



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2025 – 10:08 AM EDT

PDB ID : 9NT4 / pdb_00009nt4
Title : Crystal structure of ecLacI transcription factor ancestor 1 bound to d-fucose
Authors : Georgelin, R.L.; Frkic, R.L.; Jackson, C.J.
Deposited on : 2025-03-18
Resolution : 2.40 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

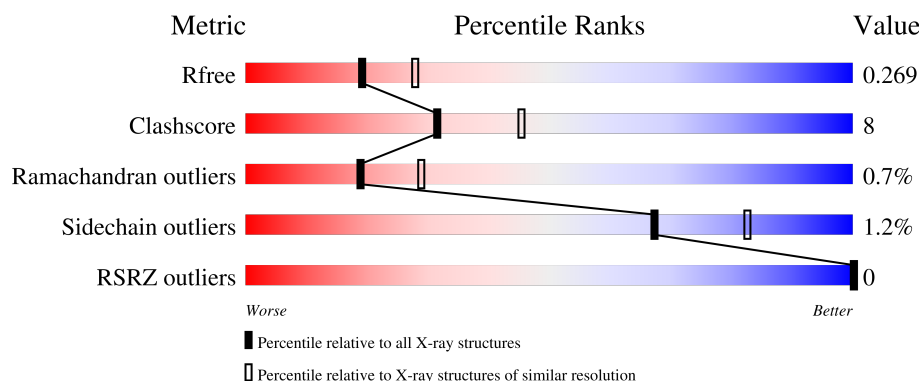
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	280	
1	B	280	
1	C	280	
1	D	280	
1	E	280	

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Mol	Chain	Length	Quality of chain
1	F	280	 71% 16% 11%
1	G	280	 75% 20% 5%
1	H	280	 72% 16% 11%

2 Entry composition

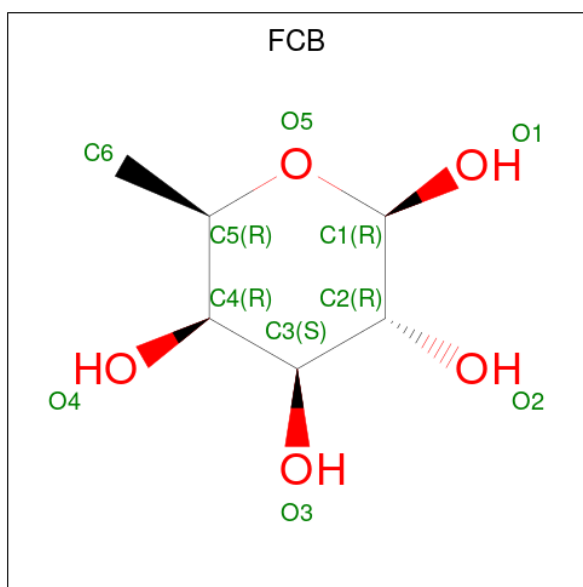
There are 3 unique types of molecules in this entry. The entry contains 16153 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LacI Transcription Factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2041	1293	358	388	2			
1	B	258	Total	C	N	O	S	0	0	0
			1988	1265	339	382	2			
1	C	264	Total	C	N	O	S	0	0	0
			2041	1295	354	390	2			
1	D	260	Total	C	N	O	S	0	0	0
			1998	1265	348	383	2			
1	E	264	Total	C	N	O	S	0	0	0
			2030	1279	353	396	2			
1	F	248	Total	C	N	O	S	0	0	0
			1915	1213	332	368	2			
1	G	265	Total	C	N	O	S	0	0	0
			2054	1299	360	393	2			
1	H	249	Total	C	N	O	S	0	0	0
			1931	1222	337	370	2			

- Molecule 2 is beta-D-fucopyranose (CCD ID: FCB) (formula: C₆H₁₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		
2	E	1	Total	C	O	0	0
			11	6	5		
2	F	1	Total	C	O	0	0
			11	6	5		
2	G	1	Total	C	O	0	0
			11	6	5		
2	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	16	Total	O	0	0
			16	16		
3	C	6	Total	O	0	0
			6	6		
3	D	7	Total	O	0	0
			7	7		

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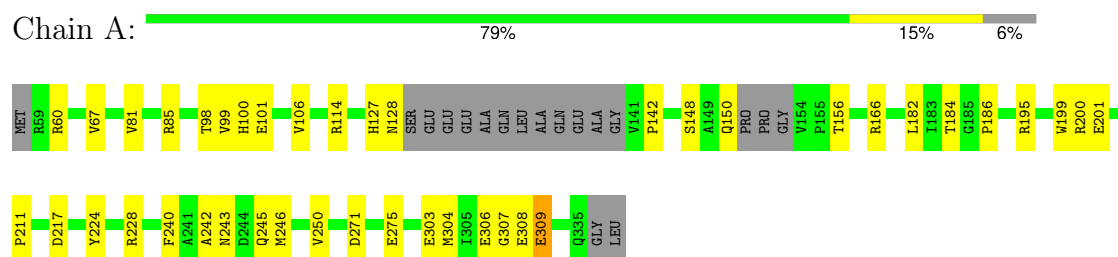
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	6	Total 6	O 6	0	0
3	F	8	Total 8	O 8	0	0
3	G	4	Total 4	O 4	0	0
3	H	11	Total 11	O 11	0	0

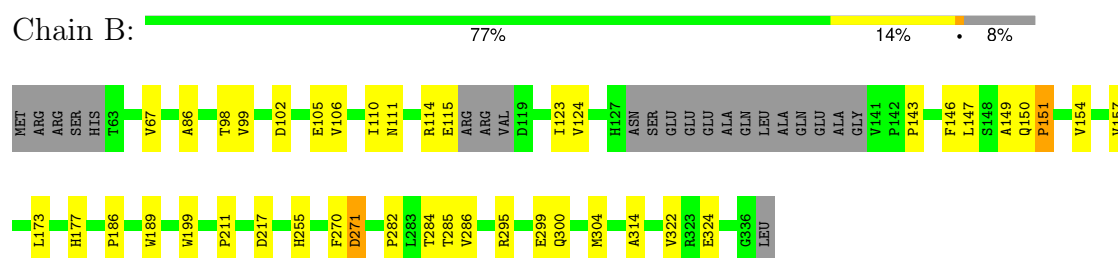
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

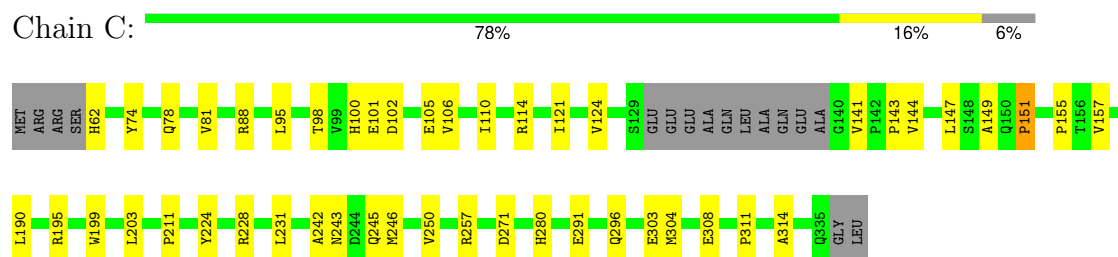
• Molecule 1: LacI Transcription Factor



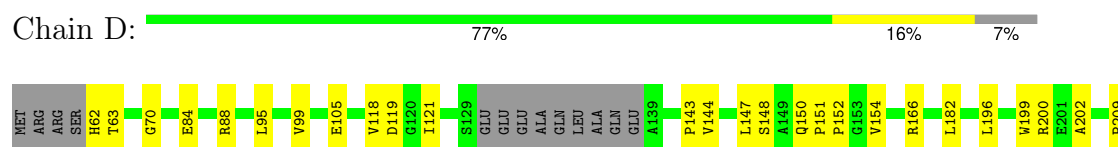
• Molecule 1: LacI Transcription Factor



• Molecule 1: LacI Transcription Factor



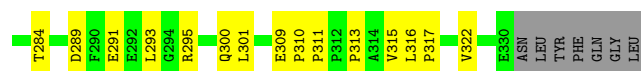
• Molecule 1: LacI Transcription Factor





• Molecule 1: LacI Transcription Factor

Chain E: 67% 27% 6%



• Molecule 1: LacI Transcription Factor

Chain F: 71% 16% 11%



• Molecule 1: LacI Transcription Factor

Chain G: 75% 20% 5%



• Molecule 1: LacI Transcription Factor

Chain H: 72% 16% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.45Å 211.00Å 87.31Å 90.00° 90.51° 90.00°	Depositor
Resolution (Å)	43.66 – 2.40 43.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.66-2.40) 96.5 (43.66-2.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.219 , 0.270 0.219 , 0.269	Depositor DCC
R_{free} test set	4413 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.237 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16153	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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: FCB

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	0.22	0/2089	0.39	0/2855
1	B	0.23	0/2037	0.40	0/2789
1	C	0.27	0/2092	0.44	1/2864 (0.0%)
1	D	0.19	0/2047	0.36	0/2803
1	E	0.19	0/2077	0.36	0/2841
1	F	0.23	0/1959	0.39	0/2678
1	G	0.22	0/2104	0.37	0/2879
1	H	0.21	0/1976	0.40	0/2702
All	All	0.22	0/16381	0.39	1/22411 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	PRO	CA-N-CD	-5.78	103.91	112.00

There are no chirality outliers.

There are no planarity outliers.

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	2041	0	2001	31	0
1	B	1988	0	1942	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2041	0	1996	32	0
1	D	1998	0	1958	29	0
1	E	2030	0	1980	58	0
1	F	1915	0	1877	31	0
1	G	2054	0	2013	35	0
1	H	1931	0	1888	29	0
2	A	11	0	12	0	0
2	B	11	0	12	1	0
2	C	11	0	11	0	0
2	D	11	0	11	1	0
2	E	11	0	12	0	0
2	F	11	0	11	1	0
2	G	11	0	11	0	0
2	H	11	0	12	0	0
3	A	9	0	0	0	0
3	B	16	0	0	0	0
3	C	6	0	0	0	0
3	D	7	0	0	0	0
3	E	6	0	0	0	0
3	F	8	0	0	0	0
3	G	4	0	0	0	0
3	H	11	0	0	0	0
All	All	16153	0	15747	254	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 8.

All (254) 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:156:THR:H	1:E:313:PRO:HG2	1.43	0.83
1:E:159:VAL:HG23	1:E:293:LEU:HD21	1.65	0.79
1:D:95:LEU:HD11	1:G:93:SER:HB3	1.70	0.74
1:A:60:ARG:NH1	1:A:306:GLU:OE2	2.21	0.73
1:B:143:PRO:HB2	1:B:304:MET:HE3	1.72	0.71
1:C:157:VAL:HG22	1:C:314:ALA:HB3	1.72	0.71
1:C:124:VAL:HG13	1:C:147:LEU:HD23	1.74	0.70
1:D:275:GLU:HG3	1:G:245:GLN:HE22	1.56	0.70
1:B:151:PRO:HG2	1:B:154:VAL:HB	1.74	0.69
1:H:272:ASP:OD2	1:H:287:ARG:NH1	2.26	0.68
1:B:111:ASN:O	1:B:114:ARG:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:THR:HG22	1:E:118:VAL:HG13	1.76	0.67
1:E:121:ILE:HB	1:E:141:VAL:HG22	1.76	0.67
1:C:88:ARG:NH2	1:E:98:THR:O	2.26	0.67
1:B:102:ASP:HB3	1:B:105:GLU:HB2	1.76	0.66
1:D:84:GLU:OE1	1:D:88:ARG:NH1	2.29	0.66
1:E:293:LEU:HD23	1:E:316:LEU:HD22	1.77	0.66
1:E:300:GLN:HE22	1:E:313:PRO:HG3	1.59	0.66
1:B:295:ARG:HG3	1:B:295:ARG:HH11	1.58	0.66
1:H:295:ARG:NH1	1:H:299:GLU:HB2	2.11	0.66
1:D:182:LEU:HD12	1:D:199:TRP:CD2	2.31	0.65
1:C:121:ILE:HB	1:C:144:VAL:HG12	1.79	0.65
1:E:74:TYR:CZ	1:E:78:GLN:HG3	2.32	0.65
1:B:99:VAL:HG13	1:B:105:GLU:HB3	1.78	0.64
1:F:106:VAL:HG12	1:F:110:ILE:HD11	1.79	0.63
1:B:67:VAL:HB	1:B:123:ILE:HD13	1.79	0.63
1:A:148:SER:HB3	1:A:150:GLN:HE21	1.63	0.63
1:E:156:THR:H	1:E:313:PRO:CG	2.10	0.62
1:A:186:PRO:HD3	1:A:217:ASP:HA	1.79	0.62
1:G:221:ALA:O	1:G:225:GLU:HG2	1.99	0.61
1:G:66:VAL:HG22	1:G:122:ILE:HB	1.82	0.61
1:A:127:HIS:CG	1:A:128:ASN:H	2.19	0.61
1:E:309:GLU:O	1:E:311:PRO:HD3	2.01	0.60
1:B:157:VAL:HG23	1:B:314:ALA:HB3	1.83	0.60
1:D:62:HIS:N	1:D:119:ASP:OD2	2.34	0.60
1:H:84:GLU:OE1	1:H:88:ARG:NH2	2.34	0.60
1:H:62:HIS:N	1:H:119:ASP:OD2	2.35	0.59
1:A:166:ARG:HH12	1:A:201:GLU:HB3	1.68	0.59
1:H:95:LEU:HD11	1:H:116:ARG:HG2	1.83	0.59
1:A:303:GLU:HG3	1:A:308:GLU:HB2	1.84	0.59
1:F:146:PHE:CE1	1:F:297:ALA:HB2	2.37	0.59
1:G:66:VAL:HG21	1:G:83:ILE:HG21	1.84	0.58
1:D:63:THR:HG23	1:D:118:VAL:HG23	1.85	0.58
1:E:121:ILE:O	1:E:142:PRO:HD2	2.03	0.58
1:H:107:GLU:HA	1:H:110:ILE:HD12	1.85	0.58
1:D:245:GLN:HE22	1:G:275:GLU:HG3	1.68	0.58
1:F:186:PRO:HG3	1:F:217:ASP:HA	1.85	0.58
1:C:147:LEU:HD12	1:C:157:VAL:O	2.04	0.58
1:H:157:VAL:HG11	1:H:296:GLN:HB2	1.86	0.58
1:H:292:GLU:O	1:H:296:GLN:HG2	2.04	0.58
1:H:304:MET:HE3	1:H:311:PRO:HD2	1.86	0.58
1:B:186:PRO:HG2	1:B:189:TRP:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:O	1:A:85:ARG:HG3	2.05	0.57
1:B:284:THR:HG23	1:B:322:VAL:HA	1.86	0.57
1:E:181:ALA:HB3	1:E:239:ILE:HG12	1.86	0.57
1:B:150:GLN:N	1:B:151:PRO:HD3	2.20	0.57
1:B:295:ARG:HG3	1:B:295:ARG:NH1	2.20	0.57
1:E:214:LEU:HD12	1:E:230:LEU:HG	1.86	0.57
1:F:159:VAL:HG23	1:F:293:LEU:HD13	1.87	0.57
1:H:231:LEU:HD13	1:H:257:ARG:HG3	1.87	0.57
1:B:124:VAL:HG13	1:B:147:LEU:HD12	1.87	0.56
1:E:177:HIS:ND1	1:E:237:THR:OG1	2.26	0.56
1:F:65:GLY:HA3	1:F:113:LEU:HD23	1.87	0.56
1:G:99:VAL:HG11	1:G:106:VAL:HA	1.87	0.56
1:H:66:VAL:HG22	1:H:122:ILE:HB	1.87	0.56
1:E:280:HIS:HB3	1:E:281:PRO:HD3	1.87	0.56
1:D:62:HIS:HD2	1:D:63:THR:HG22	1.71	0.55
1:E:182:LEU:HD23	1:E:196:LEU:HD12	1.87	0.55
1:A:106:VAL:HB	1:A:127:HIS:CD2	2.42	0.55
1:D:301:LEU:O	1:D:305:ILE:HG12	2.05	0.55
1:A:243:ASN:OD1	1:A:246:MET:HG3	2.05	0.55
1:B:299:GLU:OE2	1:B:300:GLN:NE2	2.40	0.55
1:C:100:HIS:CG	1:C:101:GLU:H	2.23	0.55
1:B:98:THR:OG1	1:F:84:GLU:OE1	2.25	0.55
1:E:145:VAL:HG11	1:E:191:GLU:HG3	1.88	0.55
1:C:195:ARG:NH1	1:C:242:ALA:O	2.40	0.55
1:D:166:ARG:HD3	1:D:202:ALA:HB2	1.87	0.55
1:F:146:PHE:CZ	1:F:297:ALA:HB2	2.42	0.54
1:E:108:GLU:N	1:E:108:GLU:OE1	2.39	0.54
1:C:102:ASP:HB2	1:C:105:GLU:CD	2.33	0.54
1:C:303:GLU:HG2	1:C:311:PRO:HG3	1.88	0.54
1:C:245:GLN:HE22	1:E:275:GLU:HG3	1.73	0.54
1:D:284:THR:HG23	1:D:322:VAL:HA	1.89	0.54
1:E:142:PRO:HB3	1:E:155:PRO:HB2	1.90	0.54
1:E:251:LEU:HD13	1:E:281:PRO:HD2	1.90	0.54
1:D:182:LEU:HD12	1:D:199:TRP:CG	2.43	0.53
1:F:106:VAL:O	1:F:110:ILE:HG13	2.07	0.53
1:G:121:ILE:HB	1:G:144:VAL:HG22	1.90	0.53
1:D:196:LEU:HD21	1:D:200:ARG:HE	1.74	0.53
1:H:66:VAL:HG21	1:H:83:ILE:HG21	1.92	0.52
1:E:300:GLN:NE2	1:E:313:PRO:HG3	2.22	0.52
1:G:102:ASP:HB3	1:G:105:GLU:HB2	1.92	0.52
1:C:100:HIS:CD2	1:C:101:GLU:H	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:HIS:CD2	1:D:63:THR:HG22	2.44	0.52
1:F:61:SER:N	1:F:119:ASP:OD1	2.42	0.52
1:E:291:GLU:O	1:E:295:ARG:HG2	2.10	0.52
1:B:149:ALA:C	1:B:151:PRO:HD3	2.34	0.52
1:E:104:ASP:OD2	1:E:104:ASP:N	2.43	0.52
1:A:67:VAL:HG11	1:A:106:VAL:HG13	1.92	0.51
1:F:107:GLU:HA	1:F:110:ILE:HD12	1.92	0.51
1:F:156:THR:HG22	1:F:313:PRO:HB3	1.92	0.51
1:F:166:ARG:HH22	1:F:205:GLU:CD	2.18	0.51
1:F:199:TRP:CZ2	1:F:211:PRO:HD2	2.46	0.51
1:E:300:GLN:HE22	1:E:313:PRO:CG	2.24	0.50
1:G:243:ASN:HD21	1:G:245:GLN:HB2	1.76	0.50
1:H:121:ILE:HB	1:H:143:PRO:HB3	1.93	0.50
1:C:224:TYR:CZ	1:C:228:ARG:HD2	2.46	0.50
1:E:102:ASP:HB3	1:E:104:ASP:OD2	2.12	0.50
1:D:243:ASN:OD1	1:D:246:MET:HG3	2.12	0.50
1:F:142:PRO:HG2	1:F:305:ILE:HG22	1.93	0.50
1:D:119:ASP:O	1:D:143:PRO:HD2	2.13	0.49
1:A:199:TRP:CE3	1:A:200:ARG:HG2	2.48	0.49
1:H:102:ASP:HB3	1:H:105:GLU:HG3	1.93	0.49
1:E:113:LEU:O	1:E:118:VAL:HG23	2.12	0.49
1:C:157:VAL:HG11	1:C:296:GLN:HB3	1.95	0.49
1:E:132:GLU:HA	1:E:136:ALA:HB3	1.95	0.48
1:G:63:THR:HG22	1:G:93:SER:HB2	1.95	0.48
1:A:275:GLU:CG	1:H:245:GLN:HE22	2.26	0.48
1:D:99:VAL:HA	1:D:105:GLU:OE2	2.13	0.48
1:E:82:GLY:O	1:E:295:ARG:HD2	2.13	0.48
1:E:142:PRO:HD3	1:E:301:LEU:HD13	1.96	0.48
1:C:155:PRO:HG3	1:C:304:MET:HE2	1.96	0.48
1:G:74:TYR:CZ	1:G:78:GLN:HG3	2.48	0.48
1:A:245:GLN:HE22	1:H:275:GLU:HG3	1.77	0.48
1:C:149:ALA:H	1:C:190:LEU:HD22	1.79	0.48
1:A:148:SER:HB3	1:A:150:GLN:NE2	2.27	0.48
1:E:113:LEU:HB3	1:E:118:VAL:HG21	1.96	0.48
1:E:224:TYR:CZ	1:E:228:ARG:HD2	2.49	0.48
1:F:92:TYR:CE2	1:F:302:LEU:HD21	2.48	0.48
1:D:221:ALA:O	1:D:225:GLU:HG3	2.14	0.48
1:C:106:VAL:O	1:C:110:ILE:HG13	2.14	0.48
1:C:143:PRO:HB2	1:C:304:MET:HE3	1.96	0.48
1:C:245:GLN:HE22	1:E:275:GLU:CG	2.27	0.48
1:E:102:ASP:OD1	1:E:103:PRO:HD2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:HIS:CG	1:A:101:GLU:H	2.31	0.47
1:C:231:LEU:HD13	1:C:257:ARG:HG3	1.96	0.47
1:D:84:GLU:OE1	1:G:98:THR:OG1	2.32	0.47
1:E:161:GLN:HB2	1:E:194:GLU:HB3	1.96	0.47
1:G:230:LEU:HB3	1:G:236:PHE:CE2	2.49	0.47
1:E:186:PRO:HD3	1:E:217:ASP:HA	1.97	0.47
1:C:228:ARG:HG2	1:C:228:ARG:HH11	1.79	0.47
1:H:63:THR:HG22	1:H:93:SER:HB2	1.97	0.47
1:E:191:GLU:CD	1:E:191:GLU:H	2.23	0.47
1:G:61:SER:OG	1:G:117:ARG:O	2.29	0.47
1:E:189:TRP:HB3	1:E:191:GLU:OE1	2.15	0.46
1:A:306:GLU:HB3	1:A:307:GLY:H	1.58	0.46
1:C:303:GLU:O	1:C:308:GLU:HB2	2.15	0.46
1:F:123:ILE:HB	1:F:145:VAL:HA	1.97	0.46
1:G:159:VAL:HG23	1:G:293:LEU:HD22	1.97	0.46
1:D:150:GLN:O	1:D:152:PRO:HD3	2.15	0.46
1:H:157:VAL:HG12	1:H:293:LEU:HD12	1.96	0.46
1:C:280:HIS:CE1	1:E:255:HIS:HB3	2.50	0.46
1:E:125:ALA:O	1:E:128:ASN:ND2	2.44	0.46
1:D:121:ILE:HB	1:D:144:VAL:HG22	1.96	0.46
1:E:284:THR:HG23	1:E:322:VAL:HA	1.98	0.46
1:G:300:GLN:HG3	1:G:311:PRO:HG2	1.97	0.46
1:E:162:TYR:CE2	1:E:194:GLU:HG2	2.51	0.46
1:A:127:HIS:CG	1:A:128:ASN:N	2.84	0.45
1:F:92:TYR:HE2	1:F:302:LEU:HD21	1.82	0.45
1:H:121:ILE:O	1:H:143:PRO:HA	2.16	0.45
1:A:199:TRP:CZ2	1:A:211:PRO:HD2	2.51	0.45
1:B:173:LEU:HD23	1:B:177:HIS:O	2.16	0.45
1:G:293:LEU:HD13	1:G:316:LEU:HD22	1.98	0.45
1:B:106:VAL:O	1:B:110:ILE:HG13	2.17	0.45
1:B:255:HIS:CE1	1:F:280:HIS:HE2	2.34	0.45
1:F:310:PRO:HA	1:F:311:PRO:HD3	1.83	0.45
1:G:224:TYR:OH	1:G:256:GLU:OE1	2.28	0.45
1:C:245:GLN:OE1	1:E:275:GLU:HG2	2.17	0.45
1:A:304:MET:HA	1:A:309:GLU:HA	1.99	0.45
1:A:306:GLU:HG3	1:E:179:ARG:HH22	1.82	0.44
1:B:86:ALA:HB2	1:B:295:ARG:HG3	1.99	0.44
1:E:162:TYR:HE1	1:E:197:GLN:HB3	1.81	0.44
1:G:199:TRP:CZ2	1:G:211:PRO:HD2	2.52	0.44
1:D:99:VAL:HG12	1:D:105:GLU:HG2	1.99	0.44
1:G:112:THR:O	1:G:116:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:PHE:C	1:B:147:LEU:HD23	2.42	0.44
1:C:199:TRP:CE2	1:C:203:LEU:HD11	2.52	0.44
1:E:186:PRO:HD2	1:E:218:TRP:CE2	2.53	0.44
1:B:186:PRO:HD3	1:B:217:ASP:HA	2.00	0.44
1:C:98:THR:HB	1:E:84:GLU:OE1	2.17	0.44
1:E:189:TRP:O	1:E:193:ARG:HG3	2.18	0.44
1:B:199:TRP:CZ2	1:B:211:PRO:HD2	2.53	0.44
1:G:328:PRO:HB3	1:G:333:TYR:HA	1.99	0.43
1:G:329:PRO:C	1:G:331:ASN:H	2.26	0.43
1:A:114:ARG:HD3	1:A:142:PRO:HD2	1.99	0.43
1:C:62:HIS:HB3	1:E:116:ARG:HH22	1.82	0.43
1:G:90:HIS:ND1	1:G:302:LEU:HD12	2.34	0.43
1:H:64:ILE:HG13	1:H:92:TYR:CD2	2.53	0.43
1:C:199:TRP:CZ2	1:C:211:PRO:HD2	2.53	0.43
1:E:280:HIS:C	1:E:280:HIS:CD2	2.95	0.43
1:F:109:ALA:O	1:F:113:LEU:HD13	2.18	0.43
1:A:224:TYR:CZ	1:A:228:ARG:HD2	2.52	0.43
1:B:98:THR:OG1	1:F:88:ARG:NH2	2.52	0.43
1:A:98:THR:OG1	1:H:88:ARG:NH2	2.51	0.43
1:A:99:VAL:HG21	1:A:106:VAL:HG22	2.00	0.43
1:G:184:THR:HA	1:G:242:ALA:HB2	2.01	0.43
1:F:162:TYR:CE2	1:F:197:GLN:HG2	2.54	0.43
1:F:187:GLN:NE2	1:F:193:ARG:HG2	2.33	0.43
1:G:293:LEU:HD12	1:G:293:LEU:HA	1.86	0.43
1:F:79:ILE:HG21	1:F:124:VAL:HG11	2.00	0.43
1:H:224:TYR:CZ	1:H:228:ARG:HD2	2.54	0.43
1:G:163:ALA:O	1:G:167:LEU:HG	2.18	0.43
1:A:148:SER:O	1:A:156:THR:OG1	2.35	0.42
1:A:195:ARG:NH1	1:A:242:ALA:O	2.52	0.42
1:B:270:PHE:O	1:B:271:ASP:HB2	2.20	0.42
1:G:66:VAL:HG23	1:G:94:LEU:HD11	1.99	0.42
1:F:218:TRP:CG	2:F:501:FCB:H63	2.55	0.42
1:G:71:LEU:HD12	1:G:98:THR:HG21	2.01	0.42
1:G:124:VAL:HG13	1:G:147:LEU:HD22	2.00	0.42
1:A:182:LEU:HD12	1:A:240:PHE:O	2.19	0.42
1:D:209:PRO:HA	1:D:210:PRO:HD3	1.89	0.42
1:E:260:ARG:HE	1:E:263:ASP:HB2	1.85	0.42
1:B:99:VAL:HG21	1:B:106:VAL:HG22	2.02	0.42
1:B:271:ASP:OD1	2:B:501:FCB:O3	2.37	0.42
1:F:218:TRP:HA	1:F:246:MET:HE2	2.02	0.42
1:D:218:TRP:CG	2:D:501:FCB:H63	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:MET:O	1:C:250:VAL:HG23	2.20	0.41
1:D:310:PRO:HA	1:D:311:PRO:HD2	1.96	0.41
1:A:98:THR:OG1	1:H:84:GLU:OE1	2.36	0.41
1:D:70:GLY:O	1:G:81:VAL:HG21	2.20	0.41
1:E:111:ASN:HA	1:E:114:ARG:HB2	2.01	0.41
1:F:121:ILE:O	1:F:143:PRO:HA	2.20	0.41
1:A:184:THR:HA	1:A:242:ALA:HB2	2.02	0.41
1:G:186:PRO:HG3	1:G:217:ASP:HA	2.02	0.41
1:F:122:ILE:HG13	1:F:301:LEU:HD22	2.01	0.41
1:H:71:LEU:HD23	1:H:71:LEU:HA	1.79	0.41
1:B:123:ILE:HD13	1:B:123:ILE:HA	1.93	0.41
1:C:114:ARG:HH21	1:C:141:VAL:HG13	1.84	0.41
1:D:84:GLU:O	1:D:88:ARG:HB2	2.20	0.41
1:E:246:MET:O	1:E:250:VAL:HG23	2.20	0.41
1:H:66:VAL:HG23	1:H:94:LEU:HD11	2.02	0.41
1:H:187:GLN:NE2	1:H:193:ARG:HG2	2.36	0.41
1:A:166:ARG:NH1	1:A:201:GLU:HB3	2.34	0.41
1:A:246:MET:O	1:A:250:VAL:HG23	2.20	0.41
1:B:282:PRO:HG2	1:B:324:GLU:CD	2.45	0.41
1:C:81:VAL:HG21	1:E:70:GLY:O	2.21	0.41
1:D:285:THR:OG1	1:D:286:VAL:N	2.53	0.41
1:E:134:GLN:HA	1:E:137:GLN:HB2	2.01	0.41
1:F:302:LEU:HA	1:F:305:ILE:HG12	2.02	0.41
1:H:188:ASP:OD1	1:H:188:ASP:N	2.53	0.41
1:H:330:GLU:O	1:H:330:GLU:CG	2.68	0.41
1:B:285:THR:OG1	1:B:286:VAL:N	2.54	0.41
1:D:246:MET:O	1:D:250:VAL:HG23	2.21	0.41
1:F:186:PRO:HD2	1:F:218:TRP:CE2	2.56	0.41
1:E:289:ASP:O	1:E:293:LEU:HG	2.22	0.40
1:C:74:TYR:CZ	1:C:78:GLN:HG3	2.56	0.40
1:G:316:LEU:HA	1:G:317:PRO:HD3	1.91	0.40
1:H:243:ASN:ND2	1:H:245:GLN:HB2	2.36	0.40
1:E:316:LEU:HA	1:E:317:PRO:HD3	1.94	0.40
1:C:243:ASN:HD21	1:C:245:GLN:HB2	1.87	0.40
1:E:270:PHE:O	1:E:271:ASP:HB2	2.21	0.40
1:F:214:LEU:HD23	1:F:214:LEU:HA	1.98	0.40
1:G:308:GLU:HA	1:G:308:GLU:OE1	2.22	0.40
1:G:309:GLU:OE1	1:G:309:GLU:HA	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 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	256/280 (91%)	238 (93%)	16 (6%)	2 (1%)	16	26
1	B	252/280 (90%)	242 (96%)	8 (3%)	2 (1%)	16	26
1	C	260/280 (93%)	247 (95%)	12 (5%)	1 (0%)	30	44
1	D	256/280 (91%)	242 (94%)	11 (4%)	3 (1%)	11	16
1	E	260/280 (93%)	239 (92%)	19 (7%)	2 (1%)	16	26
1	F	242/280 (86%)	229 (95%)	10 (4%)	3 (1%)	11	16
1	G	261/280 (93%)	247 (95%)	13 (5%)	1 (0%)	30	44
1	H	243/280 (87%)	228 (94%)	14 (6%)	1 (0%)	30	44
All	All	2030/2240 (91%)	1912 (94%)	103 (5%)	15 (1%)	19	29

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLU
1	A	271	ASP
1	B	151	PRO
1	B	271	ASP
1	C	271	ASP
1	D	271	ASP
1	E	271	ASP
1	F	271	ASP
1	G	271	ASP
1	H	271	ASP
1	D	151	PRO
1	F	143	PRO
1	E	310	PRO
1	D	211	PRO
1	F	145	VAL

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	216/228 (95%)	216 (100%)	0	100	100
1	B	210/228 (92%)	209 (100%)	1 (0%)	86	94
1	C	216/228 (95%)	213 (99%)	3 (1%)	62	79
1	D	211/228 (92%)	208 (99%)	3 (1%)	62	79
1	E	214/228 (94%)	211 (99%)	3 (1%)	62	79
1	F	202/228 (89%)	196 (97%)	6 (3%)	36	57
1	G	218/228 (96%)	217 (100%)	1 (0%)	86	94
1	H	204/228 (90%)	201 (98%)	3 (2%)	60	77
All	All	1691/1824 (93%)	1671 (99%)	20 (1%)	67	82

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	115	GLU
1	C	95	LEU
1	C	151	PRO
1	C	291	GLU
1	D	147	LEU
1	D	148	SER
1	D	154	VAL
1	E	144	VAL
1	E	196	LEU
1	E	315	VAL
1	F	77	SER
1	F	93	SER
1	F	141	VAL
1	F	144	VAL
1	F	145	VAL
1	F	146	PHE
1	G	299	GLU
1	H	98	THR
1	H	118	VAL

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Mol	Chain	Res	Type
1	H	331	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	GLN
1	B	187	GLN
1	B	215	GLN
1	C	78	GLN
1	C	100	HIS
1	C	128	ASN
1	C	197	GLN
1	C	245	GLN
1	D	90	HIS
1	D	215	GLN
1	E	134	GLN
1	E	300	GLN
1	F	171	HIS
1	F	187	GLN
1	G	187	GLN
1	H	128	ASN
1	H	187	GLN
1	H	245	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FCB	G	501	-	11,11,11	1.29	1 (9%)	16,16,16	1.06	1 (6%)
2	FCB	A	501	-	11,11,11	1.25	1 (9%)	16,16,16	1.14	2 (12%)
2	FCB	B	501	-	11,11,11	1.27	1 (9%)	16,16,16	1.31	2 (12%)
2	FCB	E	501	-	11,11,11	1.32	1 (9%)	16,16,16	0.87	0
2	FCB	H	501	-	11,11,11	1.19	1 (9%)	16,16,16	0.83	0
2	FCB	F	501	-	11,11,11	1.26	1 (9%)	16,16,16	0.92	1 (6%)
2	FCB	C	501	-	11,11,11	1.27	1 (9%)	16,16,16	0.86	1 (6%)
2	FCB	D	501	-	11,11,11	1.33	1 (9%)	16,16,16	1.43	3 (18%)

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	FCB	G	501	-	-	-	0/1/1/1
2	FCB	A	501	-	-	-	0/1/1/1
2	FCB	B	501	-	-	-	0/1/1/1
2	FCB	E	501	-	-	-	0/1/1/1
2	FCB	H	501	-	-	-	0/1/1/1
2	FCB	F	501	-	-	-	0/1/1/1
2	FCB	C	501	-	-	-	0/1/1/1
2	FCB	D	501	-	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FCB	O5-C1	3.49	1.51	1.42
2	E	501	FCB	O5-C1	3.48	1.51	1.42
2	G	501	FCB	O5-C1	3.39	1.51	1.42
2	B	501	FCB	O5-C1	3.38	1.51	1.42
2	C	501	FCB	O5-C1	3.33	1.51	1.42
2	A	501	FCB	O5-C1	3.20	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	FCB	O5-C1	3.08	1.50	1.42
2	H	501	FCB	O5-C1	3.04	1.50	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	FCB	C1-O5-C5	-3.54	108.86	114.37
2	B	501	FCB	C6-C5-C4	-2.93	107.71	113.08
2	B	501	FCB	O5-C5-C4	2.93	114.83	109.55
2	F	501	FCB	C6-C5-C4	-2.55	108.42	113.08
2	D	501	FCB	O3-C3-C2	-2.38	104.77	110.38
2	A	501	FCB	O5-C5-C4	2.32	113.73	109.55
2	C	501	FCB	C6-C5-C4	-2.16	109.14	113.08
2	A	501	FCB	C6-C5-C4	-2.15	109.15	113.08
2	G	501	FCB	O5-C5-C4	2.12	113.38	109.55
2	D	501	FCB	C1-C2-C3	2.05	114.53	110.36

There are no chirality outliers.

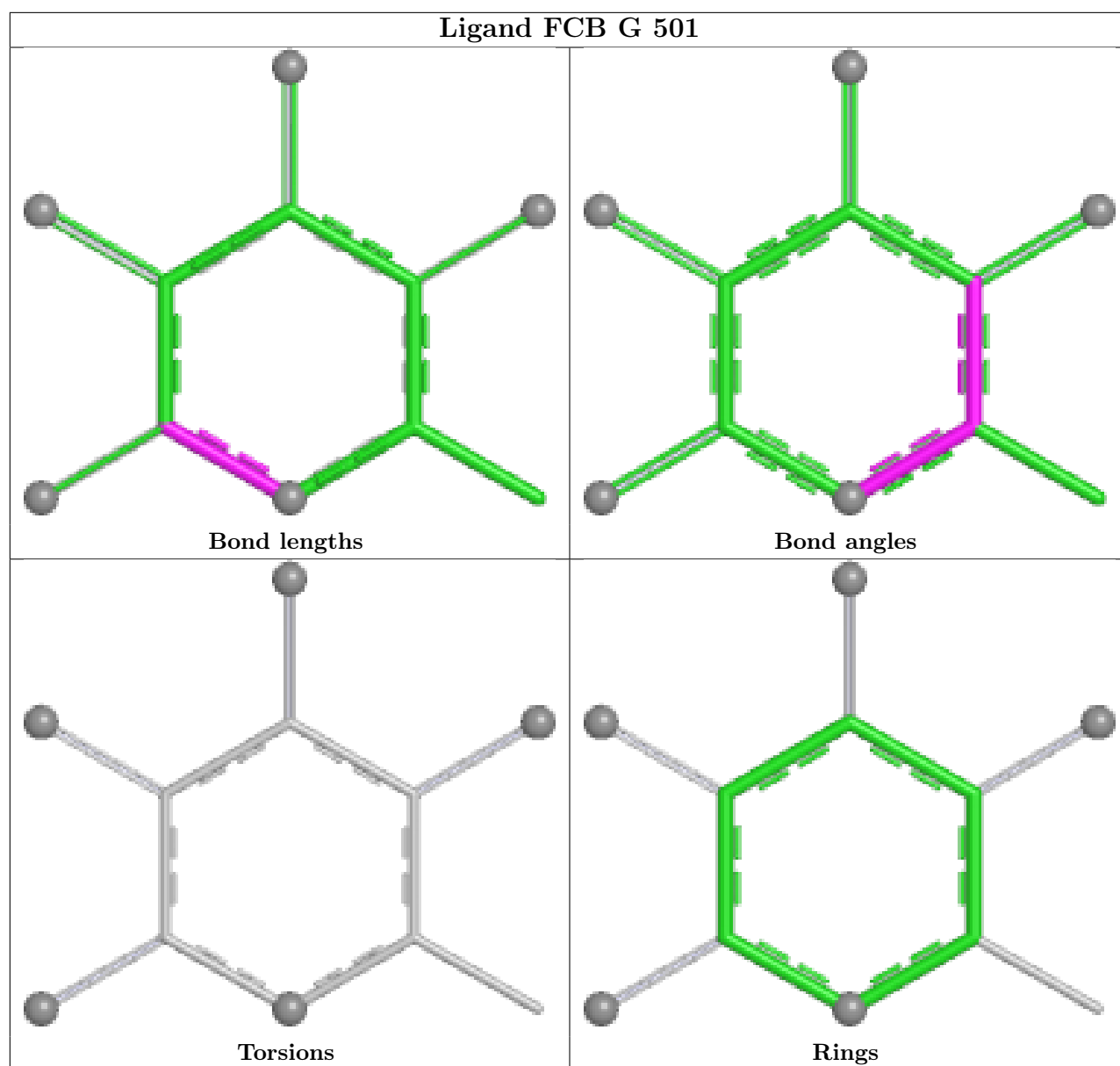
There are no torsion outliers.

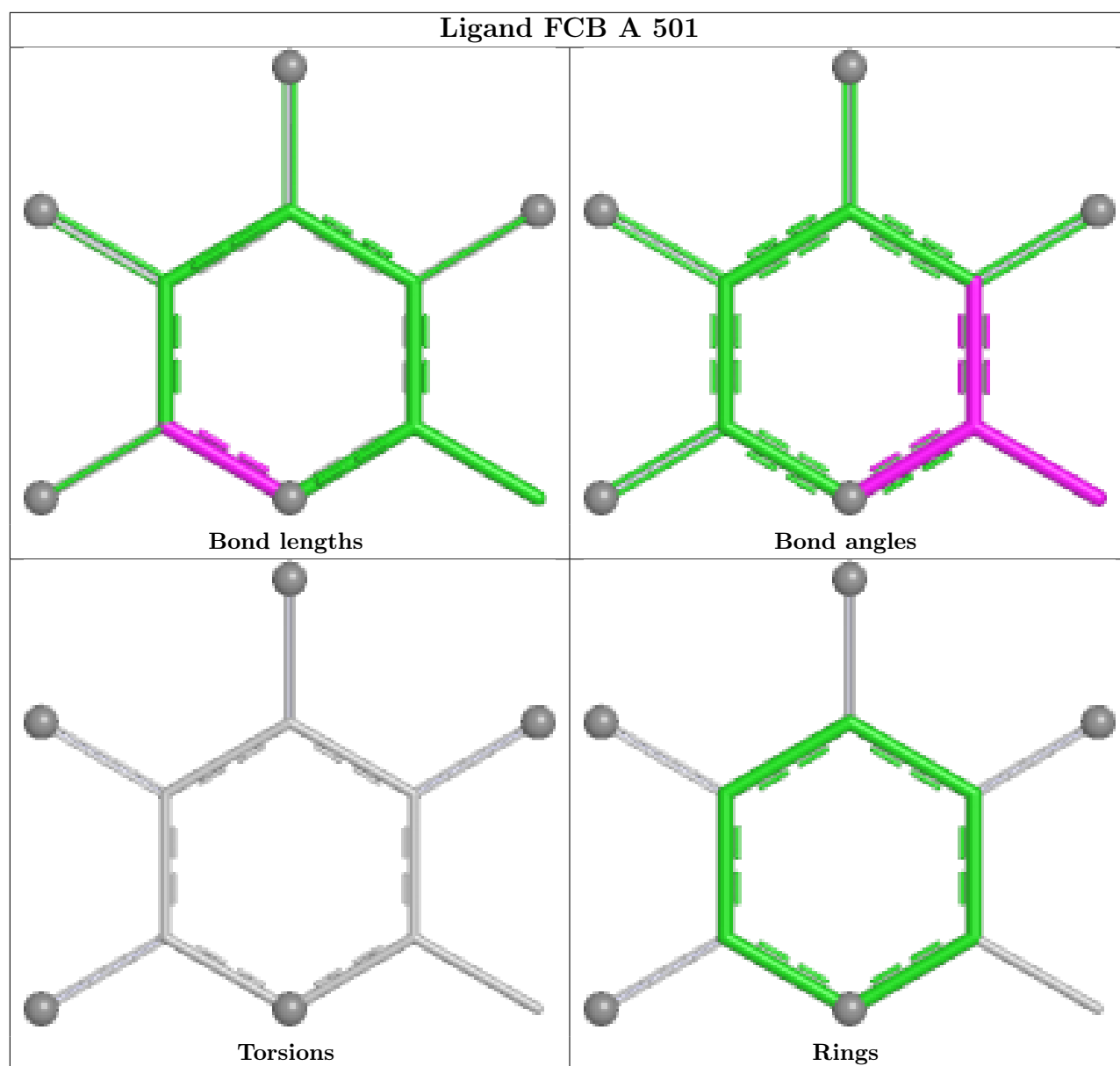
There are no ring outliers.

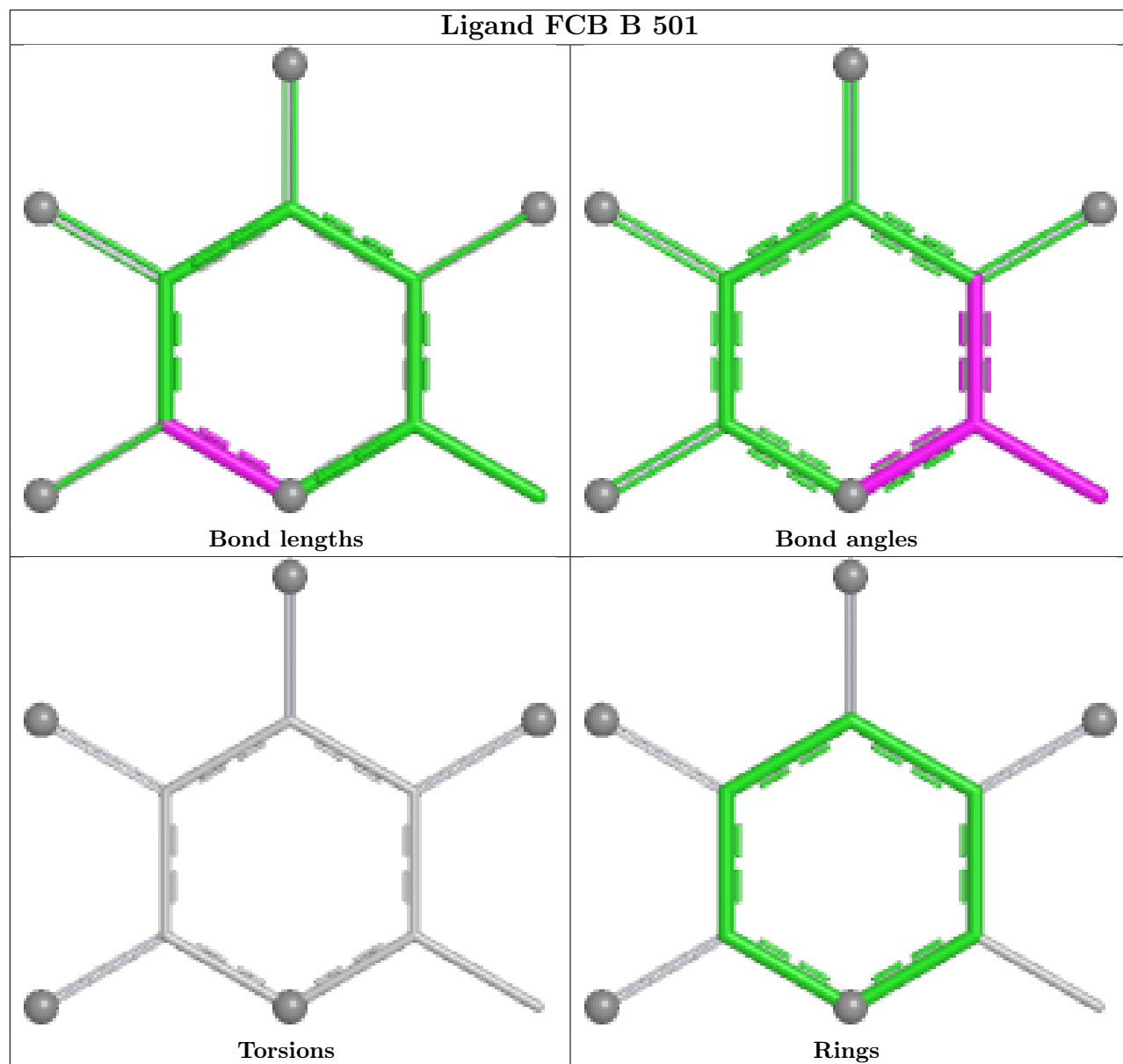
3 monomers are involved in 3 short contacts:

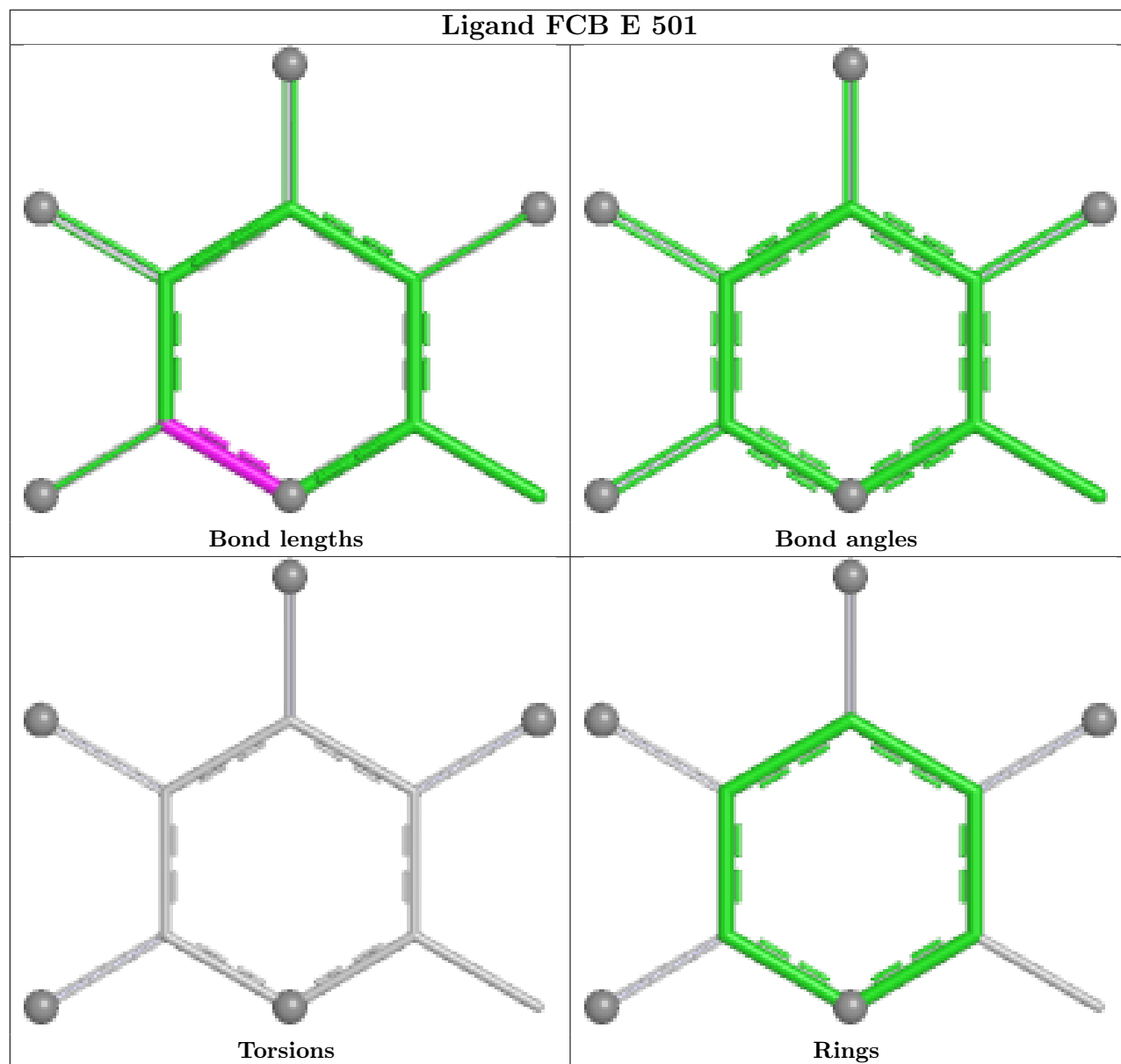
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FCB	1	0
2	F	501	FCB	1	0
2	D	501	FCB	1	0

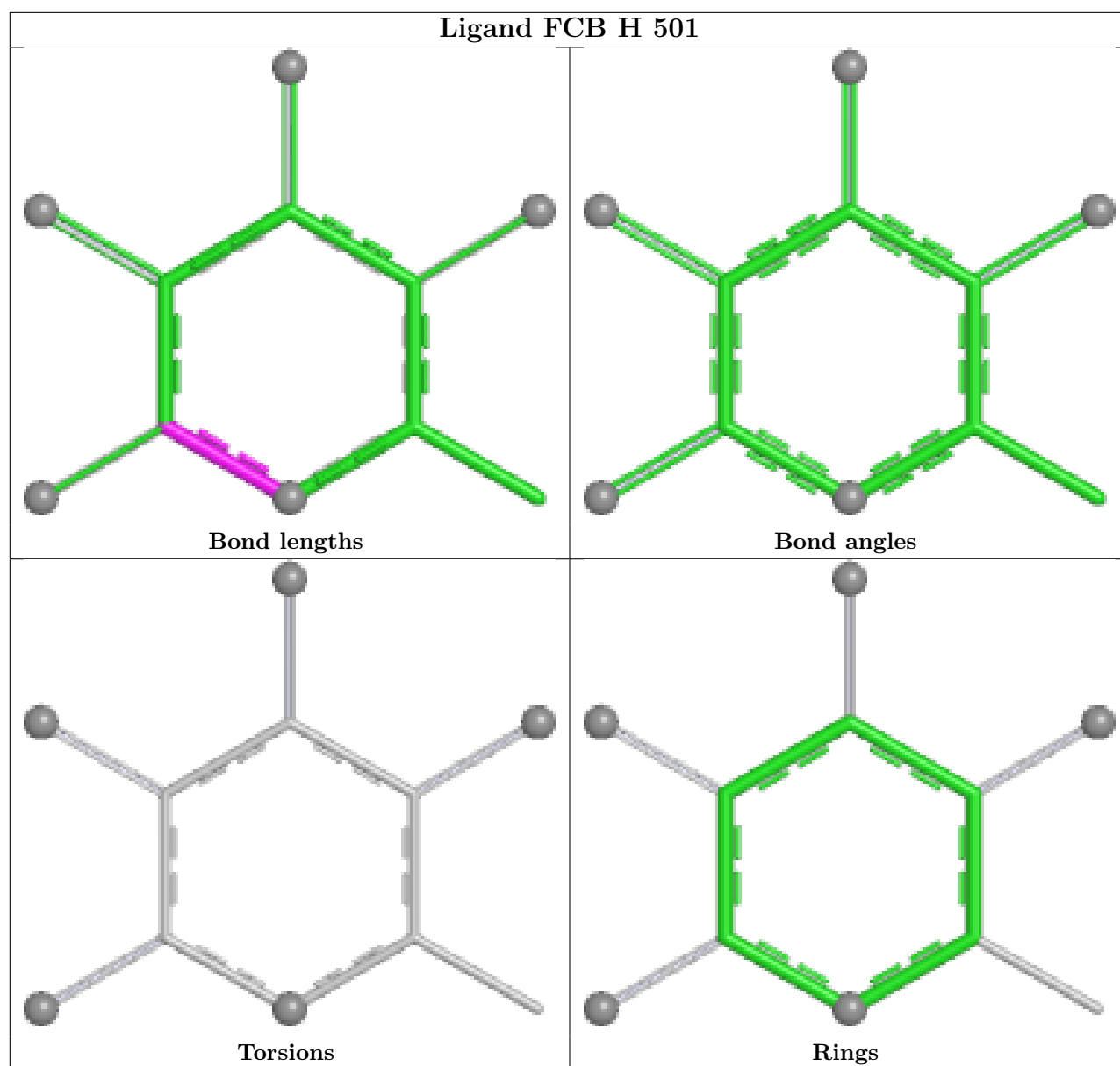
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

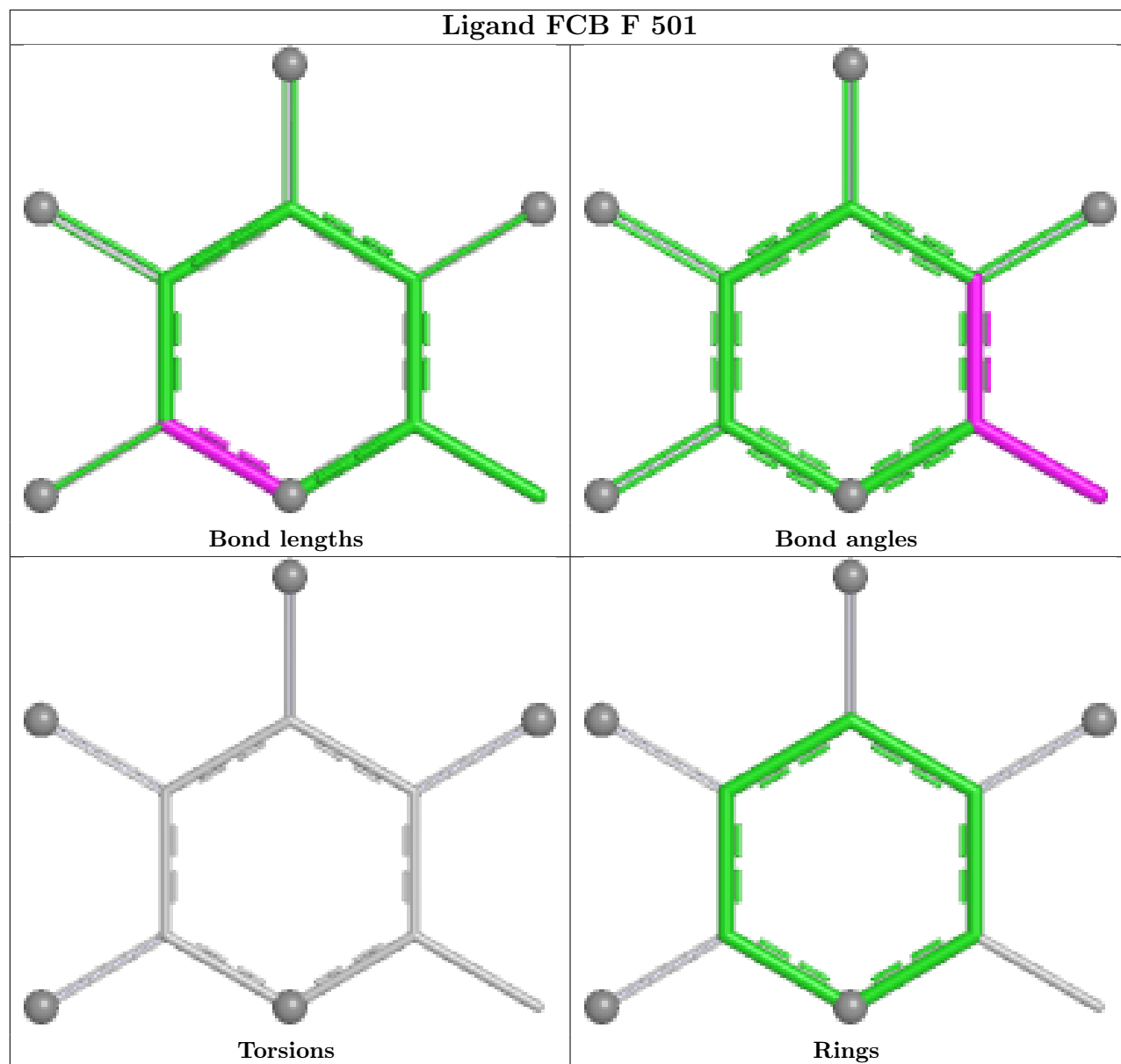


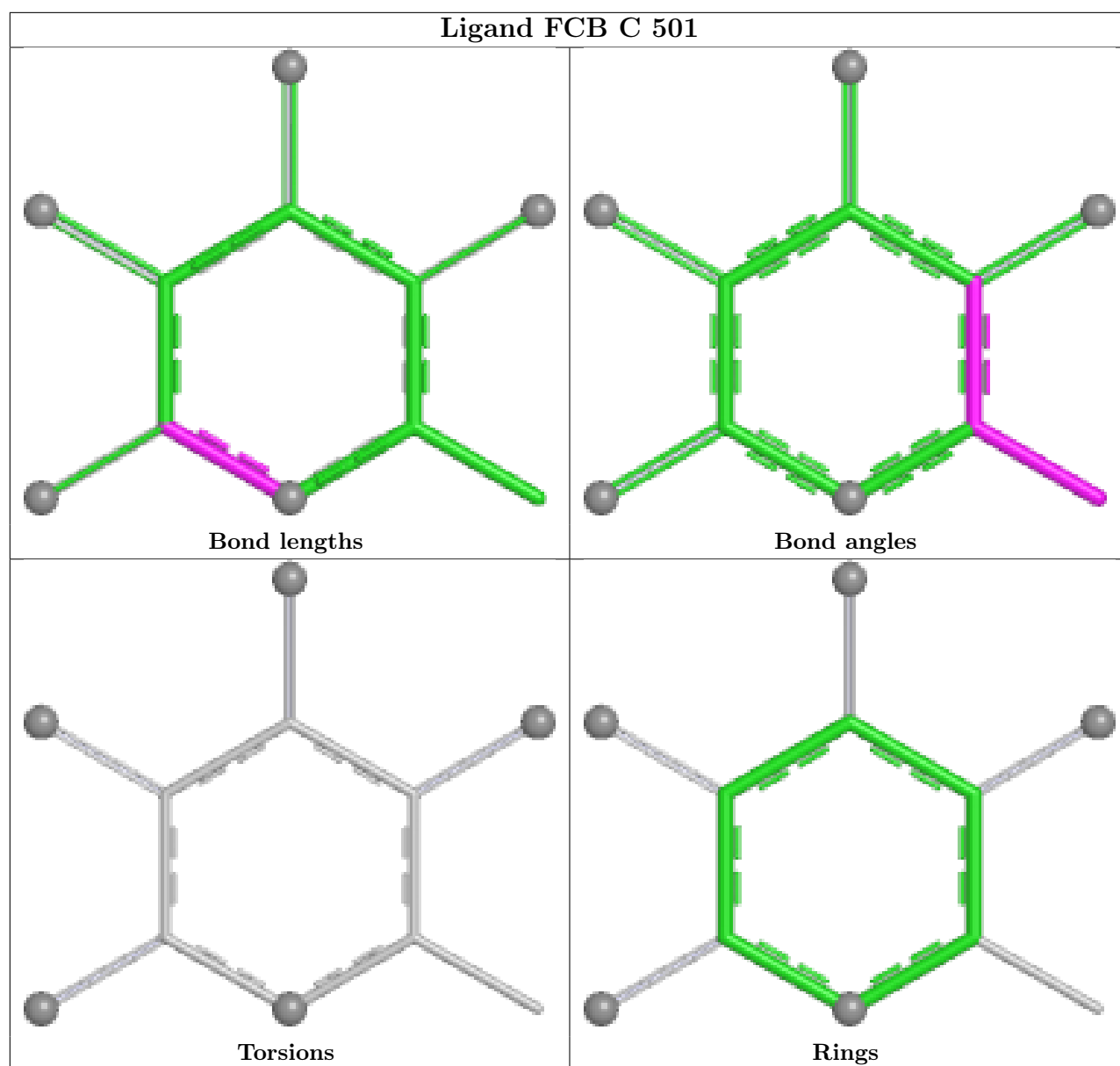


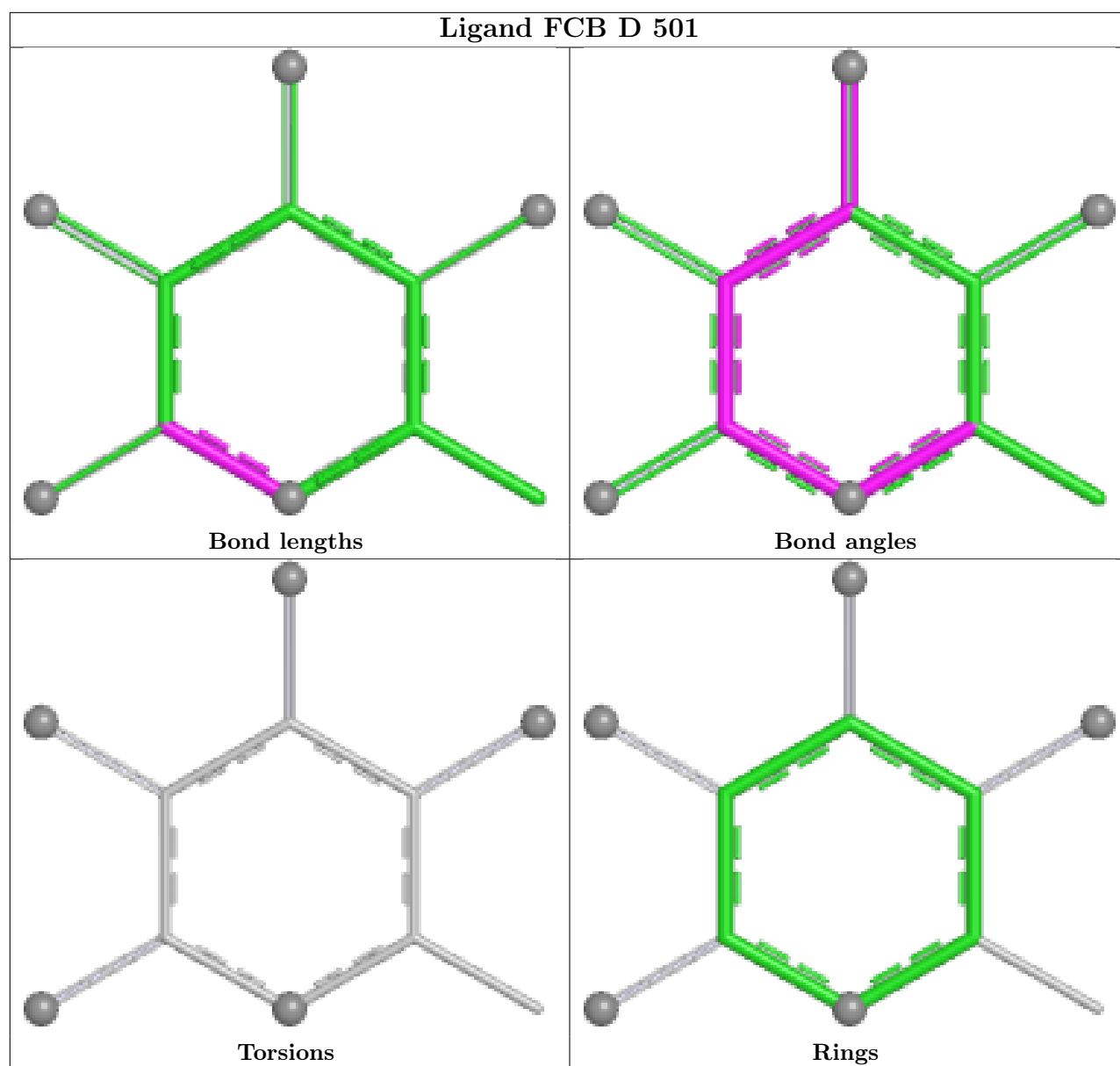












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	262/280 (93%)	-1.43	0 100 100	23, 42, 109, 146	0
1	B	258/280 (92%)	-1.44	0 100 100	22, 39, 100, 156	0
1	C	264/280 (94%)	-1.39	0 100 100	26, 43, 101, 157	0
1	D	260/280 (92%)	-1.38	0 100 100	34, 49, 104, 147	0
1	E	264/280 (94%)	-1.26	0 100 100	34, 59, 129, 154	0
1	F	248/280 (88%)	-1.41	0 100 100	26, 42, 91, 169	0
1	G	265/280 (94%)	-1.43	0 100 100	26, 43, 85, 143	0
1	H	249/280 (88%)	-1.33	0 100 100	25, 43, 102, 145	0
All	All	2070/2240 (92%)	-1.38	0 100 100	22, 45, 103, 169	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

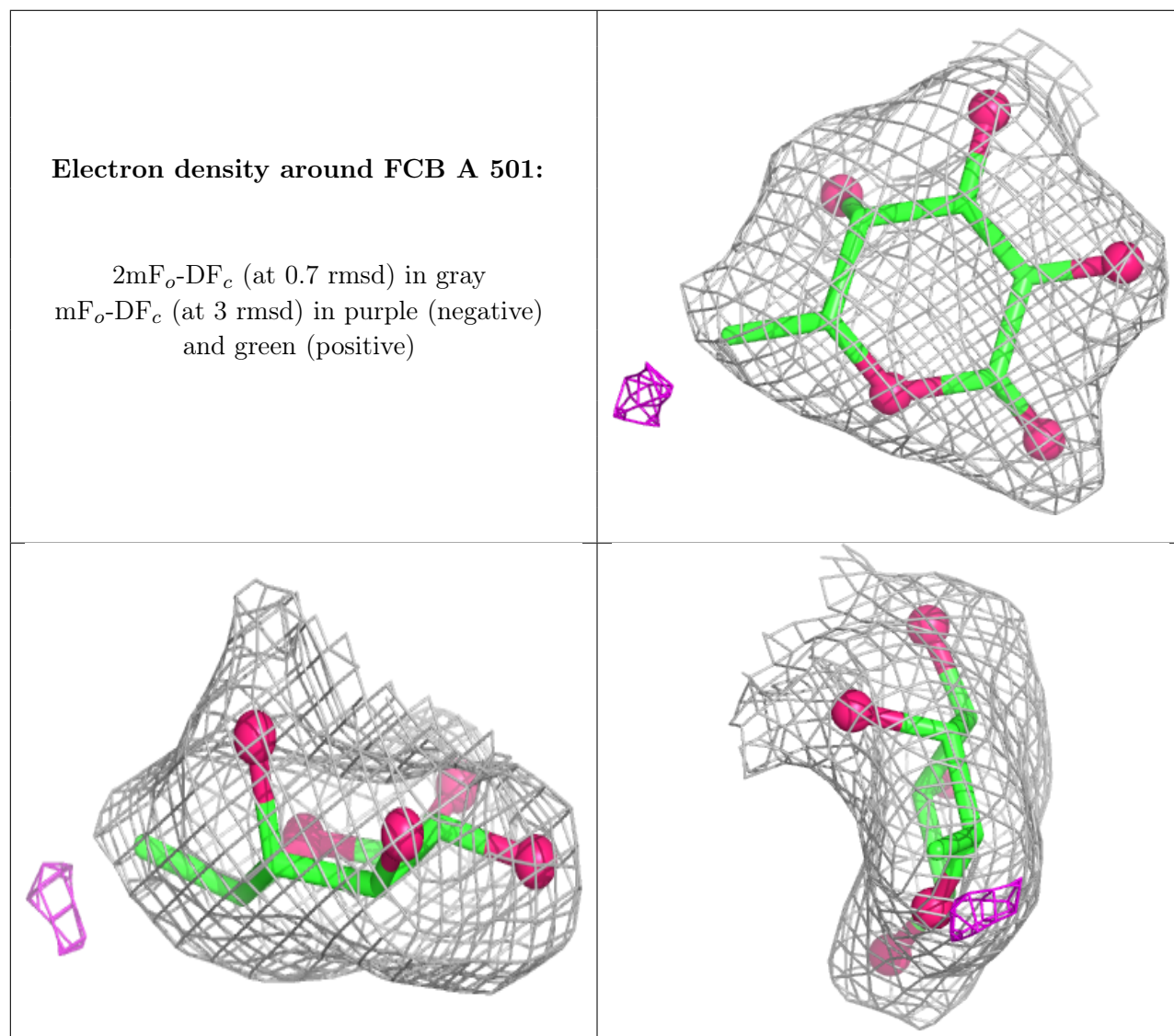
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

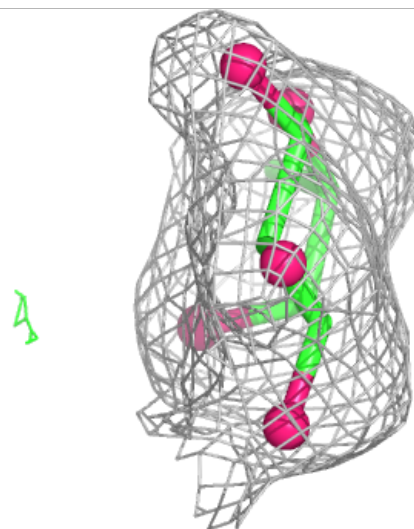
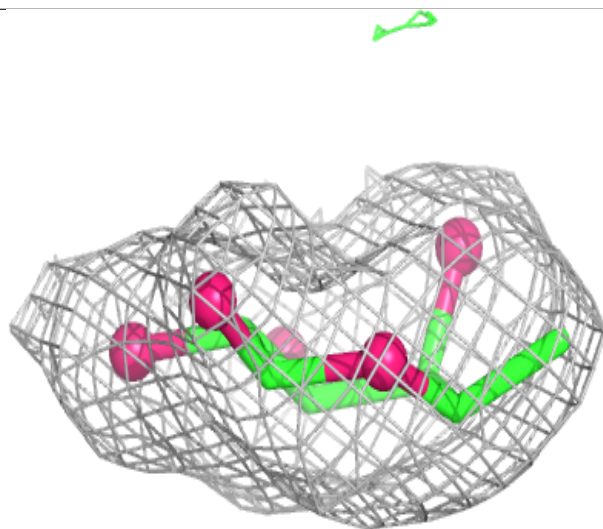
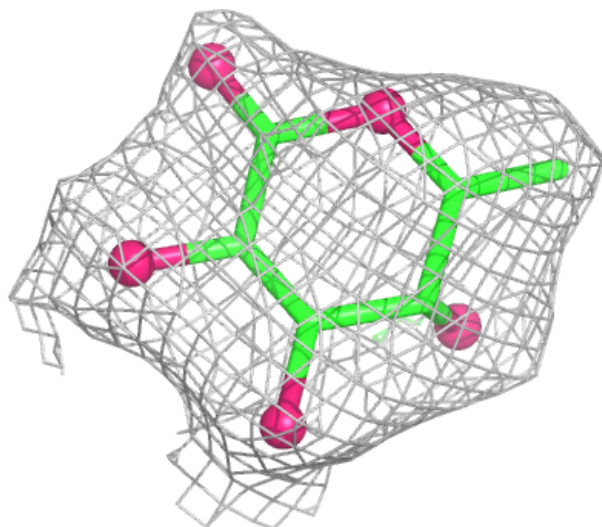
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FCB	A	501	11/11	0.99	0.03	32,37,42,43	0
2	FCB	B	501	11/11	0.99	0.03	32,38,50,51	0
2	FCB	C	501	11/11	0.99	0.03	28,33,37,40	0
2	FCB	D	501	11/11	0.99	0.04	32,38,40,43	0
2	FCB	E	501	11/11	0.99	0.03	40,44,51,53	0
2	FCB	F	501	11/11	0.99	0.03	27,29,32,34	0
2	FCB	H	501	11/11	0.99	0.03	31,34,36,39	0
2	FCB	G	501	11/11	1.00	0.03	23,28,35,36	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.



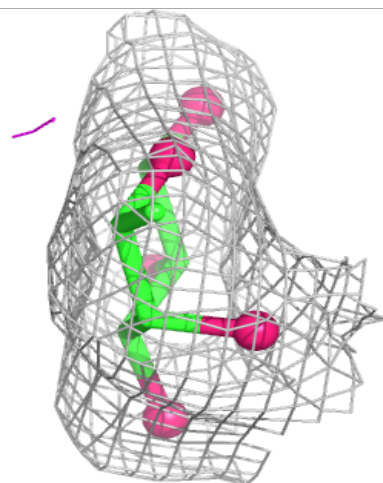
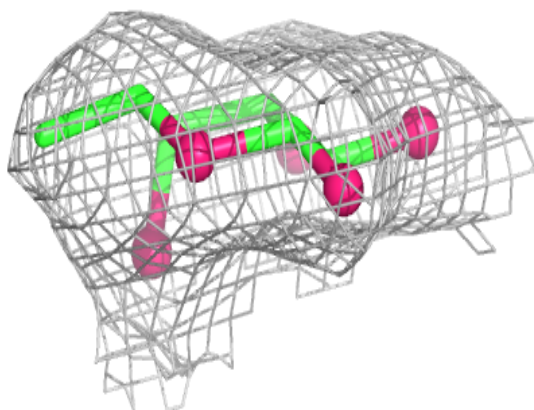
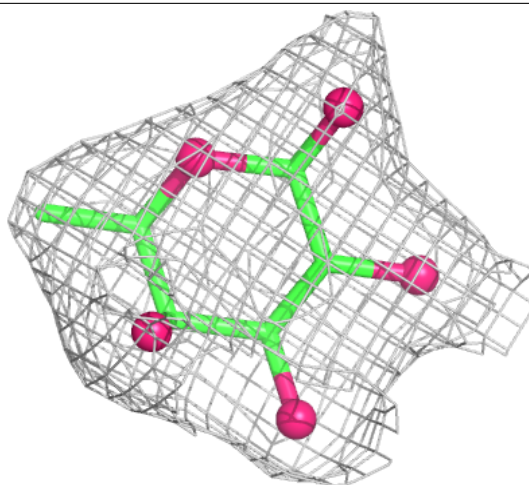
Electron density around FCB B 501:

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



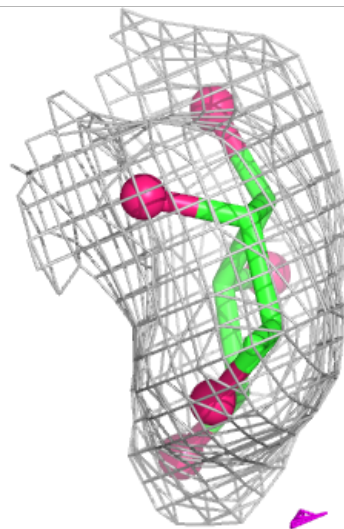
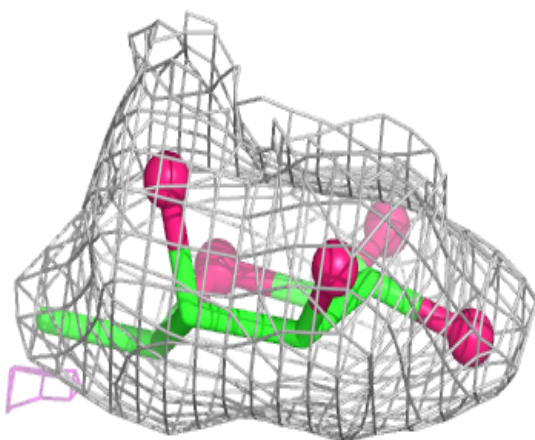
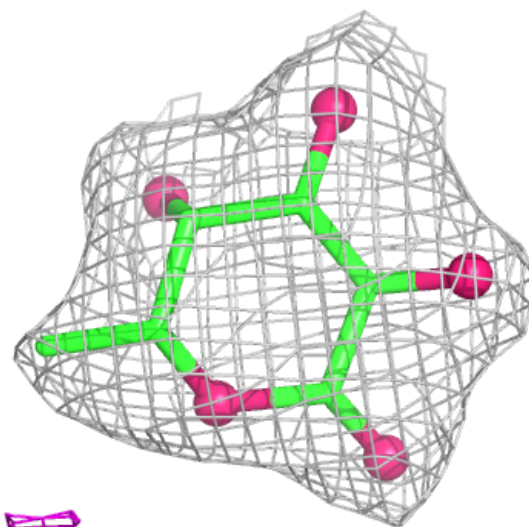
Electron density around FCB C 501:

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



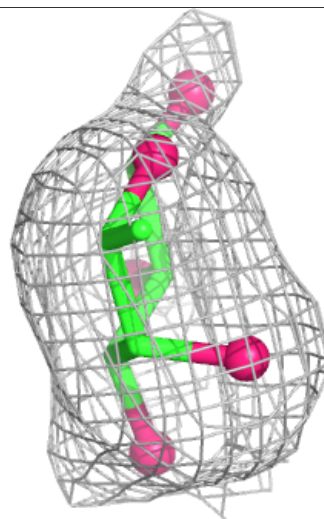
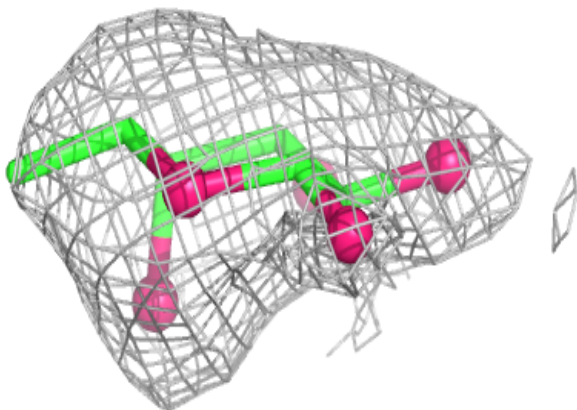
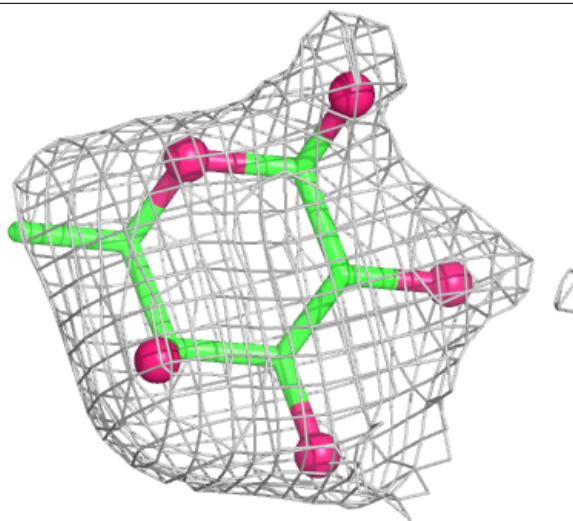
Electron density around FCB D 501:

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



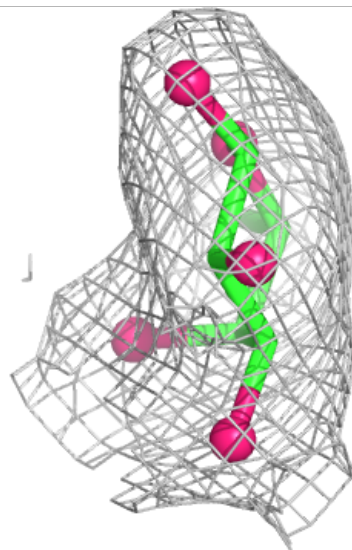
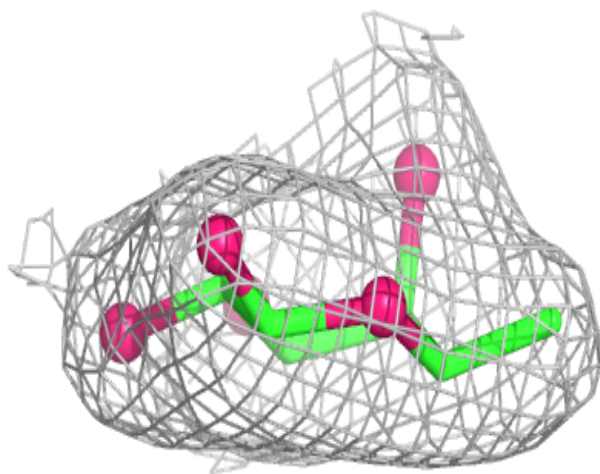
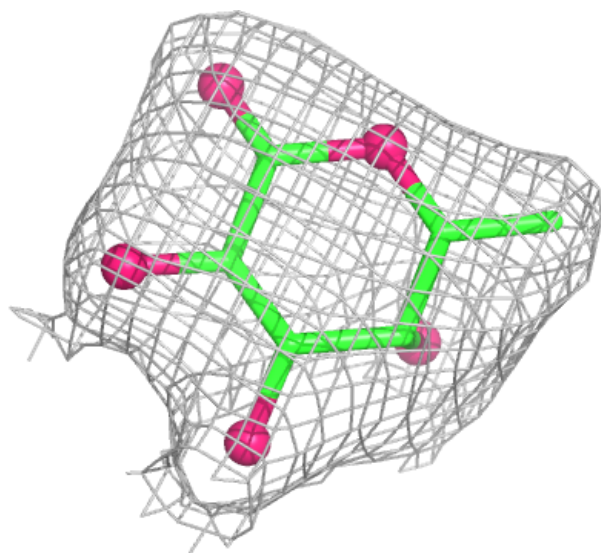
Electron density around FCB E 501:

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



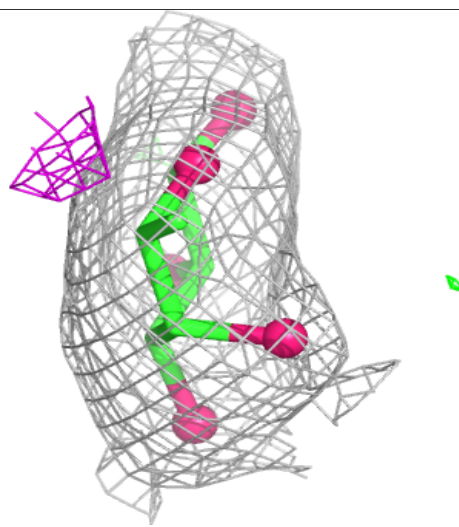
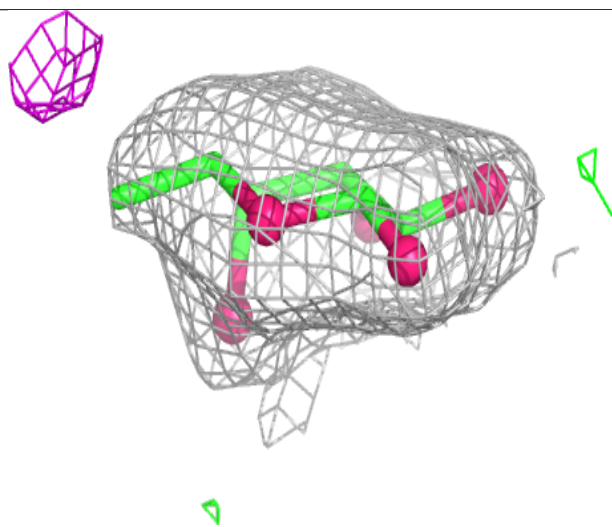
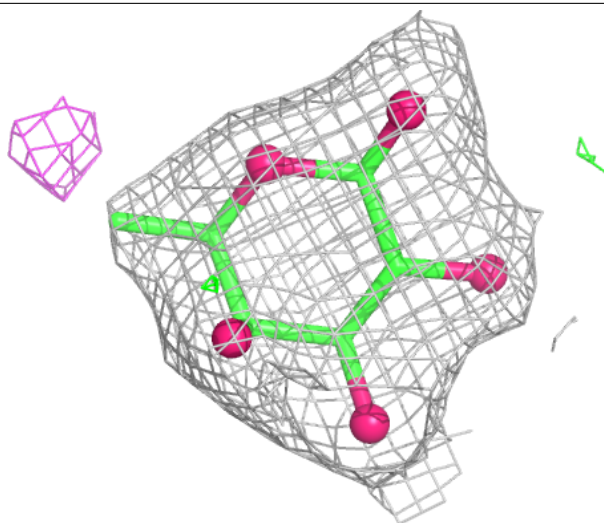
Electron density around FCB F 501:

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



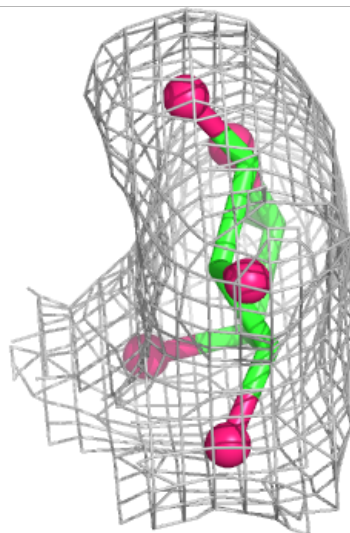
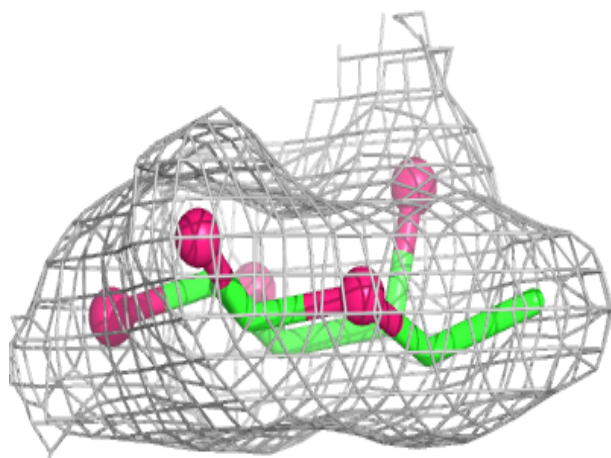
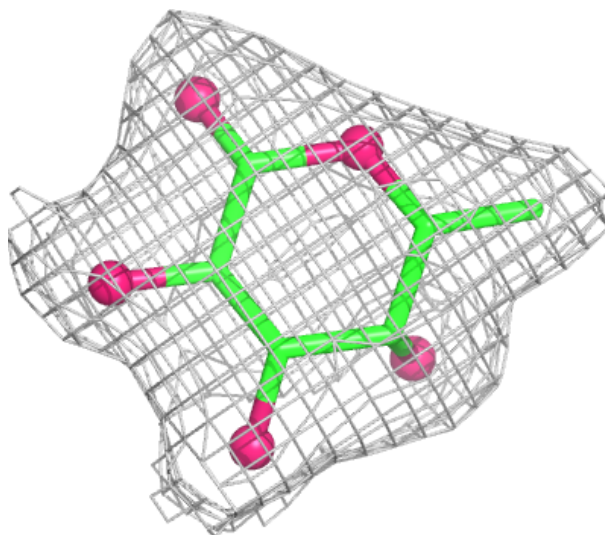
Electron density around FCB H 501:

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



Electron density around FCB G 501:

$2mF_o-DF_c$ (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.