



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:27 AM UTC

PDB ID : 8JT3 / pdb_00008jt3
Title : Crystal structure of aminotransferase CrmG from Actinoalloteichus sp. WH1-2216-6 in complex with amino donor L-Arg
Authors : Su, K.; Zhang, Y.; Xu, J.; Liu, J.
Deposited on : 2023-06-21
Resolution : 2.35 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

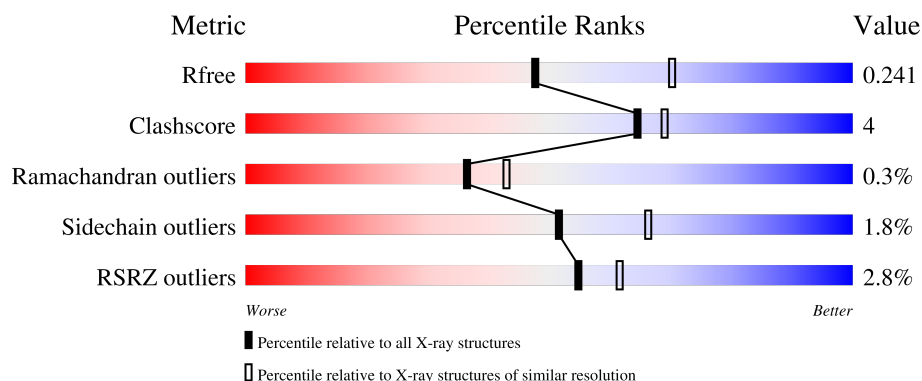
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	523	2% 86% 12% .
1	B	523	3% 88% 10% ..
1	C	523	4% 87% 10% ..
1	D	523	2% 88% 10% .

2 Entry composition [i](#)

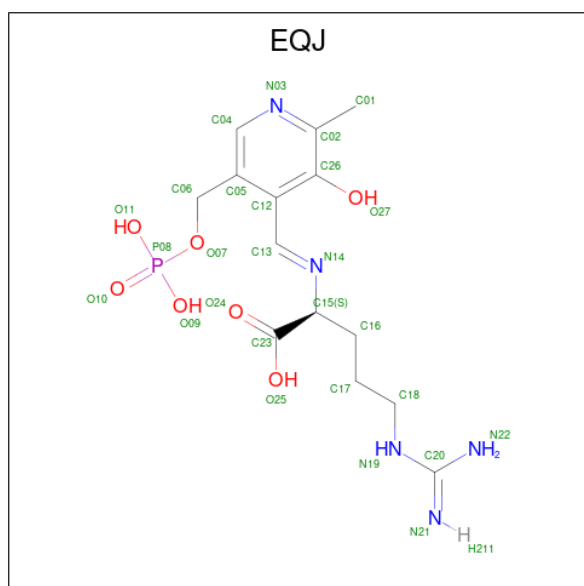
There are 5 unique types of molecules in this entry. The entry contains 16447 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CrmG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			3957	2474	716	756	11			
1	C	510	Total	C	N	O	S	0	0	0
			3942	2468	714	749	11			
1	B	512	Total	C	N	O	S	0	0	0
			3958	2476	716	755	11			
1	D	512	Total	C	N	O	S	0	0	0
			3958	2476	716	755	11			

- Molecule 2 is (E)-N 2 -({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene)-L-arginine (CCD ID: EQJ) (formula: C₁₄H₂₂N₅O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	14	5	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	14	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			27	14	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			27	14	5	7	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		

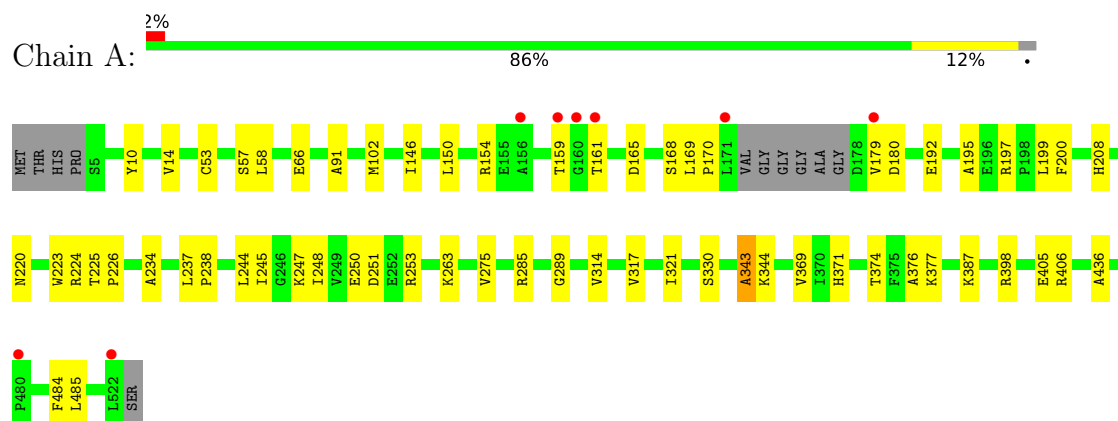
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total	O	0	0
			139	139		
5	C	103	Total	O	0	0
			103	103		
5	B	138	Total	O	0	0
			138	138		
5	D	104	Total	O	0	0
			104	104		

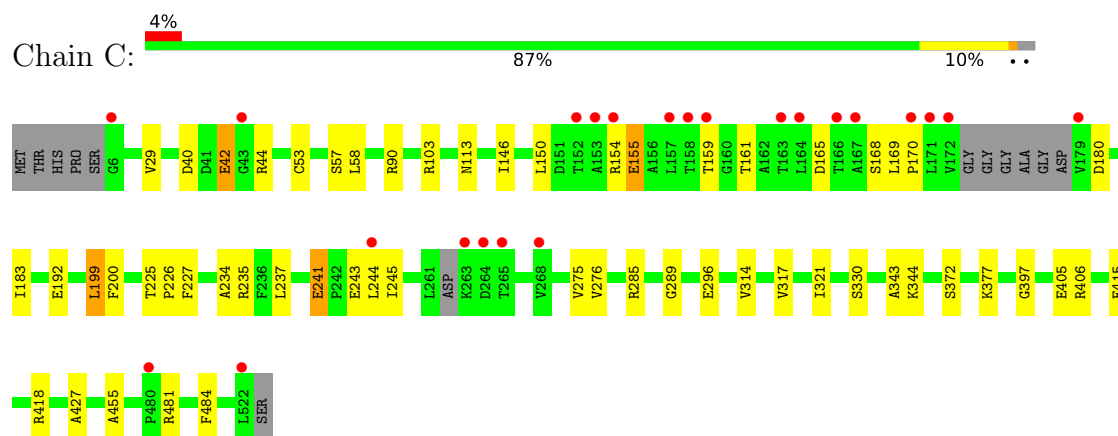
3 Residue-property plots [i](#)

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.

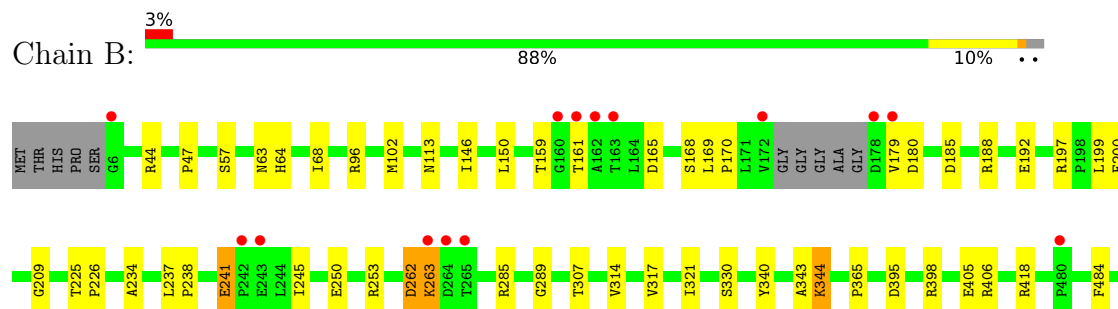
• Molecule 1: CrmG



• Molecule 1: CrmG

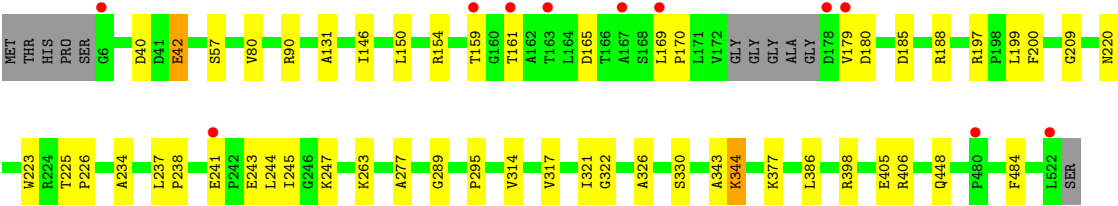
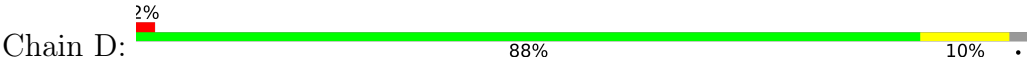


• Molecule 1: CrmG





● Molecule 1: CrmG



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.85Å 113.28Å 157.68Å 90.00° 91.74° 90.00°	Depositor
Resolution (Å)	40.19 – 2.35 40.19 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.5 (40.19-2.35) 93.5 (40.19-2.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.197 , 0.237 0.203 , 0.241	Depositor DCC
R_{free} test set	4174 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.146 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16447	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 40.30 % 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 2.7915e-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: GOL, ACT, EQJ

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	1.13	4/4024 (0.1%)	1.46	3/5451 (0.1%)
1	B	1.11	2/4025 (0.0%)	1.46	4/5453 (0.1%)
1	C	1.10	1/4008 (0.0%)	1.44	4/5428 (0.1%)
1	D	1.11	2/4025 (0.0%)	1.44	2/5453 (0.0%)
All	All	1.11	9/16082 (0.1%)	1.45	13/21785 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	238	PRO	C-O	-7.25	1.18	1.24
1	A	238	PRO	C-O	-6.22	1.19	1.24
1	A	343	ALA	C-O	-5.82	1.16	1.24
1	B	64	HIS	CE1-NE2	5.57	1.38	1.32
1	D	209	GLY	C-O	5.57	1.28	1.23
1	C	29	VAL	C-O	-5.35	1.19	1.24
1	A	208	HIS	CE1-NE2	5.17	1.37	1.32
1	B	209	GLY	C-O	5.07	1.28	1.23
1	A	371	HIS	CE1-NE2	5.07	1.37	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ARG	CA-C-N	5.90	126.66	119.99
1	A	285	ARG	C-N-CA	5.90	126.66	119.99
1	C	285	ARG	CA-C-N	5.51	126.22	119.99
1	C	285	ARG	C-N-CA	5.51	126.22	119.99
1	B	241	GLU	CB-CG-CD	5.39	121.76	112.60
1	A	369	VAL	CA-C-O	-5.37	114.17	118.90
1	B	285	ARG	CA-C-N	5.24	125.92	119.99
1	B	285	ARG	C-N-CA	5.24	125.92	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	PHE	CA-C-N	5.20	127.51	120.38
1	C	227	PHE	C-N-CA	5.20	127.51	120.38
1	D	295	PRO	CA-C-N	5.13	127.15	120.28
1	D	295	PRO	C-N-CA	5.13	127.15	120.28
1	B	307	THR	CA-C-O	-5.05	115.50	120.70

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	3957	0	3933	35	0
1	B	3958	0	3937	32	0
1	C	3942	0	3928	31	0
1	D	3958	0	3937	24	0
2	A	27	0	0	3	0
2	B	27	0	0	4	0
2	C	27	0	0	1	0
2	D	27	0	0	4	0
3	A	24	0	32	3	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
4	D	4	0	3	0	0
5	A	139	0	0	3	0
5	B	138	0	0	2	0
5	C	103	0	0	6	0
5	D	104	0	0	1	0
All	All	16447	0	15786	124	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 4.

All (124) 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:103:ARG:NH1	5:C:701:HOH:O	2.02	0.93
1:C:372:SER:OG	2:D:601:EQJ:N22	2.08	0.86
2:D:601:EQJ:N14	2:D:601:EQJ:O27	2.05	0.86
2:B:601:EQJ:N14	2:B:601:EQJ:O27	2.06	0.83
1:D:344:LYS:O	5:D:701:HOH:O	1.96	0.82
2:A:601:EQJ:O27	2:A:601:EQJ:N14	2.03	0.79
2:C:601:EQJ:N14	2:C:601:EQJ:O27	2.15	0.76
1:C:344:LYS:O	5:C:702:HOH:O	2.06	0.73
1:D:344:LYS:HZ1	2:D:601:EQJ:C13	2.05	0.69
1:A:344:LYS:O	5:A:701:HOH:O	2.11	0.68
1:B:344:LYS:O	5:B:701:HOH:O	2.10	0.68
1:A:247:LYS:NZ	1:A:251:ASP:OD2	2.27	0.66
1:B:250:GLU:OE2	1:B:253:ARG:HD2	1.95	0.66
1:A:169:LEU:N	1:A:170:PRO:HD2	2.12	0.65
1:B:169:LEU:N	1:B:170:PRO:HD2	2.12	0.64
1:C:418:ARG:HH11	1:C:427:ALA:HA	1.61	0.64
1:A:66:GLU:HG2	1:A:387:LYS:HE3	1.80	0.63
1:C:169:LEU:N	1:C:170:PRO:HD2	2.12	0.63
3:A:605:GOL:H32	1:B:63:ASN:HB3	1.80	0.63
1:C:296:GLU:HB2	5:C:787:HOH:O	2.00	0.60
1:A:195:ALA:O	5:A:702:HOH:O	2.17	0.60
1:A:344:LYS:HZ1	2:A:601:EQJ:C13	2.15	0.59
1:B:238:PRO:HB2	1:B:241:GLU:HG2	1.86	0.57
1:D:344:LYS:NZ	2:D:601:EQJ:C13	2.67	0.57
1:D:405:GLU:OE1	1:D:406:ARG:HD2	2.05	0.57
2:B:601:EQJ:C13	2:B:601:EQJ:C17	2.84	0.56
1:D:185:ASP:OD1	1:D:188:ARG:NH2	2.40	0.55
1:C:154:ARG:NH2	1:C:180:ASP:OD1	2.39	0.55
1:B:179:VAL:HG13	1:B:180:ASP:H	1.72	0.55
1:A:225:THR:N	1:A:226:PRO:CD	2.71	0.54
1:D:225:THR:N	1:D:226:PRO:CD	2.71	0.54
1:A:344:LYS:NZ	2:A:601:EQJ:C13	2.71	0.54
1:A:405:GLU:OE1	1:A:406:ARG:HD2	2.08	0.54
1:C:225:THR:N	1:C:226:PRO:CD	2.71	0.54
1:B:102:MET:HE1	1:B:340:TYR:CD1	2.42	0.54
1:A:314:VAL:HG11	1:A:330:SER:HB3	1.90	0.53
1:D:165:ASP:C	1:D:165:ASP:OD1	2.51	0.53
1:B:237:LEU:HB3	1:B:245:ILE:HG12	1.91	0.53
1:D:314:VAL:HG11	1:D:330:SER:HB3	1.90	0.52
1:C:165:ASP:OD1	1:C:165:ASP:C	2.52	0.52
1:B:185:ASP:OD1	1:B:188:ARG:NH2	2.42	0.52
1:A:165:ASP:C	1:A:165:ASP:OD1	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ASP:OD1	1:B:165:ASP:C	2.52	0.52
1:C:405:GLU:OE1	1:C:406:ARG:HD2	2.10	0.52
1:C:314:VAL:HG11	1:C:330:SER:HB3	1.90	0.52
1:B:179:VAL:HG13	1:B:180:ASP:N	2.24	0.52
1:C:241:GLU:HB3	1:C:244:LEU:HD13	1.91	0.51
1:B:225:THR:N	1:B:226:PRO:CD	2.73	0.51
1:D:237:LEU:HB3	1:D:245:ILE:HG12	1.92	0.51
1:B:405:GLU:OE1	1:B:406:ARG:HD2	2.10	0.51
1:B:314:VAL:HG11	1:B:330:SER:HB3	1.91	0.51
1:C:397:GLY:HA2	5:C:712:HOH:O	2.09	0.51
1:A:377:LYS:HG3	3:A:603:GOL:H2	1.92	0.50
1:B:197:ARG:NH1	1:B:199:LEU:HD21	2.27	0.49
1:C:200:PHE:O	1:C:234:ALA:HA	2.13	0.49
1:B:200:PHE:O	1:B:234:ALA:HA	2.12	0.49
1:C:296:GLU:CB	5:C:787:HOH:O	2.59	0.49
1:A:376:ALA:O	1:A:377:LYS:HB2	2.11	0.49
1:A:237:LEU:HB3	1:A:245:ILE:HG12	1.94	0.49
1:B:57:SER:HA	1:B:344:LYS:HB3	1.95	0.48
1:A:197:ARG:NH1	1:A:199:LEU:HD21	2.27	0.48
1:B:344:LYS:NZ	2:B:601:EQJ:C13	2.77	0.48
1:A:154:ARG:NH2	1:A:180:ASP:OD1	2.38	0.48
1:C:237:LEU:HB3	1:C:245:ILE:HG12	1.96	0.48
1:A:250:GLU:OE2	1:A:253:ARG:NH1	2.46	0.48
1:C:168:SER:C	1:C:170:PRO:HD2	2.38	0.48
1:C:199:LEU:HD11	1:C:235:ARG:HG2	1.95	0.48
1:A:220:ASN:HD22	1:A:223:TRP:CG	2.31	0.48
1:A:57:SER:HA	1:A:344:LYS:HB3	1.96	0.47
1:C:415:GLU:HG3	5:C:799:HOH:O	2.13	0.47
1:D:241:GLU:HB3	1:D:244:LEU:HD13	1.97	0.47
1:A:168:SER:C	1:A:170:PRO:HD2	2.40	0.47
1:A:200:PHE:O	1:A:234:ALA:HA	2.14	0.47
1:C:275:VAL:HG23	1:C:276:VAL:HG23	1.97	0.47
1:C:317:VAL:HG13	1:C:343:ALA:HB3	1.96	0.47
1:B:168:SER:C	1:B:170:PRO:HD2	2.40	0.47
1:D:169:LEU:N	1:D:170:PRO:CD	2.78	0.47
1:B:262:ASP:C	1:B:263:LYS:HG2	2.40	0.47
1:C:40:ASP:OD1	1:C:42:GLU:HG2	2.15	0.46
3:A:605:GOL:H11	1:B:68:ILE:HG21	1.97	0.46
1:D:197:ARG:NH1	1:D:199:LEU:HD21	2.30	0.46
1:C:146:ILE:O	1:C:150:LEU:HG	2.16	0.46
1:D:57:SER:HA	1:D:344:LYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ILE:O	1:B:150:LEU:HG	2.16	0.46
1:A:169:LEU:N	1:A:170:PRO:CD	2.79	0.46
1:B:317:VAL:HG13	1:B:343:ALA:HB3	1.98	0.46
1:C:169:LEU:N	1:C:170:PRO:CD	2.79	0.46
1:D:317:VAL:HG13	1:D:343:ALA:HB3	1.98	0.46
1:C:57:SER:HA	1:C:344:LYS:HB3	1.97	0.46
1:A:159:THR:HG22	1:A:161:THR:HG23	1.98	0.45
1:B:159:THR:HG22	1:B:161:THR:HG23	1.99	0.45
1:A:146:ILE:O	1:A:150:LEU:HG	2.17	0.45
1:B:169:LEU:N	1:B:170:PRO:CD	2.80	0.45
1:D:200:PHE:O	1:D:234:ALA:HA	2.17	0.45
1:D:159:THR:HG22	1:D:161:THR:HG23	1.99	0.45
1:D:146:ILE:O	1:D:150:LEU:HG	2.17	0.45
1:D:154:ARG:NH2	1:D:180:ASP:OD1	2.38	0.45
1:A:317:VAL:HG13	1:A:343:ALA:HB3	1.98	0.44
1:A:10:TYR:CE2	1:B:96:ARG:HG3	2.52	0.44
1:C:159:THR:HG22	1:C:161:THR:HG23	2.00	0.44
1:C:455:ALA:O	1:C:481:ARG:NH2	2.50	0.44
1:D:40:ASP:OD1	1:D:42:GLU:HG2	2.19	0.43
1:A:374:THR:OG1	2:B:601:EQJ:C18	2.67	0.43
1:A:289:GLY:HA3	1:A:484:PHE:CD2	2.54	0.43
1:C:155:GLU:OE1	1:C:155:GLU:HA	2.19	0.42
1:D:220:ASN:HD22	1:D:223:TRP:CG	2.37	0.42
1:C:289:GLY:HA3	1:C:484:PHE:CD2	2.54	0.42
1:C:44:ARG:HG2	1:B:47:PRO:HG3	2.02	0.42
1:B:289:GLY:HA3	1:B:484:PHE:CD2	2.54	0.42
1:D:322:GLY:HA2	1:D:326:ALA:O	2.20	0.42
1:A:53:CYS:HB3	1:A:58:LEU:HB2	2.02	0.41
1:A:224:ARG:C	1:A:226:PRO:HD2	2.45	0.41
1:A:91:ALA:HB2	1:A:377:LYS:HD2	2.01	0.41
1:B:418:ARG:CZ	5:B:808:HOH:O	2.68	0.41
1:D:131:ALA:HB1	1:D:277:ALA:O	2.21	0.41
1:A:436:ALA:HA	1:A:485:LEU:O	2.21	0.41
1:D:90:ARG:HD3	1:D:386:LEU:HD12	2.03	0.41
1:A:66:GLU:HG2	1:A:387:LYS:CE	2.49	0.41
1:C:53:CYS:HB3	1:C:58:LEU:HB2	2.03	0.41
1:A:102:MET:HG3	5:A:818:HOH:O	2.21	0.40
1:D:289:GLY:HA3	1:D:484:PHE:CD2	2.56	0.40
1:B:262:ASP:O	1:B:263:LYS:HG2	2.21	0.40
1:A:14:VAL:HG21	1:B:365:PRO:CB	2.51	0.40
1:B:395:ASP:O	1:B:398:ARG:NH2	2.53	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	508/523 (97%)	490 (96%)	16 (3%)	2 (0%)	30	34
1	B	508/523 (97%)	490 (96%)	16 (3%)	2 (0%)	30	34
1	C	504/523 (96%)	489 (97%)	15 (3%)	0	100	100
1	D	508/523 (97%)	490 (96%)	15 (3%)	3 (1%)	21	24
All	All	2028/2092 (97%)	1959 (97%)	62 (3%)	7 (0%)	36	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	VAL
1	A	263	LYS
1	B	344	LYS
1	D	263	LYS
1	B	263	LYS
1	D	344	LYS
1	D	179	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	416/422 (99%)	410 (99%)	6 (1%)	59	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	416/422 (99%)	411 (99%)	5 (1%)	63	77
1	C	414/422 (98%)	403 (97%)	11 (3%)	39	52
1	D	416/422 (99%)	408 (98%)	8 (2%)	50	65
All	All	1662/1688 (98%)	1632 (98%)	30 (2%)	51	66

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	GLU
1	A	244	LEU
1	A	248	ILE
1	A	275	VAL
1	A	321	ILE
1	A	398	ARG
1	C	42	GLU
1	C	90	ARG
1	C	113	ASN
1	C	155	GLU
1	C	183	ILE
1	C	192	GLU
1	C	199	LEU
1	C	241	GLU
1	C	243	GLU
1	C	321	ILE
1	C	377	LYS
1	B	44	ARG
1	B	113	ASN
1	B	192	GLU
1	B	262	ASP
1	B	321	ILE
1	D	42	GLU
1	D	80	VAL
1	D	243	GLU
1	D	247	LYS
1	D	321	ILE
1	D	377	LYS
1	D	398	ARG
1	D	448	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
1	C	421	HIS
1	B	136	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	602	-	5,5,5	0.37	0	5,5,5	0.63	0
3	GOL	A	603	-	5,5,5	0.25	0	5,5,5	0.45	0
2	EQJ	A	601	-	27,27,27	2.49	9 (33%)	32,37,37	3.01	10 (31%)
2	EQJ	D	601	-	27,27,27	2.38	9 (33%)	32,37,37	5.21	15 (46%)
3	GOL	A	605	-	5,5,5	0.26	0	5,5,5	0.74	0
2	EQJ	C	601	-	27,27,27	1.94	6 (22%)	32,37,37	2.56	9 (28%)
3	GOL	A	604	-	5,5,5	0.24	0	5,5,5	0.51	0
3	GOL	C	602	-	5,5,5	0.17	0	5,5,5	0.39	0
2	EQJ	B	601	-	27,27,27	2.52	10 (37%)	32,37,37	3.62	13 (40%)
3	GOL	B	602	-	5,5,5	0.18	0	5,5,5	0.43	0
4	ACT	D	602	-	3,3,3	1.22	0	3,3,3	1.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	602	-	-	2/4/4/4	-
3	GOL	A	603	-	-	4/4/4/4	-
2	EQJ	A	601	-	-	4/22/22/22	0/1/1/1
2	EQJ	D	601	-	-	4/22/22/22	0/1/1/1
3	GOL	A	605	-	-	2/4/4/4	-
2	EQJ	C	601	-	-	6/22/22/22	0/1/1/1
3	GOL	A	604	-	-	0/4/4/4	-
3	GOL	C	602	-	-	0/4/4/4	-
2	EQJ	B	601	-	-	6/22/22/22	0/1/1/1
3	GOL	B	602	-	-	2/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	EQJ	C15-C23	7.05	1.60	1.52
2	C	601	EQJ	C26-C02	6.74	1.48	1.41
2	D	601	EQJ	C15-C23	6.50	1.60	1.52
2	A	601	EQJ	C15-C23	5.92	1.59	1.52
2	A	601	EQJ	C13-N14	5.87	1.38	1.27
2	D	601	EQJ	C26-C02	5.66	1.46	1.41
2	B	601	EQJ	C15-N14	4.85	1.52	1.46
2	A	601	EQJ	C12-C05	4.84	1.48	1.42
2	D	601	EQJ	C12-C26	4.31	1.48	1.41
2	B	601	EQJ	C13-N14	4.28	1.35	1.27
2	A	601	EQJ	C26-C02	4.20	1.45	1.41
2	D	601	EQJ	C12-C05	4.13	1.47	1.42
2	A	601	EQJ	C16-C15	4.08	1.58	1.53
2	C	601	EQJ	C12-C13	-4.05	1.38	1.46
2	B	601	EQJ	C12-C05	3.81	1.47	1.42
2	B	601	EQJ	C12-C13	-3.79	1.38	1.46
2	B	601	EQJ	C26-C02	3.33	1.44	1.41
2	C	601	EQJ	C12-C05	2.94	1.46	1.42
2	D	601	EQJ	C13-N14	2.89	1.32	1.27
2	D	601	EQJ	C15-N14	2.85	1.50	1.46
2	A	601	EQJ	O24-C23	2.77	1.30	1.22
2	B	601	EQJ	O24-C23	2.75	1.30	1.22
2	B	601	EQJ	C12-C26	2.74	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	EQJ	C20-N19	2.74	1.38	1.33
2	C	601	EQJ	C02-N03	2.59	1.38	1.33
2	C	601	EQJ	C15-N14	2.56	1.49	1.46
2	A	601	EQJ	C15-N14	2.49	1.49	1.46
2	B	601	EQJ	C04-C05	2.39	1.42	1.37
2	A	601	EQJ	C12-C26	2.20	1.44	1.41
2	D	601	EQJ	C16-C15	-2.17	1.50	1.53
2	D	601	EQJ	O24-C23	2.17	1.28	1.22
2	B	601	EQJ	C20-N19	-2.16	1.29	1.33
2	D	601	EQJ	C04-C05	2.09	1.41	1.37
2	C	601	EQJ	C12-C26	2.01	1.44	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	EQJ	C15-N14-C13	20.85	147.75	116.77
2	D	601	EQJ	C05-C12-C13	9.27	135.78	121.47
2	B	601	EQJ	C15-N14-C13	9.26	130.53	116.77
2	D	601	EQJ	C26-C12-C05	-8.84	111.17	118.28
2	A	601	EQJ	C05-C12-C13	8.64	134.80	121.47
2	B	601	EQJ	C05-C12-C13	8.45	134.50	121.47
2	D	601	EQJ	C12-C13-N14	-7.83	107.36	122.73
2	C	601	EQJ	C12-C26-C02	-7.65	115.84	120.14
2	C	601	EQJ	C15-N14-C13	7.26	127.55	116.77
2	B	601	EQJ	C23-C15-N14	7.19	125.94	108.22
2	B	601	EQJ	C26-C12-C13	-7.17	107.45	120.40
2	B	601	EQJ	C01-C02-C26	-6.86	112.76	120.80
2	A	601	EQJ	C26-C12-C13	-6.55	108.58	120.40
2	D	601	EQJ	C12-C26-C02	6.41	123.75	120.14
2	A	601	EQJ	C15-N14-C13	6.28	126.09	116.77
2	D	601	EQJ	C23-C15-N14	6.04	123.12	108.22
2	C	601	EQJ	C12-C13-N14	-5.67	111.59	122.73
2	A	601	EQJ	C26-C12-C05	-5.21	114.09	118.28
2	D	601	EQJ	C26-C12-C13	-5.16	111.09	120.40
2	B	601	EQJ	C12-C26-C02	-5.06	117.30	120.14
2	A	601	EQJ	C01-C02-C26	-4.81	115.17	120.80
2	D	601	EQJ	C01-C02-C26	-4.60	115.41	120.80
2	D	601	EQJ	O25-C23-O24	-4.33	114.26	124.08
2	B	601	EQJ	C12-C13-N14	-4.31	114.27	122.73
2	A	601	EQJ	O25-C23-O24	-4.14	114.68	124.08
2	C	601	EQJ	O27-C26-C02	3.95	125.77	117.58
2	A	601	EQJ	C06-C05-C04	-3.89	113.03	119.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	EQJ	C01-C02-N03	3.83	124.85	117.64
2	A	601	EQJ	C01-C02-N03	3.50	124.23	117.64
2	B	601	EQJ	C01-C02-N03	3.41	124.07	117.64
2	A	601	EQJ	O27-C26-C02	3.36	124.56	117.58
2	A	601	EQJ	C23-C15-N14	3.13	115.93	108.22
2	D	601	EQJ	N22-C20-N19	-2.99	112.46	119.27
2	B	601	EQJ	O25-C23-O24	-2.93	117.44	124.08
2	D	601	EQJ	C16-C17-C18	-2.89	103.74	112.07
2	C	601	EQJ	C26-C12-C13	-2.79	115.36	120.40
2	C	601	EQJ	C04-N03-C02	2.67	124.05	119.20
2	B	601	EQJ	C06-C05-C04	-2.56	115.18	119.36
2	B	601	EQJ	N19-C20-N21	-2.50	116.38	120.67
2	B	601	EQJ	N22-C20-N19	-2.42	113.76	119.27
2	B	601	EQJ	N22-C20-N21	2.38	126.83	120.07
2	D	601	EQJ	C17-C18-N19	-2.33	105.66	112.20
2	D	601	EQJ	O07-P08-O10	2.32	112.72	106.44
2	C	601	EQJ	C05-C04-N03	-2.16	120.32	123.83
2	C	601	EQJ	O11-P08-O09	2.13	115.79	107.80
2	D	601	EQJ	C06-C05-C04	-2.10	115.94	119.36
2	C	601	EQJ	N22-C20-N19	2.02	123.86	119.27

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	EQJ	C16-C15-N14-C13
2	C	601	EQJ	N14-C15-C16-C17
2	C	601	EQJ	C16-C15-N14-C13
2	B	601	EQJ	C16-C15-N14-C13
2	B	601	EQJ	C17-C18-N19-C20
2	B	601	EQJ	N21-C20-N19-C18
2	B	601	EQJ	N22-C20-N19-C18
2	D	601	EQJ	C16-C15-N14-C13
3	A	602	GOL	O2-C2-C3-O3
3	A	603	GOL	O1-C1-C2-O2
3	A	603	GOL	C1-C2-C3-O3
3	B	602	GOL	C1-C2-C3-O3
2	C	601	EQJ	C17-C18-N19-C20
2	B	601	EQJ	C16-C17-C18-N19
2	A	601	EQJ	C16-C17-C18-N19
3	A	602	GOL	C1-C2-C3-O3
3	A	603	GOL	O1-C1-C2-C3

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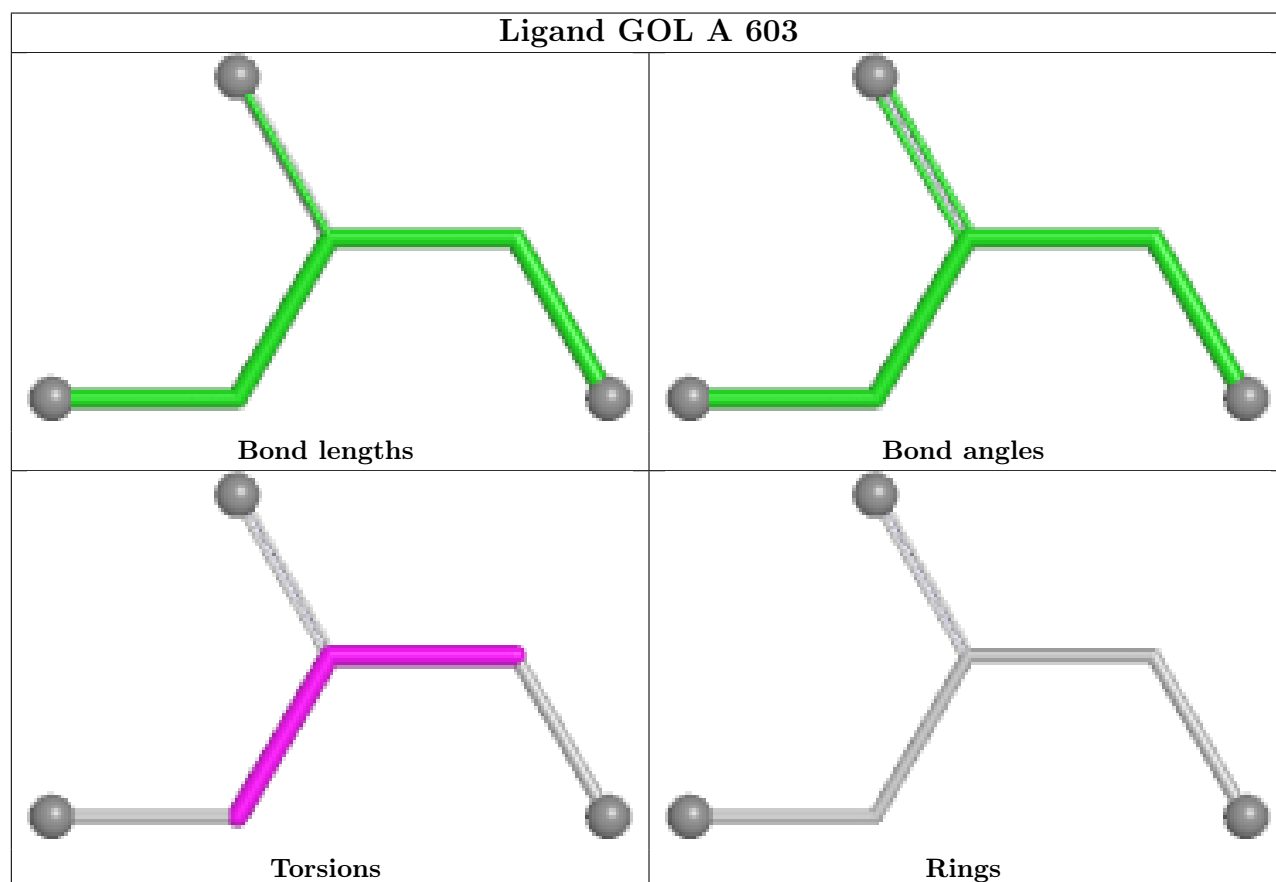
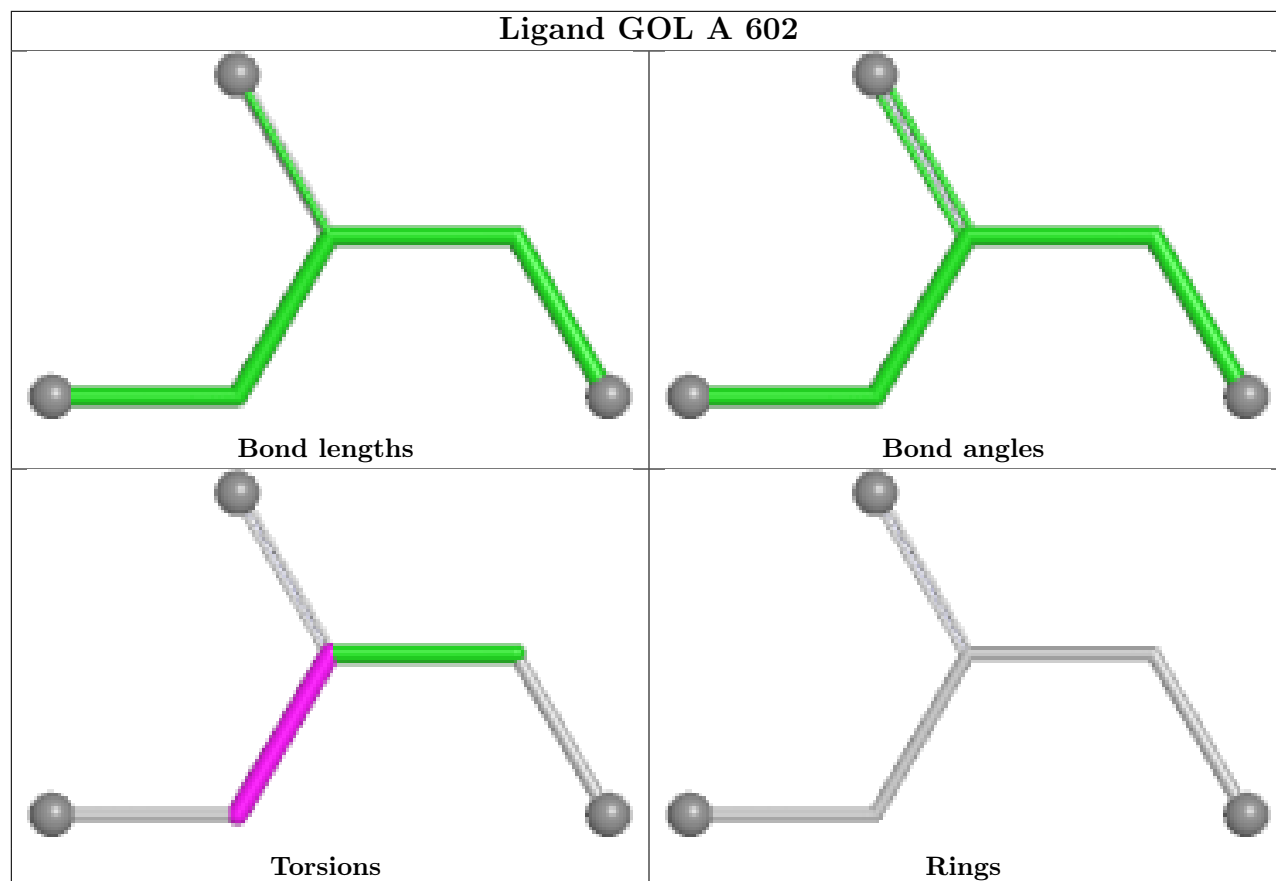
Mol	Chain	Res	Type	Atoms
3	A	605	GOL	C1-C2-C3-O3
3	A	603	GOL	O2-C2-C3-O3
2	D	601	EQJ	N14-C15-C23-O25
3	B	602	GOL	O2-C2-C3-O3
2	D	601	EQJ	C15-C16-C17-C18
2	A	601	EQJ	C17-C18-N19-C20
2	D	601	EQJ	N14-C15-C23-O24
2	C	601	EQJ	N14-C15-C23-O25
2	A	601	EQJ	C15-C16-C17-C18
3	A	605	GOL	O2-C2-C3-O3
2	C	601	EQJ	C16-C15-C23-O25
2	B	601	EQJ	C12-C05-C06-O07
2	C	601	EQJ	C16-C15-C23-O24

There are no ring outliers.

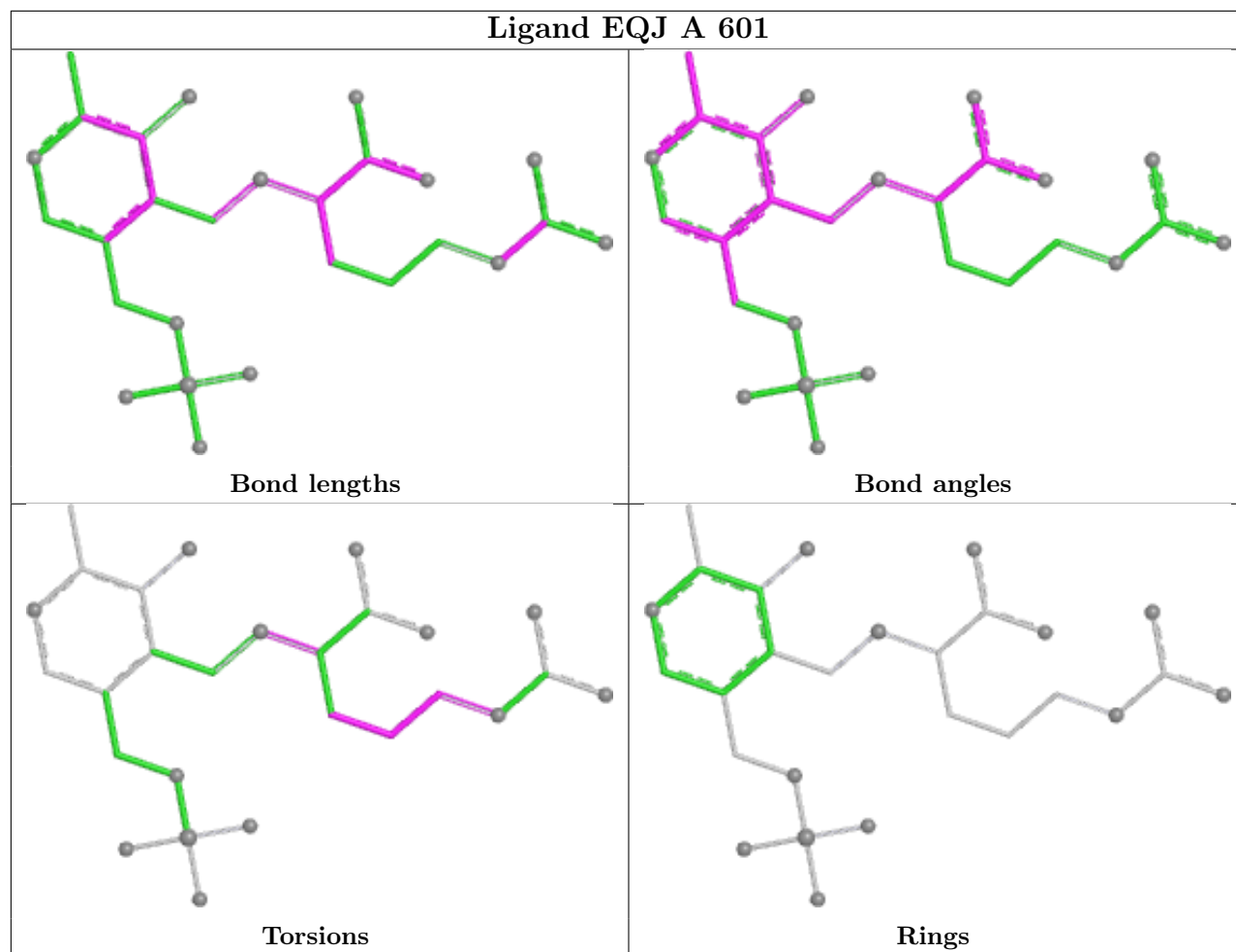
6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	GOL	1	0
2	A	601	EQJ	3	0
2	D	601	EQJ	4	0
3	A	605	GOL	2	0
2	C	601	EQJ	1	0
2	B	601	EQJ	4	0

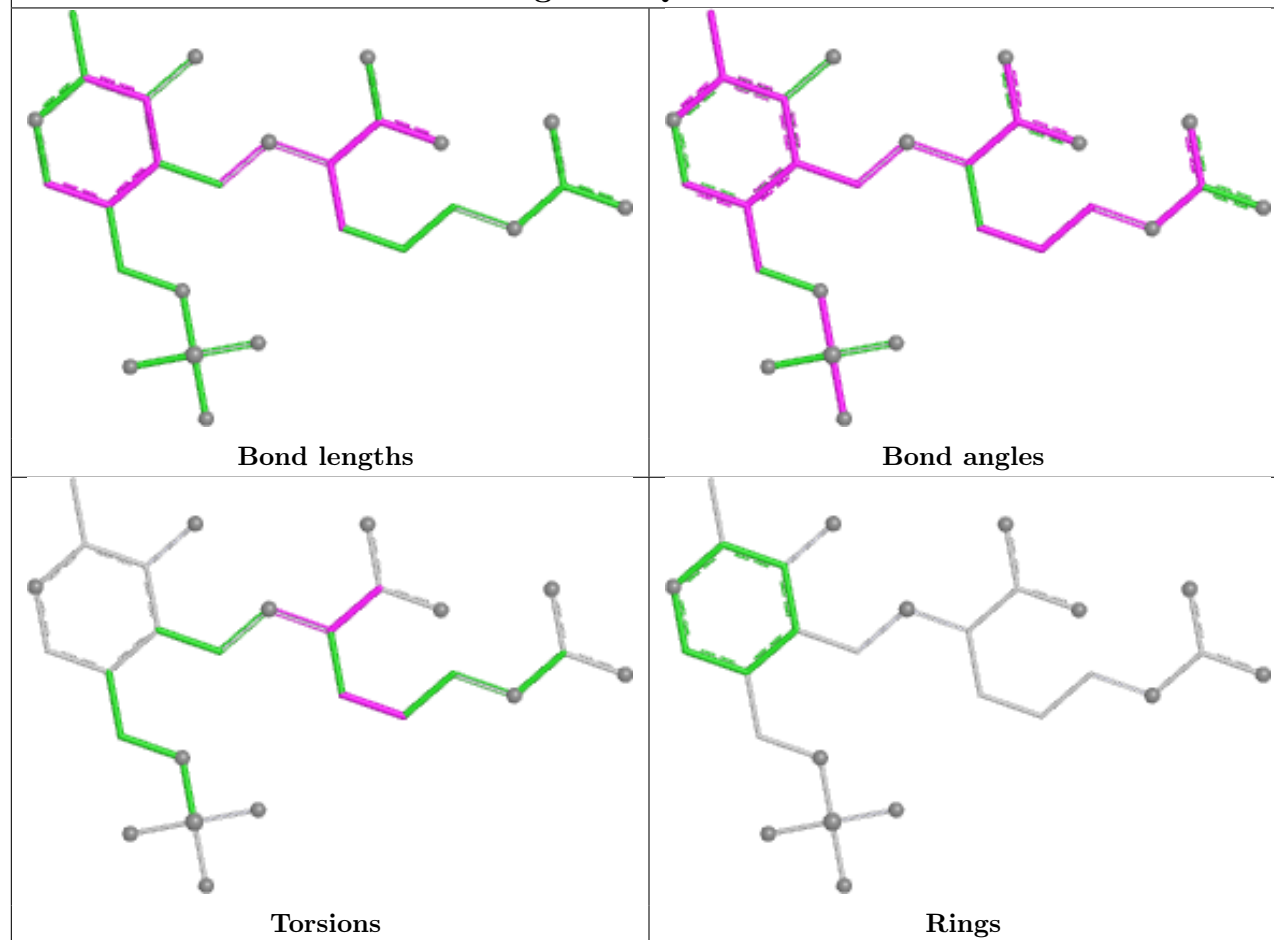
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

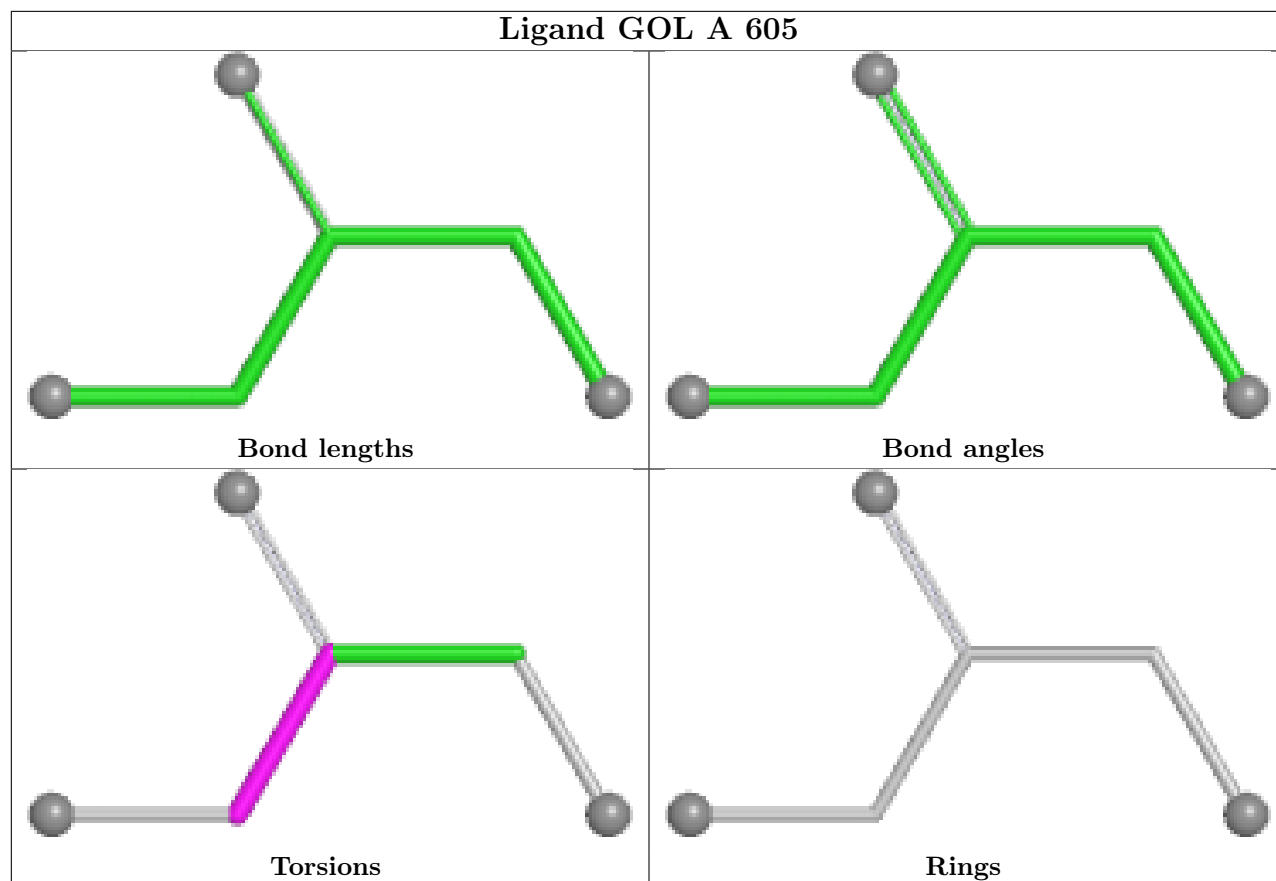


Ligand EQJ A 601

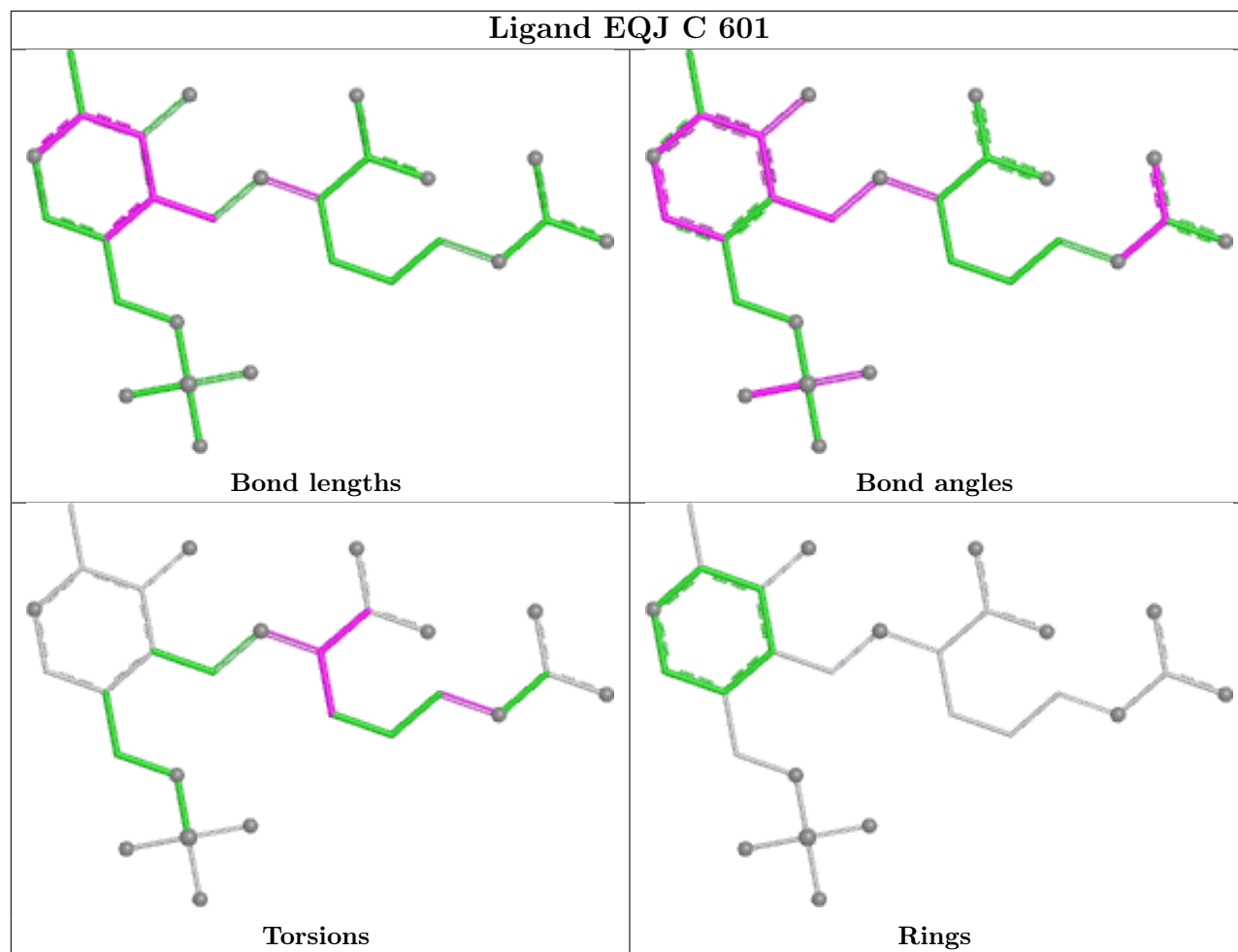


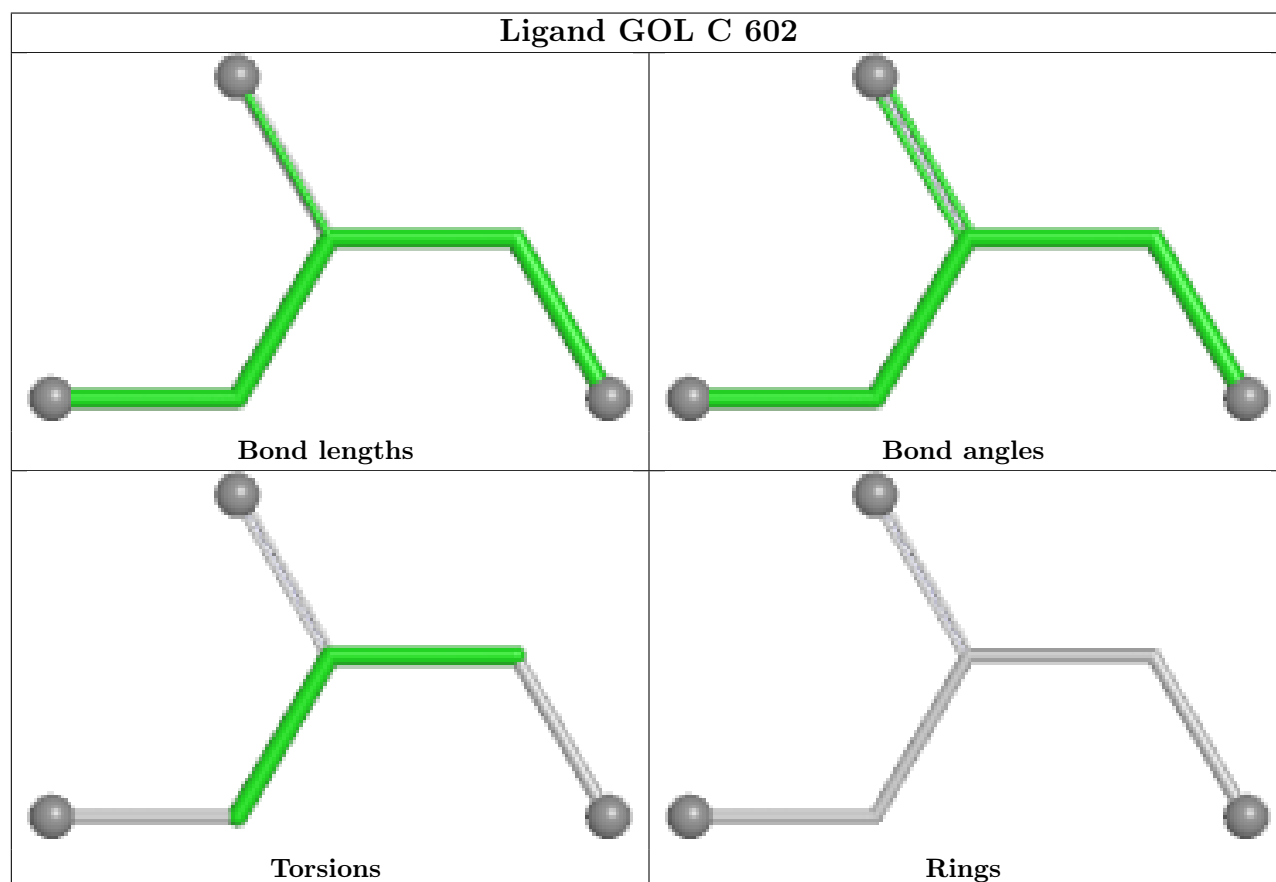
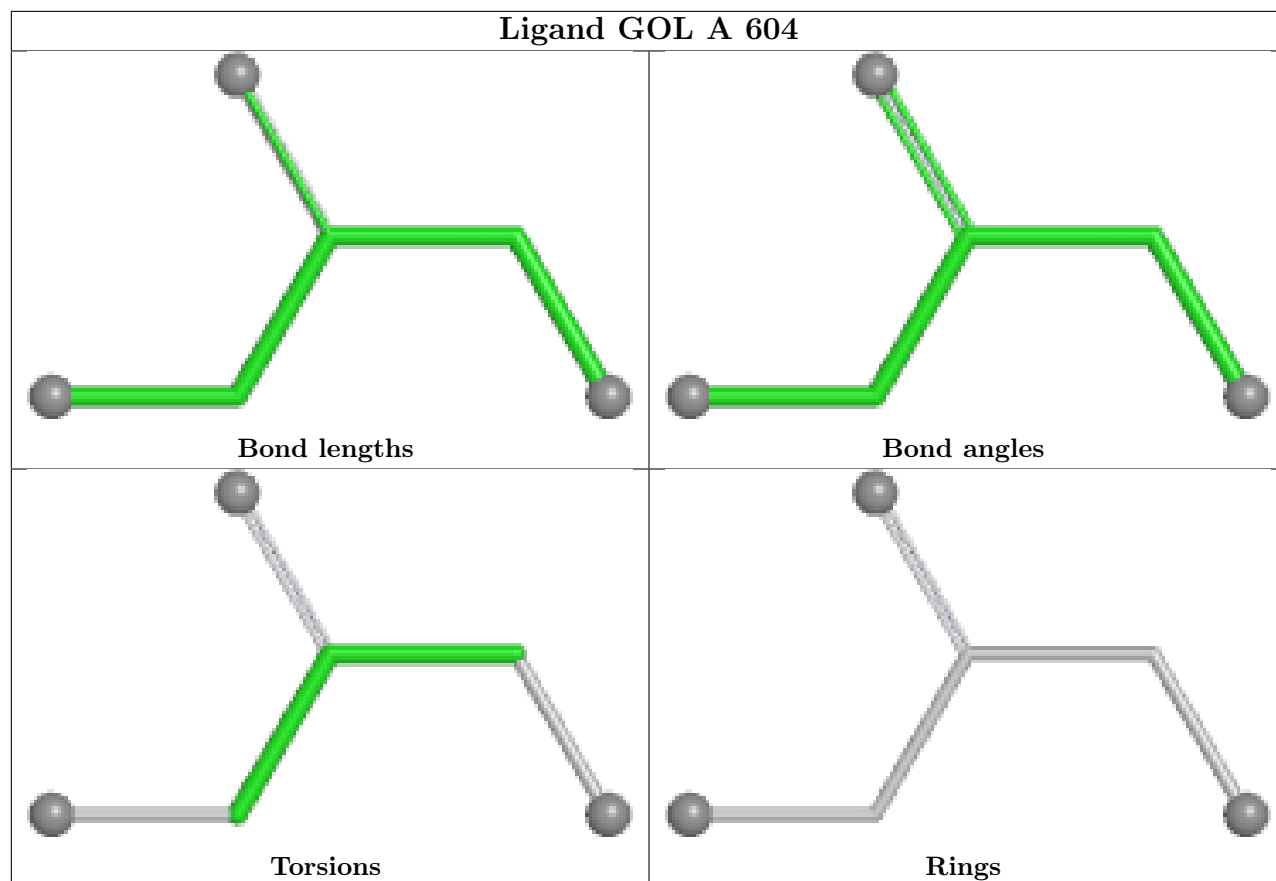
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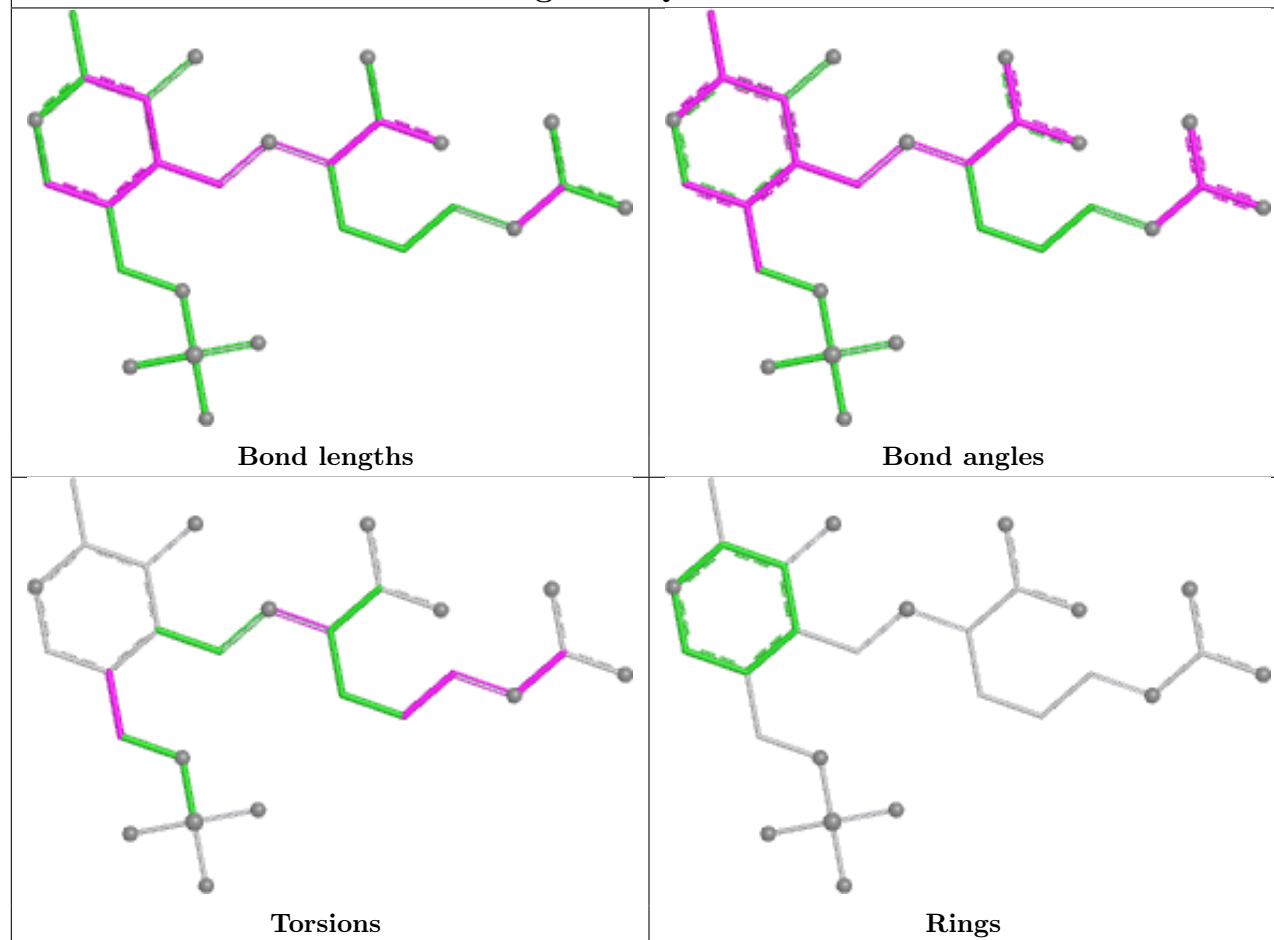


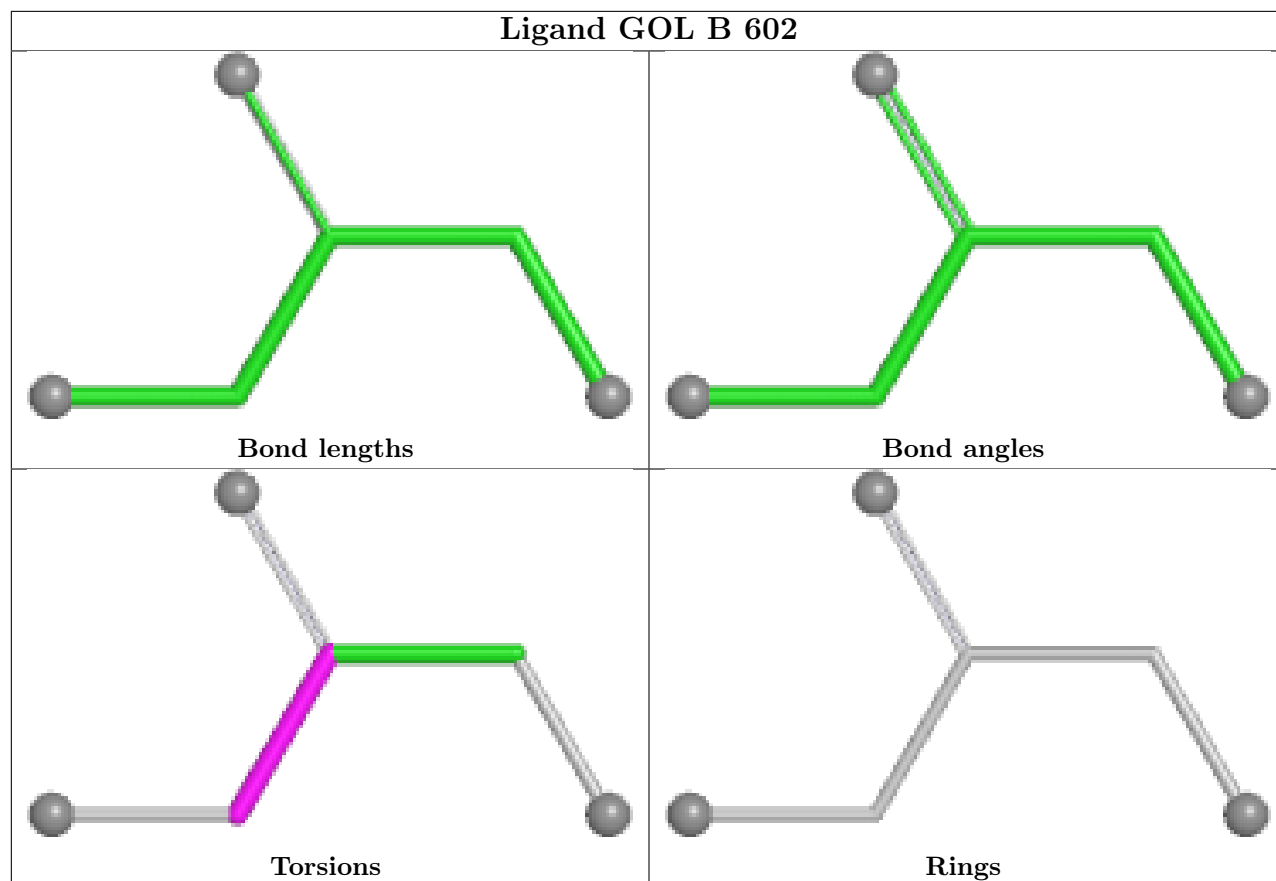
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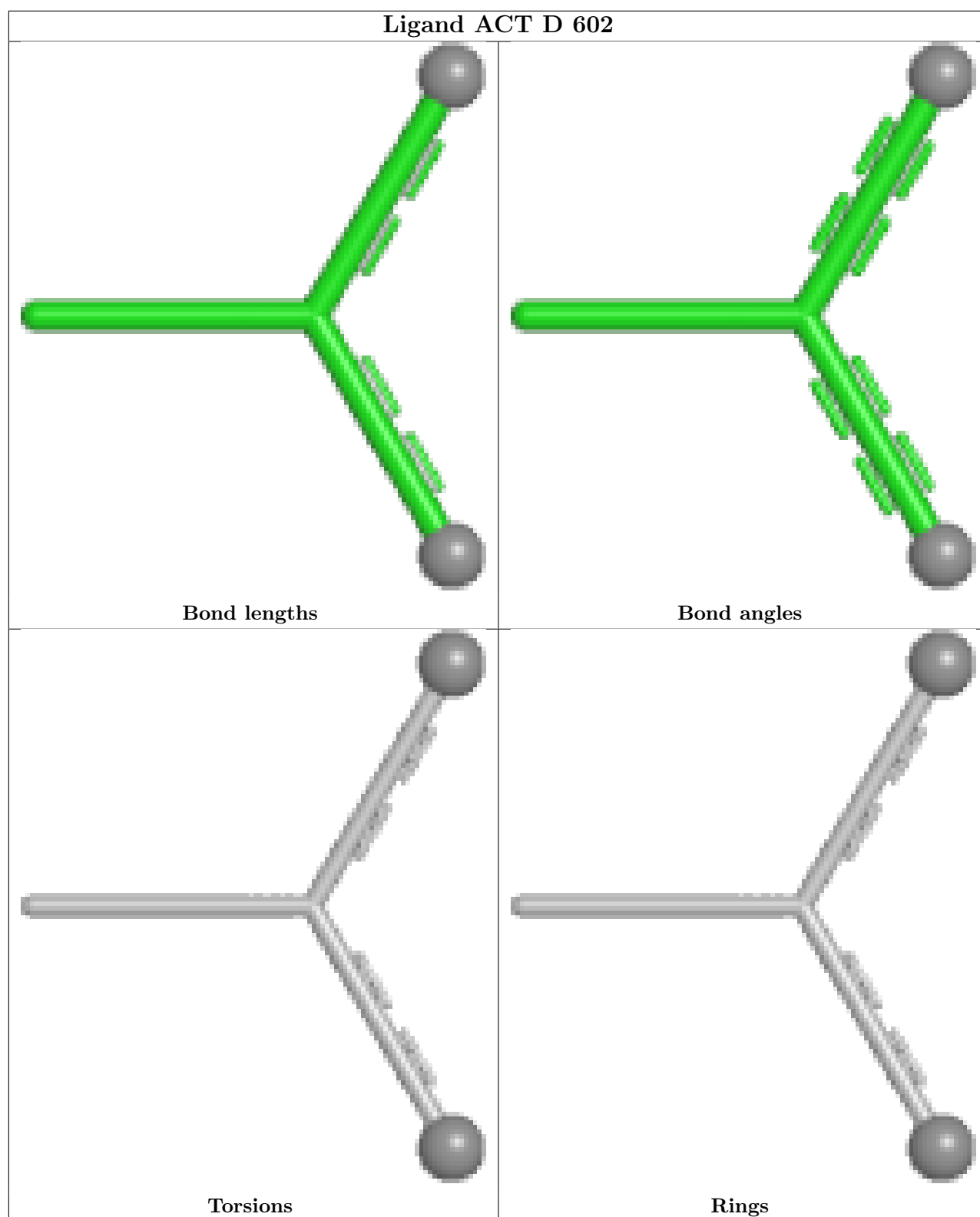




Ligand EQJ B 601







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	512/523 (97%)	-0.18	8 (1%) 70 76	10, 23, 55, 83	0
1	B	512/523 (97%)	-0.12	15 (2%) 53 60	10, 22, 56, 85	0
1	C	510/523 (97%)	0.17	23 (4%) 38 44	16, 30, 65, 92	0
1	D	512/523 (97%)	0.06	11 (2%) 63 68	15, 29, 61, 85	0
All	All	2046/2092 (97%)	-0.02	57 (2%) 55 61	10, 26, 59, 92	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	179	VAL	4.6
1	C	170	PRO	3.6
1	D	522	LEU	3.5
1	C	244	LEU	3.4
1	B	161	THR	3.4
1	C	157	LEU	3.4
1	D	6	GLY	3.3
1	C	172	VAL	3.3
1	A	161	THR	3.3
1	C	163	THR	3.2
1	A	160	GLY	3.2
1	A	159	THR	3.2
1	B	265	THR	3.2
1	B	179	VAL	3.1
1	B	522	LEU	3.0
1	B	6	GLY	2.9
1	D	161	THR	2.9
1	C	263	LYS	2.8
1	C	153	ALA	2.8
1	D	159	THR	2.8
1	B	263	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	164	LEU	2.7
1	B	162	ALA	2.7
1	A	179	VAL	2.7
1	C	268	VAL	2.7
1	B	243	GLU	2.7
1	A	522	LEU	2.7
1	C	159	THR	2.7
1	D	179	VAL	2.6
1	C	6	GLY	2.6
1	C	158	THR	2.6
1	D	167	ALA	2.5
1	B	178	ASP	2.5
1	B	264	ASP	2.5
1	C	265	THR	2.5
1	C	522	LEU	2.4
1	C	154	ARG	2.4
1	B	160	GLY	2.4
1	B	480	PRO	2.4
1	C	171	LEU	2.4
1	A	480	PRO	2.4
1	B	242	PRO	2.4
1	A	156	ALA	2.4
1	C	166	THR	2.3
1	D	163	THR	2.3
1	B	172	VAL	2.3
1	C	264	ASP	2.3
1	B	163	THR	2.3
1	D	241	GLU	2.2
1	C	480	PRO	2.2
1	D	169	LEU	2.2
1	A	171	LEU	2.2
1	C	152	THR	2.1
1	C	167	ALA	2.1
1	D	480	PRO	2.1
1	D	178	ASP	2.0
1	C	43	GLY	2.0

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

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](#)

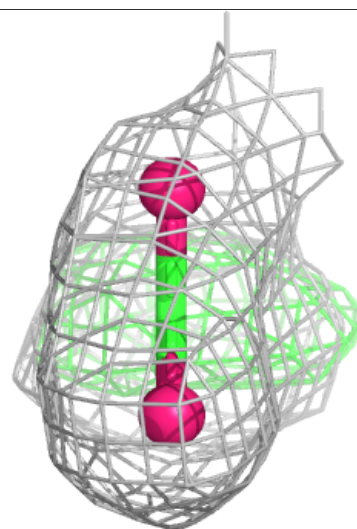
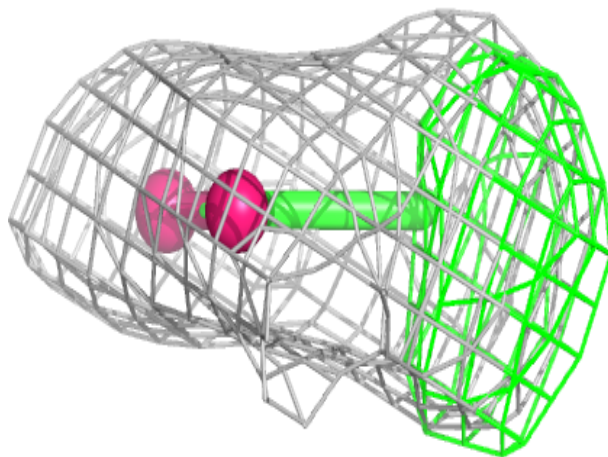
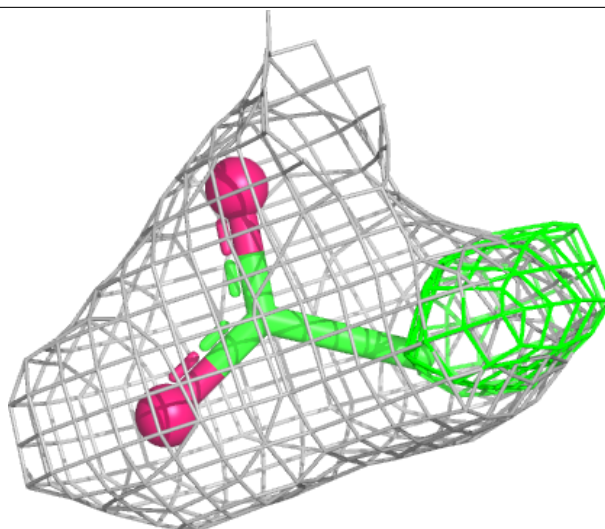
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	ACT	D	602	4/4	0.69	0.14	31,33,34,38	0
3	GOL	A	604	6/6	0.84	0.14	41,44,46,47	0
3	GOL	A	603	6/6	0.87	0.13	29,40,45,45	0
3	GOL	A	605	6/6	0.88	0.13	42,48,50,51	0
3	GOL	A	602	6/6	0.89	0.12	33,40,40,44	0
3	GOL	C	602	6/6	0.90	0.12	41,49,51,55	0
3	GOL	B	602	6/6	0.91	0.12	37,46,49,50	0
2	EQJ	D	601	27/27	0.95	0.10	19,26,61,71	0
2	EQJ	A	601	27/27	0.95	0.11	13,21,68,80	0
2	EQJ	B	601	27/27	0.96	0.08	15,17,40,44	0
2	EQJ	C	601	27/27	0.97	0.10	19,23,91,105	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.

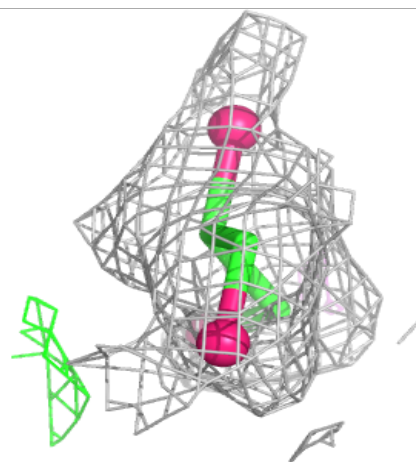
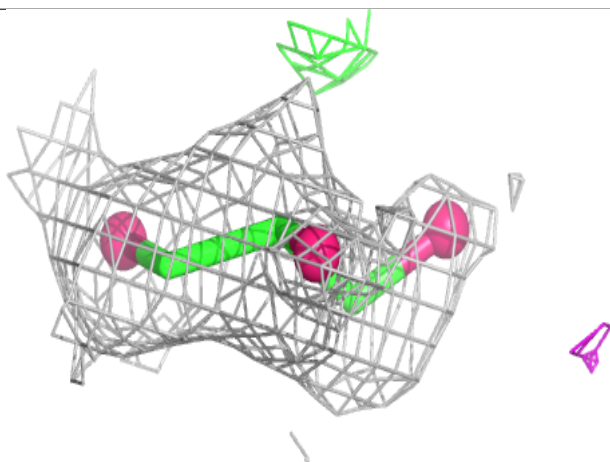
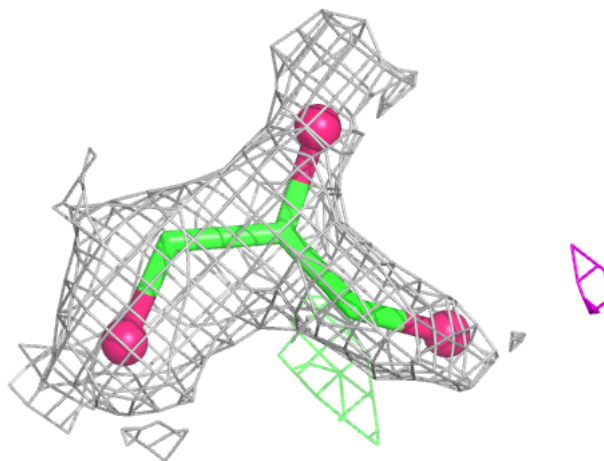
Electron density around ACT D 602:

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



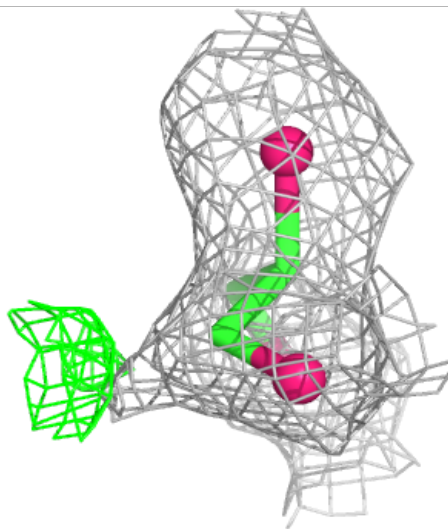
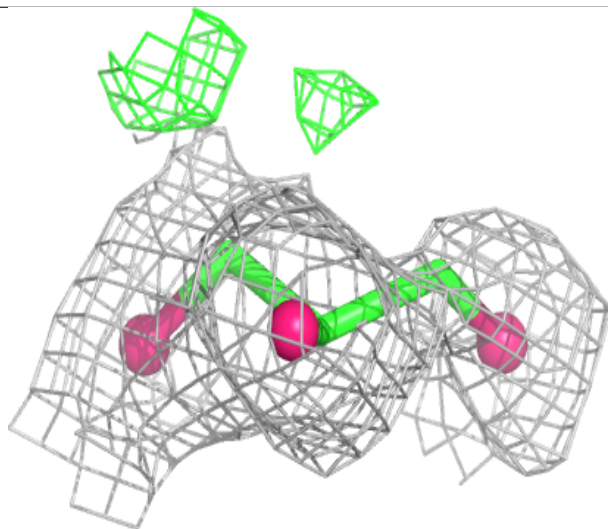
Electron density around GOL A 604:

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



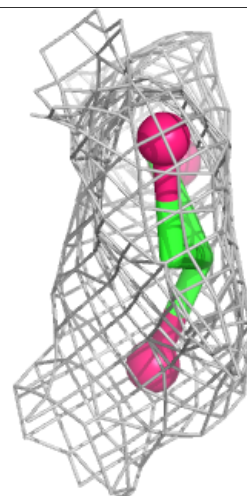
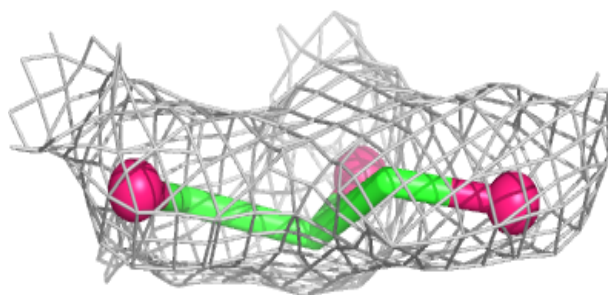
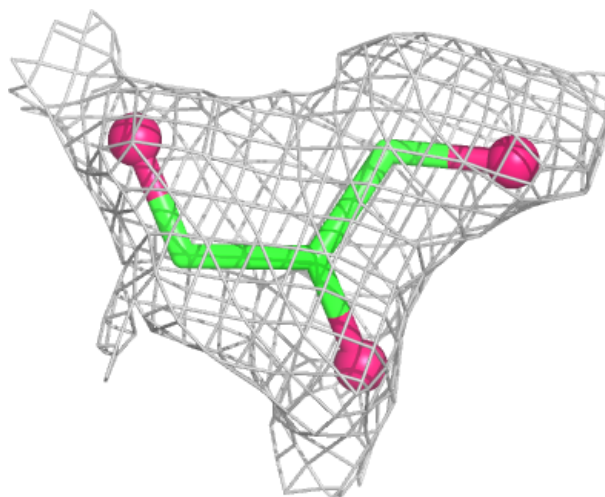
Electron density around GOL A 603:

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



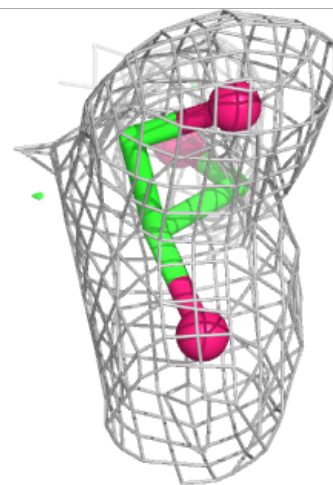
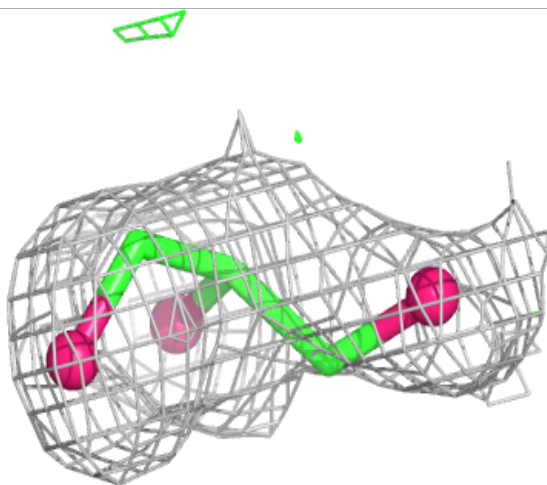
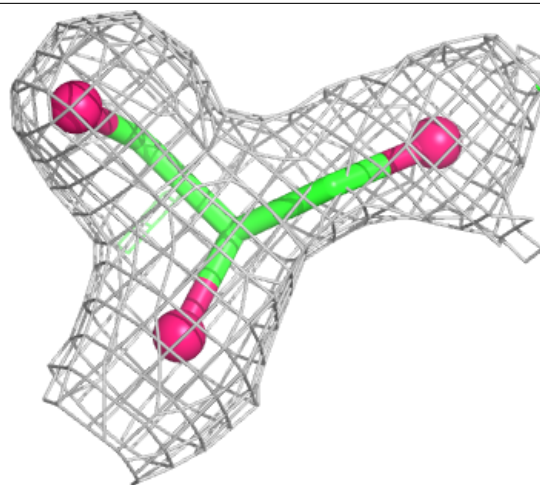
Electron density around GOL A 605:

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and green (positive)



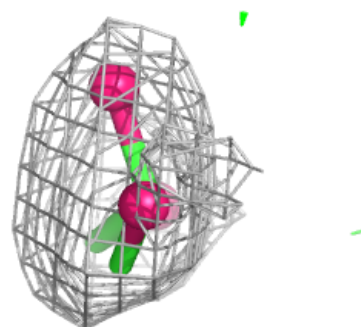
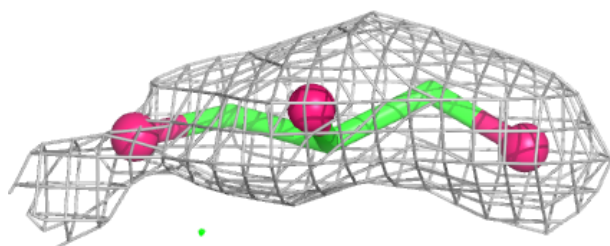
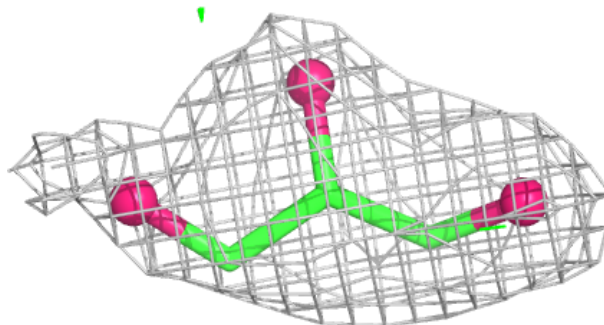
Electron density around GOL A 602:

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

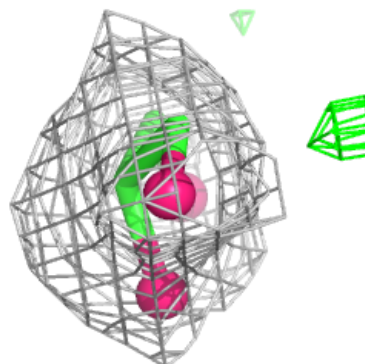
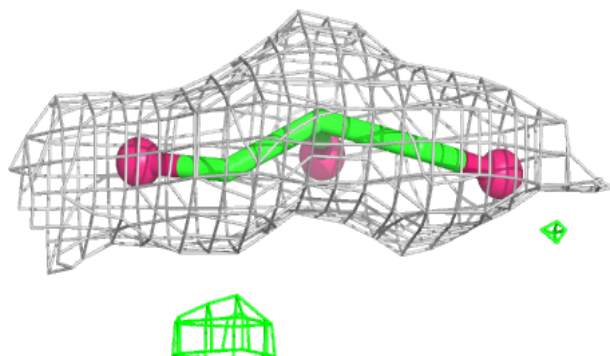
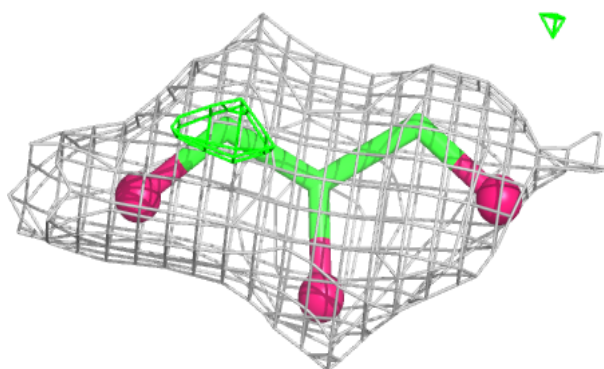


Electron density around GOL C 602:

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

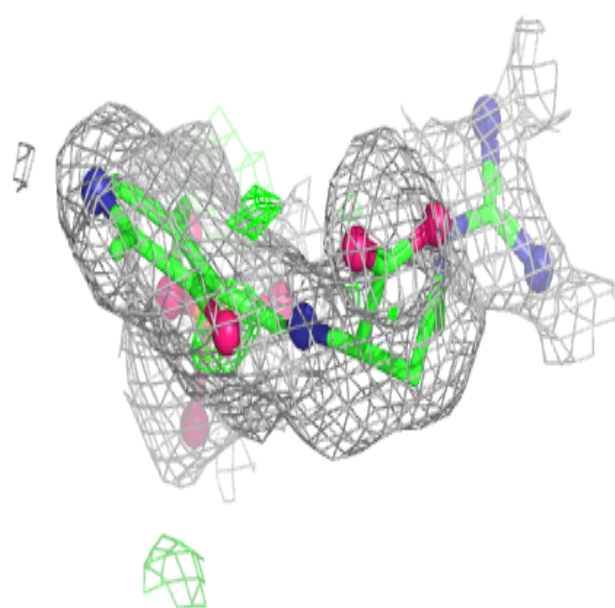
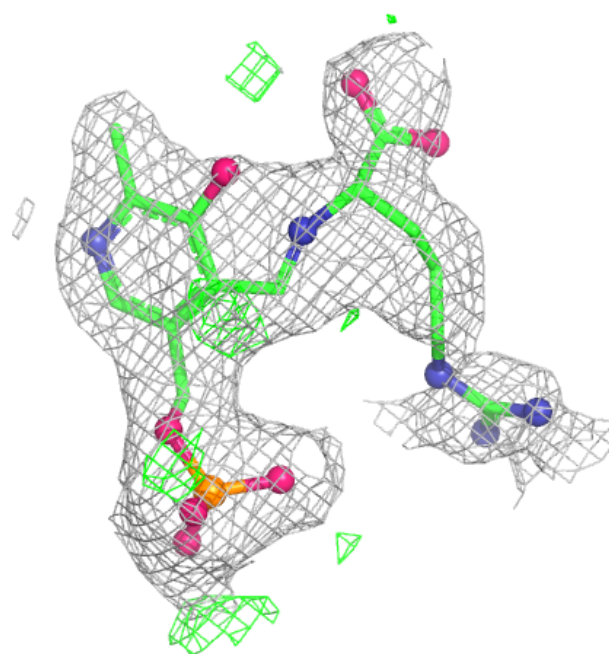
**Electron density around GOL B 602:**

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



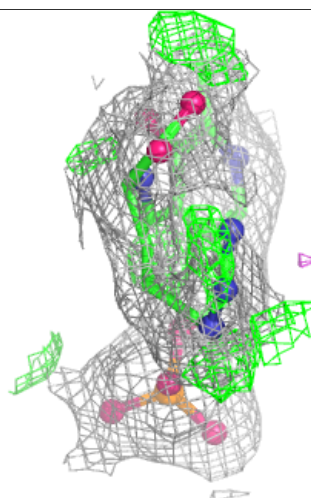
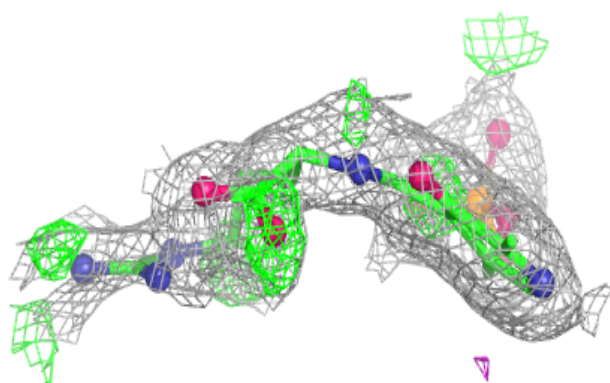
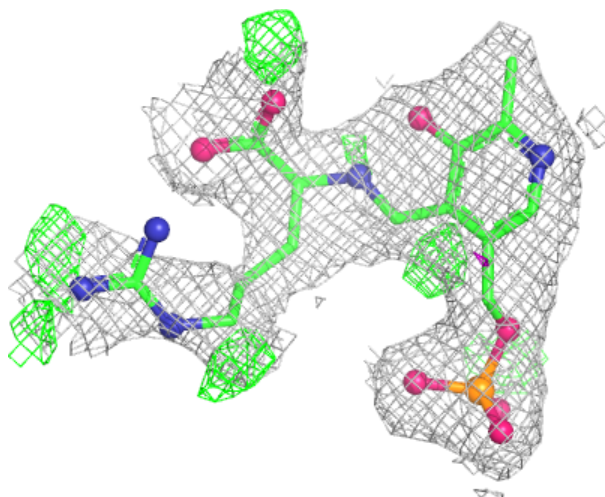
Electron density around EQJ D 601:

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



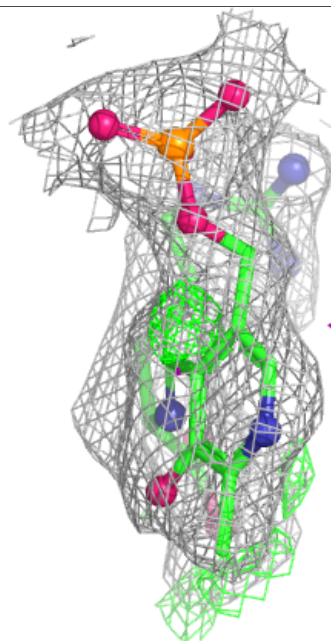
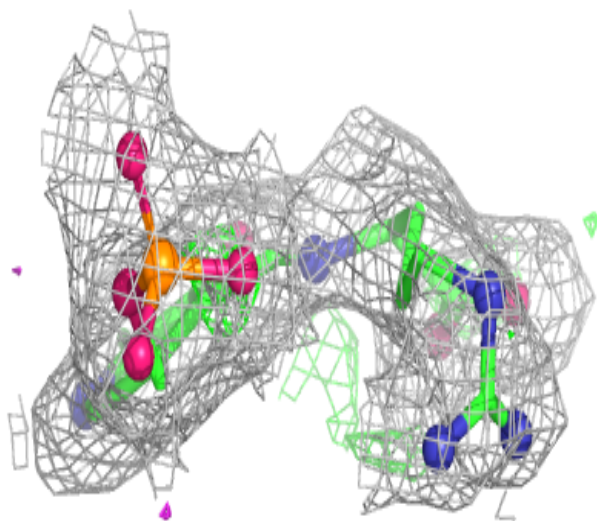
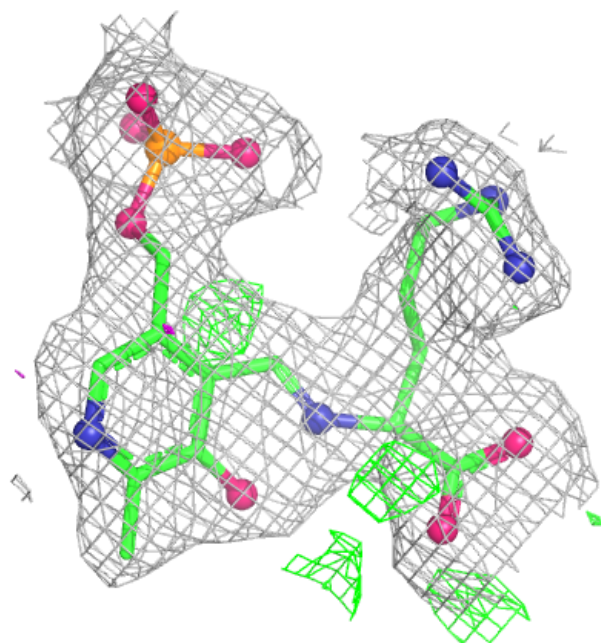
Electron density around EQJ A 601:

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



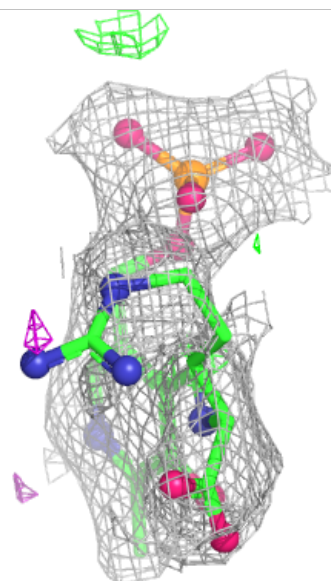
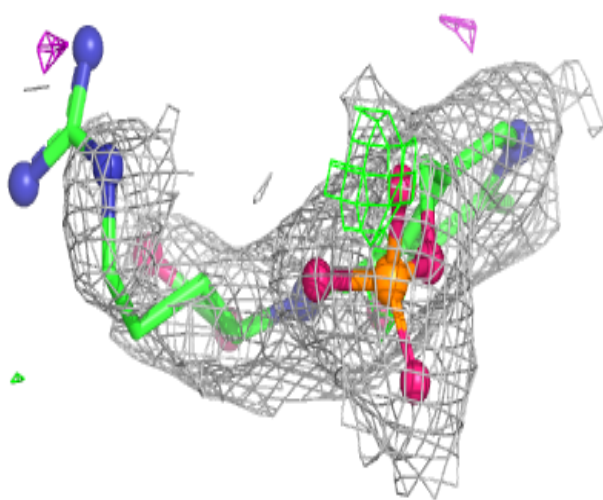
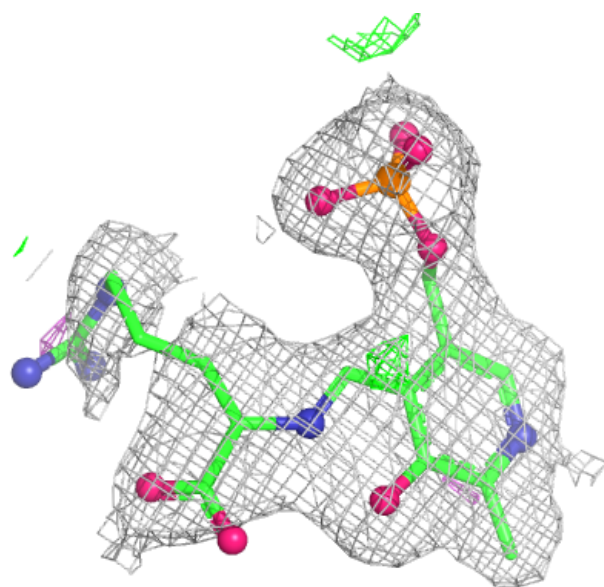
Electron density around EQJ B 601:

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



Electron density around EQJ C 601:

$2mF_o - DF_c$ (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.