



## Full wwPDB EM Validation Report ⓘ

Jul 16, 2025 – 02:48 AM JST

PDB ID : 8Z3R / pdb\_00008z3r  
EMDB ID : EMD-39752  
Title : The structure of type III CRISPR-associated deaminase in complex cA4  
Authors : Chen, M.R.; Li, Z.X.; Xiao, Y.B.  
Deposited on : 2024-04-16  
Resolution : 2.28 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

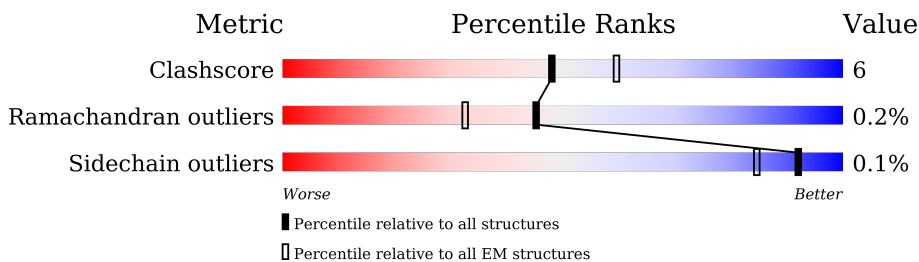
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.28 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	635	 83% 14% .
1	B	635	 85% 11% .
1	C	635	 83% 13% .
1	D	635	 84% 12% .
1	E	635	 86% 11% .
1	F	635	 81% 16% .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29190 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Adenosine deaminase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
1	B	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
1	C	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
1	D	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
1	E	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		
1	F	615	Total	C	N	O	S	0	0
			4820	3044	895	859	22		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	630	HIS	-	expression tag	UNP A0A6M1RED6
A	631	HIS	-	expression tag	UNP A0A6M1RED6
A	632	HIS	-	expression tag	UNP A0A6M1RED6
A	633	HIS	-	expression tag	UNP A0A6M1RED6
A	634	HIS	-	expression tag	UNP A0A6M1RED6
A	635	HIS	-	expression tag	UNP A0A6M1RED6
B	630	HIS	-	expression tag	UNP A0A6M1RED6
B	631	HIS	-	expression tag	UNP A0A6M1RED6
B	632	HIS	-	expression tag	UNP A0A6M1RED6
B	633	HIS	-	expression tag	UNP A0A6M1RED6
B	634	HIS	-	expression tag	UNP A0A6M1RED6
B	635	HIS	-	expression tag	UNP A0A6M1RED6
C	630	HIS	-	expression tag	UNP A0A6M1RED6
C	631	HIS	-	expression tag	UNP A0A6M1RED6
C	632	HIS	-	expression tag	UNP A0A6M1RED6
C	633	HIS	-	expression tag	UNP A0A6M1RED6
C	634	HIS	-	expression tag	UNP A0A6M1RED6
C	635	HIS	-	expression tag	UNP A0A6M1RED6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	630	HIS	-	expression tag	UNP A0A6M1RED6
D	631	HIS	-	expression tag	UNP A0A6M1RED6
D	632	HIS	-	expression tag	UNP A0A6M1RED6
D	633	HIS	-	expression tag	UNP A0A6M1RED6
D	634	HIS	-	expression tag	UNP A0A6M1RED6
D	635	HIS	-	expression tag	UNP A0A6M1RED6
E	630	HIS	-	expression tag	UNP A0A6M1RED6
E	631	HIS	-	expression tag	UNP A0A6M1RED6
E	632	HIS	-	expression tag	UNP A0A6M1RED6
E	633	HIS	-	expression tag	UNP A0A6M1RED6
E	634	HIS	-	expression tag	UNP A0A6M1RED6
E	635	HIS	-	expression tag	UNP A0A6M1RED6
F	630	HIS	-	expression tag	UNP A0A6M1RED6
F	631	HIS	-	expression tag	UNP A0A6M1RED6
F	632	HIS	-	expression tag	UNP A0A6M1RED6
F	633	HIS	-	expression tag	UNP A0A6M1RED6
F	634	HIS	-	expression tag	UNP A0A6M1RED6
F	635	HIS	-	expression tag	UNP A0A6M1RED6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Zn 1 1	0
2	B	1	Total Zn 1 1	0
2	C	1	Total Zn 1 1	0
2	D	1	Total Zn 1 1	0
2	E	1	Total Zn 1 1	0
2	F	1	Total Zn 1 1	0

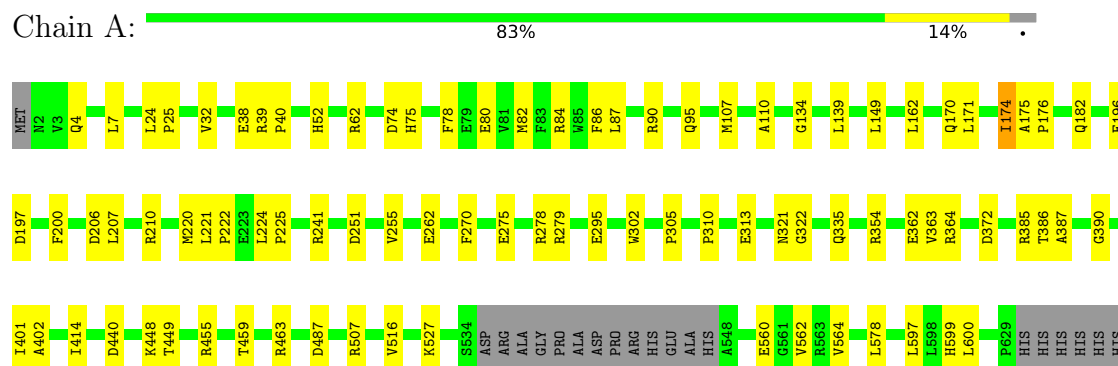
- Molecule 3 is 3'-O-[(R)-{[(2S,3aS,4S,6S,6aS)-6-(6-amino-9H-purin-9-yl)-2-hydroxy-2-oxotetrahydro-2H-2lambda 5 -furo[3,4-d][1,3,2]dioxaphosphol-4-yl]methoxy}(hydroxy)phosphoryl]adenosine (CCD ID: LQJ) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>10</sub>O<sub>12</sub>P<sub>2</sub>).



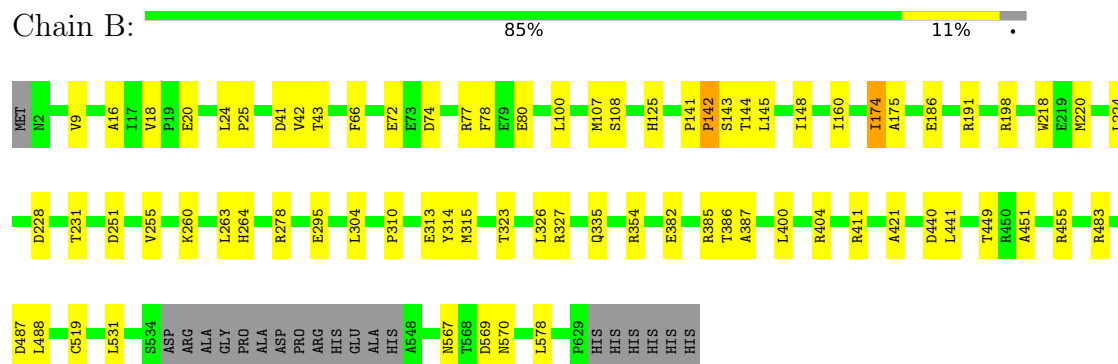
### 3 Residue-property plots

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

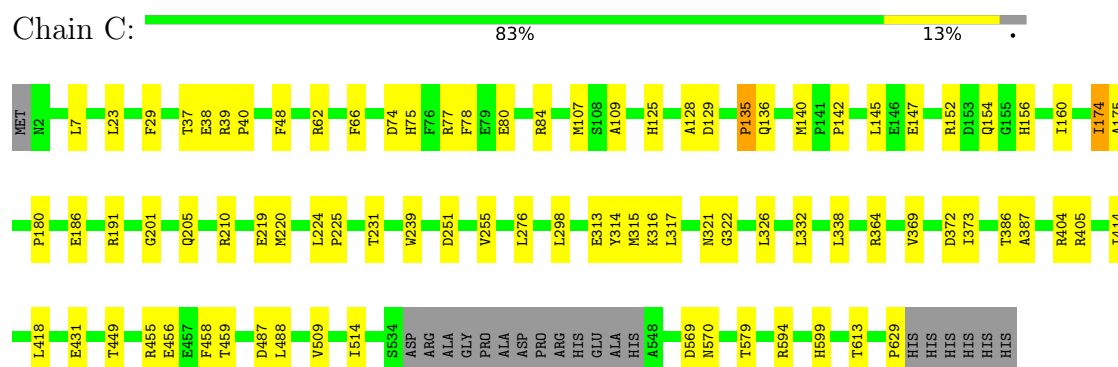
- Molecule 1: Adenosine deaminase domain-containing protein



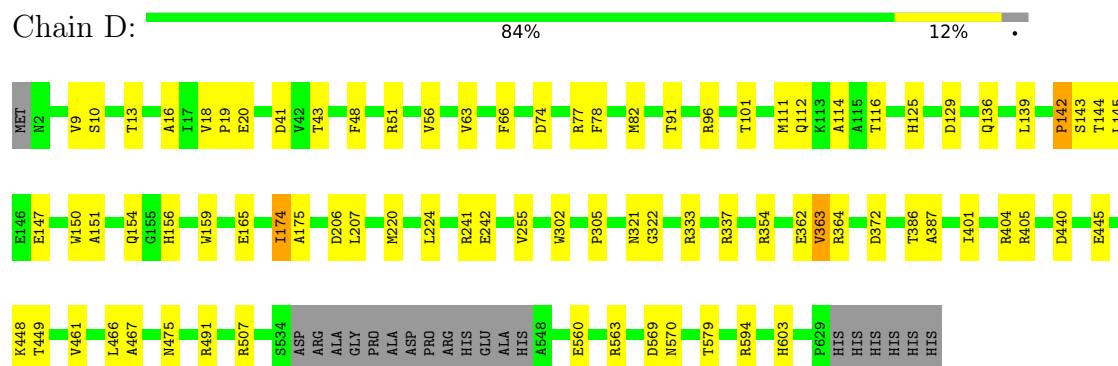
- Molecule 1: Adenosine deaminase domain-containing protein



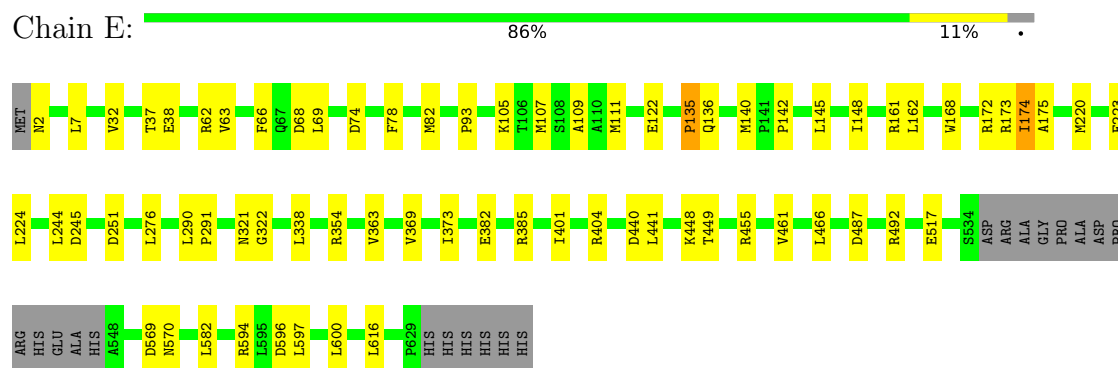
- Molecule 1: Adenosine deaminase domain-containing protein



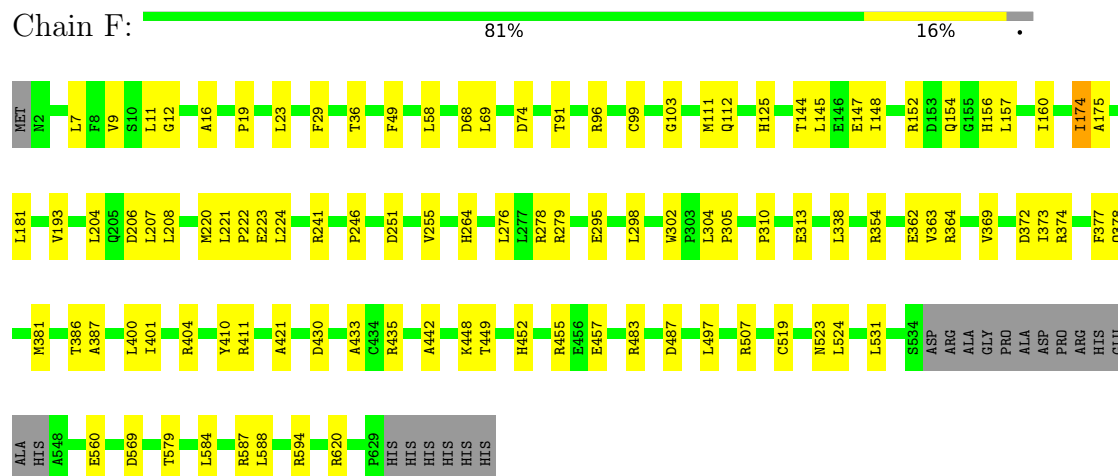
- Molecule 1: Adenosine deaminase domain-containing protein



- Molecule 1: Adenosine deaminase domain-containing protein



- Molecule 1: Adenosine deaminase domain-containing protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1005809	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.14	0/4936	0.37	0/6712
1	B	0.14	0/4936	0.38	1/6712 (0.0%)
1	C	0.14	0/4936	0.39	2/6712 (0.0%)
1	D	0.15	0/4936	0.40	3/6712 (0.0%)
1	E	0.15	0/4936	0.40	2/6712 (0.0%)
1	F	0.14	0/4936	0.39	0/6712
All	All	0.14	0/29616	0.39	8/40272 (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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	PRO	CA-N-CD	-10.65	97.09	112.00
1	B	142	PRO	CA-N-CD	-9.35	98.91	112.00
1	E	135	PRO	CA-N-CD	-8.33	100.34	112.00
1	D	142	PRO	CA-N-CD	-8.20	100.52	112.00
1	D	363	VAL	N-CA-C	-6.01	107.64	113.53
1	C	135	PRO	N-CD-CG	-5.66	94.71	103.20
1	E	363	VAL	N-CA-C	-5.62	108.02	113.53
1	D	142	PRO	N-CD-CG	-5.43	95.06	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	63	VAL	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4820	0	4786	59	0
1	B	4820	0	4786	48	0
1	C	4820	0	4786	56	0
1	D	4820	0	4786	57	0
1	E	4820	0	4786	46	0
1	F	4820	0	4786	66	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	44	0	0	1	0
3	B	44	0	0	1	0
3	C	44	0	0	1	0
3	D	44	0	0	2	0
3	F	88	0	0	2	0
All	All	29190	0	28716	330	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 6.

All (330) 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)
3:F:703:LQJ:O2	3:F:703:LQJ:C2	1.68	1.24
3:A:702:LQJ:O2	3:A:702:LQJ:C2	1.68	1.23
3:B:702:LQJ:O2	3:B:702:LQJ:C2	1.68	1.22
3:D:702:LQJ:O2	3:D:702:LQJ:C2	1.68	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:702:LQJ:C2	3:C:702:LQJ:O2	1.68	1.21
3:F:702:LQJ:O2	3:F:702:LQJ:C2	1.68	1.18
1:B:142:PRO:HD2	1:B:143:SER:H	1.30	0.94
1:E:135:PRO:HD2	1:E:136:GLN:H	1.37	0.88
1:C:135:PRO:HD2	1:C:136:GLN:H	1.41	0.84
1:D:174:ILE:HG13	1:D:175:ALA:H	1.43	0.83
1:E:82:MET:HE1	1:E:111:MET:HA	1.60	0.83
1:A:90:ARG:HE	1:A:176:PRO:HG3	1.45	0.82
1:A:182:GLN:NE2	1:A:196:GLU:OE2	2.13	0.82
1:A:174:ILE:HG22	1:A:175:ALA:H	1.48	0.79
1:A:38:GLU:HA	1:A:62:ARG:HD3	1.64	0.78
1:D:116:THR:HA	1:D:165:GLU:HG2	1.66	0.77
1:D:142:PRO:HD2	1:D:143:SER:H	1.50	0.76
1:E:38:GLU:HA	1:E:62:ARG:HH11	1.50	0.76
1:F:278:ARG:NH1	1:F:295:GLU:OE1	2.18	0.75
1:C:38:GLU:HA	1:C:62:ARG:HH11	1.50	0.74
1:C:135:PRO:HD2	1:C:136:GLN:N	2.01	0.74
1:D:220:MET:HE3	1:D:241:ARG:HH22	1.52	0.73
1:C:174:ILE:HG22	1:C:175:ALA:H	1.55	0.72
1:E:135:PRO:HD2	1:E:136:GLN:N	2.04	0.71
1:A:278:ARG:NH1	1:A:295:GLU:OE2	2.19	0.70
1:D:10:SER:HB3	1:D:111:MET:HE3	1.74	0.69
1:D:151:ALA:HA	1:D:154:GLN:HE21	1.56	0.69
1:A:386:THR:HG22	1:A:387:ALA:H	1.59	0.68
1:B:386:THR:HG22	1:B:387:ALA:H	1.57	0.68
1:D:386:THR:HG22	1:D:387:ALA:H	1.58	0.67
1:D:101:THR:OG1	1:D:125:HIS:ND1	2.24	0.67
1:C:142:PRO:HD2	1:C:147:GLU:HG2	1.77	0.67
1:D:142:PRO:HD2	1:D:143:SER:N	2.10	0.67
1:A:7:LEU:HB3	1:A:32:VAL:HG12	1.76	0.67
1:F:386:THR:HG22	1:F:387:ALA:H	1.60	0.66
1:B:264:HIS:HA	1:B:354:ARG:HH12	1.60	0.66
1:D:364:ARG:NH1	1:D:372:ASP:OD2	2.29	0.66
1:F:264:HIS:HA	1:F:354:ARG:HH12	1.61	0.66
1:A:402:ALA:HB1	1:A:414:ILE:HG12	1.78	0.65
1:E:174:ILE:HG22	1:E:175:ALA:H	1.61	0.65
1:D:333:ARG:HG2	1:D:337:ARG:NH1	2.12	0.64
1:D:66:PHE:HD1	1:D:74:ASP:HB2	1.63	0.63
1:B:278:ARG:NH1	1:B:295:GLU:OE2	2.18	0.63
1:B:323:THR:O	1:B:327:ARG:NH1	2.32	0.62
1:A:364:ARG:NH1	1:A:372:ASP:OD2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:PRO:HD2	1:B:143:SER:N	1.99	0.62
1:C:386:THR:HG22	1:C:387:ALA:H	1.64	0.62
1:F:364:ARG:NH1	1:F:372:ASP:OD2	2.30	0.62
1:E:66:PHE:CE1	1:E:74:ASP:HB3	2.35	0.61
1:C:66:PHE:HD1	1:C:74:ASP:HB2	1.66	0.61
1:E:66:PHE:HE1	1:E:74:ASP:HB3	1.66	0.60
1:F:298:LEU:HD22	1:F:302:TRP:CD1	2.37	0.60
1:A:206:ASP:OD2	1:A:207:LEU:N	2.35	0.59
1:D:129:ASP:HB2	1:D:156:HIS:CD2	2.36	0.59
1:D:91:THR:HG23	1:D:96:ARG:HE	1.66	0.59
1:C:364:ARG:NH1	1:C:372:ASP:OD2	2.35	0.59
1:C:255:VAL:HG12	1:C:579:THR:HG23	1.84	0.59
1:C:455:ARG:NH1	1:C:487:ASP:O	2.36	0.59
1:F:255:VAL:HG12	1:F:579:THR:HG23	1.84	0.59
1:B:66:PHE:HD1	1:B:74:ASP:HB2	1.69	0.58
1:A:354:ARG:NH1	1:A:440:ASP:OD1	2.37	0.58
1:A:38:GLU:HA	1:A:62:ARG:HH11	1.68	0.58
1:B:326:LEU:HD21	1:B:335:GLN:HG3	1.87	0.57
1:A:52:HIS:CE1	1:A:149:LEU:HD11	2.40	0.57
1:F:246:PRO:HG3	1:F:587:ARG:HG3	1.86	0.57
1:C:386:THR:HG22	1:C:387:ALA:N	2.19	0.57
1:D:48:PHE:HA	1:D:145:LEU:HD21	1.85	0.57
1:B:404:ARG:NH1	1:B:449:THR:O	2.38	0.57
1:A:385:ARG:NH1	1:A:390:GLY:O	2.35	0.57
1:F:156:HIS:O	1:F:157:LEU:HD23	2.04	0.57
1:E:37:THR:HB	1:E:66:PHE:HD2	1.69	0.57
1:E:105:LYS:NZ	1:F:103:GLY:O	2.38	0.56
1:E:354:ARG:NH1	1:E:440:ASP:OD2	2.38	0.56
1:E:455:ARG:NH1	1:E:487:ASP:O	2.38	0.56
1:D:129:ASP:HB2	1:D:156:HIS:HD2	1.71	0.56
1:F:386:THR:HG22	1:F:387:ALA:N	2.21	0.56
1:D:404:ARG:NH1	1:D:449:THR:O	2.38	0.56
1:D:354:ARG:HB3	1:D:401:ILE:HD11	1.88	0.55
1:E:223:GLU:OE2	1:F:620:ARG:NH2	2.37	0.55
1:B:440:ASP:OD2	1:B:441:LEU:N	2.39	0.55
1:B:9:VAL:HG11	1:B:18:VAL:HG13	1.89	0.55
1:D:74:ASP:HA	1:D:77:ARG:HG2	1.88	0.55
1:F:302:TRP:O	1:F:305:PRO:HD3	2.07	0.55
1:A:302:TRP:O	1:A:305:PRO:HD3	2.07	0.55
1:C:405:ARG:HG2	1:C:405:ARG:HH11	1.72	0.55
1:A:386:THR:HG22	1:A:387:ALA:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:THR:O	1:A:463:ARG:HG2	2.06	0.55
1:C:74:ASP:HA	1:C:77:ARG:HG2	1.88	0.55
1:F:145:LEU:HD13	1:F:148:ILE:HD12	1.88	0.55
1:C:210:ARG:HG3	1:C:231:THR:HG23	1.89	0.55
1:B:228:ASP:O	1:B:231:THR:OG1	2.25	0.54
1:B:41:ASP:OD1	1:B:43:THR:HG23	2.07	0.54
1:C:48:PHE:HD1	1:C:145:LEU:HD22	1.71	0.54
1:D:386:THR:HG22	1:D:387:ALA:N	2.23	0.54
1:B:174:ILE:HG13	1:B:175:ALA:H	1.72	0.54
1:F:174:ILE:HG12	1:F:175:ALA:H	1.73	0.54
1:D:16:ALA:HA	1:D:19:PRO:HG2	1.90	0.54
1:A:210:ARG:HH22	1:B:218:TRP:CD1	2.25	0.53
1:B:386:THR:HG22	1:B:387:ALA:N	2.23	0.53
1:D:507:ARG:NH2	1:D:560:GLU:HB3	2.23	0.53
1:C:37:THR:HB	1:C:66:PHE:HD2	1.73	0.53
1:A:24:LEU:HD12	1:A:25:PRO:HD2	1.90	0.53
1:D:136:GLN:NE2	1:D:139:LEU:HD13	2.24	0.52
1:E:354:ARG:HB3	1:E:401:ILE:HD11	1.90	0.52
1:B:310:PRO:HG2	1:B:313:GLU:OE1	2.09	0.52
1:E:82:MET:HE3	1:E:111:MET:HE2	1.90	0.52
1:F:279:ARG:HD2	1:F:338:LEU:HD21	1.92	0.52
1:F:524:LEU:HD12	1:F:588:LEU:HD21	1.92	0.52
1:B:314:TYR:HD2	1:B:315:MET:HE2	1.75	0.52
1:C:298:LEU:HD23	1:C:317:LEU:HD22	1.90	0.52
1:E:37:THR:O	1:E:38:GLU:HG2	2.10	0.52
1:F:455:ARG:NH1	1:F:487:ASP:O	2.43	0.52
1:A:170:GLN:HG2	1:A:171:LEU:HD12	1.92	0.52
1:C:66:PHE:CD1	1:C:74:ASP:HB2	2.44	0.51
1:C:404:ARG:NH1	1:C:449:THR:O	2.43	0.51
1:D:144:THR:O	1:D:147:GLU:HG2	2.10	0.51
1:E:276:LEU:HD22	1:E:338:LEU:HD13	1.91	0.51
1:F:354:ARG:HB3	1:F:401:ILE:HD11	1.92	0.51
1:F:483:ARG:O	1:F:487:ASP:HB2	2.10	0.51
1:F:23:LEU:HD22	1:F:152:ARG:HH12	1.75	0.51
1:D:321:ASN:OD1	1:D:322:GLY:N	2.43	0.51
1:F:507:ARG:NH2	1:F:560:GLU:OE1	2.44	0.51
1:F:181:LEU:HD22	1:F:193:VAL:HB	1.92	0.51
1:A:174:ILE:HG22	1:A:175:ALA:N	2.22	0.50
1:B:66:PHE:CD1	1:B:74:ASP:HB2	2.46	0.50
1:B:74:ASP:HA	1:B:77:ARG:HG2	1.92	0.50
1:C:129:ASP:HB2	1:C:156:HIS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:310:PRO:HD2	1:F:313:GLU:OE2	2.10	0.50
1:A:562:VAL:HG12	1:A:564:VAL:HG13	1.92	0.50
1:D:405:ARG:HG2	1:D:405:ARG:HH11	1.76	0.50
1:A:197:ASP:OD2	1:A:197:ASP:N	2.45	0.50
1:E:162:LEU:HD12	1:E:162:LEU:O	2.10	0.50
1:E:290:LEU:HD12	1:E:291:PRO:HD2	1.93	0.50
1:D:448:LYS:HG3	1:D:449:THR:HG23	1.93	0.50
1:C:314:TYR:HD1	1:C:315:MET:HE2	1.75	0.50
1:A:220:MET:HE3	1:A:241:ARG:HH22	1.76	0.50
1:C:313:GLU:HA	1:C:316:LYS:HG2	1.94	0.50
1:B:483:ARG:O	1:B:487:ASP:HB2	2.12	0.50
1:F:91:THR:O	1:F:96:ARG:NH1	2.44	0.50
1:A:463:ARG:HH12	1:F:411:ARG:HD3	1.77	0.49
1:E:220:MET:HE1	1:E:224:LEU:HD21	1.93	0.49
1:A:310:PRO:HG2	1:A:313:GLU:OE1	2.11	0.49
1:C:80:GLU:OE2	1:C:84:ARG:NE	2.45	0.49
1:C:509:VAL:HG13	1:C:514:ILE:HB	1.93	0.49
1:D:66:PHE:CD1	1:D:74:ASP:HB2	2.44	0.49
1:F:448:LYS:HG3	1:F:449:THR:HG23	1.95	0.49
1:A:39:ARG:HB3	1:A:40:PRO:HD3	1.94	0.49
1:E:174:ILE:HG22	1:E:175:ALA:N	2.27	0.49
1:A:4:GLN:HB2	1:A:95:GLN:HE21	1.78	0.49
1:A:134:GLY:HA3	1:A:139:LEU:HD12	1.95	0.49
1:B:186:GLU:HB2	1:B:191:ARG:HG2	1.95	0.49
1:D:174:ILE:HG13	1:D:175:ALA:N	2.21	0.49
1:B:80:GLU:HG3	1:B:198:ARG:HD3	1.94	0.49
1:F:362:GLU:HG2	1:F:363:VAL:N	2.27	0.49
1:F:369:VAL:O	1:F:373:ILE:HG13	2.13	0.49
1:A:87:LEU:HD11	1:A:200:PHE:CE1	2.48	0.48
1:A:262:GLU:OE1	1:A:578:LEU:HD21	2.13	0.48
1:A:597:LEU:HA	1:A:600:LEU:HD12	1.94	0.48
1:E:78:PHE:CZ	1:E:107:MET:HG2	2.48	0.48
1:E:440:ASP:OD1	1:E:441:LEU:N	2.47	0.48
1:B:74:ASP:O	1:B:77:ARG:HG2	2.13	0.48
1:B:455:ARG:NH1	1:B:487:ASP:O	2.47	0.48
1:C:135:PRO:CD	1:C:136:GLN:H	2.21	0.48
1:C:414:ILE:O	1:C:418:LEU:HG	2.13	0.48
1:F:125:HIS:CE1	1:F:160:ILE:HD13	2.49	0.48
1:F:11:LEU:HB3	1:F:36:THR:HB	1.94	0.48
1:D:354:ARG:NH1	1:D:440:ASP:OD2	2.45	0.48
1:B:251:ASP:O	1:B:255:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ILE:HG22	1:C:175:ALA:N	2.24	0.48
1:D:20:GLU:O	1:D:159:TRP:HH2	1.96	0.48
1:F:524:LEU:HD13	1:F:584:LEU:HD21	1.95	0.48
1:F:452:HIS:ND1	1:F:483:ARG:HD2	2.28	0.48
1:F:497:LEU:HD11	1:F:523:ASN:ND2	2.29	0.48
1:B:304:LEU:HD12	1:B:531:LEU:HD11	1.95	0.48
1:C:23:LEU:HD22	1:C:152:ARG:NH1	2.29	0.48
1:F:16:ALA:HA	1:F:19:PRO:HG2	1.95	0.48
1:F:206:ASP:OD2	1:F:207:LEU:N	2.47	0.48
1:C:276:LEU:HD22	1:C:338:LEU:HD13	1.96	0.48
1:A:270:PHE:HB3	1:A:335:GLN:NE2	2.28	0.47
1:B:569:ASP:OD2	1:B:570:ASN:OD1	2.31	0.47
1:C:74:ASP:OD1	1:C:75:HIS:N	2.47	0.47
1:C:135:PRO:CD	1:C:136:GLN:N	2.75	0.47
1:D:206:ASP:OD2	1:D:207:LEU:N	2.46	0.47
1:E:122:GLU:OE2	1:E:161:ARG:HB2	2.15	0.47
1:A:455:ARG:NH1	1:A:487:ASP:O	2.48	0.47
1:D:445:GLU:OE2	1:D:475:ASN:N	2.42	0.47
1:E:321:ASN:OD1	1:E:322:GLY:N	2.47	0.47
1:F:9:VAL:HG23	1:F:99:CYS:HB3	1.97	0.47
1:F:519:CYS:SG	1:F:569:ASP:HB2	2.54	0.47
1:B:519:CYS:SG	1:B:569:ASP:HB2	2.55	0.47
1:D:9:VAL:HG11	1:D:18:VAL:HG13	1.96	0.47
1:D:255:VAL:HG12	1:D:579:THR:HG23	1.97	0.47
1:B:264:HIS:HA	1:B:354:ARG:NH1	2.28	0.47
1:D:82:MET:HE3	1:D:114:ALA:HB2	1.96	0.47
1:A:162:LEU:O	1:A:162:LEU:HD12	2.14	0.47
1:C:84:ARG:NH1	1:C:180:PRO:O	2.47	0.47
1:E:596:ASP:O	1:E:600:LEU:HG	2.15	0.47
1:F:220:MET:HE1	1:F:224:LEU:HD21	1.97	0.47
1:A:225:PRO:HG3	1:A:599:HIS:CD2	2.49	0.46
1:F:374:ARG:HH22	1:F:433:ALA:HB1	1.81	0.46
1:E:68:ASP:OD2	1:E:68:ASP:N	2.46	0.46
1:F:264:HIS:HA	1:F:354:ARG:NH1	2.30	0.46
1:F:304:LEU:HD12	1:F:531:LEU:HD11	1.98	0.46
1:B:145:LEU:HD23	1:B:148:ILE:HD12	1.97	0.46
1:D:154:GLN:HE22	1:D:156:HIS:CE1	2.34	0.46
1:C:431:GLU:OE2	1:C:613:THR:OG1	2.33	0.46
1:A:74:ASP:OD1	1:A:75:HIS:N	2.49	0.46
1:C:386:THR:CG2	1:C:387:ALA:H	2.29	0.46
1:E:7:LEU:HB3	1:E:32:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLU:O	1:C:220:MET:HG2	2.16	0.45
1:F:174:ILE:CG1	1:F:175:ALA:H	2.29	0.45
1:B:263:LEU:H	1:B:567:ASN:ND2	2.15	0.45
1:A:321:ASN:OD1	1:A:322:GLY:N	2.49	0.45
1:A:507:ARG:NH2	1:A:560:GLU:OE2	2.49	0.45
1:B:24:LEU:HD12	1:B:25:PRO:HD2	1.99	0.45
1:F:220:MET:HE3	1:F:241:ARG:NH2	2.31	0.45
1:C:109:ALA:HB1	1:D:112:GLN:OE1	2.16	0.45
1:D:63:VAL:HG21	1:D:78:PHE:HD1	1.81	0.45
1:A:463:ARG:NH1	1:F:411:ARG:HD3	2.31	0.45
1:B:41:ASP:OD1	1:B:42:VAL:N	2.50	0.45
1:D:136:GLN:HE21	1:D:139:LEU:HD13	1.81	0.45
1:B:143:SER:O	1:B:144:THR:OG1	2.33	0.45
1:F:68:ASP:OD1	1:F:68:ASP:N	2.50	0.45
1:F:152:ARG:HD2	1:F:152:ARG:C	2.41	0.45
1:A:78:PHE:CE2	1:A:107:MET:HG2	2.53	0.44
1:E:448:LYS:HG3	1:E:449:THR:HG23	1.99	0.44
1:A:251:ASP:O	1:A:255:VAL:HG23	2.17	0.44
1:F:276:LEU:HD22	1:F:338:LEU:HD23	1.99	0.44
1:A:52:HIS:HE1	1:A:149:LEU:HD11	1.83	0.44
1:B:16:ALA:O	1:B:20:GLU:HG3	2.17	0.44
1:E:109:ALA:HB1	1:F:112:GLN:OE1	2.17	0.44
1:F:457:GLU:N	1:F:457:GLU:OE1	2.50	0.44
1:B:382:GLU:OE1	1:B:385:ARG:NH2	2.51	0.44
1:A:221:LEU:N	1:A:222:PRO:HD2	2.33	0.44
1:C:239:TRP:CE3	1:C:629:PRO:HG3	2.53	0.44
1:D:41:ASP:OD2	1:D:43:THR:HG23	2.17	0.44
1:E:582:LEU:HD22	1:E:597:LEU:HD22	2.00	0.44
1:F:377:PHE:O	1:F:381:MET:HG3	2.18	0.44
1:A:354:ARG:HB3	1:A:401:ILE:HD11	2.00	0.44
1:D:242:GLU:HB2	1:D:594:ARG:HH12	1.82	0.44
1:D:150:TRP:O	1:D:154:GLN:HG3	2.17	0.43
1:E:140:MET:O	1:E:142:PRO:HD3	2.18	0.43
1:E:168:TRP:O	1:E:172:ARG:HG3	2.18	0.43
1:E:492:ARG:NE	1:E:517:GLU:OE2	2.51	0.43
1:F:111:MET:HA	1:F:111:MET:HE2	2.00	0.43
1:C:225:PRO:HG3	1:C:599:HIS:CD2	2.53	0.43
1:A:220:MET:HE1	1:A:224:LEU:HD21	1.99	0.43
1:B:451:ALA:HB1	1:B:488:LEU:HD12	2.00	0.43
1:F:7:LEU:HB2	1:F:29:PHE:CE2	2.54	0.43
1:D:461:VAL:HG13	1:D:466:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD11	1:A:207:LEU:HD13	2.00	0.43
1:A:174:ILE:HD12	1:A:174:ILE:HG23	1.79	0.43
1:D:220:MET:HE1	1:D:224:LEU:HD21	1.99	0.43
1:C:7:LEU:HB2	1:C:29:PHE:CD2	2.53	0.43
1:D:51:ARG:HH21	1:D:145:LEU:HD22	1.83	0.43
1:E:244:LEU:HD12	1:E:245:ASP:H	1.84	0.43
1:E:404:ARG:NH1	1:E:449:THR:O	2.51	0.43
1:F:204:LEU:O	1:F:208:LEU:HG	2.18	0.43
1:D:563:ARG:HH11	1:D:603:HIS:CE1	2.37	0.43
1:E:616:LEU:HD21	1:F:223:GLU:OE2	2.18	0.43
1:A:516:VAL:HB	1:A:564:VAL:HG12	2.00	0.43
1:E:461:VAL:HG13	1:E:466:LEU:HB3	1.99	0.43
1:C:174:ILE:HD12	1:C:174:ILE:HG23	1.80	0.43
1:F:11:LEU:HD12	1:F:12:GLY:N	2.33	0.43
1:C:125:HIS:HB3	1:C:160:ILE:HD11	2.01	0.42
1:D:405:ARG:HG2	1:D:405:ARG:NH1	2.34	0.42
1:B:141:PRO:HA	1:B:142:PRO:HD3	1.92	0.42
1:C:78:PHE:CE1	1:C:107:MET:HE3	2.54	0.42
1:D:302:TRP:O	1:D:305:PRO:HD3	2.19	0.42
1:E:69:LEU:HD12	1:E:69:LEU:HA	1.88	0.42
1:F:400:LEU:HD12	1:F:421:ALA:HB2	2.01	0.42
1:A:275:GLU:O	1:A:279:ARG:HG3	2.19	0.42
1:A:448:LYS:HG3	1:A:449:THR:HG23	2.01	0.42
1:B:125:HIS:CE1	1:B:160:ILE:HD13	2.54	0.42
1:F:221:LEU:N	1:F:222:PRO:HD2	2.34	0.42
1:F:374:ARG:NH1	1:F:378:GLN:HB2	2.33	0.42
1:B:220:MET:HE1	1:B:224:LEU:HD21	2.01	0.42
1:C:39:ARG:HB3	1:C:40:PRO:HD3	2.02	0.42
1:D:56:VAL:HG12	1:D:56:VAL:O	2.20	0.42
1:F:251:ASP:OD1	1:F:594:ARG:NH2	2.37	0.42
1:A:362:GLU:HG2	1:A:363:VAL:N	2.35	0.42
1:C:201:GLY:O	1:C:205:GLN:HG2	2.19	0.42
1:A:507:ARG:NH2	1:A:560:GLU:HB3	2.33	0.42
1:D:569:ASP:HB3	1:D:570:ASN:H	1.58	0.42
1:E:135:PRO:CD	1:E:136:GLN:N	2.77	0.42
1:C:456:GLU:O	1:C:459:THR:HG22	2.20	0.42
1:E:369:VAL:O	1:E:373:ILE:HG13	2.20	0.42
1:C:186:GLU:HG3	1:C:191:ARG:HB3	2.02	0.41
1:C:321:ASN:OD1	1:C:322:GLY:N	2.51	0.41
1:F:404:ARG:HG2	1:F:442:ALA:O	2.20	0.41
1:A:82:MET:HE1	1:A:110:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HD13	1:B:108:SER:HB3	2.02	0.41
1:C:326:LEU:HB3	1:C:332:LEU:HD13	2.03	0.41
1:E:251:ASP:CG	1:E:594:ARG:HH21	2.24	0.41
1:A:82:MET:HG2	1:A:86:PHE:HE2	1.85	0.41
1:C:37:THR:HB	1:C:66:PHE:CD2	2.54	0.41
1:C:458:PHE:CG	1:C:488:LEU:HD11	2.56	0.41
1:C:251:ASP:CG	1:C:594:ARG:HH21	2.28	0.41
1:C:369:VAL:O	1:C:373:ILE:HG13	2.21	0.41
1:D:142:PRO:CD	1:D:143:SER:H	2.26	0.41
1:C:128:ALA:HB3	1:C:140:MET:HE1	2.02	0.41
1:E:93:PRO:HD2	1:E:173:ARG:HH12	1.86	0.41
1:E:569:ASP:HB3	1:E:570:ASN:H	1.68	0.41
1:A:174:ILE:CG2	1:A:175:ALA:H	2.23	0.41
1:D:63:VAL:HG21	1:D:78:PHE:CD1	2.55	0.41
1:E:382:GLU:OE1	1:E:385:ARG:NH2	2.52	0.41
1:B:569:ASP:OD2	1:B:570:ASN:N	2.54	0.41
1:A:527:LYS:HB3	1:A:527:LYS:HE3	1.84	0.41
1:B:260:LYS:HD3	1:B:578:LEU:HD23	2.03	0.41
1:E:145:LEU:HD23	1:E:148:ILE:HD12	2.02	0.41
1:F:49:PHE:CD2	1:F:58:LEU:HD22	2.55	0.41
1:C:569:ASP:HB3	1:C:570:ASN:H	1.58	0.41
1:D:467:ALA:HB2	1:D:491:ARG:HH11	1.86	0.41
1:E:174:ILE:HD12	1:E:174:ILE:HG23	1.84	0.41
1:B:78:PHE:CZ	1:B:107:MET:HG2	2.56	0.41
1:B:400:LEU:HD12	1:B:421:ALA:HB2	2.03	0.41
1:F:69:LEU:HA	1:F:74:ASP:OD2	2.21	0.41
1:F:160:ILE:HD12	1:F:160:ILE:H	1.86	0.41
1:F:404:ARG:HA	1:F:410:TYR:CD1	2.56	0.40
1:D:362:GLU:HG2	1:D:363:VAL:N	2.37	0.40
1:F:144:THR:O	1:F:147:GLU:HG2	2.22	0.40
1:A:80:GLU:OE2	1:A:84:ARG:NE	2.50	0.40
1:B:72:GLU:CD	1:B:72:GLU:H	2.30	0.40
1:B:411:ARG:HE	1:B:411:ARG:HB3	1.76	0.40
1:C:154:GLN:HB3	1:C:156:HIS:HE1	1.86	0.40
1:C:220:MET:O	1:C:224:LEU:HG	2.22	0.40
1:D:13:THR:HG22	3:D:702:LQJ:O8	2.22	0.40
1:D:51:ARG:NH2	1:D:145:LEU:HD22	2.36	0.40
1:A:386:THR:CG2	1:A:387:ALA:H	2.31	0.40
1:F:430:ASP:O	1:F:435:ARG:HD2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	611/635 (96%)	575 (94%)	35 (6%)	1 (0%)	44	53
1	B	611/635 (96%)	584 (96%)	26 (4%)	1 (0%)	44	53
1	C	611/635 (96%)	578 (95%)	32 (5%)	1 (0%)	44	53
1	D	611/635 (96%)	578 (95%)	32 (5%)	1 (0%)	44	53
1	E	611/635 (96%)	572 (94%)	38 (6%)	1 (0%)	44	53
1	F	611/635 (96%)	578 (95%)	32 (5%)	1 (0%)	44	53
All	All	3666/3810 (96%)	3465 (94%)	195 (5%)	6 (0%)	45	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	Ile
1	D	174	Ile
1	F	174	Ile
1	A	174	Ile
1	C	174	Ile
1	E	174	Ile

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	495/511 (97%)	495 (100%)	0	100	100
1	B	495/511 (97%)	495 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	495/511 (97%)	495 (100%)	0	100	100
1	D	495/511 (97%)	495 (100%)	0	100	100
1	E	495/511 (97%)	494 (100%)	1 (0%)	92	96
1	F	495/511 (97%)	494 (100%)	1 (0%)	92	96
All	All	2970/3066 (97%)	2968 (100%)	2 (0%)	92	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2	ASN
1	F	154	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	335	GLN
1	A	342	HIS
1	A	601	GLN
1	B	6	HIS
1	B	33	HIS
1	B	136	GLN
1	B	286	ASN
1	B	307	GLN
1	B	489	ASN
1	B	567	ASN
1	B	570	ASN
1	B	601	GLN
1	B	603	HIS
1	C	75	HIS
1	C	156	HIS
1	C	307	GLN
1	C	335	GLN
1	C	603	HIS
1	D	136	GLN
1	D	154	GLN
1	D	209	GLN
1	D	570	ASN
1	E	182	GLN
1	E	307	GLN

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Mol	Chain	Res	Type
1	E	342	HIS
1	F	75	HIS
1	F	335	GLN
1	F	489	ASN
1	F	495	HIS
1	F	601	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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
3	LQJ	F	702	-	41,50,50	3.60	15 (36%)	44,78,78	1.36	5 (11%)
3	LQJ	B	702	-	41,50,50	3.60	15 (36%)	44,78,78	1.40	6 (13%)
3	LQJ	C	702	-	41,50,50	3.59	14 (34%)	44,78,78	1.43	5 (11%)
3	LQJ	D	702	-	41,50,50	3.60	15 (36%)	44,78,78	1.37	6 (13%)
3	LQJ	F	703	-	41,50,50	3.59	14 (34%)	44,78,78	1.35	5 (11%)
3	LQJ	A	702	-	41,50,50	3.60	15 (36%)	44,78,78	1.37	5 (11%)

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	LQJ	F	702	-	-	6/13/63/63	0/7/7/7
3	LQJ	B	702	-	-	5/13/63/63	0/7/7/7
3	LQJ	C	702	-	-	5/13/63/63	0/7/7/7
3	LQJ	D	702	-	-	6/13/63/63	0/7/7/7
3	LQJ	F	703	-	-	7/13/63/63	0/7/7/7
3	LQJ	A	702	-	-	5/13/63/63	0/7/7/7

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	LQJ	O2-C2	10.44	1.68	1.45
3	B	702	LQJ	O2-C2	10.43	1.68	1.45
3	D	702	LQJ	O2-C2	10.40	1.68	1.45
3	F	703	LQJ	O2-C2	10.37	1.68	1.45
3	C	702	LQJ	O2-C2	10.36	1.68	1.45
3	F	702	LQJ	O2-C2	10.35	1.68	1.45
3	F	703	LQJ	C20-C12	-9.32	1.27	1.52
3	F	702	LQJ	C20-C12	-9.26	1.28	1.52
3	A	702	LQJ	C20-C12	-9.21	1.28	1.52
3	C	702	LQJ	C20-C12	-9.20	1.28	1.52
3	D	702	LQJ	C20-C12	-9.19	1.28	1.52
3	B	702	LQJ	C20-C12	-9.11	1.28	1.52
3	A	702	LQJ	O2-C3	-7.95	1.30	1.41
3	B	702	LQJ	O2-C3	-7.92	1.30	1.41
3	D	702	LQJ	O2-C3	-7.88	1.30	1.41
3	F	703	LQJ	O2-C3	-7.86	1.30	1.41
3	C	702	LQJ	O2-C3	-7.85	1.30	1.41
3	F	702	LQJ	O2-C3	-7.85	1.30	1.41
3	B	702	LQJ	O7-C12	7.16	1.61	1.45
3	C	702	LQJ	C10-C2	-7.12	1.33	1.52
3	F	703	LQJ	C10-C2	-7.10	1.33	1.52
3	D	702	LQJ	O7-C12	7.09	1.60	1.45
3	C	702	LQJ	O7-C12	7.04	1.60	1.45
3	F	702	LQJ	C10-C2	-7.03	1.34	1.52
3	F	702	LQJ	O7-C12	7.02	1.60	1.45
3	A	702	LQJ	O7-C12	7.01	1.60	1.45
3	D	702	LQJ	C10-C2	-6.99	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	LQJ	C10-C2	-6.97	1.34	1.52
3	A	702	LQJ	C10-C2	-6.96	1.34	1.52
3	F	703	LQJ	O7-C12	6.92	1.60	1.45
3	A	702	LQJ	C19-C20	5.11	1.64	1.53
3	F	702	LQJ	C9-C3	5.07	1.61	1.53
3	C	702	LQJ	C19-C20	5.04	1.64	1.53
3	F	703	LQJ	C19-C20	5.03	1.64	1.53
3	F	702	LQJ	C19-C20	5.03	1.64	1.53
3	D	702	LQJ	C19-C20	4.99	1.64	1.53
3	D	702	LQJ	C9-C3	4.96	1.61	1.53
3	B	702	LQJ	C9-C3	4.95	1.61	1.53
3	B	702	LQJ	C19-C20	4.92	1.63	1.53
3	A	702	LQJ	C9-C3	4.91	1.61	1.53
3	C	702	LQJ	C9-C3	4.88	1.61	1.53
3	B	702	LQJ	O9-C20	-4.86	1.34	1.45
3	D	702	LQJ	O9-C20	-4.81	1.34	1.45
3	F	702	LQJ	O9-C20	-4.81	1.34	1.45
3	C	702	LQJ	O9-C20	-4.80	1.34	1.45
3	F	703	LQJ	C9-C3	4.77	1.61	1.53
3	F	703	LQJ	O9-C20	-4.77	1.34	1.45
3	A	702	LQJ	O9-C20	-4.71	1.35	1.45
3	F	703	LQJ	O3-C9	-4.36	1.32	1.43
3	A	702	LQJ	O3-C9	-4.34	1.32	1.43
3	B	702	LQJ	O3-C9	-4.33	1.32	1.43
3	D	702	LQJ	O3-C9	-4.32	1.32	1.43
3	F	702	LQJ	O3-C9	-4.31	1.32	1.43
3	C	702	LQJ	O3-C9	-4.30	1.32	1.43
3	D	702	LQJ	P2-O10	3.91	1.64	1.50
3	B	702	LQJ	P2-O10	3.90	1.64	1.50
3	A	702	LQJ	P2-O10	3.89	1.64	1.50
3	F	703	LQJ	P2-O10	3.89	1.64	1.50
3	C	702	LQJ	P2-O10	3.88	1.64	1.50
3	F	702	LQJ	P2-O10	3.87	1.64	1.50
3	F	703	LQJ	C8-N5	3.85	1.48	1.34
3	F	702	LQJ	C8-N5	3.82	1.48	1.34
3	D	702	LQJ	C8-N5	3.82	1.48	1.34
3	B	702	LQJ	C8-N5	3.81	1.48	1.34
3	C	702	LQJ	C8-N5	3.81	1.48	1.34
3	A	702	LQJ	C8-N5	3.80	1.47	1.34
3	B	702	LQJ	C18-N10	3.30	1.46	1.34
3	C	702	LQJ	C18-N10	3.30	1.46	1.34
3	A	702	LQJ	C18-N10	3.30	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	702	LQJ	C18-N10	3.29	1.46	1.34
3	F	703	LQJ	C18-N10	3.29	1.46	1.34
3	D	702	LQJ	C18-N10	3.29	1.46	1.34
3	F	703	LQJ	P2-O11	-2.39	1.44	1.55
3	D	702	LQJ	P2-O11	-2.39	1.44	1.55
3	A	702	LQJ	P2-O11	-2.39	1.44	1.55
3	F	702	LQJ	P2-O11	-2.39	1.44	1.55
3	C	702	LQJ	P2-O11	-2.38	1.44	1.55
3	B	702	LQJ	P2-O11	-2.38	1.44	1.55
3	A	702	LQJ	C11-C12	2.33	1.58	1.51
3	F	702	LQJ	C11-C12	2.32	1.58	1.51
3	B	702	LQJ	C11-C12	2.32	1.58	1.51
3	C	702	LQJ	C11-C12	2.30	1.58	1.51
3	D	702	LQJ	C11-C12	2.28	1.58	1.51
3	F	703	LQJ	C11-C12	2.26	1.58	1.51
3	A	702	LQJ	P1-O4	2.19	1.66	1.60
3	B	702	LQJ	P1-O4	2.16	1.66	1.60
3	D	702	LQJ	P1-O4	2.13	1.66	1.60
3	F	702	LQJ	P1-O4	2.11	1.66	1.60

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	702	LQJ	N3-C7-N4	-4.97	120.91	128.68
3	F	702	LQJ	N8-C17-N9	-4.50	121.64	128.68
3	A	702	LQJ	N8-C17-N9	-4.50	121.65	128.68
3	C	702	LQJ	N8-C17-N9	-4.49	121.66	128.68
3	D	702	LQJ	N8-C17-N9	-4.48	121.67	128.68
3	B	702	LQJ	N8-C17-N9	-4.48	121.67	128.68
3	F	703	LQJ	N8-C17-N9	-4.48	121.68	128.68
3	A	702	LQJ	N3-C7-N4	-4.44	121.74	128.68
3	B	702	LQJ	N3-C7-N4	-4.43	121.76	128.68
3	D	702	LQJ	N3-C7-N4	-4.40	121.80	128.68
3	F	702	LQJ	N3-C7-N4	-4.39	121.81	128.68
3	F	703	LQJ	N3-C7-N4	-4.39	121.82	128.68
3	F	703	LQJ	O9-P2-O10	-2.47	109.24	115.76
3	F	702	LQJ	O9-P2-O10	-2.41	109.41	115.76
3	B	702	LQJ	O9-P2-O10	-2.41	109.41	115.76
3	C	702	LQJ	O9-P2-O10	-2.41	109.41	115.76
3	D	702	LQJ	O8-P2-O10	-2.39	109.45	115.76
3	D	702	LQJ	O9-P2-O10	-2.38	109.48	115.76
3	A	702	LQJ	O9-P2-O10	-2.38	109.48	115.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	LQJ	C16-C15-N7	-2.36	106.94	109.40
3	B	702	LQJ	O8-P2-O10	-2.35	109.55	115.76
3	F	703	LQJ	C16-C15-N7	-2.35	106.95	109.40
3	B	702	LQJ	C16-C15-N7	-2.34	106.96	109.40
3	D	702	LQJ	C16-C15-N7	-2.34	106.96	109.40
3	C	702	LQJ	O8-P2-O10	-2.33	109.60	115.76
3	F	702	LQJ	C16-C15-N7	-2.33	106.97	109.40
3	C	702	LQJ	C16-C15-N7	-2.31	106.99	109.40
3	A	702	LQJ	O8-P2-O10	-2.28	109.74	115.76
3	F	702	LQJ	O8-P2-O10	-2.28	109.75	115.76
3	B	702	LQJ	O7-C13-C19	-2.27	102.66	106.59
3	F	703	LQJ	O8-P2-O10	-2.26	109.79	115.76
3	D	702	LQJ	O7-C13-C19	-2.08	102.98	106.59

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	LQJ	C10-O4-P1-O6
3	A	702	LQJ	C11-O6-P1-O5
3	A	702	LQJ	C11-O6-P1-O12
3	B	702	LQJ	C10-O4-P1-O6
3	D	702	LQJ	C10-O4-P1-O6
3	D	702	LQJ	C11-O6-P1-O12
3	F	702	LQJ	C11-O6-P1-O12
3	F	703	LQJ	C10-O4-P1-O6
3	F	703	LQJ	C11-O6-P1-O4
3	F	703	LQJ	C11-O6-P1-O5
3	F	703	LQJ	C11-O6-P1-O12
3	C	702	LQJ	O1-C1-C2-O2
3	C	702	LQJ	O1-C1-C2-C10
3	F	702	LQJ	O1-C1-C2-O2
3	F	703	LQJ	O1-C1-C2-O2
3	F	703	LQJ	O1-C1-C2-C10
3	D	702	LQJ	O1-C1-C2-C10
3	B	702	LQJ	O1-C1-C2-C10
3	F	702	LQJ	O1-C1-C2-C10
3	D	702	LQJ	O1-C1-C2-O2
3	A	702	LQJ	C11-O6-P1-O4
3	B	702	LQJ	C11-O6-P1-O4
3	C	702	LQJ	C11-O6-P1-O4
3	D	702	LQJ	C11-O6-P1-O4

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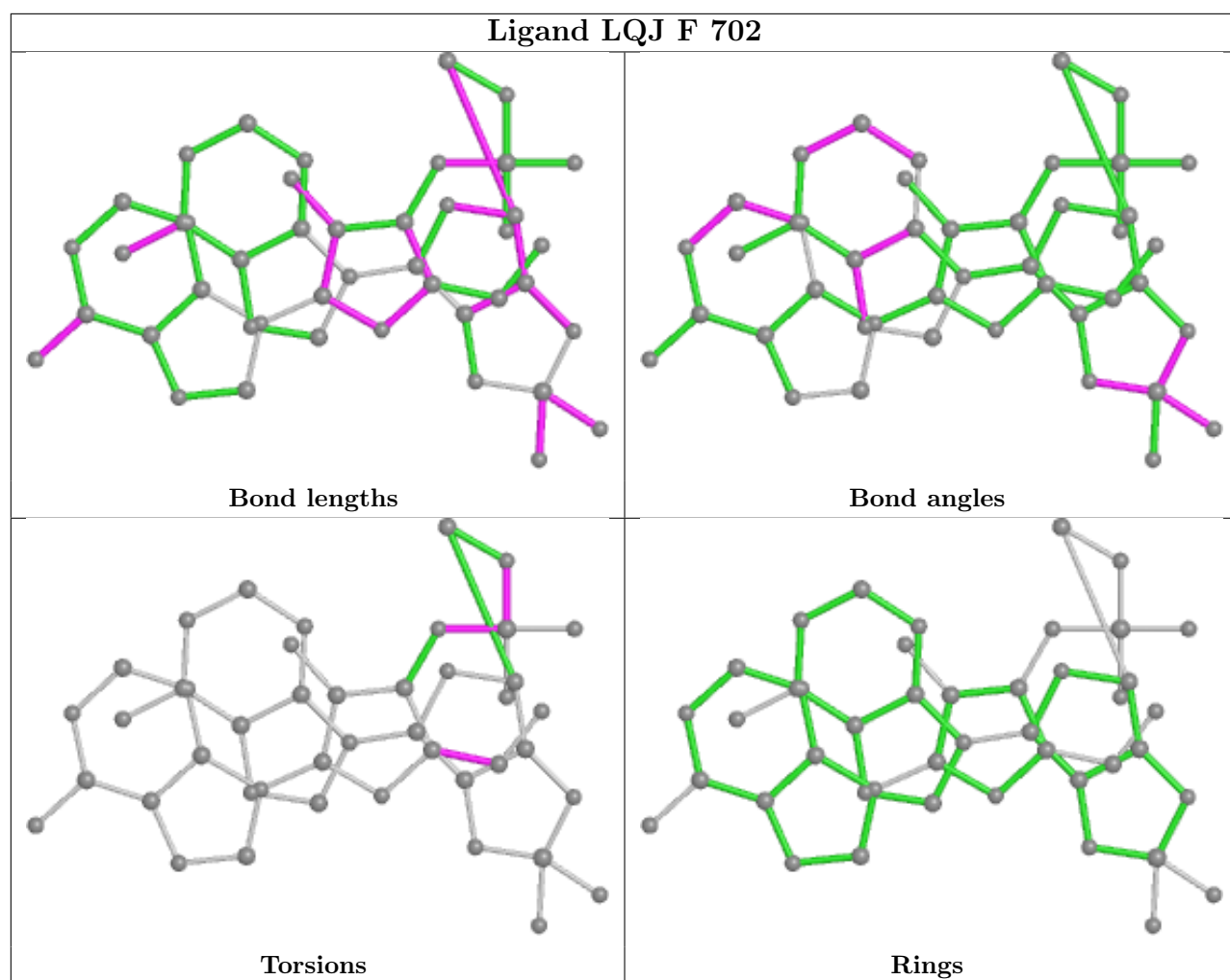
Mol	Chain	Res	Type	Atoms
3	F	702	LQJ	C11-O6-P1-O4
3	F	702	LQJ	C10-O4-P1-O6
3	B	702	LQJ	O1-C1-C2-O2
3	C	702	LQJ	C10-O4-P1-O6
3	F	703	LQJ	C10-O4-P1-O5
3	B	702	LQJ	C11-O6-P1-O5
3	C	702	LQJ	C11-O6-P1-O12
3	D	702	LQJ	C11-O6-P1-O5
3	F	702	LQJ	C11-O6-P1-O5
3	A	702	LQJ	O1-C1-C2-O2

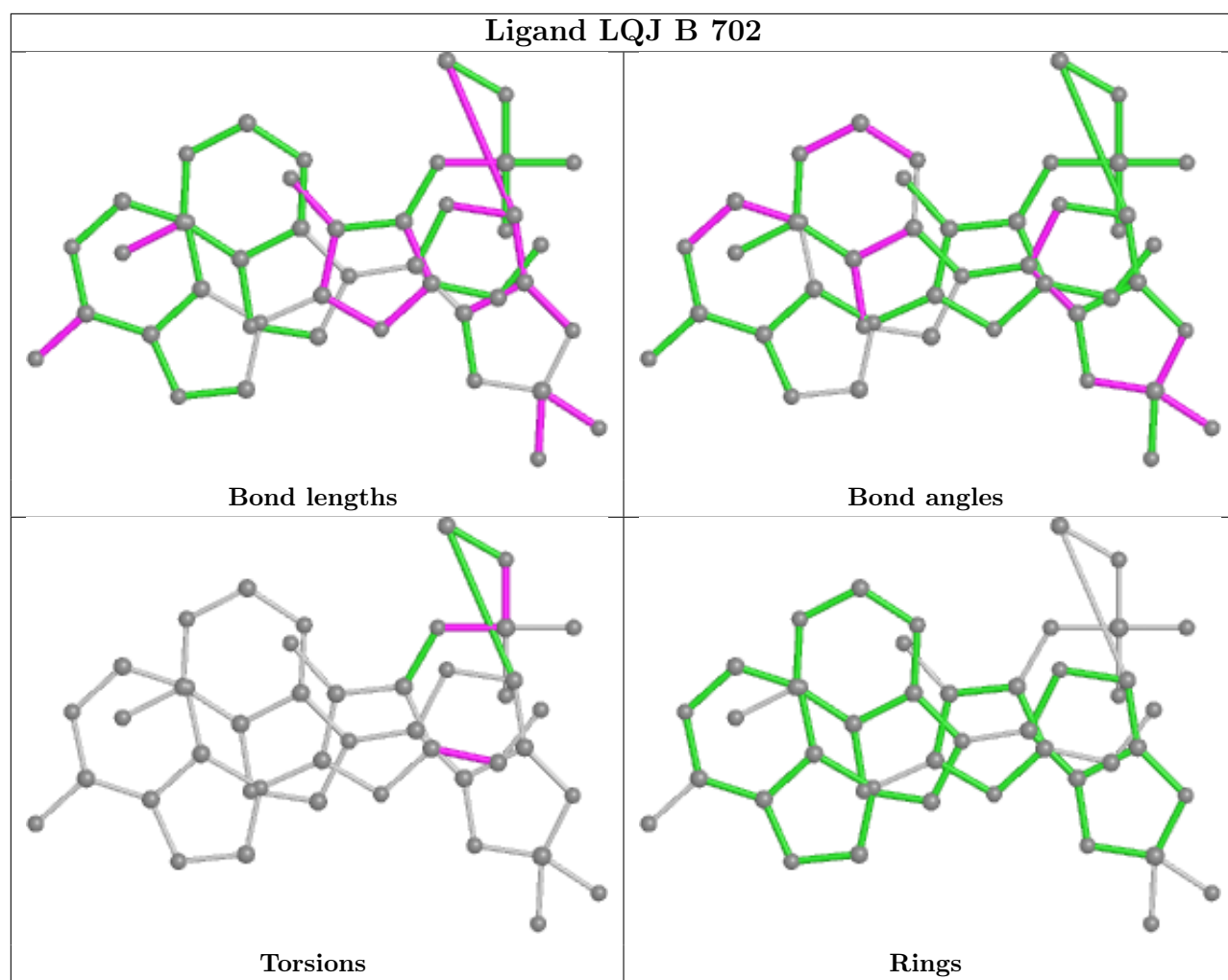
There are no ring outliers.

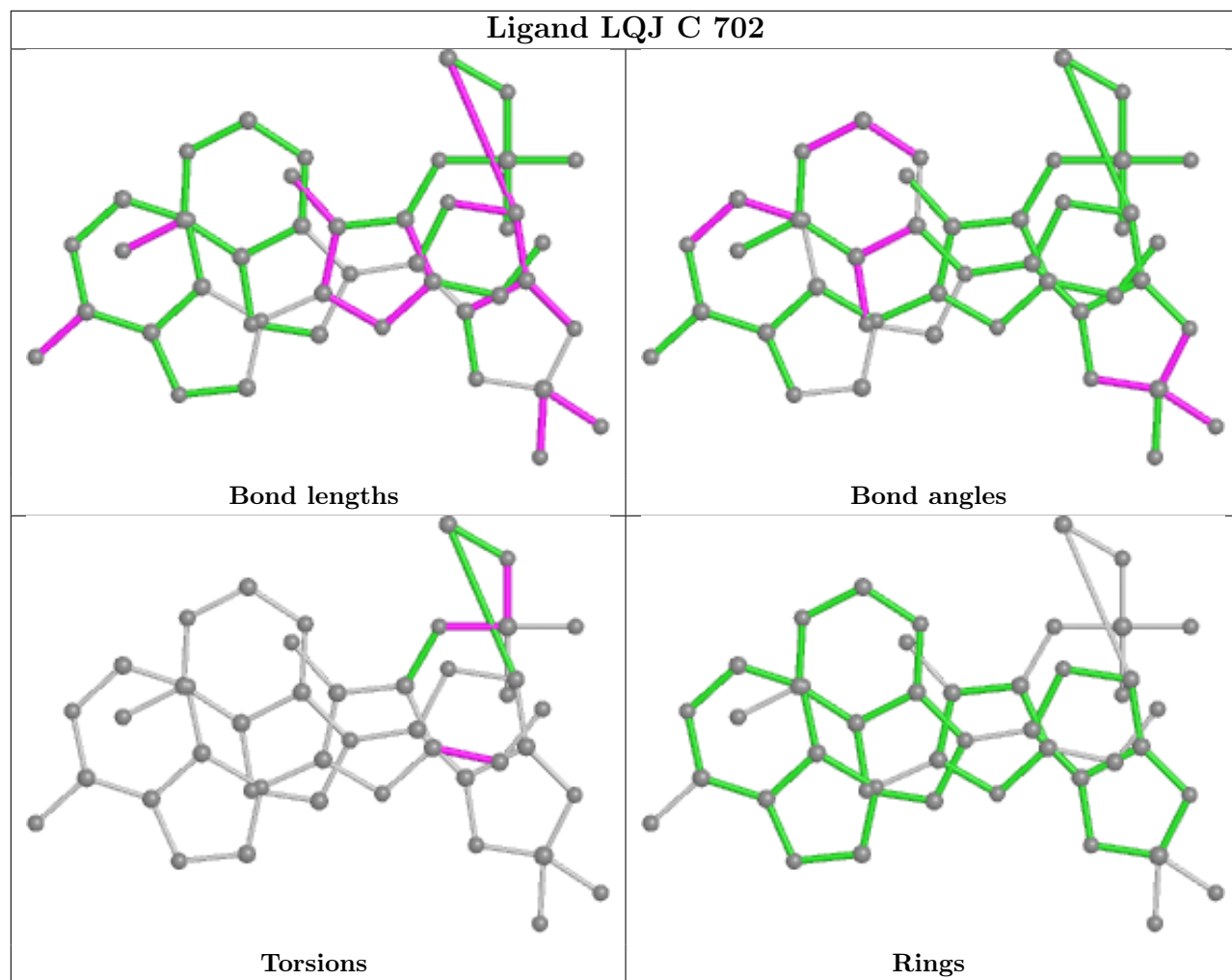
6 monomers are involved in 7 short contacts:

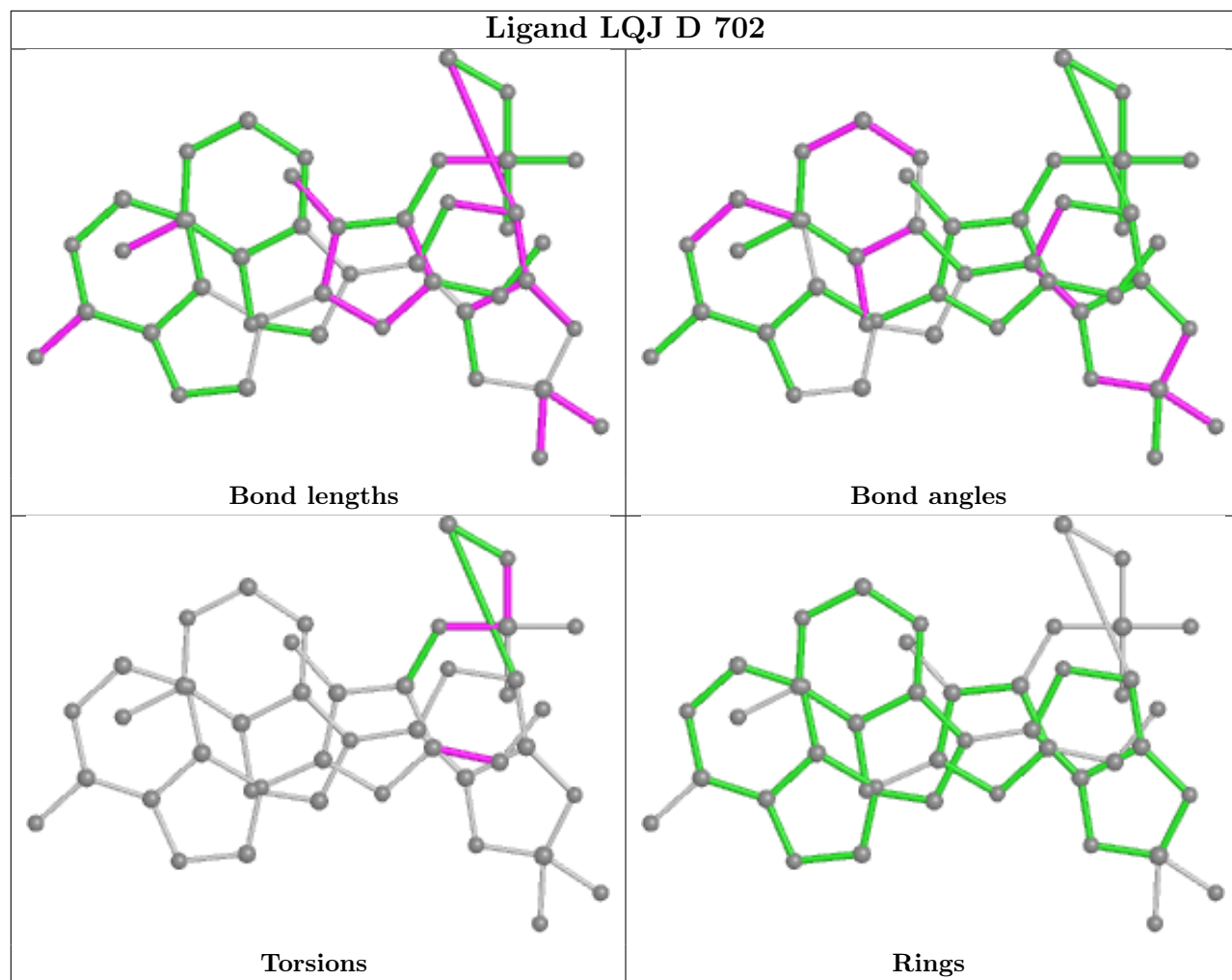
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	702	LQJ	1	0
3	B	702	LQJ	1	0
3	C	702	LQJ	1	0
3	D	702	LQJ	2	0
3	F	703	LQJ	1	0
3	A	702	LQJ	1	0

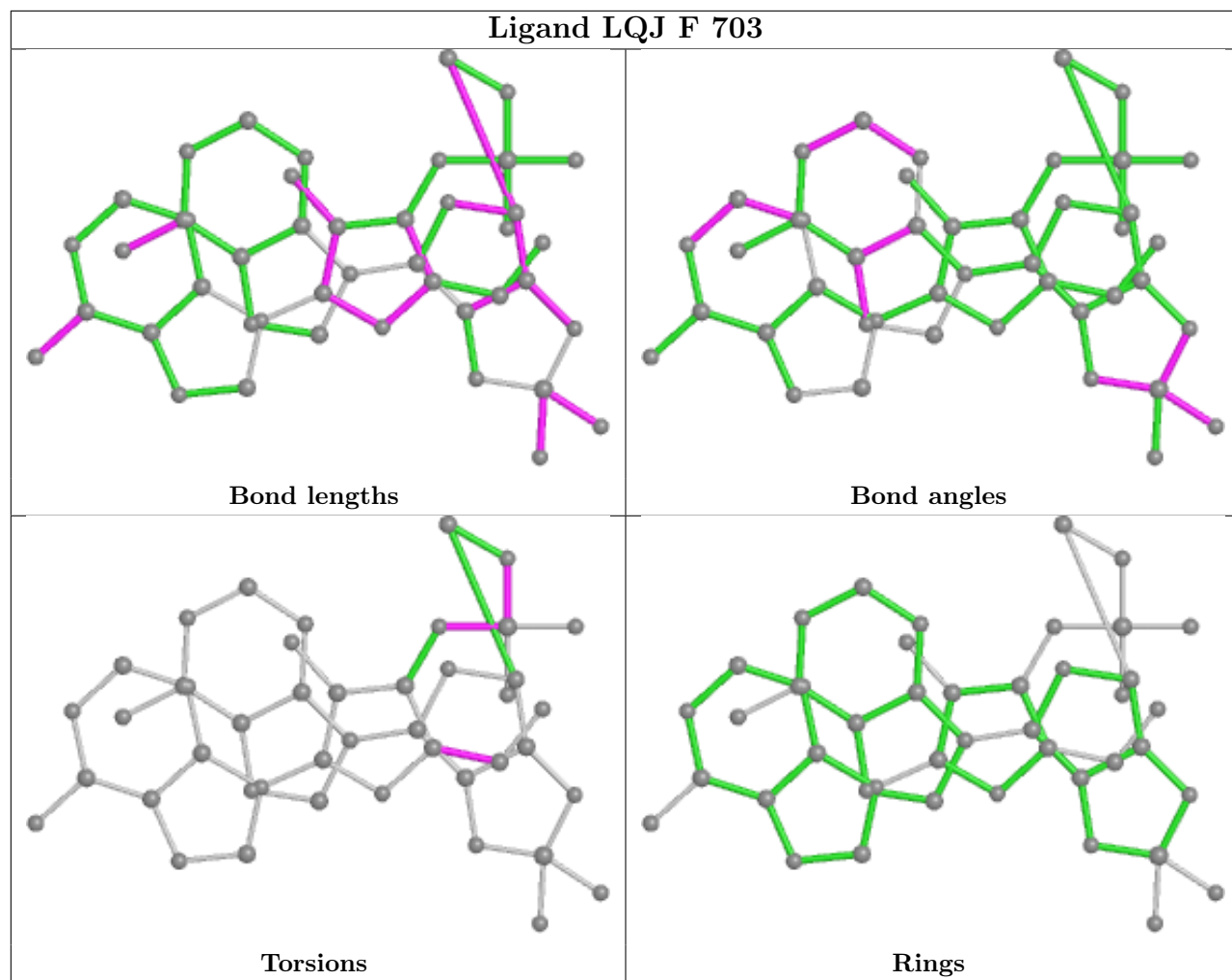
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

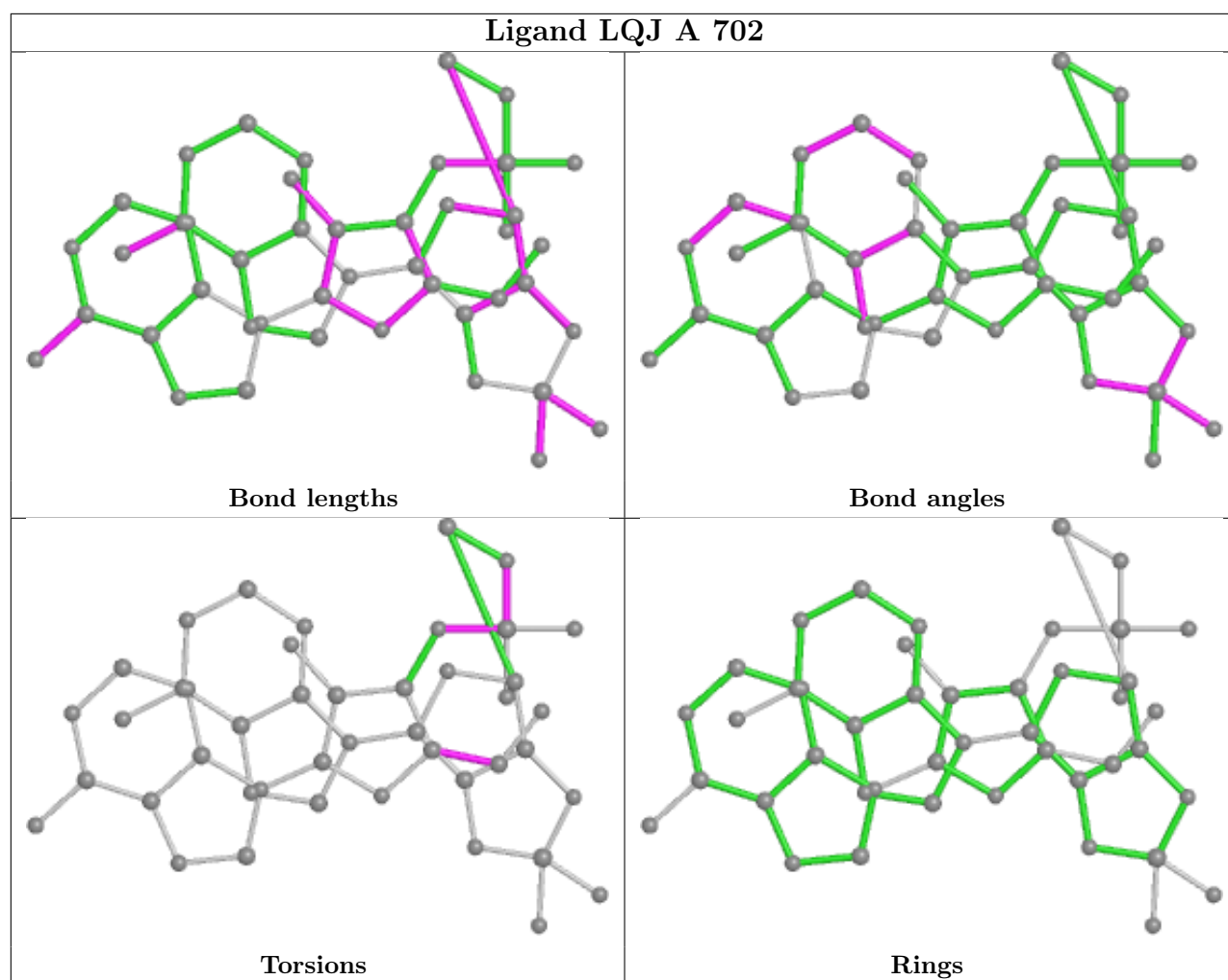












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.