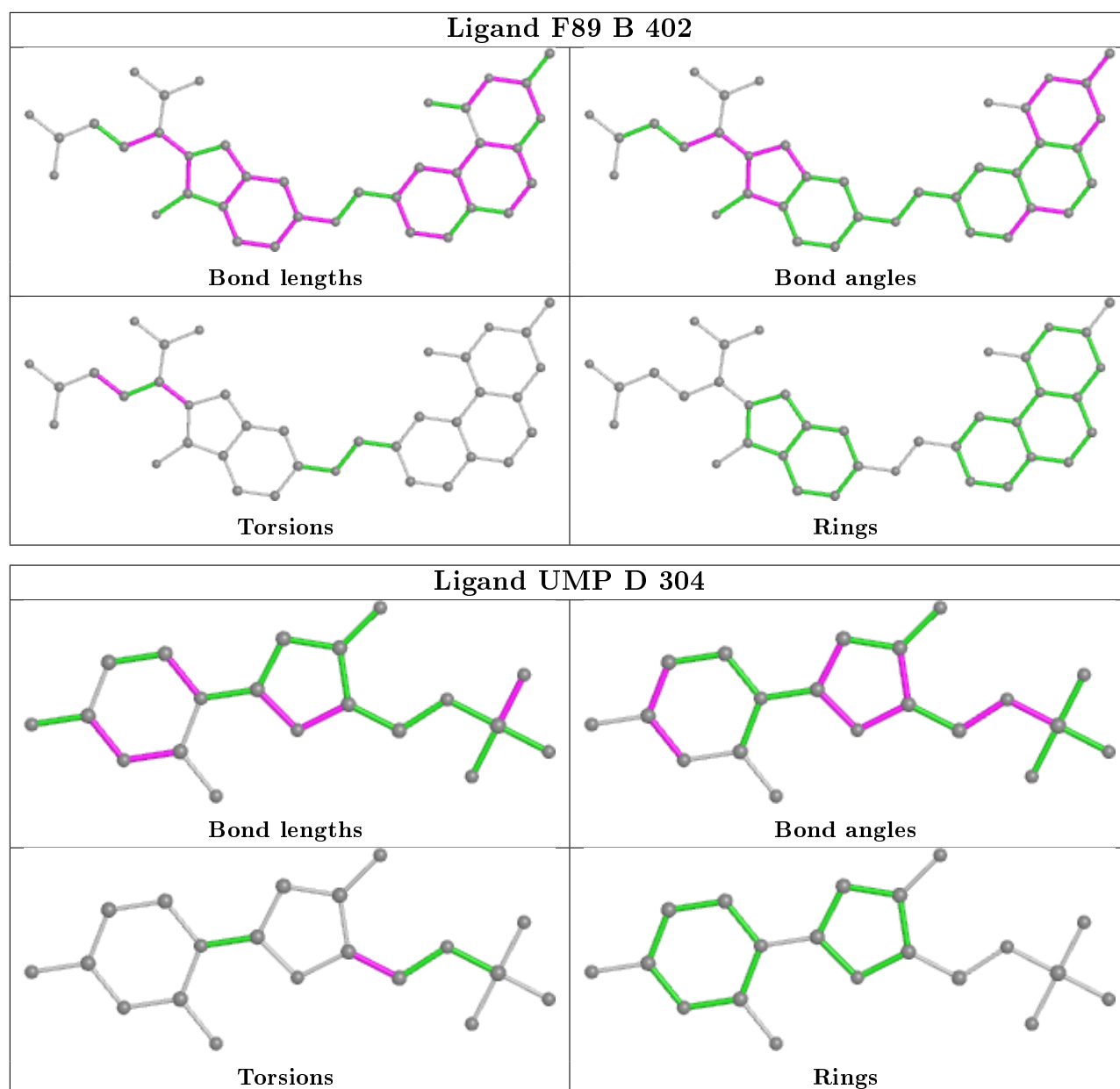
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.