



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:13 AM UTC

PDB ID : 9NY7 / pdb_00009ny7
Title : Crystal structure of the ribose operon repressor, RbsR, bound to ribose
Authors : Wells, M.L.; Lu, C.; Sultanov, D.; Weber, K.C.; Gong, Z.; Glasgow, A.
Deposited on : 2025-03-26
Resolution : 2.07 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

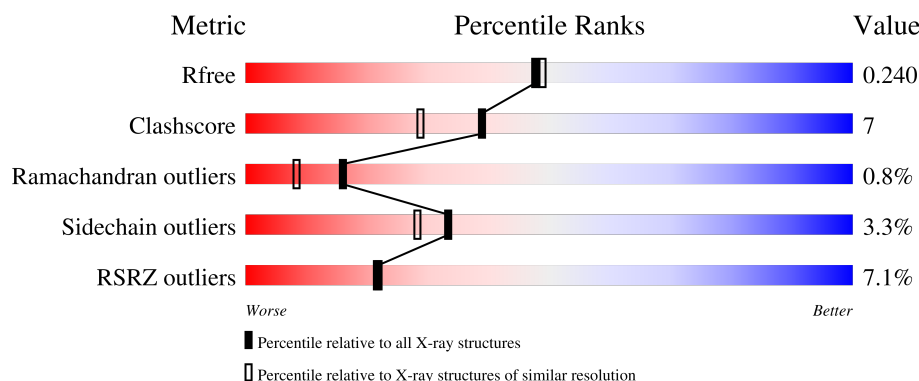
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	330	4% 69% 12% 15%
1	B	330	12% 79% 18%
1	C	330	2% 73% 10% 16%
1	D	330	11% 66% 15% 17%
1	E	330	3% 73% 10% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	330	

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
2	RIP	E	401	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13879 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.

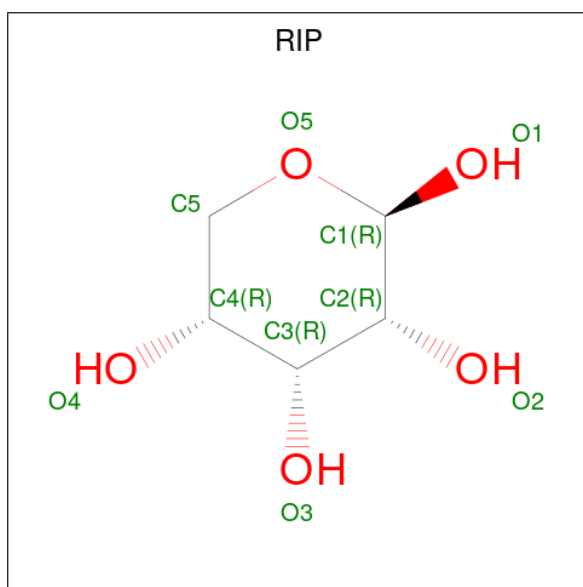
- Molecule 1 is a protein called Ribose operon repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2190	1372	383	420	15			
1	B	326	Total	C	N	O	S	0	0	0
			2539	1590	444	489	16			
1	C	278	Total	C	N	O	S	0	1	0
			2190	1372	383	420	15			
1	D	273	Total	C	N	O	S	0	1	0
			2149	1346	374	414	15			
1	E	279	Total	C	N	O	S	0	0	0
			2190	1372	383	420	15			
1	F	273	Total	C	N	O	S	0	0	0
			2140	1341	372	412	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P0ACQ0
B	1	SER	-	expression tag	UNP P0ACQ0
C	1	SER	-	expression tag	UNP P0ACQ0
D	1	SER	-	expression tag	UNP P0ACQ0
E	1	SER	-	expression tag	UNP P0ACQ0
F	1	SER	-	expression tag	UNP P0ACQ0

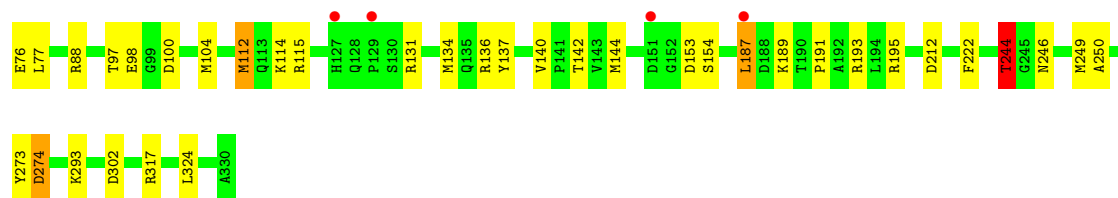
- Molecule 2 is beta-D-ribose (CCD ID: RIP) (formula: C₅H₁₀O₅) (labeled as "Ligand of Interest" by depositor).



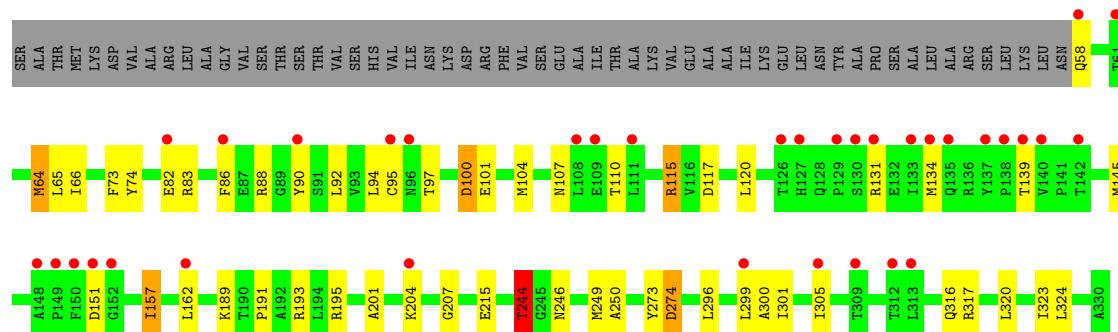
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	1	Total	C	O	0	0
			10	5	5		
2	E	1	Total	C	O	0	0
			10	5	5		
2	F	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is water.

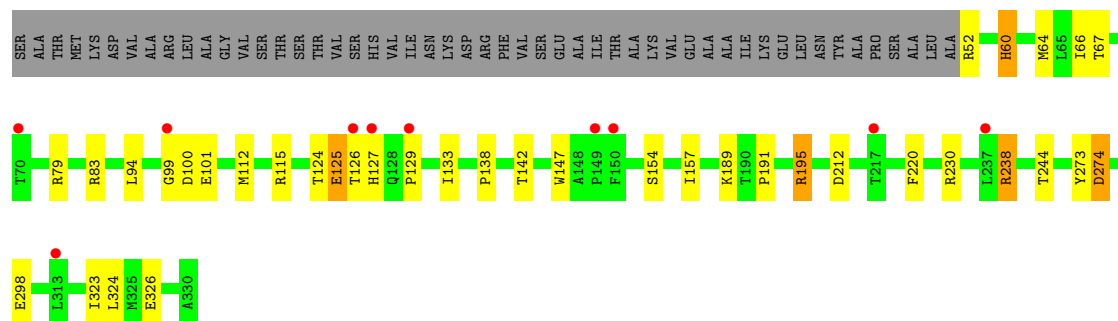
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	82	Total	O	0	0
			82	82		
3	B	74	Total	O	0	0
			74	74		
3	C	103	Total	O	0	0
			103	103		
3	D	44	Total	O	0	0
			44	44		
3	E	69	Total	O	0	0
			69	69		
3	F	49	Total	O	0	0
			49	49		



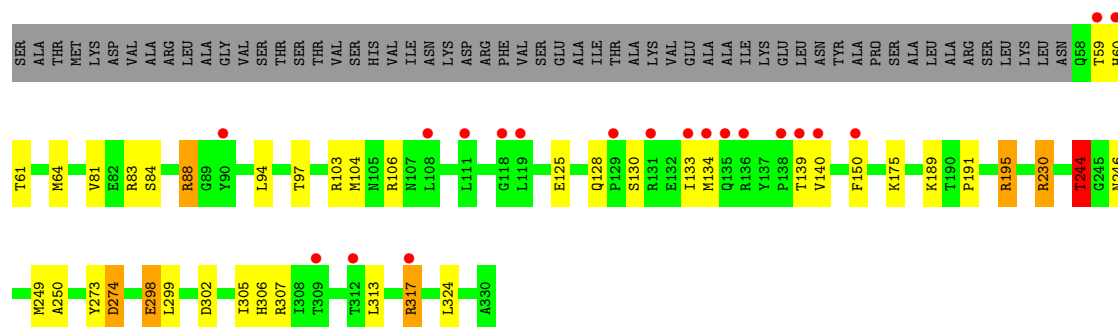
- Molecule 1: Ribose operon repressor



- Molecule 1: Ribose operon repressor



- Molecule 1: Ribose operon repressor



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.46Å 87.35Å 130.94Å 90.00° 100.38° 90.00°	Depositor
Resolution (Å)	33.82 – 2.07 33.82 – 2.07	Depositor EDS
% Data completeness (in resolution range)	61.4 (33.82-2.07) 61.6 (33.82-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8	Depositor
R, R_{free}	0.191 , 0.234 0.201 , 0.240	Depositor DCC
R_{free} test set	3661 reflections (3.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13879	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9824e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.68	3/2230 (0.1%)	0.93	6/3024 (0.2%)
1	B	0.66	0/2582	0.93	2/3500 (0.1%)
1	C	0.71	2/2230 (0.1%)	0.92	4/3024 (0.1%)
1	D	0.67	2/2189 (0.1%)	0.90	2/2970 (0.1%)
1	E	0.67	2/2230 (0.1%)	0.92	2/3024 (0.1%)
1	F	0.64	1/2180 (0.0%)	0.89	1/2958 (0.0%)
All	All	0.67	10/13641 (0.1%)	0.92	17/18500 (0.1%)

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	A	0	8
1	B	0	5
1	C	0	4
1	D	0	6
1	E	0	7
1	F	0	5
All	All	0	35

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	112	MET	SD-CE	-12.00	1.49	1.79
1	D	157	ILE	CG1-CD1	-9.51	1.14	1.51
1	A	64	MET	SD-CE	-8.34	1.58	1.79
1	F	305	ILE	CG1-CD1	-7.14	1.24	1.51
1	E	112	MET	SD-CE	6.15	1.95	1.79
1	C	64	MET	SD-CE	-6.09	1.64	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	MET	SD-CE	-5.81	1.65	1.79
1	E	157	ILE	CG1-CD1	-5.19	1.31	1.51
1	D	64	MET	SD-CE	-5.18	1.66	1.79
1	A	133	ILE	CG1-CD1	-5.04	1.32	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	ASP	CA-CB-CG	7.42	120.02	112.60
1	A	57	ASN	CA-CB-CG	-6.72	105.88	112.60
1	A	102	GLN	N-CA-C	-6.22	97.56	110.80
1	B	127	HIS	CA-CB-CG	5.85	119.65	113.80
1	B	244	THR	N-CA-C	-5.81	99.05	108.52
1	E	244	THR	N-CA-C	-5.71	99.21	108.52
1	A	230	ARG	CB-CA-C	-5.69	101.35	110.79
1	C	140	VAL	N-CA-C	5.60	112.66	107.56
1	C	187	LEU	CB-CA-C	-5.37	101.56	110.68
1	A	244	THR	N-CA-C	5.35	119.91	113.17
1	F	244	THR	N-CA-C	5.34	119.95	113.38
1	C	222	PHE	CA-CB-CG	5.32	119.12	113.80
1	D	244	THR	N-CA-C	5.30	119.90	113.38
1	A	140	VAL	N-CA-C	5.25	112.33	107.56
1	E	220	PHE	CA-CB-CG	5.11	118.91	113.80
1	C	244	THR	N-CA-C	5.07	119.61	113.38
1	A	222	PHE	CA-CB-CG	5.03	118.83	113.80

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ARG	Sidechain
1	A	131	ARG	Sidechain
1	A	195	ARG	Sidechain
1	A	205	ARG	Sidechain
1	A	230	ARG	Sidechain
1	A	52	ARG	Sidechain
1	A	79	ARG	Sidechain
1	A	83	ARG	Sidechain
1	B	103	ARG	Sidechain
1	B	115	ARG	Sidechain
1	B	195	ARG	Sidechain
1	B	230	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	52	ARG	Sidechain
1	C	115	ARG	Sidechain
1	C	193	ARG	Sidechain
1	C	195	ARG	Sidechain
1	C	317	ARG	Sidechain
1	D	115	ARG	Sidechain
1	D	193	ARG	Sidechain
1	D	195	ARG	Sidechain
1	D	207	GLY	Peptide
1	D	317	ARG	Sidechain
1	D	83	ARG	Sidechain
1	E	115	ARG	Sidechain
1	E	195	ARG	Sidechain
1	E	230	ARG	Sidechain
1	E	238	ARG	Sidechain
1	E	52	ARG	Sidechain
1	E	79	ARG	Sidechain
1	E	83	ARG	Sidechain
1	F	195	ARG	Sidechain
1	F	230	ARG	Sidechain
1	F	317	ARG	Sidechain
1	F	83	ARG	Sidechain
1	F	88	ARG	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	2190	0	2178	30	0
1	B	2539	0	2542	43	0
1	C	2190	0	2177	15	0
1	D	2149	0	2126	35	0
1	E	2190	0	2178	35	0
1	F	2140	0	2119	31	0
2	A	10	0	10	0	0
2	B	10	0	10	0	0
2	C	10	0	10	0	0
2	D	10	0	10	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	10	0	10	7	0
2	F	10	0	10	5	0
3	A	82	0	0	0	0
3	B	74	0	0	2	0
3	C	103	0	0	1	0
3	D	44	0	0	1	0
3	E	69	0	0	3	0
3	F	49	0	0	0	0
All	All	13879	0	13380	182	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 7.

All (182) 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:E:124:THR:O	1:E:126:THR:N	1.85	1.07
1:F:307:ARG:HH21	1:F:313:LEU:HD23	1.16	1.04
1:A:130:SER:O	1:A:133:ILE:HD13	1.55	1.04
1:E:195:ARG:HH22	2:E:401:RIP:H3	1.35	0.91
1:F:195:ARG:HH22	2:F:401:RIP:H3	1.38	0.89
1:F:274:ASP:OD1	2:F:401:RIP:O2	1.90	0.88
1:E:125:GLU:O	1:E:126:THR:OG1	1.97	0.82
1:B:126:THR:O	1:B:127:HIS:ND1	2.13	0.81
1:E:67:THR:HG21	1:E:124:THR:HG23	1.63	0.81
1:E:274:ASP:OD1	2:E:401:RIP:O2	1.98	0.80
1:E:195:ARG:NH2	2:E:401:RIP:H3	1.98	0.78
1:D:157:ILE:CD1	1:D:300:ALA:HA	2.15	0.77
1:A:106:ARG:HH11	1:A:106:ARG:HG3	1.49	0.77
1:F:307:ARG:HH21	1:F:313:LEU:CD2	1.97	0.74
1:E:67:THR:HG21	1:E:124:THR:CG2	2.17	0.74
1:A:93:VAL:HG13	1:B:93:VAL:HG13	1.69	0.74
1:E:124:THR:C	1:E:126:THR:N	2.46	0.72
1:D:58:GLN:HG3	1:D:117:ASP:OD2	1.90	0.71
1:E:124:THR:C	1:E:126:THR:H	1.97	0.71
1:D:82:GLU:CD	1:D:92:LEU:HD23	2.15	0.70
1:A:99:GLY:O	1:A:100:ASP:HB2	1.92	0.68
1:E:125:GLU:C	1:E:127:HIS:H	2.02	0.68
1:D:157:ILE:HD13	1:D:300:ALA:HA	1.75	0.67
1:D:82:GLU:OE2	1:D:92:LEU:HD23	1.94	0.67
1:B:106:ARG:HH11	1:B:106:ARG:HG2	1.60	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:ARG:HH12	2:E:401:RIP:H2	1.61	0.65
1:E:326:GLU:OE1	3:E:501:HOH:O	2.15	0.65
1:A:102:GLN:O	1:A:104:MET:N	2.28	0.65
1:F:195:ARG:NH2	2:F:401:RIP:H3	2.10	0.65
1:B:26:ARG:NH2	1:B:153:ASP:OD2	2.31	0.64
1:A:101:GLU:C	1:A:102:GLN:O	2.37	0.62
1:D:296:LEU:HD23	1:D:320:LEU:HD13	1.81	0.62
1:D:201:ALA:O	1:D:204:LYS:HG2	2.00	0.62
1:A:91:SER:CB	1:B:110:THR:HG21	2.30	0.62
1:E:238:ARG:HH11	1:E:238:ARG:HG2	1.65	0.61
1:C:244:THR:HG21	1:C:250:ALA:HB2	1.83	0.61
1:F:106:ARG:HG3	1:F:106:ARG:HH11	1.66	0.61
1:B:125:GLU:HG2	1:B:186:PRO:HG2	1.84	0.60
1:D:73:PHE:CD2	2:D:401:RIP:H4	2.37	0.60
1:F:64:MET:HE1	1:F:81:VAL:HG21	1.82	0.60
1:E:195:ARG:HH22	2:E:401:RIP:C3	2.13	0.60
1:D:64:MET:HE3	1:D:145:MET:CE	2.32	0.59
1:A:193:ARG:HH11	1:A:193:ARG:HB3	1.68	0.59
1:A:91:SER:HB2	1:B:110:THR:HG21	1.85	0.58
1:F:317:ARG:HG2	1:F:317:ARG:O	2.01	0.58
1:A:128:GLN:OE1	1:A:129:PRO:HD2	2.03	0.58
1:E:125:GLU:C	1:E:126:THR:HG1	2.08	0.58
1:F:307:ARG:NH2	1:F:313:LEU:HD23	2.02	0.58
1:E:124:THR:O	1:E:125:GLU:C	2.45	0.58
1:B:177:HIS:HE1	3:B:556:HOH:O	1.86	0.57
1:F:244:THR:HG21	1:F:250:ALA:HB2	1.86	0.57
1:F:128:GLN:OE1	1:F:150:PHE:HB2	2.05	0.56
1:F:189:LYS:NZ	2:F:401:RIP:H51	2.20	0.56
1:A:244:THR:O	1:A:249:MET:HE3	2.05	0.56
1:B:238:ARG:HD3	1:B:239:PRO:HD2	1.87	0.56
1:E:126:THR:HA	1:E:147:TRP:CZ2	2.40	0.56
1:C:76:GLU:OE1	1:C:293:LYS:HE3	2.06	0.56
1:F:103:ARG:HH11	1:F:103:ARG:HG3	1.71	0.56
1:A:130:SER:O	1:A:133:ILE:CD1	2.42	0.56
1:A:131:ARG:NH2	1:A:134:MET:HG3	2.21	0.56
1:B:10:LEU:HD12	1:B:43:LEU:CD1	2.36	0.56
1:B:4:MET:HE1	1:B:19:SER:HA	1.88	0.55
1:B:41:LYS:O	1:B:42:GLU:CB	2.54	0.55
1:D:131:ARG:HA	1:D:134:MET:HE2	1.88	0.55
1:D:244:THR:HG21	1:D:250:ALA:HB2	1.88	0.55
1:D:64:MET:HE3	1:D:145:MET:HE1	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:THR:O	1:F:249:MET:HE3	2.07	0.55
1:C:244:THR:O	1:C:249:MET:HE3	2.07	0.55
1:A:100:ASP:O	1:A:101:GLU:HB2	2.06	0.54
1:F:88:ARG:NH2	1:F:298:GLU:OE2	2.39	0.54
1:D:244:THR:O	1:D:249:MET:HE3	2.07	0.54
1:C:88:ARG:HH22	1:C:302:ASP:HB2	1.73	0.54
1:D:100:ASP:CG	1:D:101:GLU:H	2.16	0.54
1:E:125:GLU:C	1:E:127:HIS:N	2.67	0.53
1:A:112:MET:HE2	1:A:137:TYR:HB2	1.91	0.53
1:F:88:ARG:HH22	1:F:302:ASP:HB2	1.73	0.53
1:E:124:THR:OG1	1:E:125:GLU:N	2.41	0.52
1:D:86:PHE:C	1:D:86:PHE:CD1	2.87	0.52
1:E:101:GLU:HB2	1:E:127:HIS:CE1	2.45	0.52
1:B:20:HIS:CE1	1:B:26:ARG:HD3	2.44	0.51
1:B:112:MET:HE3	1:B:137:TYR:HB2	1.92	0.51
1:E:238:ARG:HD3	3:E:505:HOH:O	2.12	0.50
1:B:10:LEU:HD12	1:B:43:LEU:HD13	1.93	0.50
1:F:88:ARG:HH21	1:F:298:GLU:CD	2.20	0.50
1:E:67:THR:CG2	1:E:124:THR:HG23	2.39	0.50
1:B:32:ILE:O	1:B:36:VAL:HG23	2.12	0.49
1:B:226:PHE:CZ	1:B:230:ARG:HD3	2.48	0.49
1:C:136:ARG:HD3	1:D:215:GLU:O	2.12	0.49
1:F:189:LYS:HG2	1:F:191:PRO:HD2	1.95	0.49
1:B:64:MET:HB3	1:B:94:LEU:HD23	1.94	0.48
1:F:84:SER:OG	1:F:298:GLU:OE1	2.31	0.48
1:C:189:LYS:HG2	1:C:191:PRO:HD2	1.95	0.48
1:D:157:ILE:HD13	1:D:300:ALA:CA	2.44	0.48
1:A:106:ARG:HG3	1:A:106:ARG:NH1	2.21	0.48
1:E:195:ARG:HH12	2:E:401:RIP:C2	2.26	0.48
1:F:84:SER:OG	1:F:298:GLU:HA	2.13	0.48
1:A:103:ARG:NH2	1:B:82:GLU:OE2	2.37	0.48
1:D:64:MET:HB3	1:D:94:LEU:HD23	1.96	0.48
1:D:90:TYR:CZ	1:D:305:ILE:HD12	2.49	0.48
1:B:21:VAL:HG11	1:B:36:VAL:HB	1.95	0.48
1:D:316:GLN:HA	3:D:526:HOH:O	2.13	0.48
1:F:244:THR:HG22	1:F:246:ASN:O	2.14	0.48
1:A:189:LYS:HG2	1:A:191:PRO:HD2	1.95	0.47
1:B:67:THR:HG21	1:B:124:THR:HG23	1.96	0.47
1:A:187:LEU:H	1:A:187:LEU:CD2	2.26	0.47
1:C:97:THR:OG1	1:C:104:MET:HG2	2.13	0.47
1:E:99:GLY:O	1:E:100:ASP:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LYS:HG2	1:B:191:PRO:HD2	1.95	0.47
1:F:189:LYS:HZ3	2:F:401:RIP:H51	1.79	0.47
1:A:193:ARG:HB3	1:A:193:ARG:NH1	2.30	0.47
1:A:132:GLU:O	1:A:136:ARG:HG2	2.14	0.47
1:C:244:THR:HG22	1:C:246:ASN:O	2.15	0.47
1:C:98:GLU:OE1	3:C:501:HOH:O	2.20	0.46
1:A:100:ASP:O	1:A:101:GLU:CB	2.62	0.46
1:D:244:THR:HG22	1:D:246:ASN:O	2.14	0.46
1:D:74:TYR:OH	2:D:401:RIP:H51	2.16	0.46
1:D:120:LEU:HB3	1:D:145:MET:HE2	1.97	0.46
1:D:88:ARG:HD2	1:D:301:ILE:HG22	1.97	0.46
1:B:41:LYS:O	1:B:42:GLU:HB3	2.15	0.46
1:B:124:THR:O	1:B:127:HIS:CG	2.69	0.46
1:E:64:MET:HB3	1:E:94:LEU:HD23	1.96	0.46
1:E:238:ARG:HG2	1:E:238:ARG:NH1	2.31	0.46
1:A:187:LEU:H	1:A:187:LEU:HD23	1.81	0.46
1:F:64:MET:HB3	1:F:94:LEU:HD23	1.98	0.46
1:B:104:MET:HE1	1:B:127:HIS:HB3	1.98	0.45
1:E:189:LYS:HG2	1:E:191:PRO:HD2	1.97	0.45
1:F:97:THR:OG1	1:F:104:MET:HG2	2.17	0.45
1:A:187:LEU:HD23	1:A:187:LEU:N	2.32	0.45
1:B:131:ARG:NH2	1:B:150:PHE:O	2.49	0.45
1:E:60:HIS:HE1	3:E:503:HOH:O	2.00	0.45
1:A:306:HIS:ND1	1:A:313:LEU:HD22	2.32	0.44
1:B:8:ALA:HB2	1:B:18:VAL:HG21	1.99	0.44
1:D:189:LYS:HG2	1:D:191:PRO:HD2	2.00	0.44
1:E:189:LYS:HZ3	2:E:401:RIP:H51	1.82	0.43
1:F:104:MET:HE1	1:F:125:GLU:HB2	1.99	0.43
1:B:21:VAL:HG21	1:B:36:VAL:HG21	2.00	0.43
1:F:130:SER:O	1:F:134:MET:HG3	2.18	0.43
1:E:99:GLY:O	1:E:100:ASP:CB	2.66	0.43
1:F:273:TYR:O	1:F:274:ASP:CB	2.66	0.43
1:C:131:ARG:HA	1:C:134:MET:HE2	2.01	0.43
1:D:273:TYR:O	1:D:274:ASP:CB	2.67	0.43
1:B:125:GLU:CD	1:B:186:PRO:HG2	2.44	0.43
1:B:125:GLU:CG	1:B:186:PRO:HG2	2.48	0.43
1:D:97:THR:OG1	1:D:104:MET:HG2	2.18	0.43
1:A:131:ARG:NE	1:A:131:ARG:HA	2.33	0.42
1:D:100:ASP:O	1:D:104:MET:HE2	2.19	0.42
1:D:162:LEU:C	1:D:162:LEU:HD23	2.44	0.42
1:A:273:TYR:O	1:A:274:ASP:CB	2.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:THR:HA	1:E:147:TRP:CH2	2.54	0.42
1:E:273:TYR:O	1:E:274:ASP:CB	2.67	0.42
1:C:273:TYR:O	1:C:274:ASP:CB	2.67	0.42
1:A:97:THR:OG1	1:A:104:MET:HG2	2.20	0.42
1:B:273:TYR:O	1:B:274:ASP:CB	2.66	0.42
1:D:64:MET:HG2	1:D:66:ILE:HG23	2.02	0.42
1:B:10:LEU:HD12	1:B:43:LEU:HD11	2.01	0.42
1:D:90:TYR:CE2	1:D:305:ILE:HD12	2.54	0.42
1:A:315:GLN:OE1	1:A:317:ARG:NH1	2.53	0.42
1:C:112:MET:HE2	1:C:137:TYR:HB2	2.02	0.42
1:D:64:MET:CE	1:D:145:MET:HE1	2.49	0.42
1:F:130:SER:O	1:F:133:ILE:HG22	2.20	0.42
1:B:306:HIS:ND1	1:B:313:LEU:HD22	2.35	0.42
1:C:212:ASP:OD1	1:E:138:PRO:HD2	2.20	0.42
1:D:64:MET:HE3	1:D:145:MET:HE3	2.02	0.41
1:B:29:SER:HB3	1:B:32:ILE:CD1	2.50	0.41
1:B:125:GLU:O	1:B:147:TRP:CZ2	2.73	0.41
1:B:65:LEU:HD12	1:B:95:CYS:HB3	2.01	0.41
1:B:125:GLU:O	1:B:147:TRP:HZ2	2.03	0.41
1:B:134:MET:HE1	1:B:150:PHE:CZ	2.55	0.41
1:E:142:THR:O	1:E:154:SER:OG	2.38	0.41
1:C:100:ASP:O	1:C:104:MET:HE2	2.21	0.41
1:D:107:ASN:O	1:D:110:THR:OG1	2.33	0.41
1:A:112:MET:CE	1:A:137:TYR:CB	2.99	0.41
1:B:142:THR:O	1:B:154:SER:OG	2.39	0.41
1:D:65:LEU:HD12	1:D:95:CYS:HB3	2.02	0.41
1:B:264:VAL:HA	1:B:265:PRO:HA	1.91	0.41
1:F:244:THR:HG21	1:F:250:ALA:CA	2.51	0.41
1:B:97:THR:OG1	1:B:104:MET:HG2	2.21	0.40
1:F:59:THR:HG23	1:F:61:THR:HB	2.02	0.40
1:B:104:MET:HE2	1:B:129:PRO:HG3	2.03	0.40
1:C:187:LEU:HD11	1:E:133:ILE:HD11	2.02	0.40
1:B:60:HIS:HE1	3:B:530:HOH:O	2.05	0.40
1:F:175:LYS:HA	1:F:175:LYS:HD2	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	277/330 (84%)	268 (97%)	4 (1%)	5 (2%)	6	2
1	B	322/330 (98%)	309 (96%)	10 (3%)	3 (1%)	14	7
1	C	277/330 (84%)	271 (98%)	5 (2%)	1 (0%)	30	23
1	D	272/330 (82%)	265 (97%)	6 (2%)	1 (0%)	30	23
1	E	277/330 (84%)	267 (96%)	7 (2%)	3 (1%)	11	4
1	F	271/330 (82%)	266 (98%)	4 (2%)	1 (0%)	30	23
All	All	1696/1980 (86%)	1646 (97%)	36 (2%)	14 (1%)	16	8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	103	ARG
1	B	42	GLU
1	E	125	GLU
1	E	129	PRO
1	A	101	GLU
1	A	102	GLN
1	A	274	ASP
1	B	274	ASP
1	C	274	ASP
1	D	274	ASP
1	E	274	ASP
1	F	274	ASP
1	B	53	SER

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/280 (86%)	230 (96%)	10 (4%)	26	20
1	B	278/280 (99%)	270 (97%)	8 (3%)	37	33
1	C	240/280 (86%)	231 (96%)	9 (4%)	29	23
1	D	235/280 (84%)	228 (97%)	7 (3%)	36	32
1	E	240/280 (86%)	234 (98%)	6 (2%)	42	38
1	F	234/280 (84%)	225 (96%)	9 (4%)	29	23
All	All	1467/1680 (87%)	1418 (97%)	49 (3%)	33	28

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	77	LEU
1	A	119	LEU
1	A	133	ILE
1	A	136	ARG
1	A	142	THR
1	A	144	MET
1	A	314	GLN
1	A	321	THR
1	A	324	LEU
1	B	10	LEU
1	B	44	ASN
1	B	60	HIS
1	B	66	ILE
1	B	82	GLU
1	B	167	LEU
1	B	223	ASN
1	B	324	LEU
1	C	60	HIS
1	C	77	LEU
1	C	114	LYS
1	C	142	THR
1	C	144	MET
1	C	153	ASP
1	C	154	SER
1	C	244	THR
1	C	324	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	115	ARG
1	D	139	THR
1	D	151	ASP
1	D	244	THR
1	D	299	LEU
1	D	323	ILE
1	D	324	LEU
1	E	60	HIS
1	E	66	ILE
1	E	212	ASP
1	E	298	GLU
1	E	323	ILE
1	E	324	LEU
1	F	60	HIS
1	F	139	THR
1	F	140	VAL
1	F	230	ARG
1	F	244	THR
1	F	298	GLU
1	F	299	LEU
1	F	306	HIS
1	F	324	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	96	ASN
1	A	105	ASN
1	A	177	HIS
1	B	60	HIS
1	B	177	HIS
1	B	316	GLN
1	C	107	ASN
1	D	102	GLN
1	D	177	HIS
1	D	310	GLN
1	E	60	HIS
1	E	96	ASN
1	E	127	HIS
1	E	158	GLN
1	E	223	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	319	GLN
1	F	105	ASN
1	F	177	HIS
1	F	235	HIS
1	F	255	GLN
1	F	259	GLN
1	F	290	HIS

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 ⓘ

6 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	$\# Z > 2$
2	RIP	A	401	-	10,10,10	0.33	0	14,14,14	0.86	0
2	RIP	D	401	-	10,10,10	0.39	0	14,14,14	0.65	0
2	RIP	F	401	-	10,10,10	0.28	0	14,14,14	0.77	0
2	RIP	C	401	-	10,10,10	0.24	0	14,14,14	0.48	0
2	RIP	B	401	-	10,10,10	0.16	0	14,14,14	0.63	0
2	RIP	E	401	-	10,10,10	0.59	0	14,14,14	1.34	2 (14%)

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
2	RIP	A	401	-	-	-	0/1/1/1
2	RIP	D	401	-	-	-	0/1/1/1
2	RIP	F	401	-	-	-	0/1/1/1
2	RIP	C	401	-	-	-	0/1/1/1
2	RIP	B	401	-	-	-	0/1/1/1
2	RIP	E	401	-	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	RIP	C5-C4-C3	2.91	113.88	109.64
2	E	401	RIP	O1-C1-C2	2.14	115.18	108.98

There are no chirality outliers.

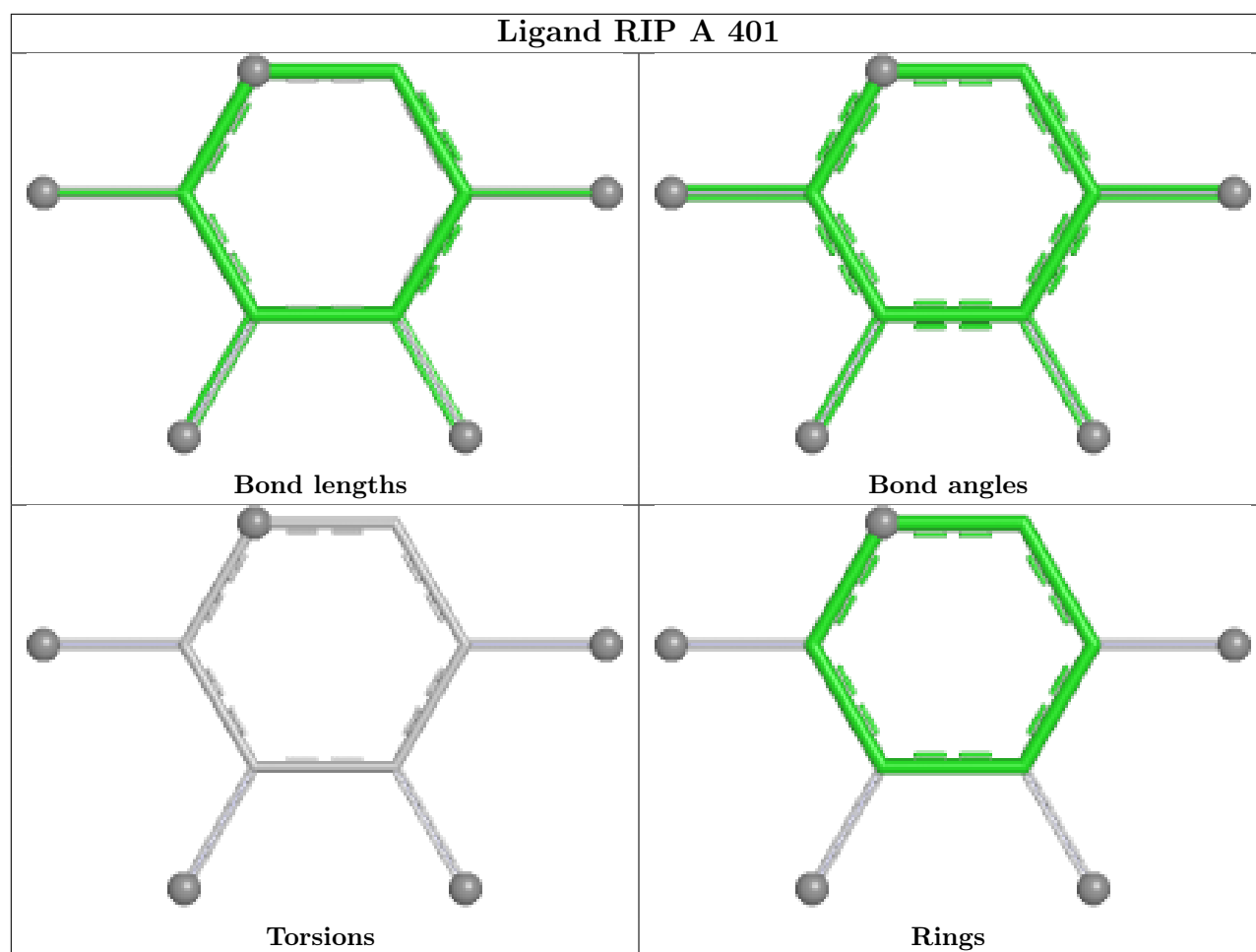
There are no torsion outliers.

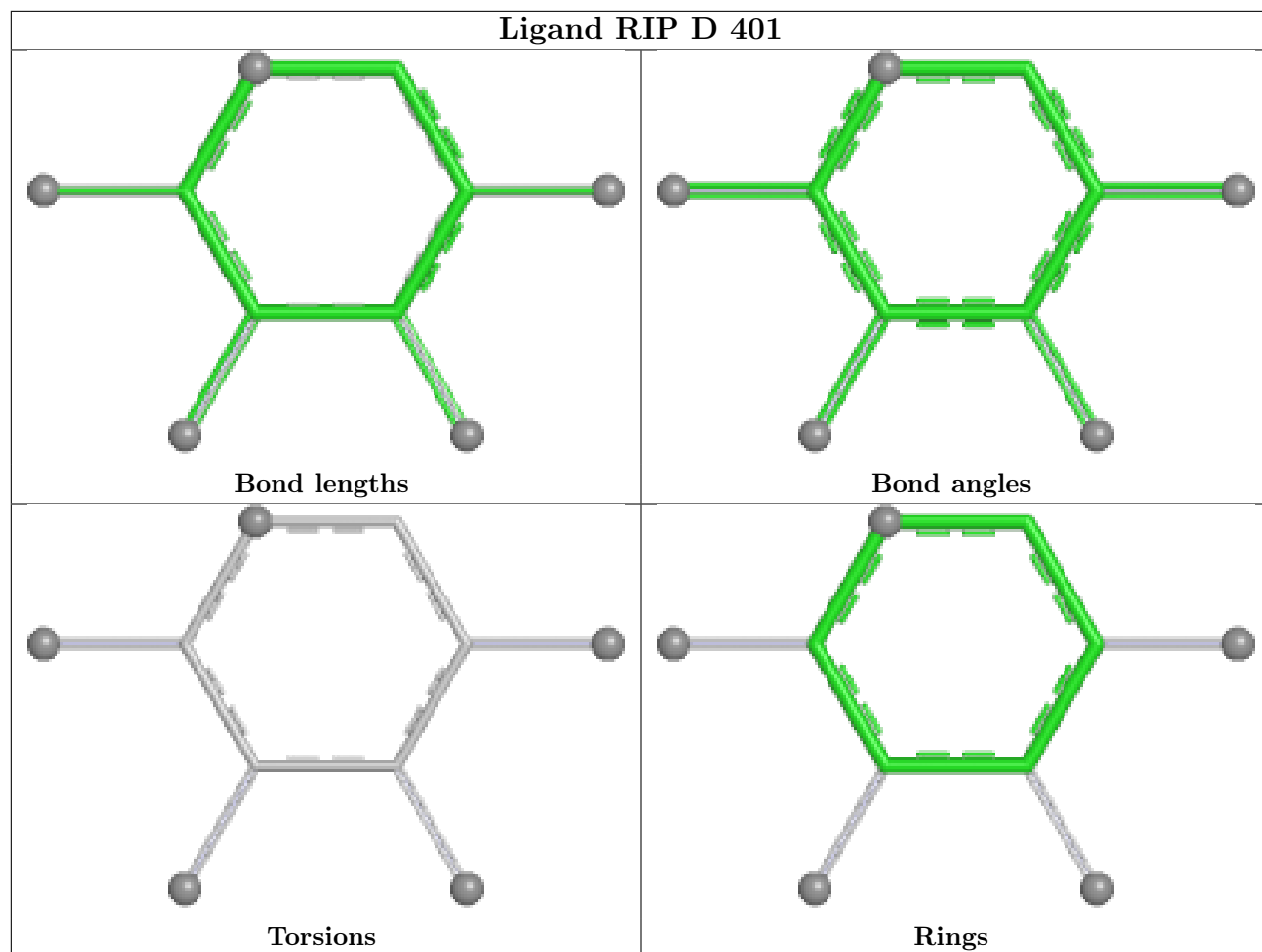
There are no ring outliers.

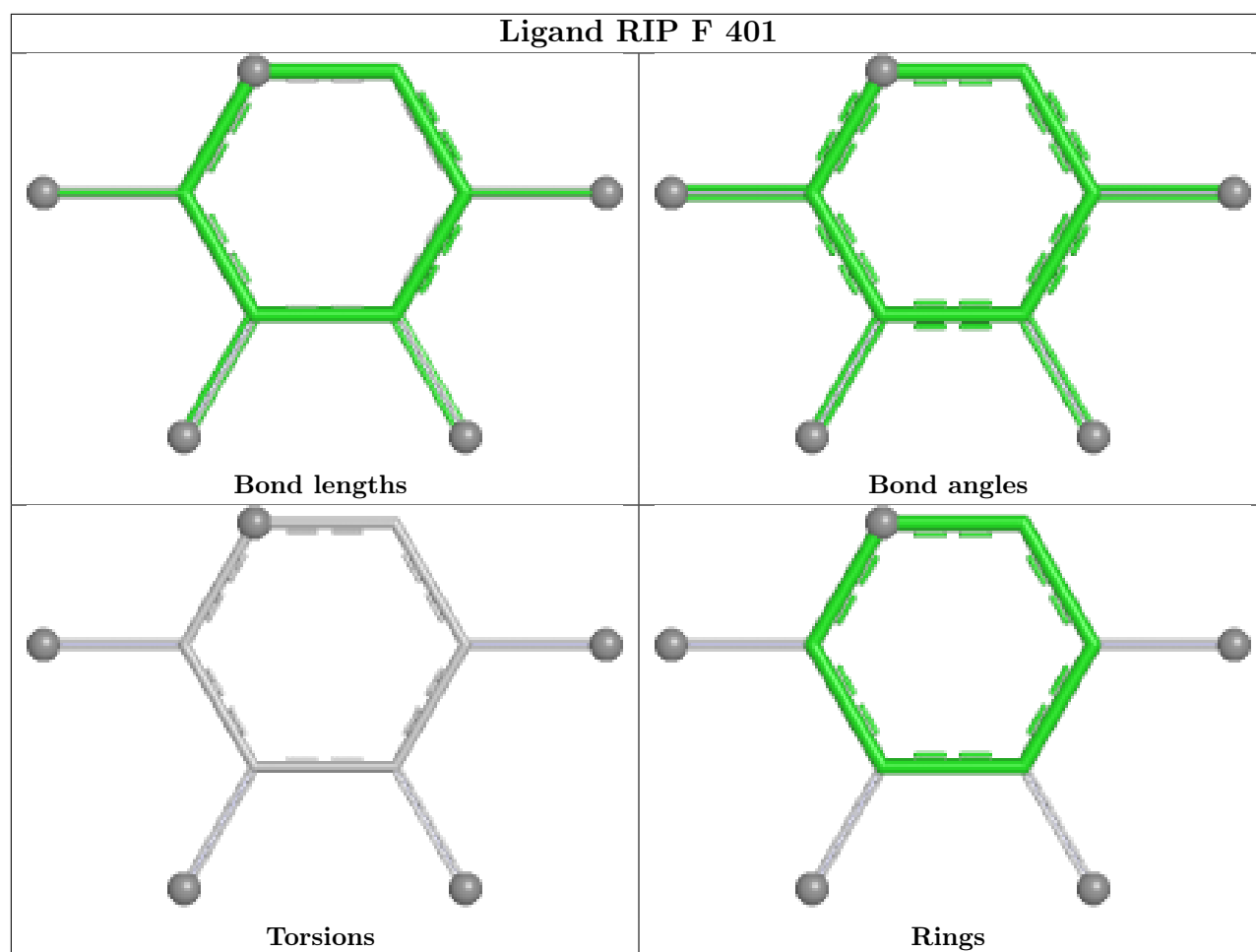
3 monomers are involved in 14 short contacts:

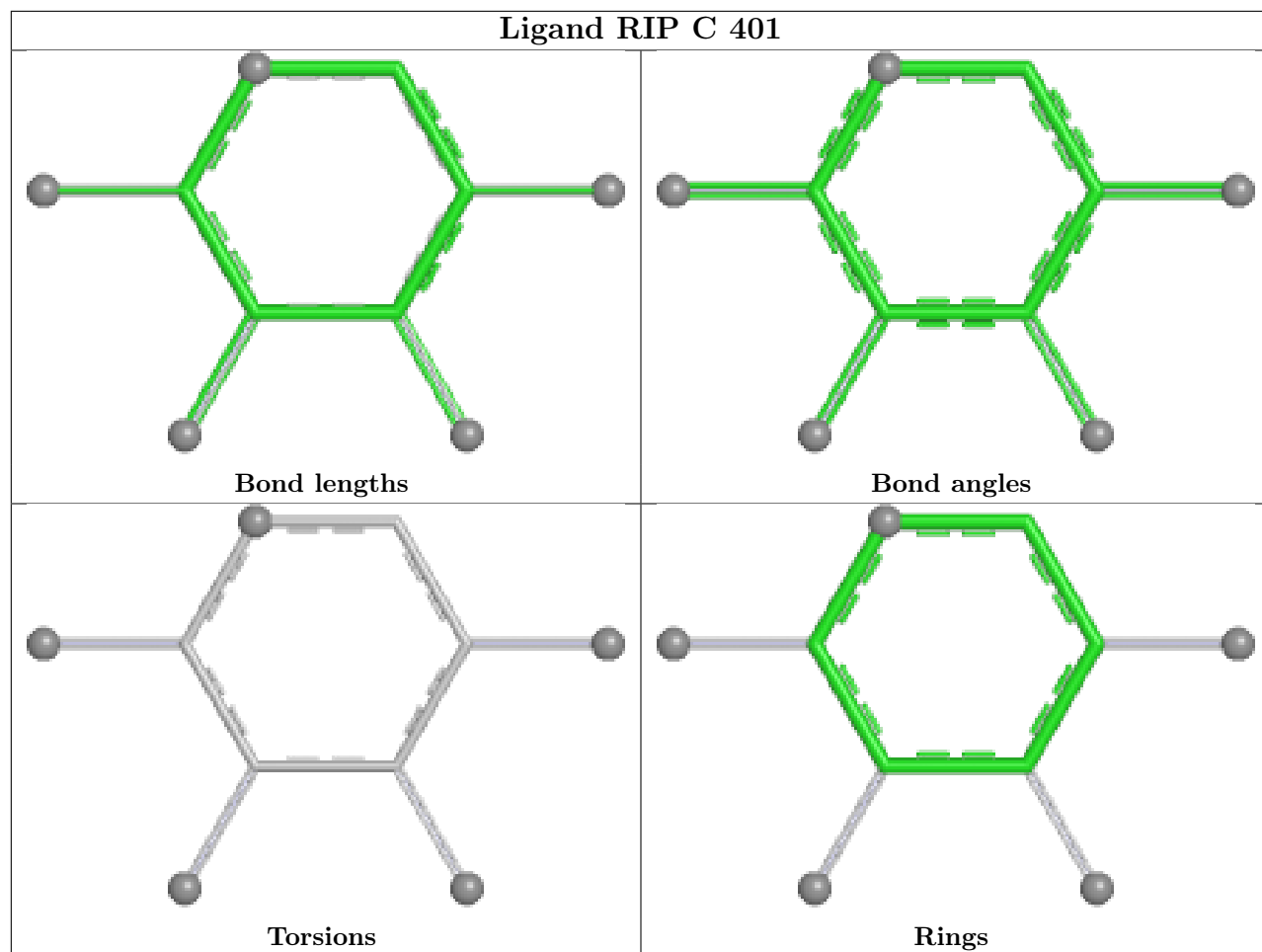
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	RIP	2	0
2	F	401	RIP	5	0
2	E	401	RIP	7	0

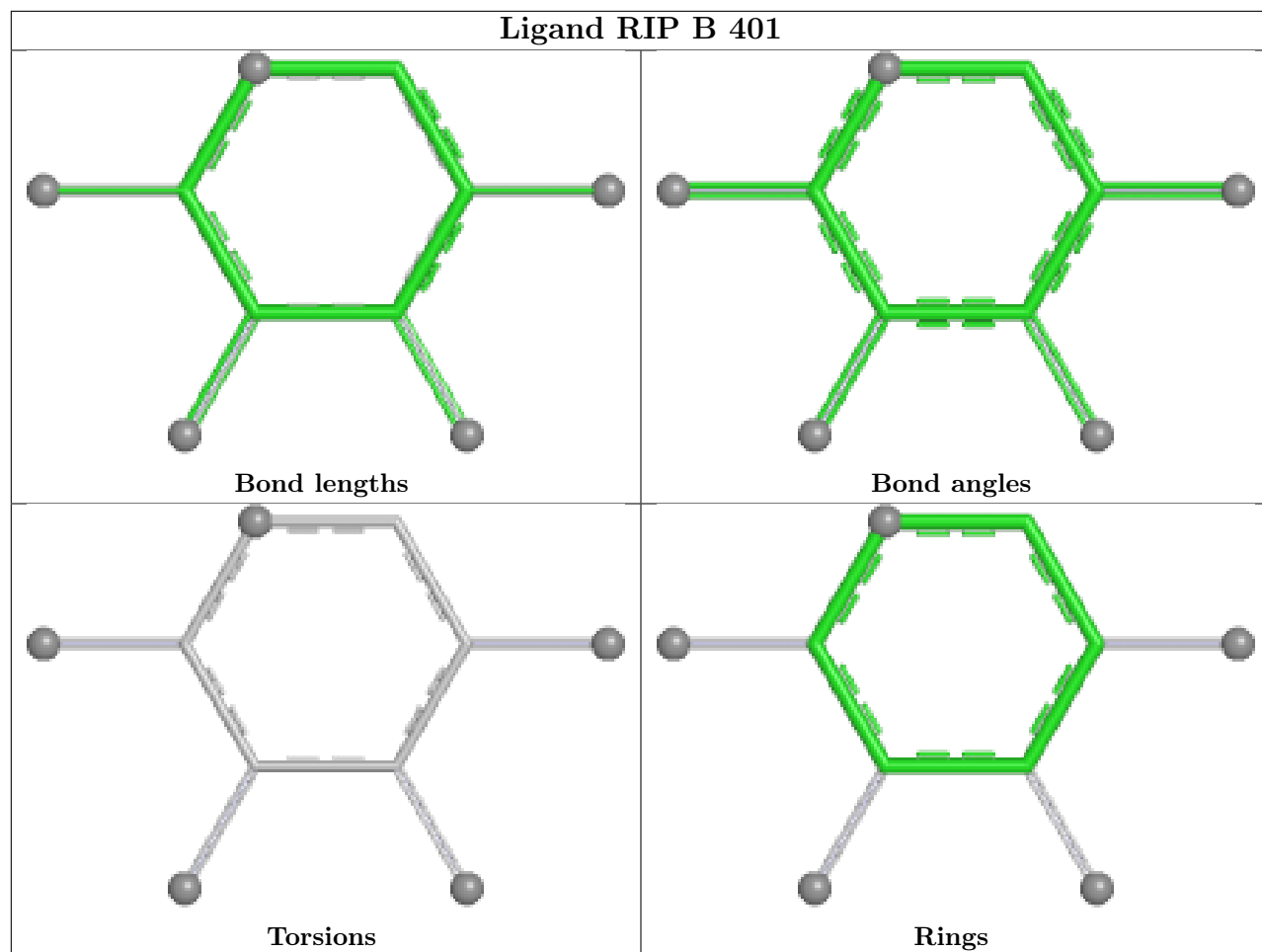
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

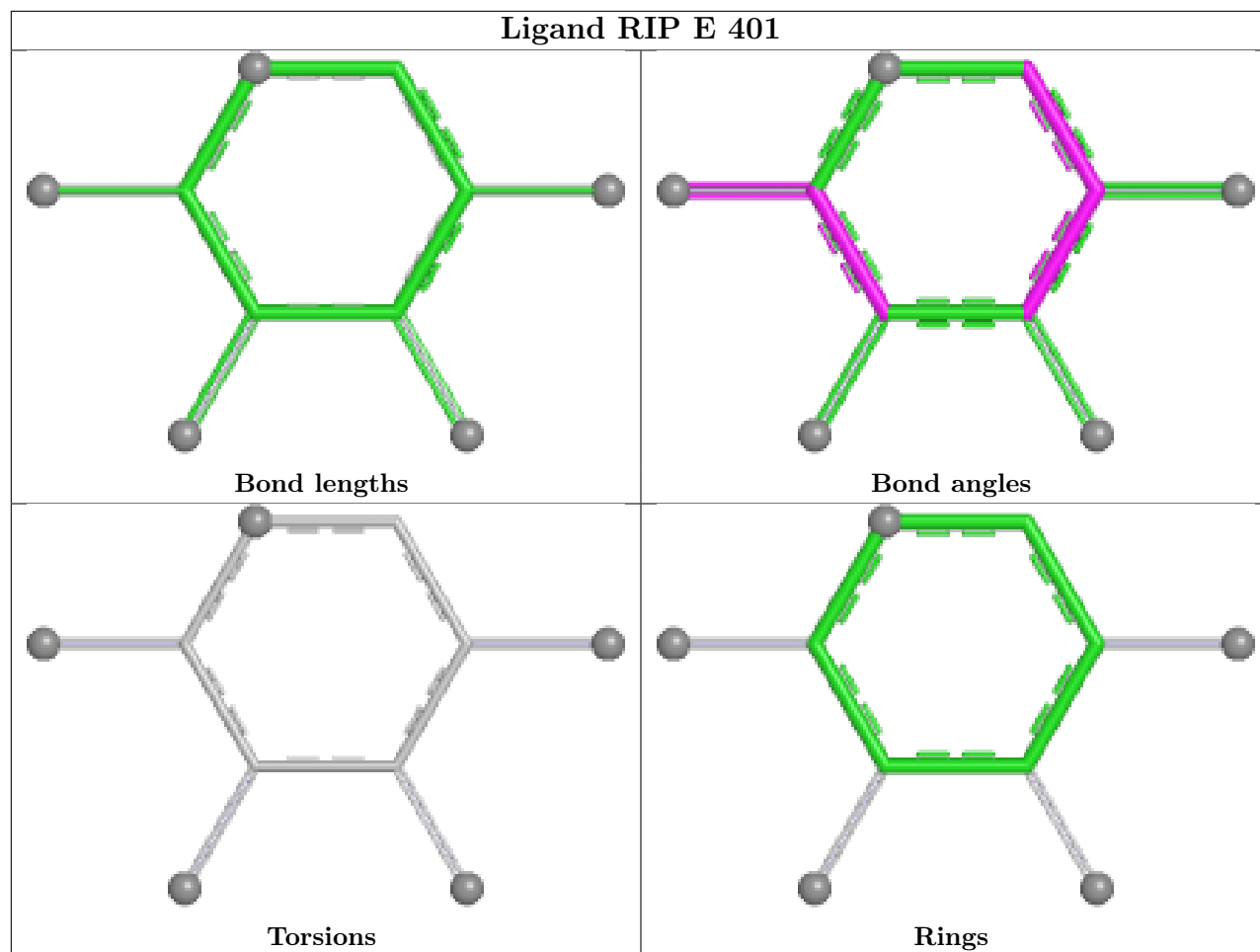












5.7 Other polymers [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	279/330 (84%)	0.08	13 (4%) 36 36	14, 31, 101, 134	0
1	B	326/330 (98%)	0.38	38 (11%) 9 9	15, 37, 97, 150	0
1	C	278/330 (84%)	-0.08	6 (2%) 62 64	9, 28, 77, 124	1 (0%)
1	D	273/330 (82%)	0.62	35 (12%) 7 7	10, 52, 115, 140	1 (0%)
1	E	279/330 (84%)	0.05	10 (3%) 46 47	15, 32, 79, 123	0
1	F	273/330 (82%)	0.46	20 (7%) 21 21	16, 46, 108, 123	0
All	All	1708/1980 (86%)	0.25	122 (7%) 22 21	9, 36, 104, 150	2 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	VAL	5.3
1	B	129	PRO	4.8
1	C	129	PRO	4.7
1	E	150	PHE	4.6
1	F	139	THR	4.5
1	B	11	ALA	4.4
1	B	127	HIS	4.3
1	B	47	PRO	3.9
1	A	150	PHE	3.8
1	A	137	TYR	3.8
1	B	150	PHE	3.6
1	A	99	GLY	3.5
1	E	99	GLY	3.5
1	F	129	PRO	3.4
1	B	125	GLU	3.3
1	F	131	ARG	3.2
1	B	126	THR	3.2
1	B	12	GLY	3.2
1	F	119	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	138	PRO	3.1
1	B	52	ARG	3.1
1	E	127	HIS	3.1
1	B	7	VAL	3.1
1	B	39	ALA	3.1
1	A	139	THR	3.1
1	E	129	PRO	3.0
1	F	111	LEU	3.0
1	F	312	THR	3.0
1	F	133	ILE	2.9
1	A	126	THR	2.9
1	E	149	PRO	2.9
1	B	102	GLN	2.9
1	D	149	PRO	2.9
1	B	34	ALA	2.9
1	B	43	LEU	2.8
1	C	187	LEU	2.8
1	D	131	ARG	2.8
1	D	134	MET	2.8
1	D	139	THR	2.8
1	A	187	LEU	2.8
1	B	10	LEU	2.8
1	D	133	ILE	2.8
1	F	134	MET	2.8
1	D	150	PHE	2.8
1	B	31	ALA	2.8
1	D	61	THR	2.8
1	E	126	THR	2.8
1	D	305	ILE	2.8
1	D	309	THR	2.7
1	A	52	ARG	2.7
1	D	129	PRO	2.7
1	D	140	VAL	2.7
1	B	70	THR	2.7
1	D	126	THR	2.7
1	B	36	VAL	2.7
1	C	127	HIS	2.6
1	D	142	THR	2.6
1	F	59	THR	2.6
1	A	129	PRO	2.6
1	D	162	LEU	2.6
1	D	137	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	38	ALA	2.6
1	D	135	GLN	2.6
1	B	35	LYS	2.6
1	D	108	LEU	2.6
1	D	82	GLU	2.5
1	B	32	ILE	2.5
1	C	53	SER	2.5
1	D	109	GLU	2.5
1	D	86	PHE	2.5
1	B	99	GLY	2.5
1	F	60	HIS	2.5
1	B	45	TYR	2.5
1	B	236	PRO	2.5
1	F	108	LEU	2.5
1	F	150	PHE	2.5
1	A	133	ILE	2.5
1	D	58	GLN	2.5
1	D	127	HIS	2.5
1	B	40	ILE	2.5
1	D	152	GLY	2.4
1	A	53	SER	2.4
1	D	130	SER	2.4
1	D	312	THR	2.4
1	B	46	ALA	2.4
1	F	136	ARG	2.4
1	E	70	THR	2.4
1	E	217	THR	2.4
1	F	317	ARG	2.4
1	C	57	ASN	2.4
1	D	95	CYS	2.4
1	B	18	VAL	2.3
1	F	140	VAL	2.3
1	B	149	PRO	2.3
1	A	313	LEU	2.3
1	B	41	LYS	2.3
1	D	148	ALA	2.3
1	C	151	ASP	2.2
1	D	151	ASP	2.2
1	D	111	LEU	2.2
1	D	313	LEU	2.2
1	E	237	LEU	2.2
1	F	135	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	138	PRO	2.2
1	D	96	ASN	2.2
1	D	138	PRO	2.2
1	D	299	LEU	2.2
1	D	204	LYS	2.2
1	B	22	ILE	2.2
1	A	149	PRO	2.1
1	F	90	TYR	2.1
1	B	3	THR	2.1
1	B	17	THR	2.1
1	F	309	THR	2.1
1	B	9	ARG	2.1
1	B	8	ALA	2.1
1	E	313	LEU	2.0
1	B	151	ASP	2.0
1	F	118	GLY	2.0
1	B	23	ASN	2.0
1	B	96	ASN	2.0
1	D	90	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	RIP	F	401	10/10	0.92	0.09	29,36,57,57	0
2	RIP	E	401	10/10	0.94	0.07	17,22,32,35	0
2	RIP	D	401	10/10	0.94	0.08	21,41,50,58	0
2	RIP	C	401	10/10	0.97	0.05	13,17,19,21	0

Continued on next page...

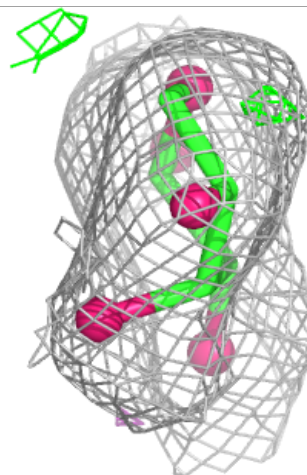
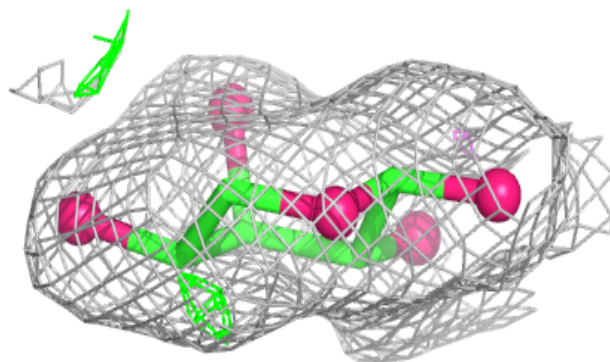
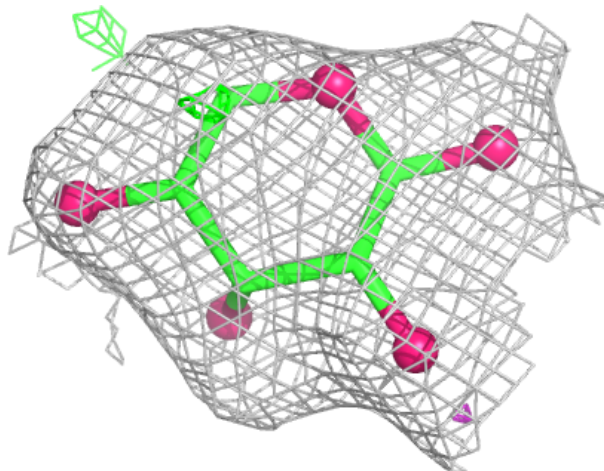
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	RIP	A	401	10/10	0.98	0.05	13,22,33,34	0
2	RIP	B	401	10/10	0.98	0.04	14,17,23,24	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.

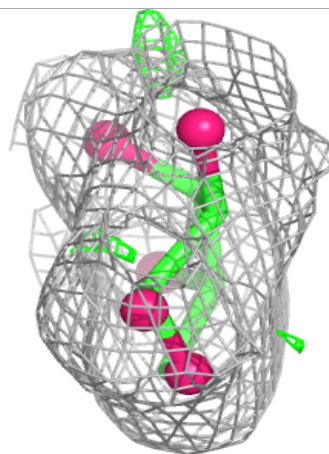
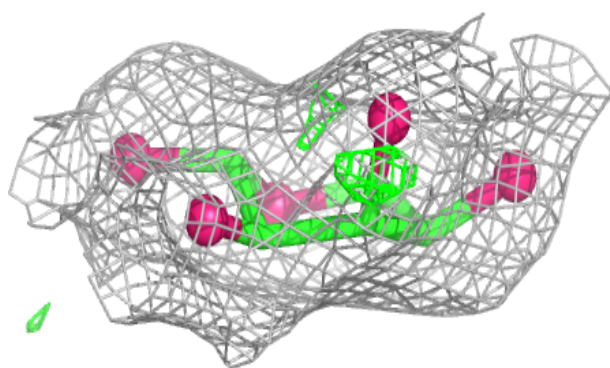
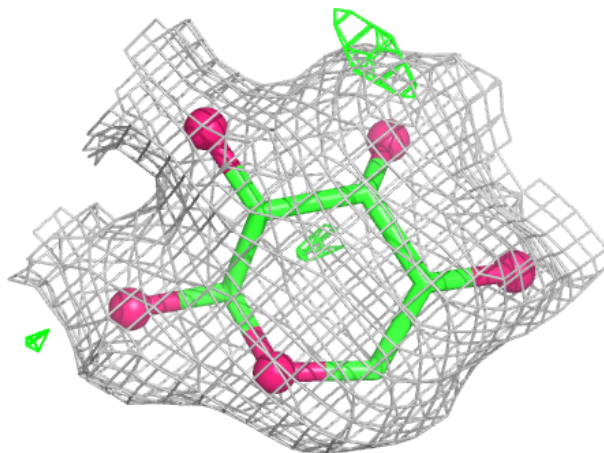
Electron density around RIP F 401:

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



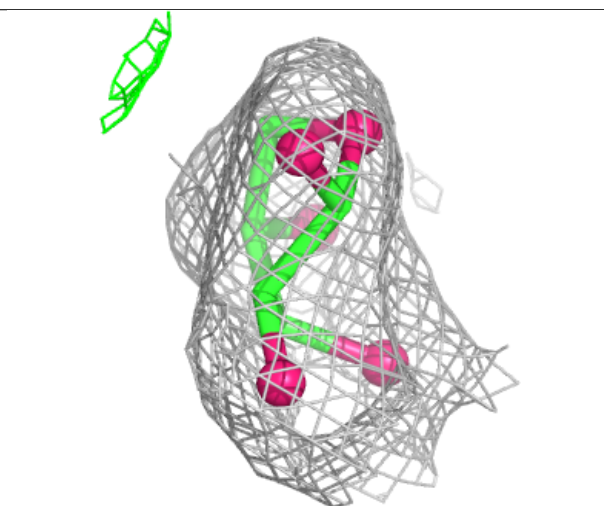
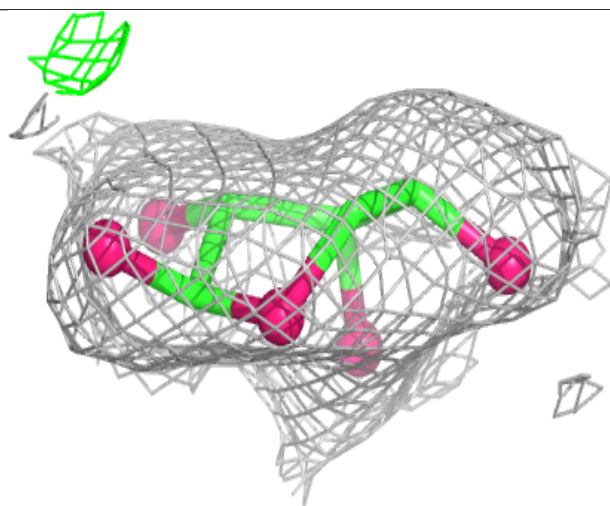
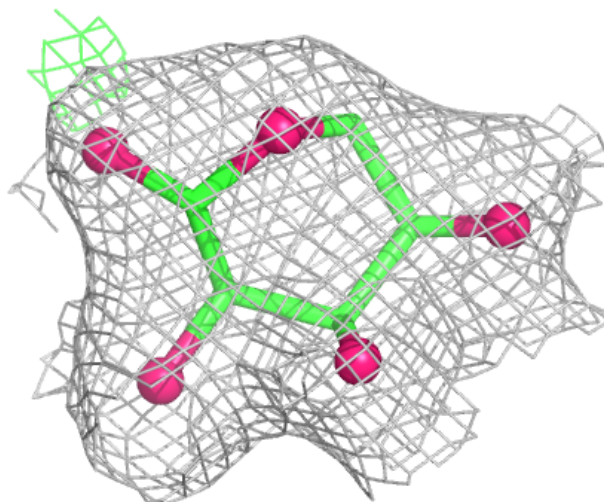
Electron density around RIP E 401:

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



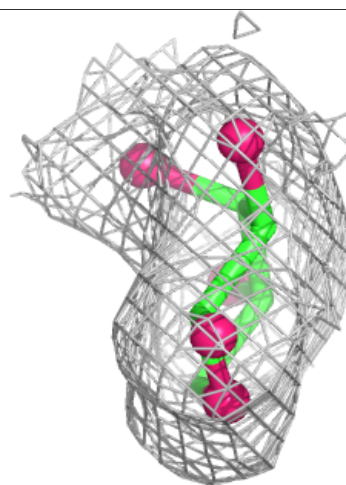
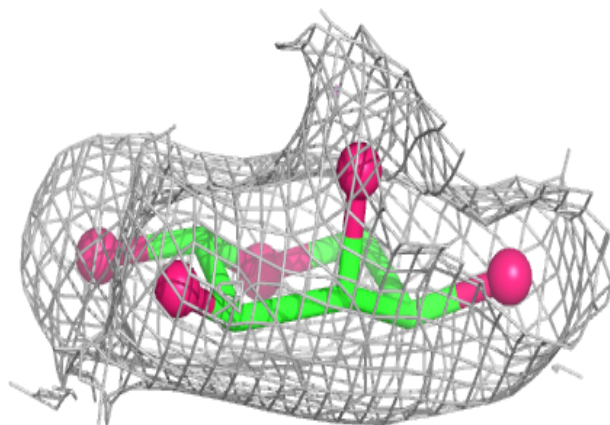
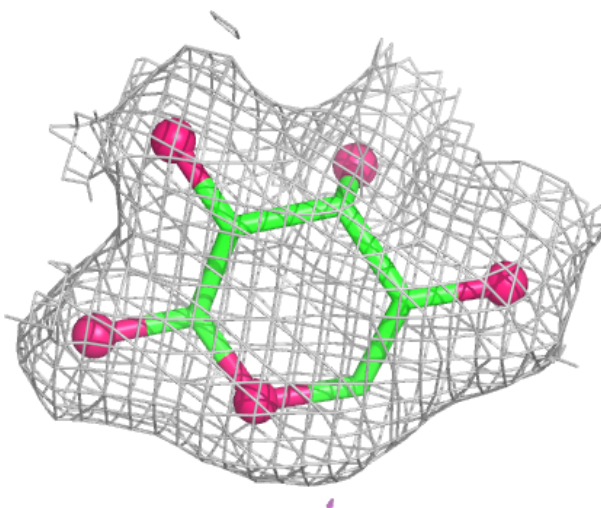
Electron density around RIP D 401:

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



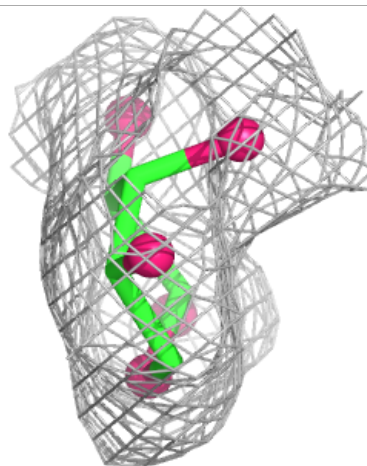
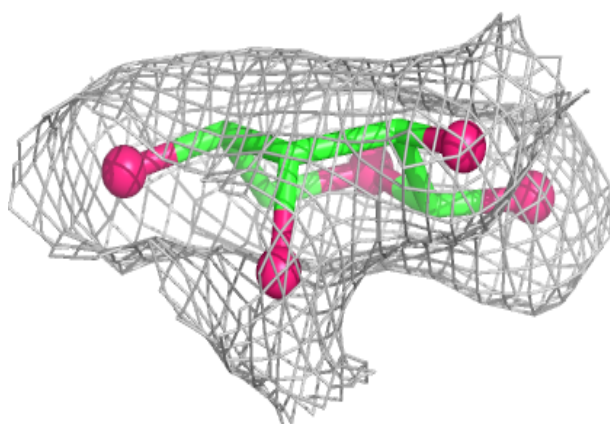
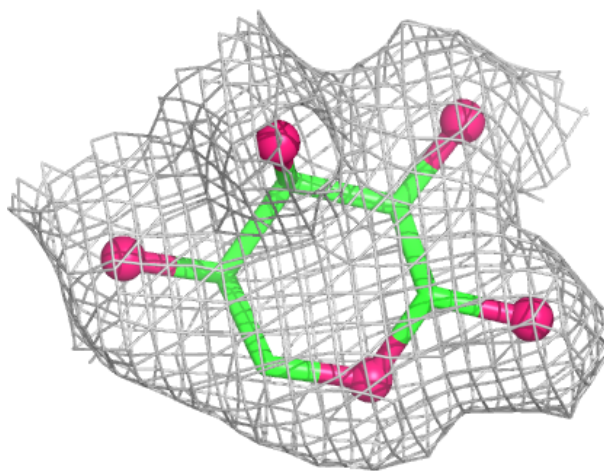
Electron density around RIP C 401:

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



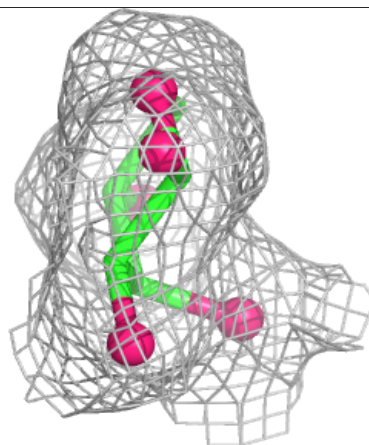
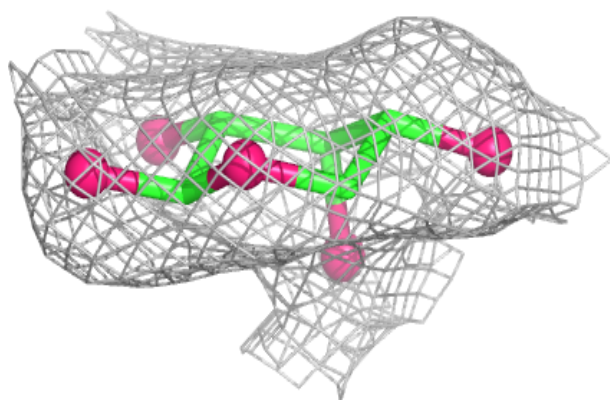
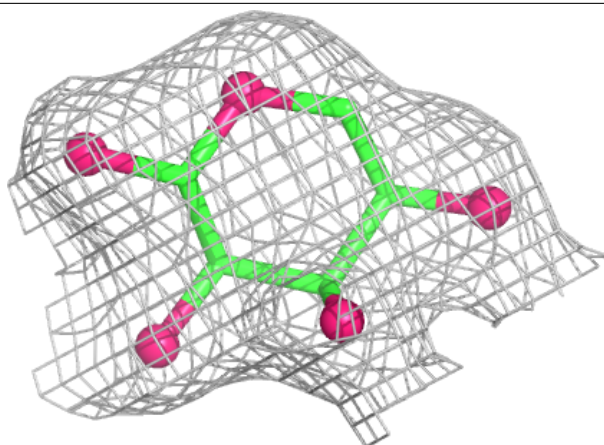
Electron density around RIP A 401:

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



Electron density around RIP B 401:

$2mF_o-DF_c$ (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.