



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:52 AM UTC

PDB ID : 8XFY / pdb_00008xfy
Title : The Crystal Structure of RSK2 from Biortus.
Authors : Wang, F.; Cheng, W.; Lv, Z.; Lin, D.; Pan, W.
Deposited on : 2023-12-14
Resolution : 3.20 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:

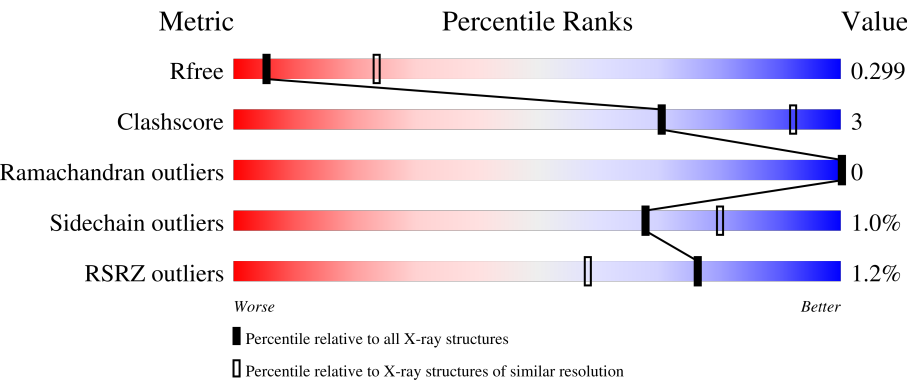
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	320	% 81% 9% 10%
1	B	320	% 79% 7% 13%
1	C	320	% 77% 8% 15%
1	D	320	% 73% 8% 19%
1	E	320	% 75% 7% 18%

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Mol	Chain	Length	Quality of chain
1	F	320	%73%6%20%
1	G	320	%78%8%14%
1	H	320	%76%11%13%
1	I	320	2%71%10%19%
1	J	320	2%74%6%20%

2 Entry composition

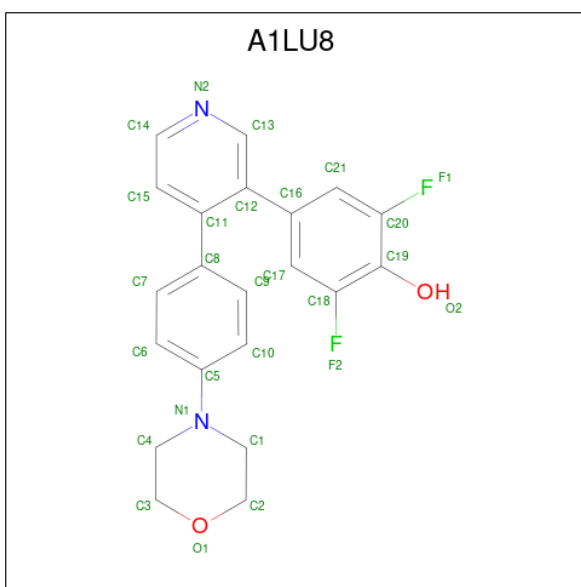
There are 3 unique types of molecules in this entry. The entry contains 22210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribosomal protein S6 kinase alpha-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2354	1521	403	419	11			
1	B	277	Total	C	N	O	S	0	0	0
			2251	1460	380	401	10			
1	C	272	Total	C	N	O	S	0	0	0
			2208	1435	369	394	10			
1	D	260	Total	C	N	O	S	0	0	0
			2102	1367	353	372	10			
1	E	261	Total	C	N	O	S	0	0	0
			2112	1373	355	374	10			
1	F	255	Total	C	N	O	S	0	0	0
			2066	1346	348	362	10			
1	G	276	Total	C	N	O	S	0	0	0
			2244	1452	387	394	11			
1	H	277	Total	C	N	O	S	0	0	0
			2245	1454	385	395	11			
1	I	260	Total	C	N	O	S	0	0	0
			2102	1367	353	372	10			
1	J	257	Total	C	N	O	S	0	0	0
			2084	1356	352	366	10			

- Molecule 2 is 2,6-bis(fluoranyl)-4-[4-(4-morpholin-4-ylphenyl)pyridin-3-yl]phenol (CCD ID: A1LU8) (formula: C₂₁H₁₈F₂N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			27	21	2	2	2		
2	B	1	Total	C	F	N	O	0	0
			27	21	2	2	2		
2	C	1	Total	C	F	N	O	0	0
			27	21	2	2	2		
2	D	1	Total	C	F	N	O	0	0
			27	21	2	2	2		
2	E	1	Total	C	F	N	O	0	0
			27	21	2	2	2		
2	F	1	Total	C	F	N	O	0	0
			27	21	2	2	2		
2	G	1	Total	C	F	N	O	0	0
			27	21	2	2	2		
2	H	1	Total	C	F	N	O	0	0
			27	21	2	2	2		
2	I	1	Total	C	F	N	O	0	0
			27	21	2	2	2		
2	J	1	Total	C	F	N	O	0	0
			27	21	2	2	2		

- Molecule 3 is water.

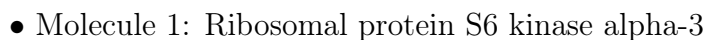
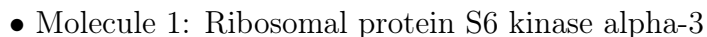
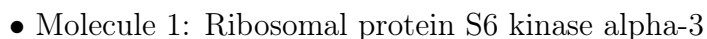
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	B	22	Total	O	0	0
			22	22		

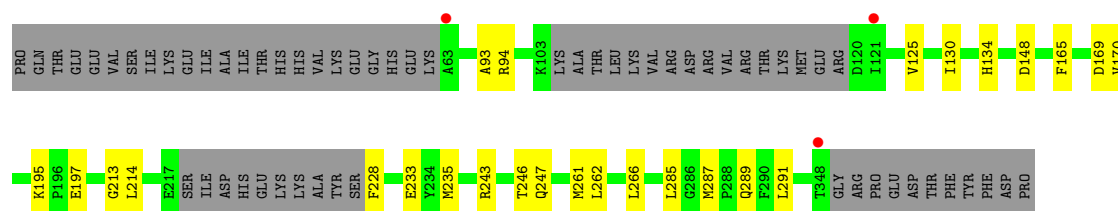
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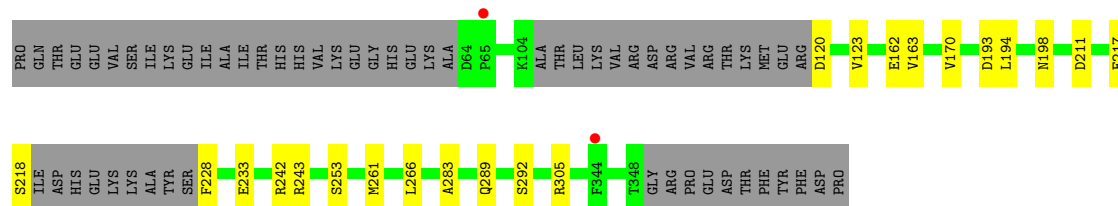
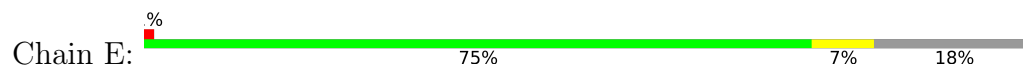
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	16	Total 16	O 16	0	0
3	D	15	Total 15	O 15	0	0
3	E	15	Total 15	O 15	0	0
3	F	15	Total 15	O 15	0	0
3	G	13	Total 13	O 13	0	0
3	H	30	Total 30	O 30	0	0
3	I	11	Total 11	O 11	0	0
3	J	7	Total 7	O 7	0	0

- Molecule 1: Ribosomal protein S6 kinase alpha-3

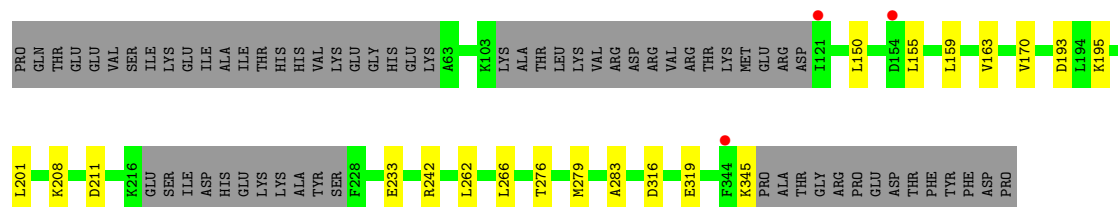
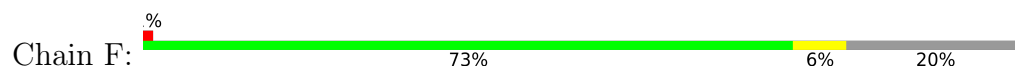




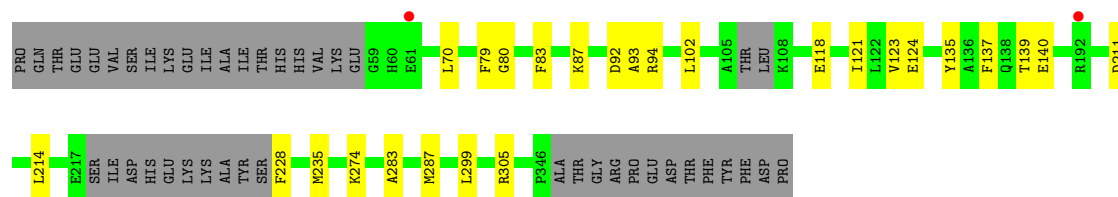
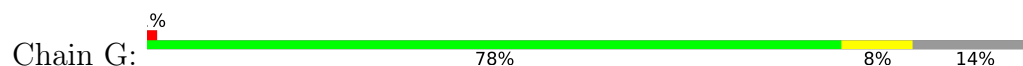
• Molecule 1: Ribosomal protein S6 kinase alpha-3



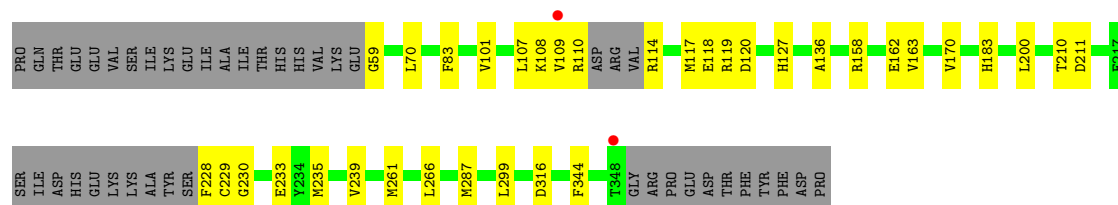
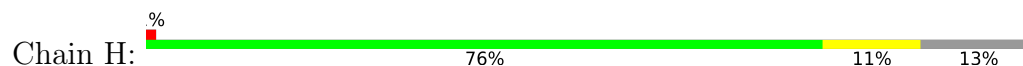
• Molecule 1: Ribosomal protein S6 kinase alpha-3



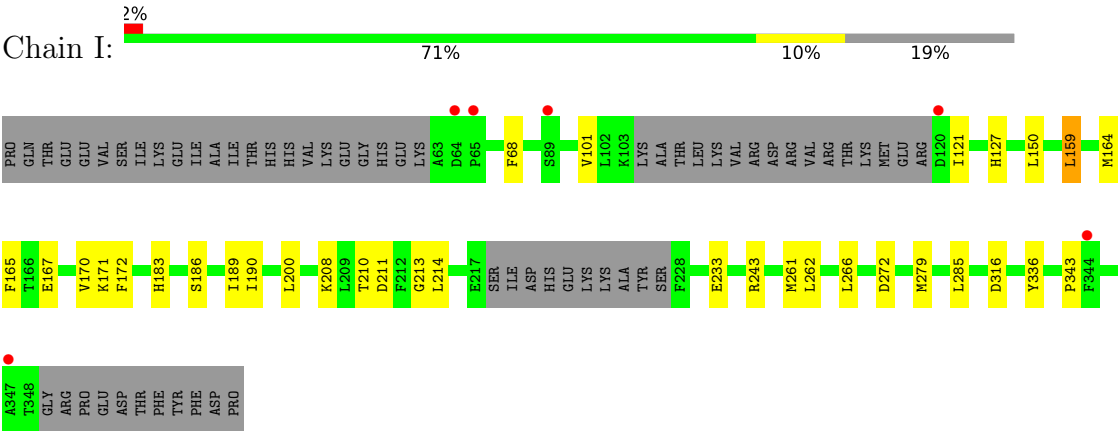
• Molecule 1: Ribosomal protein S6 kinase alpha-3



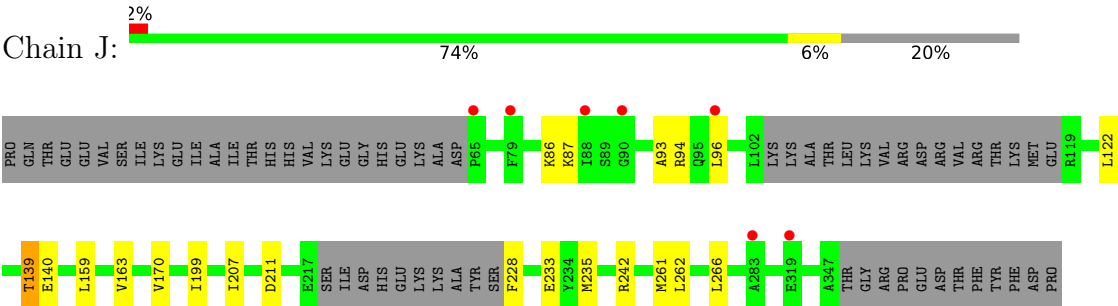
• Molecule 1: Ribosomal protein S6 kinase alpha-3



● Molecule 1: Ribosomal protein S6 kinase alpha-3



● Molecule 1: Ribosomal protein S6 kinase alpha-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	34.06Å 273.37Å 170.34Å 90.00° 92.14° 90.00°	Depositor
Resolution (Å)	48.21 – 3.20 48.21 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.21-3.20) 99.4 (48.21-3.20)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.229 , 0.303 0.231 , 0.299	Depositor DCC
R_{free} test set	2573 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22210	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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 32.56 % 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 9.2073e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1LU8

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	0.43	0/2408	0.83	0/3234
1	B	0.43	0/2305	0.82	0/3099
1	C	0.43	0/2261	0.80	0/3042
1	D	0.43	0/2151	0.80	0/2894
1	E	0.43	0/2161	0.81	0/2906
1	F	0.42	0/2114	0.79	0/2842
1	G	0.43	0/2294	0.79	0/3079
1	H	0.42	0/2295	0.81	0/3082
1	I	0.42	0/2151	0.79	0/2894
1	J	0.43	0/2133	0.80	0/2868
All	All	0.43	0/22273	0.80	0/29940

There are no bond length outliers.

There are no bond angle outliers.

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	2354	0	2375	13	0
1	B	2251	0	2261	17	0
1	C	2208	0	2219	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2102	0	2129	17	0
1	E	2112	0	2142	13	0
1	F	2066	0	2100	12	0
1	G	2244	0	2286	15	0
1	H	2245	0	2290	20	0
1	I	2102	0	2129	20	0
1	J	2084	0	2114	12	0
2	A	27	0	0	0	0
2	B	27	0	0	1	0
2	C	27	0	0	1	0
2	D	27	0	0	0	0
2	E	27	0	0	1	0
2	F	27	0	0	1	0
2	G	27	0	0	1	0
2	H	27	0	0	1	0
2	I	27	0	0	1	0
2	J	27	0	0	0	0
3	A	28	0	0	0	0
3	B	22	0	0	1	0
3	C	16	0	0	1	0
3	D	15	0	0	0	0
3	E	15	0	0	0	0
3	F	15	0	0	0	0
3	G	13	0	0	0	0
3	H	30	0	0	1	0
3	I	11	0	0	0	0
3	J	7	0	0	0	0
All	All	22210	0	22045	151	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 3.

All (151) 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:C:122:LEU:HD21	1:C:211:ASP:HB3	1.77	0.66
1:H:287:MET:HE1	1:H:299:LEU:HB2	1.77	0.65
1:F:316:ASP:HB3	1:F:319:GLU:HB2	1.80	0.64
1:H:59:GLY:HA3	1:H:136:ALA:HB3	1.79	0.64
1:C:228:PHE:CZ	1:C:235:MET:HE1	2.33	0.63
1:B:190:ILE:HD11	1:B:247:GLN:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:159:LEU:HD12	1:I:165:PHE:CZ	2.36	0.61
1:H:211:ASP:OD1	2:H:401:A1LU8:O2	2.20	0.59
1:J:233:GLU:HG2	1:J:266:LEU:HD13	1.84	0.59
1:B:190:ILE:HD11	1:B:247:GLN:CA	2.36	0.56
1:B:119:ARG:NH1	3:B:501:HOH:O	2.39	0.56
1:I:159:LEU:HD11	1:I:261:MET:HG2	1.87	0.56
1:A:217:GLU:O	1:A:218:SER:C	2.48	0.56
1:E:228:PHE:HB2	1:E:242:ARG:HH21	1.69	0.56
1:A:151:ARG:HB2	1:A:348:THR:HG23	1.86	0.56
1:H:228:PHE:CZ	1:H:235:MET:HE1	2.41	0.55
1:H:109:VAL:O	1:H:114:ARG:N	2.40	0.54
1:G:123:VAL:HG23	1:G:124:GLU:HG2	1.89	0.54
1:D:233:GLU:HG2	1:D:266:LEU:HD13	1.89	0.54
1:I:121:ILE:HD11	1:I:189:ILE:HG12	1.88	0.54
1:A:283:ALA:O	1:A:305:ARG:NH1	2.41	0.54
1:C:235:MET:HE3	1:C:239:VAL:HG12	1.88	0.54
1:E:211:ASP:OD1	2:E:401:A1LU8:O2	2.27	0.52
1:F:211:ASP:OD1	2:F:401:A1LU8:O2	2.28	0.52
1:F:233:GLU:HG2	1:F:266:LEU:HD13	1.90	0.52
1:E:283:ALA:O	1:E:305:ARG:NH1	2.43	0.51
1:I:164:MET:HE3	1:I:262:LEU:O	2.09	0.51
1:E:170:VAL:HG22	1:E:261:MET:HB3	1.92	0.51
1:H:59:GLY:CA	1:H:136:ALA:HB3	2.40	0.51
1:H:235:MET:HE3	1:H:239:VAL:HG12	1.91	0.51
1:G:121:ILE:HG21	1:G:214:LEU:HB3	1.93	0.51
1:I:233:GLU:HG2	1:I:266:LEU:HD13	1.93	0.51
1:E:120:ASP:O	1:E:123:VAL:HG22	2.12	0.50
1:G:287:MET:HE1	1:G:299:LEU:HB2	1.93	0.50
1:I:279:MET:HE2	1:I:285:LEU:HD11	1.94	0.49
1:B:150:LEU:HD12	1:B:200:LEU:HD13	1.95	0.49
1:H:228:PHE:CE2	1:H:235:MET:HE1	2.47	0.49
1:B:155:LEU:HD13	1:B:201:LEU:HD21	1.94	0.49
1:J:159:LEU:O	1:J:163:VAL:N	2.45	0.48
1:G:87:LYS:HG2	1:G:92:ASP:HB2	1.95	0.48
1:A:59:GLY:HA3	1:A:136:ALA:HB3	1.96	0.48
1:B:85:VAL:HG11	1:B:99:MET:HE3	1.95	0.48
1:C:63:ALA:HB2	1:C:135:TYR:HB3	1.94	0.48
1:C:85:VAL:HG11	1:C:99:MET:HE3	1.96	0.47
1:J:199:ILE:HG23	1:J:207:ILE:HG23	1.95	0.47
1:C:228:PHE:CE2	1:C:235:MET:HE1	2.50	0.47
1:H:118:GLU:O	1:H:119:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:LEU:HD22	1:C:208:LYS:HG3	1.96	0.47
1:D:165:PHE:HB3	1:D:169:ASP:HB2	1.96	0.47
1:D:170:VAL:HG21	1:D:262:LEU:CD2	2.45	0.47
1:E:233:GLU:HG2	1:E:266:LEU:HD13	1.96	0.47
1:F:150:LEU:HD21	1:F:208:LYS:HB2	1.97	0.47
1:D:170:VAL:HG21	1:D:262:LEU:HD23	1.97	0.46
1:I:172:PHE:CD2	1:I:343:PRO:HD3	2.51	0.46
1:D:289:GLN:HG3	1:J:228:PHE:CD2	2.51	0.46
1:A:85:VAL:HG11	1:A:99:MET:HE3	1.97	0.46
1:D:125:VAL:HG11	1:D:130:ILE:HG21	1.97	0.46
1:J:139:THR:HG22	1:J:140:GLU:HG2	1.98	0.46
1:B:194:LEU:HD23	1:B:253:SER:HB2	1.97	0.46
1:B:194:LEU:HD23	1:B:253:SER:CB	2.46	0.46
1:C:154:ASP:HA	1:C:200:LEU:HA	1.98	0.46
1:I:127:HIS:HB2	1:I:183:HIS:CD2	2.51	0.46
1:B:211:ASP:OD1	2:B:401:A1LU8:O2	2.34	0.46
1:B:336:TYR:CD1	1:B:336:TYR:C	2.93	0.46
1:C:190:ILE:HD11	1:C:247:GLN:HA	1.97	0.45
1:D:125:VAL:CG1	1:D:130:ILE:HG21	2.47	0.45
1:E:194:LEU:HD23	1:E:253:SER:HB2	1.98	0.45
1:B:190:ILE:HD11	1:B:247:GLN:CB	2.47	0.45
1:H:70:LEU:HD23	1:H:83:PHE:CE2	2.52	0.45
1:E:289:GLN:HG3	1:G:228:PHE:CD2	2.51	0.45
1:H:200:LEU:HD13	1:H:210:THR:CG2	2.47	0.45
1:A:233:GLU:HG2	1:A:266:LEU:HD13	1.98	0.45
1:I:213:GLY:O	1:I:214:LEU:C	2.59	0.45
1:E:292:SER:HA	1:G:274:LYS:HE2	1.98	0.45
1:D:228:PHE:CZ	1:D:235:MET:HE1	2.52	0.44
1:G:228:PHE:CZ	1:G:235:MET:HE1	2.53	0.44
1:C:159:LEU:HD23	1:C:165:PHE:CE1	2.52	0.44
1:H:119:ARG:HG2	3:H:509:HOH:O	2.17	0.44
1:D:134:HIS:NE2	1:D:148:ASP:OD1	2.50	0.44
1:H:233:GLU:HG2	1:H:266:LEU:HD13	1.99	0.44
1:A:162:GLU:O	1:A:163:VAL:HB	2.16	0.44
1:D:170:VAL:HG22	1:D:261:MET:HB3	2.00	0.44
1:I:211:ASP:OD1	2:I:401:A1LU8:O2	2.36	0.43
1:B:342:PRO:HA	1:B:343:PRO:HD3	1.92	0.43
1:H:127:HIS:HB2	1:H:183:HIS:CD2	2.53	0.43
1:H:158:ARG:HD2	1:H:344:PHE:CD2	2.53	0.43
1:I:183:HIS:O	1:I:186:SER:OG	2.36	0.43
1:J:93:ALA:O	1:J:94:ARG:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ASP:O	1:C:198:ASN:ND2	2.52	0.43
1:G:102:LEU:HD13	1:G:118:GLU:HG3	1.99	0.43
1:I:200:LEU:HD13	1:I:210:THR:CG2	2.49	0.43
1:B:356:TYR:CE2	1:H:110:ARG:HG2	2.54	0.43
1:A:170:VAL:HG21	1:A:262:LEU:HD23	2.00	0.43
1:B:286:GLY:HA3	1:F:242:ARG:HH21	1.84	0.43
1:C:211:ASP:OD1	2:C:401:A1LU8:O2	2.37	0.43
1:G:287:MET:HE1	1:G:299:LEU:CB	2.49	0.43
1:F:159:LEU:O	1:F:163:VAL:N	2.49	0.42
1:F:345:LYS:HD3	1:F:345:LYS:C	2.42	0.42
1:D:285:LEU:CD1	1:D:287:MET:HE2	2.49	0.42
1:A:113:VAL:HG11	3:C:506:HOH:O	2.20	0.42
1:C:246:THR:OG1	1:C:247:GLN:N	2.52	0.42
1:G:79:PHE:CG	1:G:80:GLY:N	2.87	0.42
1:G:139:THR:HG22	1:G:140:GLU:N	2.34	0.42
1:G:211:ASP:OD1	2:G:401:A1LU8:O2	2.38	0.42
1:E:162:GLU:O	1:E:163:VAL:HB	2.20	0.42
1:F:193:ASP:OD2	1:F:195:LYS:NZ	2.52	0.42
1:G:70:LEU:HD23	1:G:83:PHE:CD2	2.54	0.42
1:H:170:VAL:HG22	1:H:261:MET:HB3	2.00	0.42
1:I:272:ASP:OD1	1:I:272:ASP:N	2.53	0.42
1:C:213:GLY:O	1:C:214:LEU:C	2.62	0.42
1:J:228:PHE:CZ	1:J:235:MET:HE1	2.55	0.42
1:E:217:GLU:O	1:E:218:SER:C	2.61	0.42
1:G:93:ALA:O	1:G:94:ARG:HB2	2.19	0.42
1:H:162:GLU:O	1:H:163:VAL:HB	2.20	0.42
1:E:242:ARG:HB3	1:E:242:ARG:NH1	2.35	0.42
1:A:79:PHE:CG	1:A:80:GLY:N	2.88	0.41
1:I:150:LEU:HD21	1:I:208:LYS:HD2	2.02	0.41
1:I:167:GLU:O	1:I:171:LYS:HB2	2.20	0.41
1:C:348:THR:HG23	1:C:350:ARG:HG2	2.02	0.41
1:I:170:VAL:HG13	1:I:261:MET:HE3	2.01	0.41
1:J:170:VAL:HG22	1:J:261:MET:HB3	2.01	0.41
1:A:183:HIS:O	1:A:186:SER:OG	2.33	0.41
1:J:170:VAL:HG21	1:J:262:LEU:HD23	2.02	0.41
1:C:122:LEU:HD21	1:C:211:ASP:CB	2.47	0.41
1:C:211:ASP:HA	1:C:214:LEU:HG	2.03	0.41
1:E:193:ASP:O	1:E:198:ASN:ND2	2.54	0.41
1:H:117:MET:O	1:H:120:ASP:HB2	2.21	0.41
1:H:229:CYS:SG	1:H:230:GLY:N	2.94	0.41
1:I:336:TYR:CD1	1:I:336:TYR:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:LYS:HA	1:B:305:ARG:HH12	1.85	0.41
1:D:195:LYS:HD3	1:D:197:GLU:HB2	2.02	0.41
1:D:262:LEU:HD13	1:D:291:LEU:HD22	2.03	0.41
1:A:70:LEU:HD23	1:A:83:PHE:CE2	2.55	0.41
1:D:246:THR:OG1	1:D:247:GLN:N	2.54	0.41
1:C:266:LEU:O	1:I:243:ARG:NH2	2.51	0.41
1:D:93:ALA:O	1:D:94:ARG:HB2	2.19	0.41
1:D:213:GLY:O	1:D:214:LEU:C	2.64	0.41
1:D:228:PHE:CE1	1:D:235:MET:HE1	2.56	0.41
1:F:279:MET:O	1:F:283:ALA:HB3	2.21	0.41
1:J:228:PHE:HB2	1:J:242:ARG:HH21	1.85	0.41
1:G:283:ALA:O	1:G:305:ARG:NH1	2.51	0.41
1:B:99:MET:HE2	1:B:146:ILE:HD11	2.03	0.40
1:I:211:ASP:HA	1:I:214:LEU:HG	2.03	0.40
1:I:211:ASP:HB2	1:I:214:LEU:HD12	2.03	0.40
1:J:86:LYS:HG2	1:J:96:LEU:HD23	2.02	0.40
1:B:59:GLY:HA3	1:B:136:ALA:HB3	2.03	0.40
1:J:122:LEU:HD21	1:J:211:ASP:HB2	2.02	0.40
1:F:155:LEU:HD13	1:F:201:LEU:HD21	2.03	0.40
1:F:233:GLU:HG3	1:F:276:THR:HG21	2.02	0.40
1:A:151:ARG:HE	1:A:350:ARG:HH11	1.70	0.40
1:F:170:VAL:HG21	1:F:262:LEU:CD2	2.51	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	283/320 (88%)	268 (95%)	15 (5%)	0	100	100
1	B	271/320 (85%)	258 (95%)	13 (5%)	0	100	100
1	C	266/320 (83%)	253 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	254/320 (79%)	241 (95%)	13 (5%)	0	100	100
1	E	255/320 (80%)	242 (95%)	13 (5%)	0	100	100
1	F	249/320 (78%)	237 (95%)	12 (5%)	0	100	100
1	G	270/320 (84%)	255 (94%)	15 (6%)	0	100	100
1	H	271/320 (85%)	253 (93%)	18 (7%)	0	100	100
1	I	254/320 (79%)	246 (97%)	8 (3%)	0	100	100
1	J	251/320 (78%)	239 (95%)	12 (5%)	0	100	100
All	All	2624/3200 (82%)	2492 (95%)	132 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	254/282 (90%)	249 (98%)	5 (2%)	48	72
1	B	242/282 (86%)	240 (99%)	2 (1%)	73	82
1	C	238/282 (84%)	237 (100%)	1 (0%)	84	86
1	D	227/282 (80%)	226 (100%)	1 (0%)	84	86
1	E	229/282 (81%)	228 (100%)	1 (0%)	84	86
1	F	223/282 (79%)	223 (100%)	0	100	100
1	G	242/282 (86%)	240 (99%)	2 (1%)	73	82
1	H	242/282 (86%)	238 (98%)	4 (2%)	53	75
1	I	227/282 (80%)	222 (98%)	5 (2%)	45	71
1	J	225/282 (80%)	223 (99%)	2 (1%)	70	81
All	All	2349/2820 (83%)	2326 (99%)	23 (1%)	68	80

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	101	VAL
1	A	109	VAL
1	A	154	ASP
1	A	243	ARG
1	B	151	ARG
1	B	190	ILE
1	C	101	VAL
1	D	243	ARG
1	E	243	ARG
1	G	135	TYR
1	G	137	PHE
1	H	101	VAL
1	H	107	LEU
1	H	108	LYS
1	H	316	ASP
1	I	68	PHE
1	I	101	VAL
1	I	159	LEU
1	I	190	ILE
1	I	316	ASP
1	J	87	LYS
1	J	139	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	241	ASN
1	C	269	GLN
1	E	138	GLN
1	E	183	HIS
1	E	198	ASN
1	F	247	GLN
1	F	333	ASN
1	G	76	GLN
1	G	134	HIS
1	H	198	ASN
1	J	289	GLN
1	J	341	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 ⓘ

10 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	A1LU8	J	401	-	30,30,30	0.50	0	42,42,42	1.04	4 (9%)
2	A1LU8	D	401	-	30,30,30	0.45	0	42,42,42	0.94	5 (11%)
2	A1LU8	A	401	-	30,30,30	0.47	0	42,42,42	1.03	5 (11%)
2	A1LU8	B	401	-	30,30,30	0.44	0	42,42,42	1.12	4 (9%)
2	A1LU8	C	401	-	30,30,30	0.48	0	42,42,42	1.04	4 (9%)
2	A1LU8	G	401	-	30,30,30	0.43	0	42,42,42	1.01	4 (9%)
2	A1LU8	F	401	-	30,30,30	0.48	0	42,42,42	1.05	4 (9%)
2	A1LU8	H	401	-	30,30,30	0.45	0	42,42,42	1.07	4 (9%)
2	A1LU8	E	401	-	30,30,30	0.45	0	42,42,42	1.08	5 (11%)
2	A1LU8	I	401	-	30,30,30	0.49	0	42,42,42	0.99	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
2	A1LU8	J	401	-	-	0/12/20/20	0/4/4/4
2	A1LU8	D	401	-	-	0/12/20/20	0/4/4/4
2	A1LU8	A	401	-	-	0/12/20/20	0/4/4/4
2	A1LU8	B	401	-	-	0/12/20/20	0/4/4/4
2	A1LU8	C	401	-	-	0/12/20/20	0/4/4/4
2	A1LU8	G	401	-	-	0/12/20/20	0/4/4/4
2	A1LU8	F	401	-	-	0/12/20/20	0/4/4/4
2	A1LU8	H	401	-	-	0/12/20/20	0/4/4/4
2	A1LU8	E	401	-	-	0/12/20/20	0/4/4/4
2	A1LU8	I	401	-	-	0/12/20/20	0/4/4/4

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	A1LU8	F1-C20-C19	3.51	119.67	117.13
2	B	401	A1LU8	F1-C20-C19	3.49	119.65	117.13
2	B	401	A1LU8	F2-C18-C19	3.25	119.48	117.13
2	C	401	A1LU8	F1-C20-C19	3.20	119.44	117.13
2	E	401	A1LU8	F1-C20-C19	3.15	119.41	117.13
2	E	401	A1LU8	F2-C18-C19	3.10	119.37	117.13
2	J	401	A1LU8	F2-C18-C19	2.99	119.29	117.13
2	A	401	A1LU8	F2-C18-C19	2.99	119.29	117.13
2	H	401	A1LU8	F1-C20-C19	2.94	119.25	117.13
2	D	401	A1LU8	F2-C18-C19	2.88	119.21	117.13
2	A	401	A1LU8	F1-C20-C19	2.87	119.20	117.13
2	G	401	A1LU8	F1-C20-C19	2.87	119.20	117.13
2	G	401	A1LU8	F2-C18-C19	2.78	119.13	117.13
2	C	401	A1LU8	F2-C18-C19	2.76	119.12	117.13
2	H	401	A1LU8	F2-C18-C19	2.70	119.08	117.13
2	J	401	A1LU8	F1-C20-C19	2.70	119.08	117.13
2	F	401	A1LU8	F2-C18-C19	2.67	119.06	117.13
2	I	401	A1LU8	F1-C20-C19	2.67	119.06	117.13
2	I	401	A1LU8	F2-C18-C19	2.62	119.02	117.13
2	B	401	A1LU8	C21-C20-C19	-2.60	121.76	123.79
2	B	401	A1LU8	C17-C18-C19	-2.60	121.76	123.79
2	H	401	A1LU8	C17-C18-C19	-2.56	121.78	123.79
2	H	401	A1LU8	C21-C20-C19	-2.51	121.82	123.79
2	F	401	A1LU8	C21-C20-C19	-2.46	121.86	123.79
2	E	401	A1LU8	C21-C20-C19	-2.45	121.87	123.79
2	C	401	A1LU8	C21-C20-C19	-2.43	121.89	123.79
2	D	401	A1LU8	F1-C20-C19	2.43	118.89	117.13
2	J	401	A1LU8	C21-C20-C19	-2.43	121.89	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	A1LU8	C17-C18-C19	-2.41	121.91	123.79
2	A	401	A1LU8	C21-C20-C19	-2.41	121.91	123.79
2	F	401	A1LU8	C17-C18-C19	-2.33	121.97	123.79
2	C	401	A1LU8	C17-C18-C19	-2.32	121.97	123.79
2	G	401	A1LU8	C21-C20-C19	-2.31	121.98	123.79
2	A	401	A1LU8	C17-C18-C19	-2.30	121.99	123.79
2	E	401	A1LU8	C17-C18-C19	-2.24	122.04	123.79
2	I	401	A1LU8	C17-C18-C19	-2.21	122.06	123.79
2	D	401	A1LU8	C17-C18-C19	-2.20	122.06	123.79
2	D	401	A1LU8	C4-N1-C5	2.17	124.03	118.11
2	I	401	A1LU8	C21-C20-C19	-2.15	122.11	123.79
2	E	401	A1LU8	C1-N1-C5	2.11	123.87	118.11
2	D	401	A1LU8	C21-C20-C19	-2.10	122.15	123.79
2	A	401	A1LU8	C4-N1-C5	2.06	123.71	118.11
2	I	401	A1LU8	C4-N1-C5	2.06	123.71	118.11
2	J	401	A1LU8	C17-C18-C19	-2.02	122.21	123.79

There are no chirality outliers.

There are no torsion outliers.

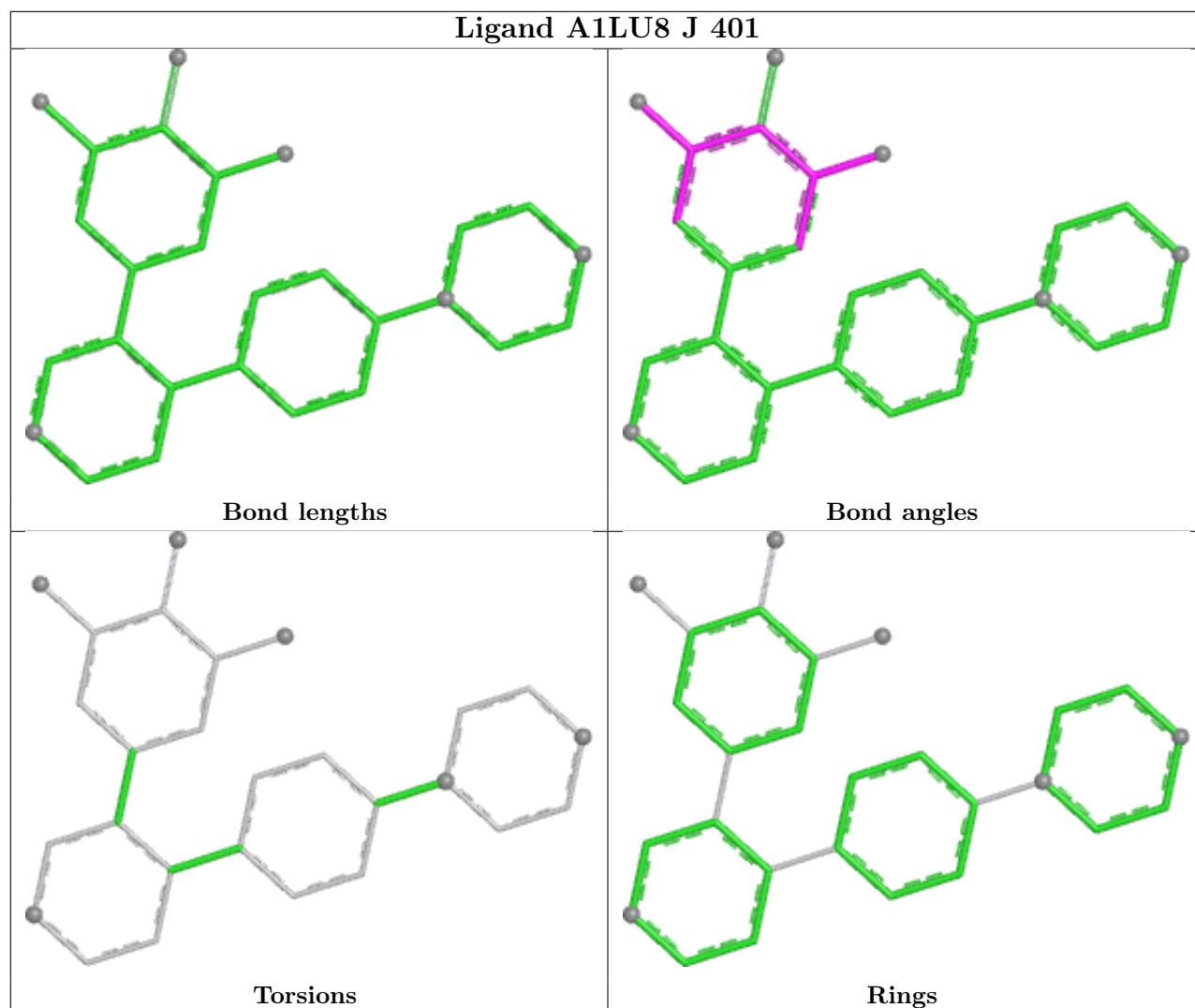
There are no ring outliers.

7 monomers are involved in 7 short contacts:

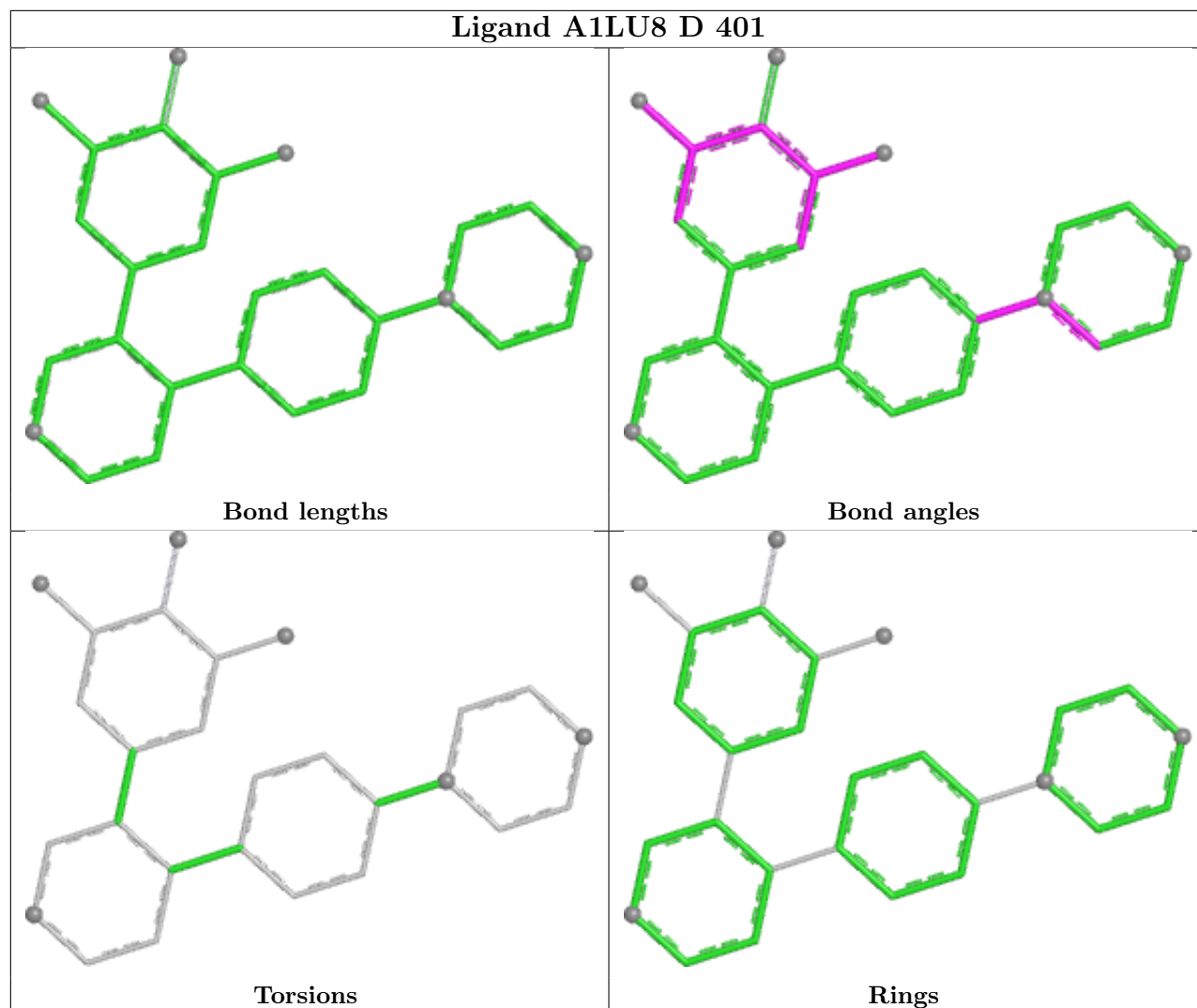
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	A1LU8	1	0
2	C	401	A1LU8	1	0
2	G	401	A1LU8	1	0
2	F	401	A1LU8	1	0
2	H	401	A1LU8	1	0
2	E	401	A1LU8	1	0
2	I	401	A1LU8	1	0

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

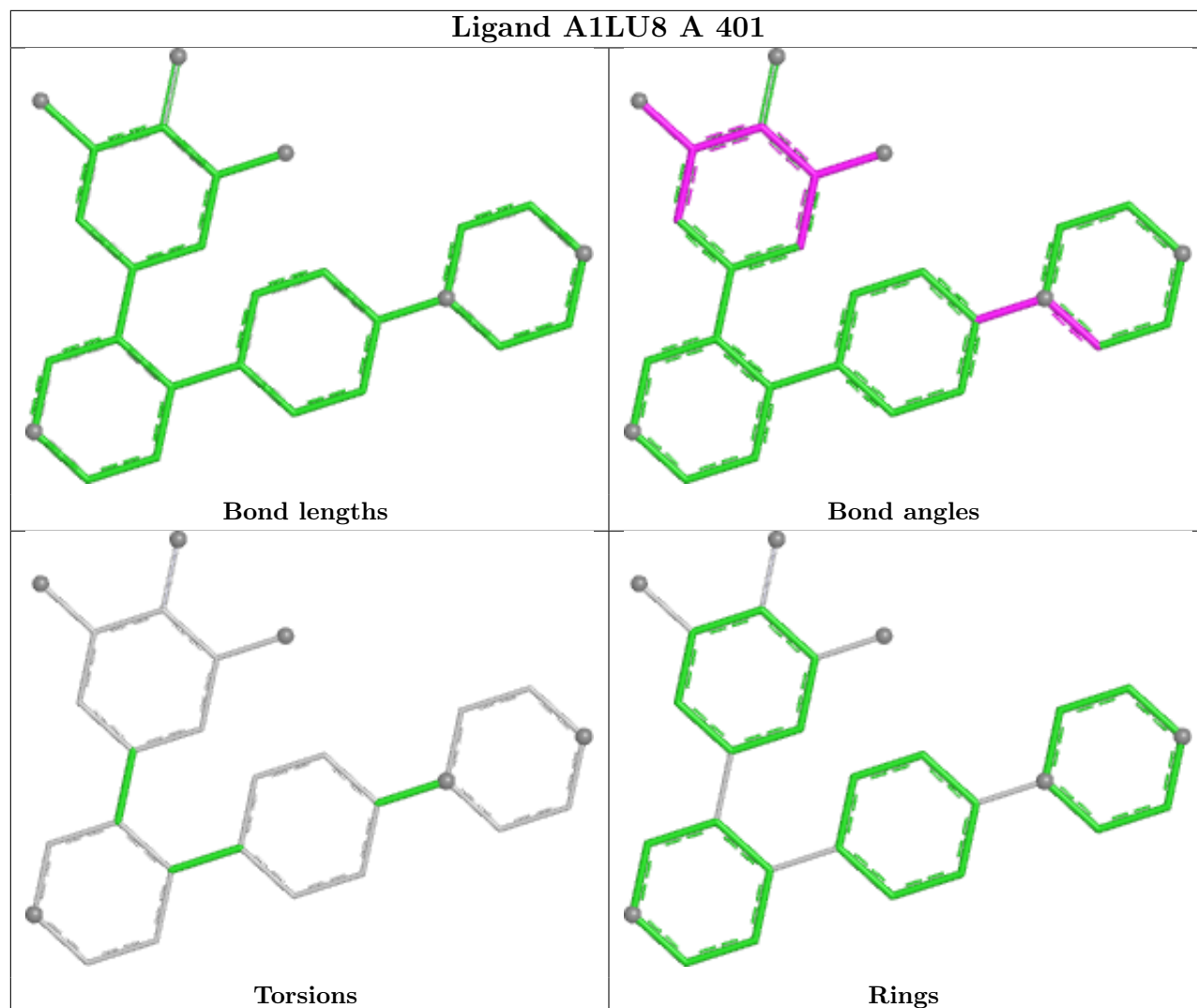
equivalents in the CSD to analyse the geometry.



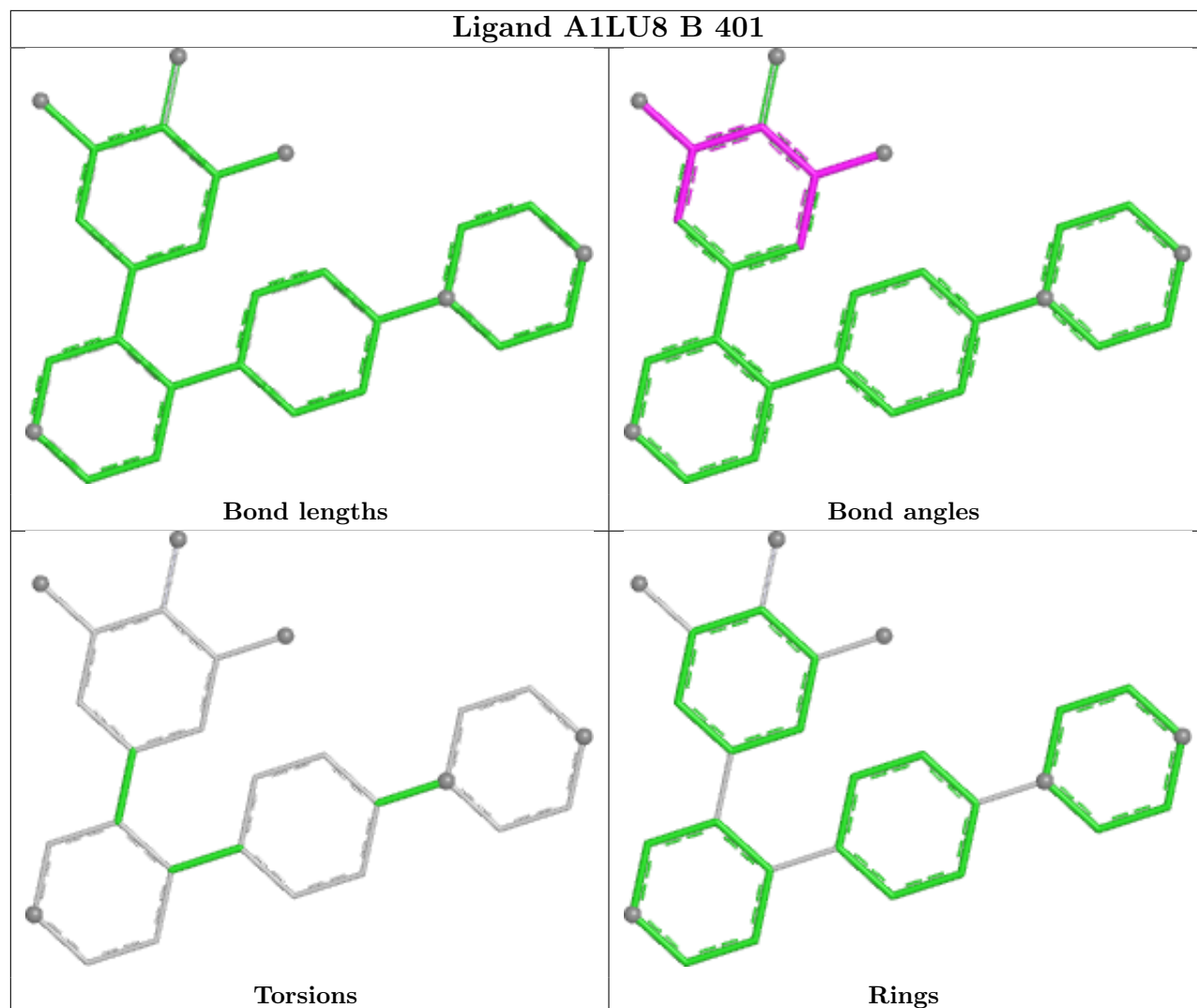
Ligand A1LU8 D 401



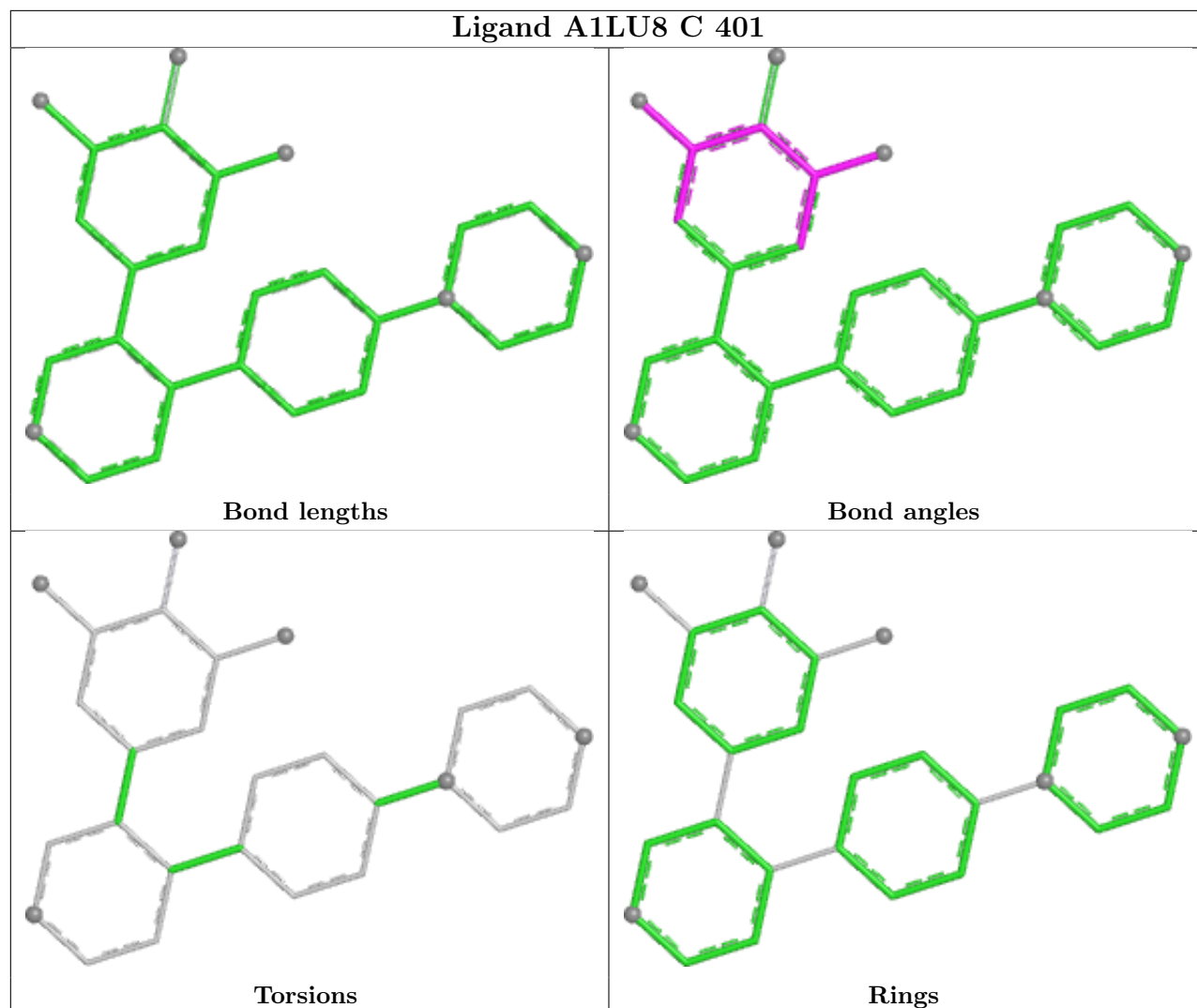
Ligand A1LU8 A 401



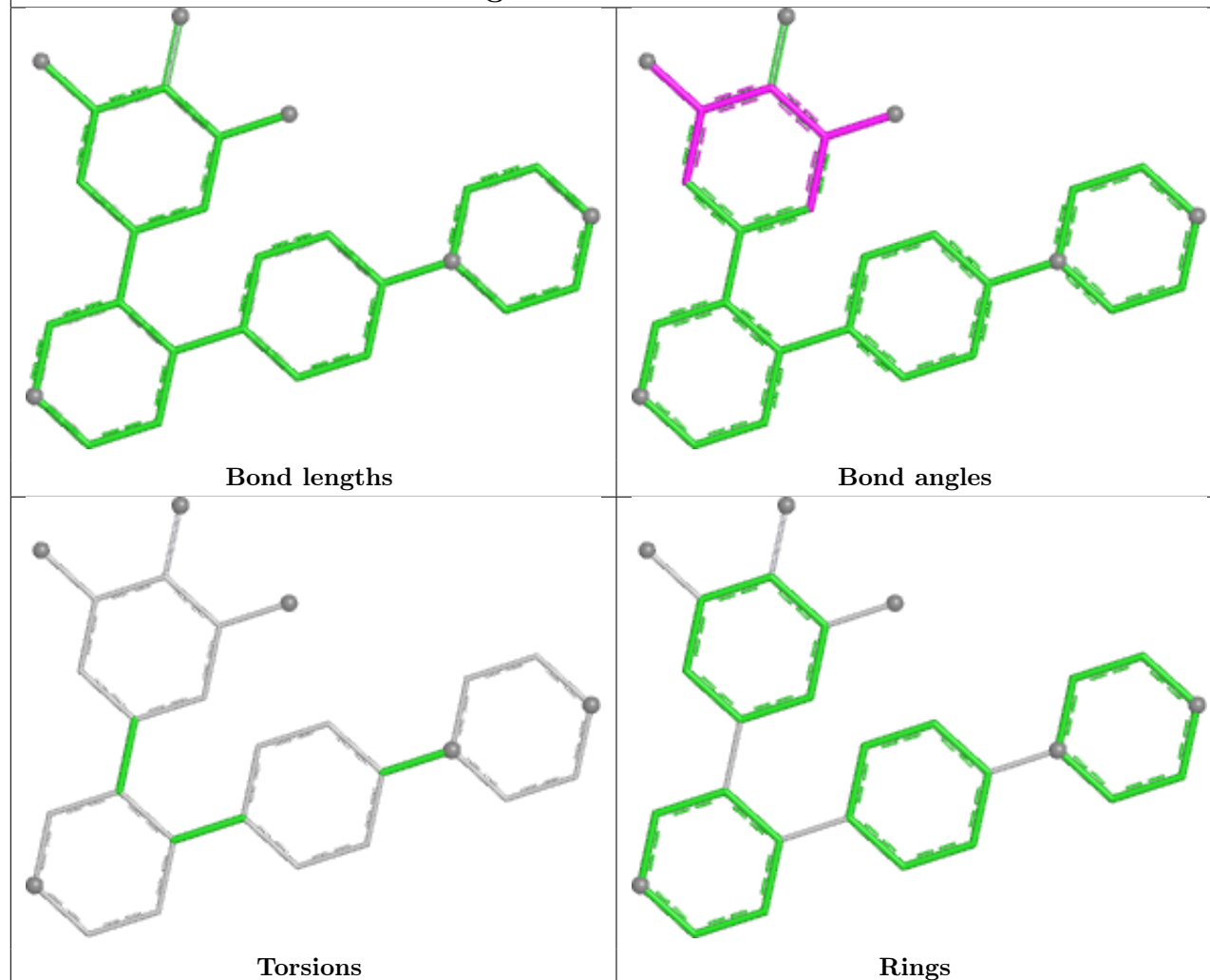
Ligand A1LU8 B 401



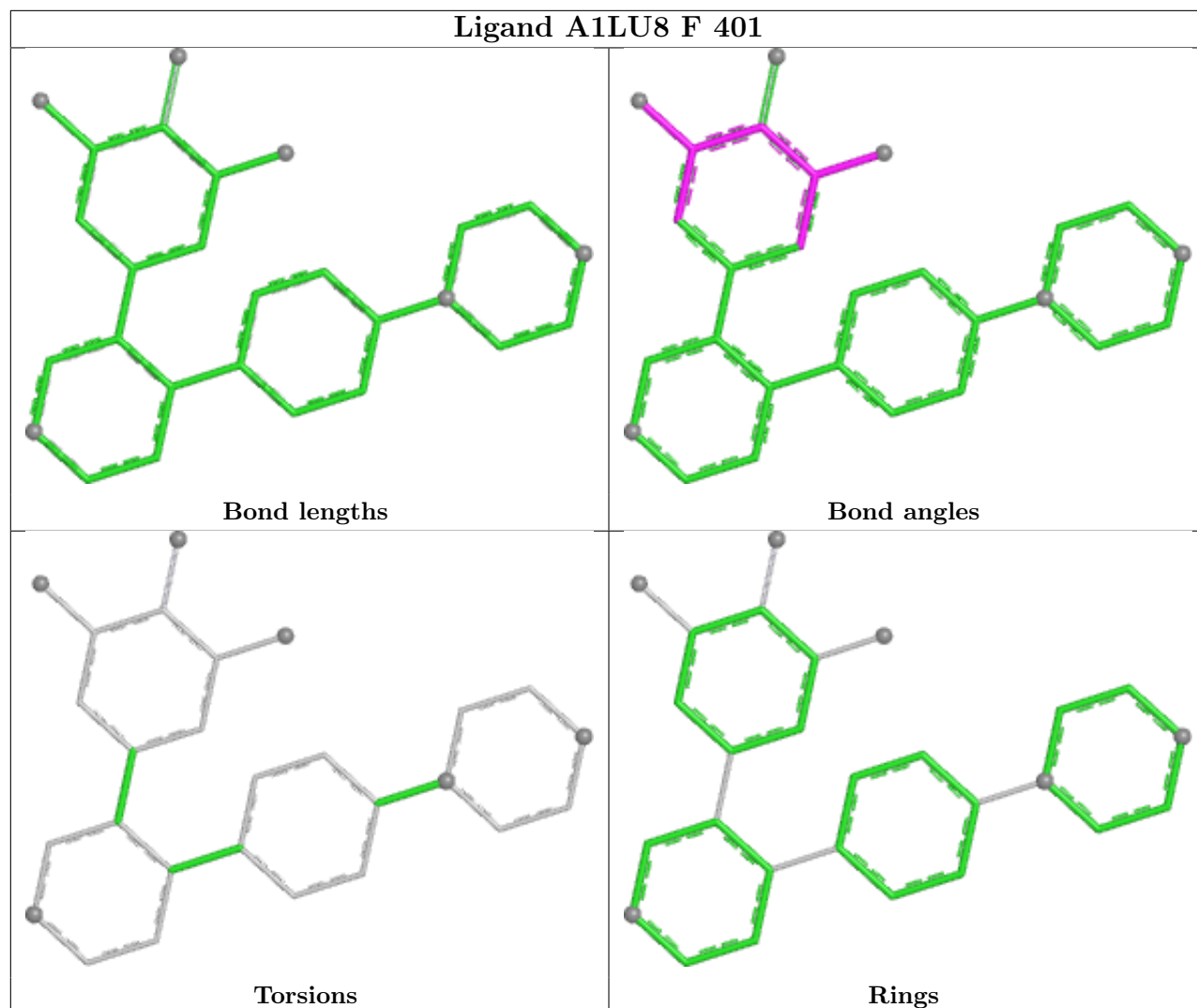
Ligand A1LU8 C 401



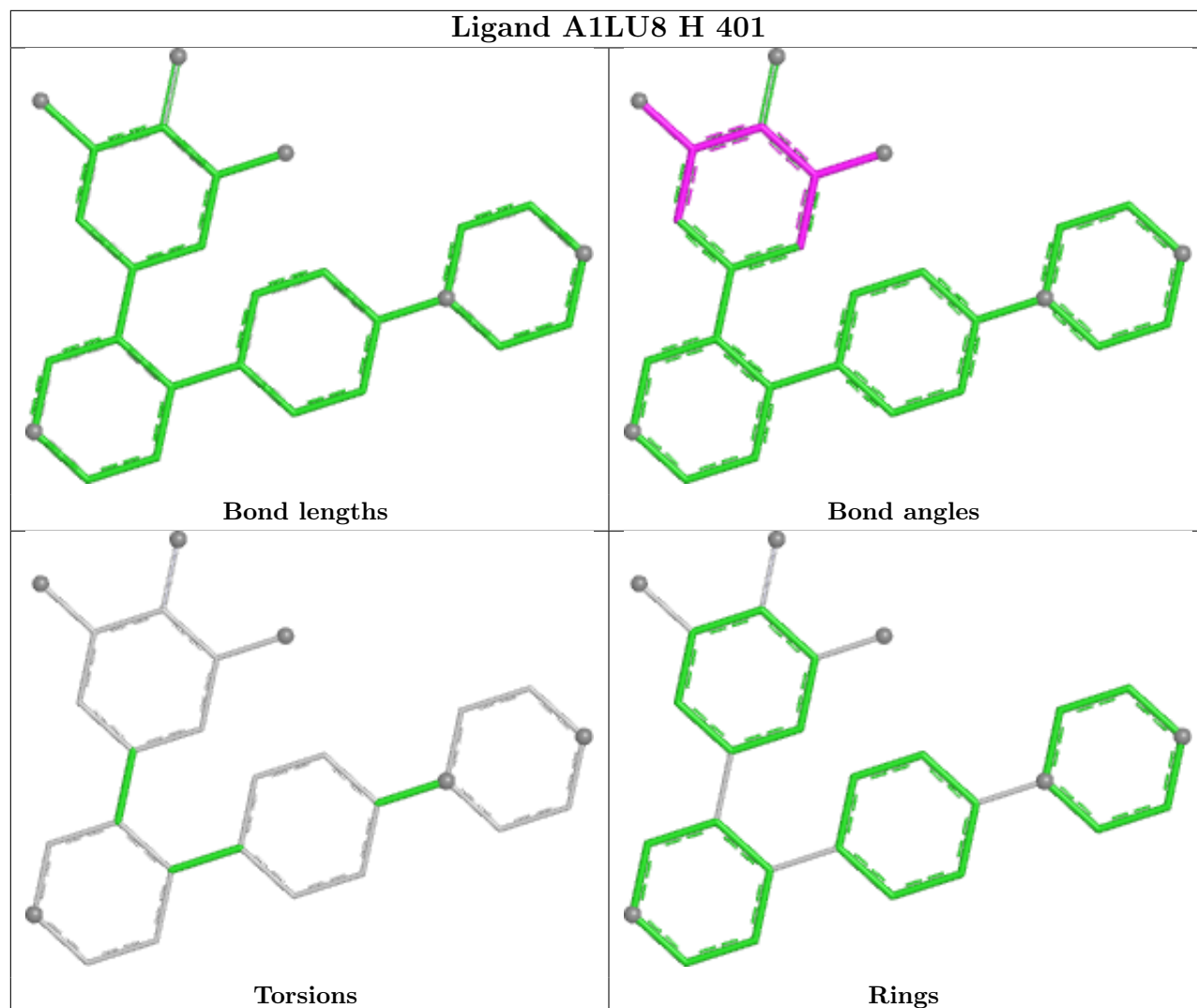
Ligand A1LU8 G 401



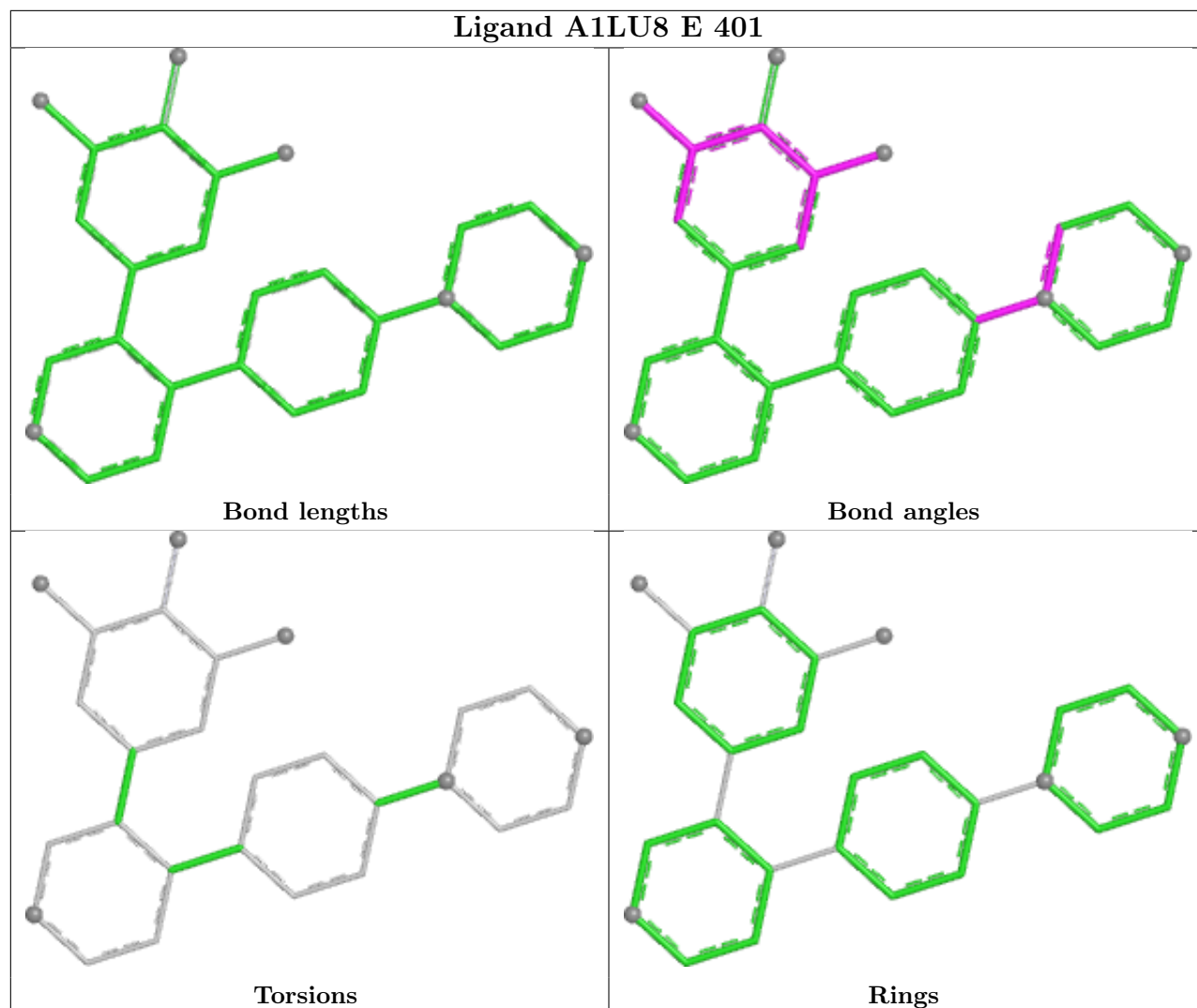
Ligand A1LU8 F 401

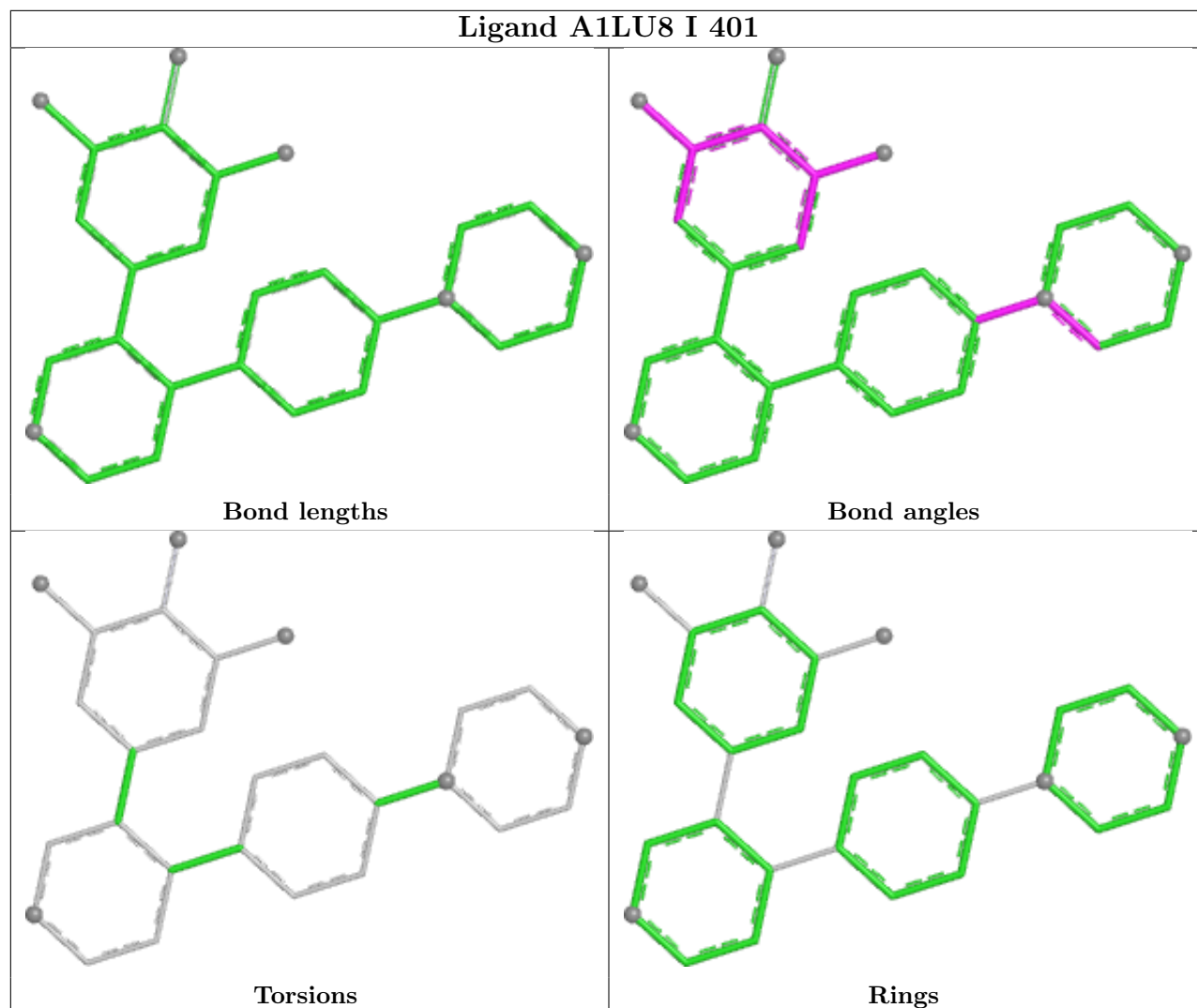


Ligand A1LU8 H 401



Ligand A1LU8 E 401





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	289/320 (90%)	0.05	2 (0%) 84 69	22, 39, 76, 103	0
1	B	277/320 (86%)	0.10	3 (1%) 78 61	27, 48, 77, 113	0
1	C	272/320 (85%)	0.21	3 (1%) 78 61	33, 57, 90, 116	0
1	D	260/320 (81%)	0.18	3 (1%) 76 58	33, 55, 91, 122	0
1	E	261/320 (81%)	0.29	2 (0%) 82 67	32, 57, 98, 122	0
1	F	255/320 (79%)	0.20	3 (1%) 76 58	31, 54, 85, 125	0
1	G	276/320 (86%)	0.20	2 (0%) 84 69	30, 50, 80, 101	0
1	H	277/320 (86%)	0.05	2 (0%) 84 69	23, 41, 74, 100	0
1	I	260/320 (81%)	0.20	6 (2%) 61 41	28, 52, 96, 136	0
1	J	257/320 (80%)	0.29	7 (2%) 56 36	37, 61, 108, 137	0
All	All	2684/3200 (83%)	0.17	33 (1%) 76 58	22, 51, 90, 137	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	121	ILE	3.5
1	C	121	ILE	2.9
1	J	283	ALA	2.8
1	H	109	VAL	2.7
1	J	65	PRO	2.7
1	A	113	VAL	2.7
1	J	88	ILE	2.6
1	B	316	ASP	2.5
1	A	109	VAL	2.4
1	G	61	GLU	2.4
1	B	118	GLU	2.4
1	D	121	ILE	2.4
1	D	63	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	192	ARG	2.3
1	F	344	PHE	2.3
1	I	347	ALA	2.3
1	E	65	PRO	2.3
1	J	79	PHE	2.2
1	B	59	GLY	2.2
1	I	64	ASP	2.2
1	E	344	PHE	2.2
1	I	344	PHE	2.2
1	I	89	SER	2.1
1	H	348	THR	2.1
1	J	319	GLU	2.1
1	C	159	LEU	2.1
1	F	154	ASP	2.1
1	J	90	GLY	2.1
1	C	79	PHE	2.1
1	I	65	PRO	2.1
1	I	120	ASP	2.1
1	D	348	THR	2.0
1	J	96	LEU	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(Å ²)	Q<0.9
2	A1LU8	D	401	27/27	0.88	0.13	52,59,63,64	0
2	A1LU8	C	401	27/27	0.90	0.12	50,55,57,57	0
2	A1LU8	I	401	27/27	0.90	0.11	41,42,51,52	0

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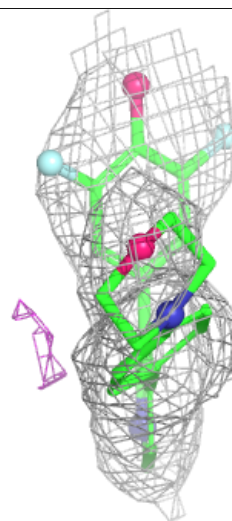
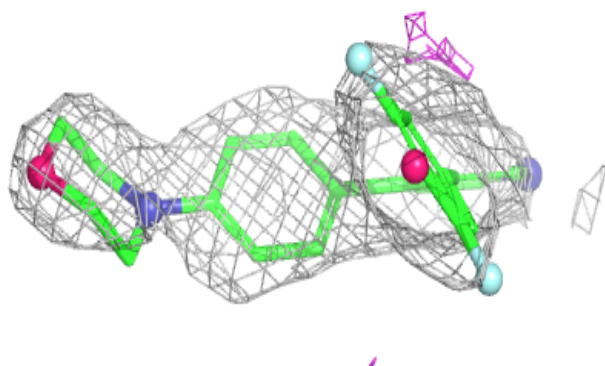
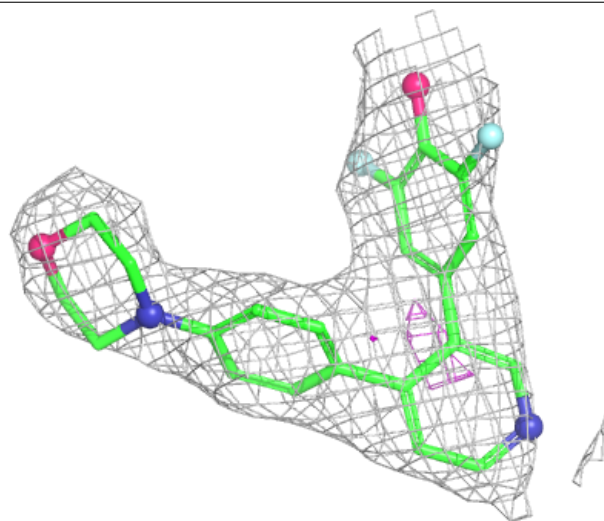
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1LU8	F	401	27/27	0.92	0.10	42,48,69,69	0
2	A1LU8	J	401	27/27	0.92	0.11	48,51,55,56	0
2	A1LU8	G	401	27/27	0.93	0.10	38,43,53,54	0
2	A1LU8	E	401	27/27	0.94	0.09	44,50,67,68	0
2	A1LU8	H	401	27/27	0.95	0.08	28,32,46,46	0
2	A1LU8	B	401	27/27	0.95	0.09	38,41,44,45	0
2	A1LU8	A	401	27/27	0.95	0.08	30,33,44,45	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.

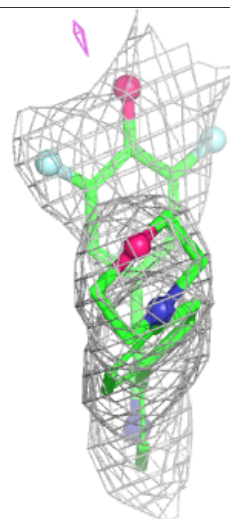
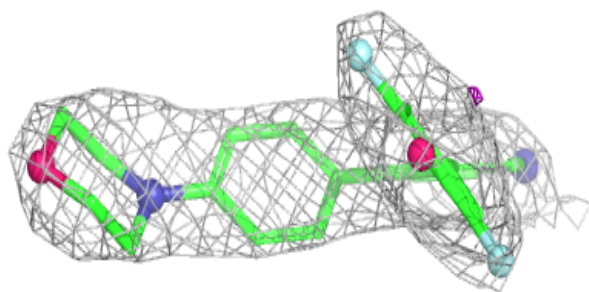
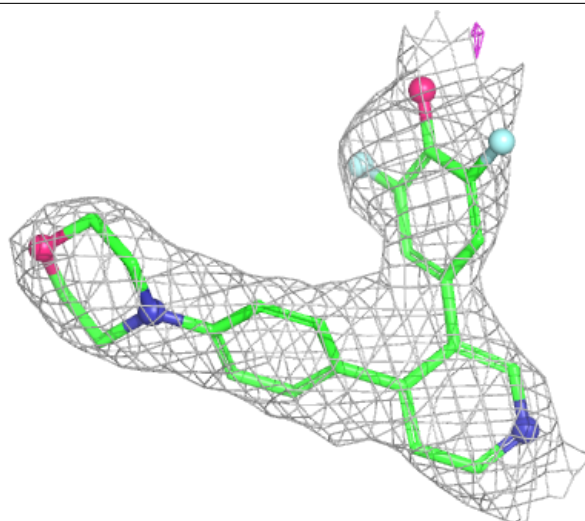
Electron density around A1LU8 D 401:

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



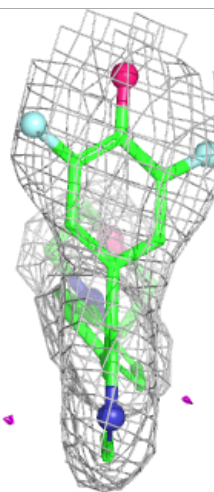
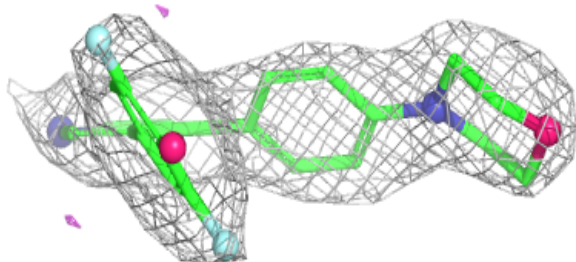
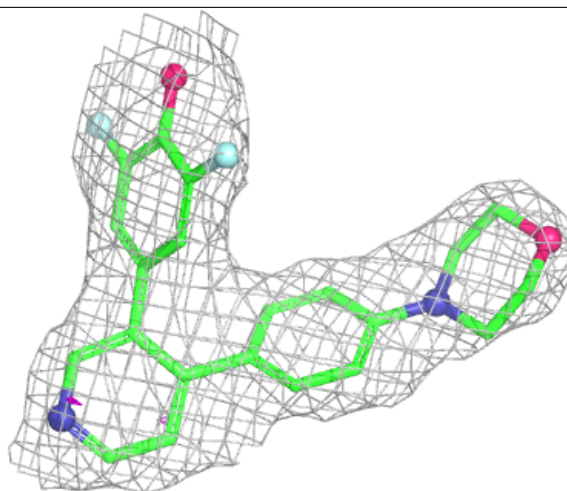
Electron density around A1LU8 C 401:

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and green (positive)



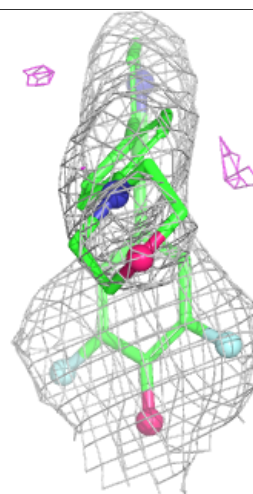
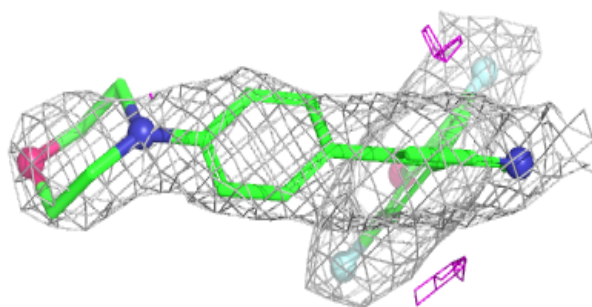
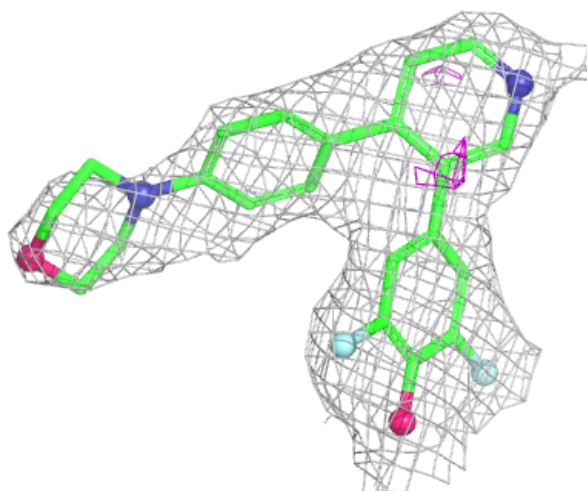
Electron density around A1LU8 I 401:

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and green (positive)



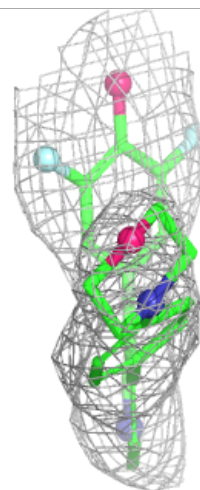
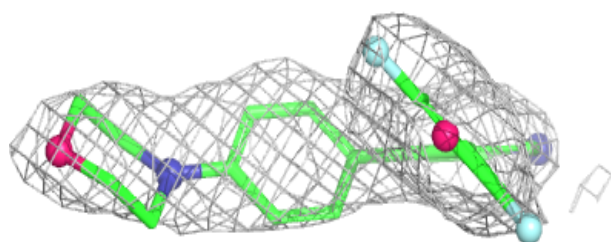
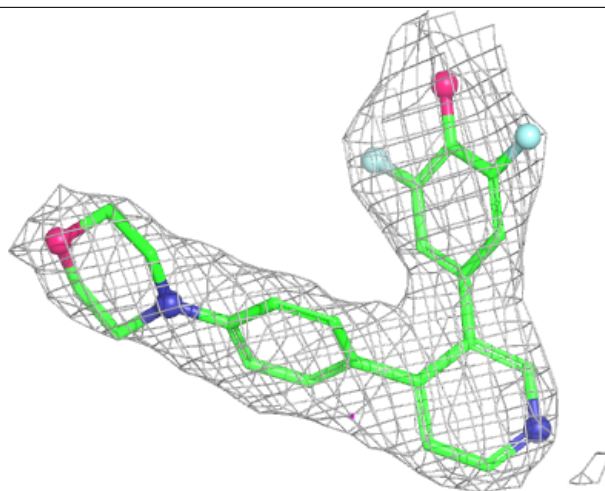
Electron density around A1LU8 F 401:

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and green (positive)



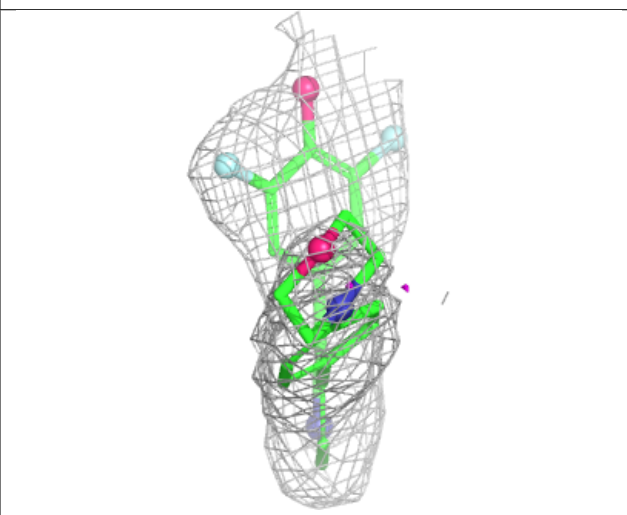
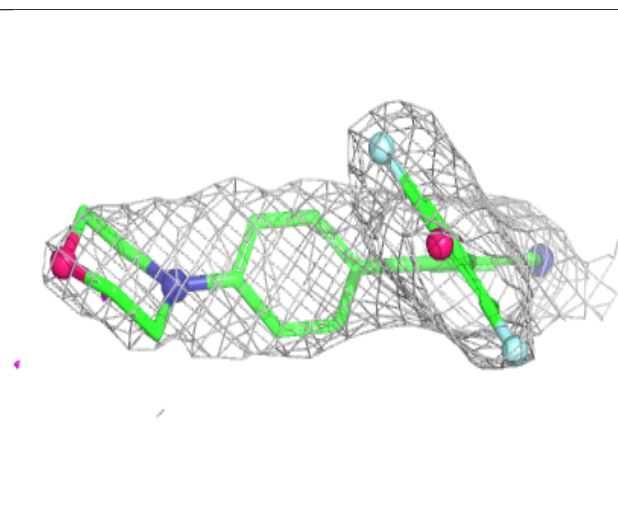
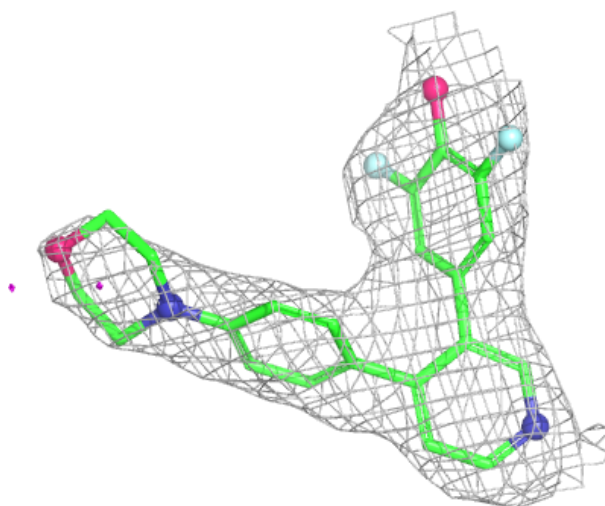
Electron density around A1LU8 J 401:

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and green (positive)



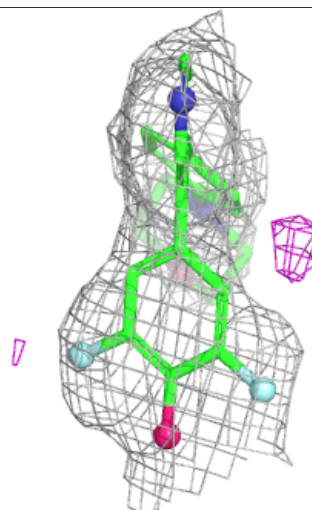
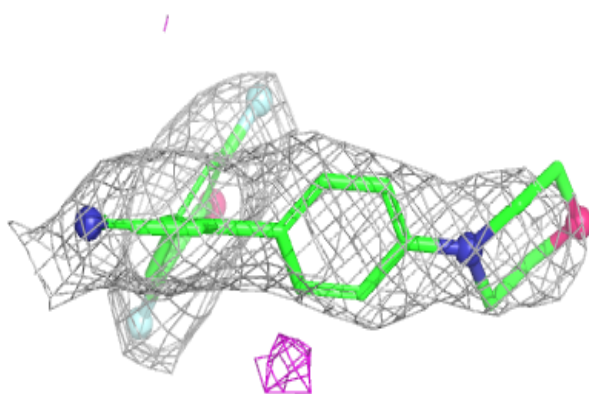
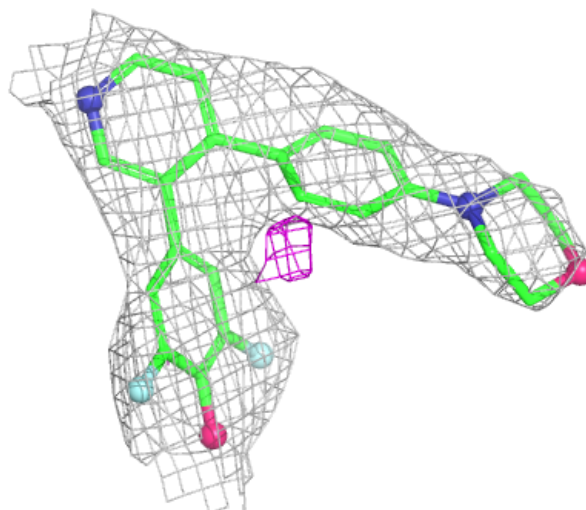
Electron density around A1LU8 G 401:

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and green (positive)



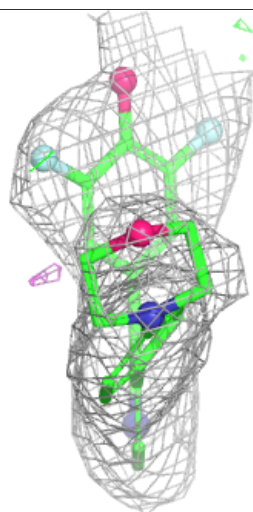
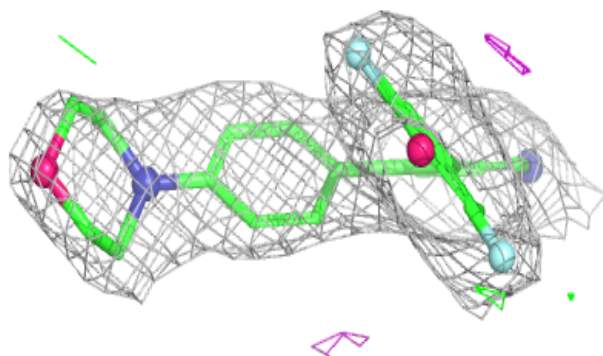
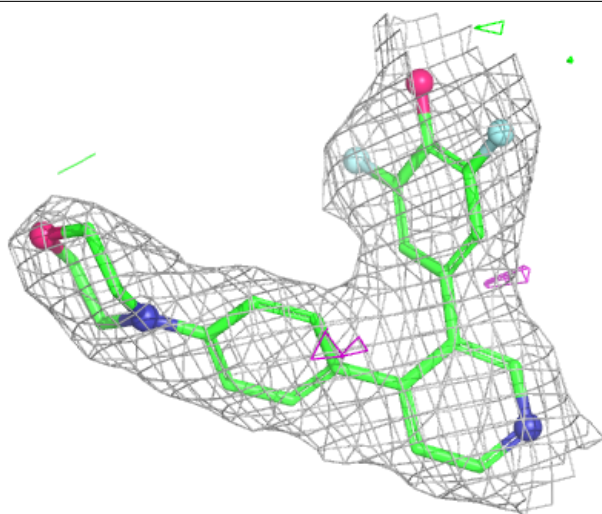
Electron density around A1LU8 E 401:

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



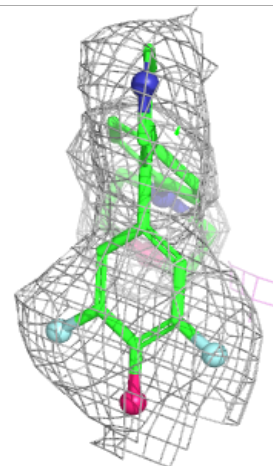
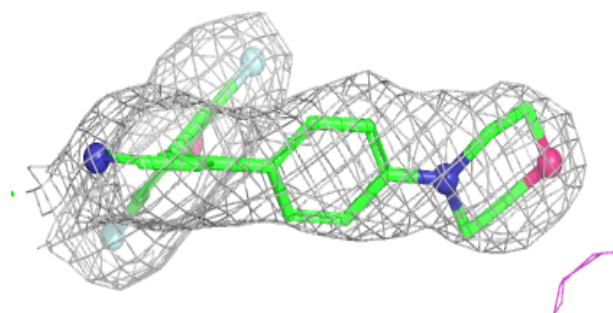
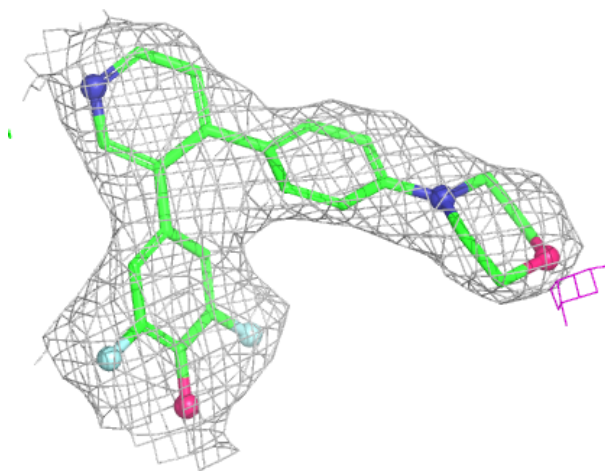
Electron density around A1LU8 H 401:

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and green (positive)



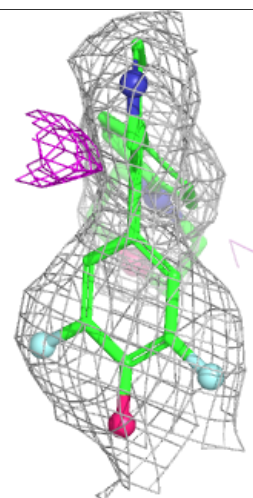
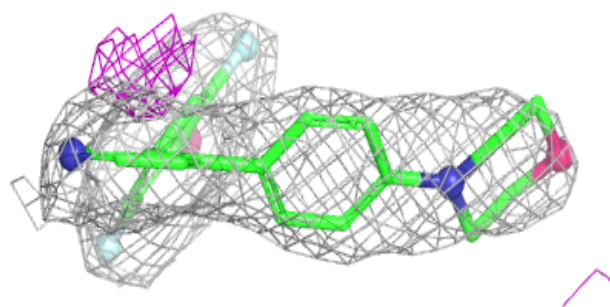
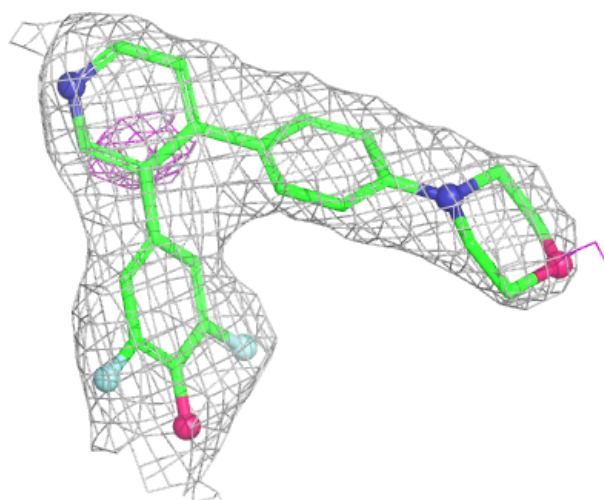
Electron density around A1LU8 B 401:

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and green (positive)



Electron density around A1LU8 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.