



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:23 AM BST

PDB ID : 6VCH
Title : Crystal structure of Nitrosotalea devanatterra carotenoid cleavage dioxygenase
in complex with 3-hydroxy-beta-apo-14'-carotenal
Authors : Daruwalla, A.; Shi, W.; Kiser, P.D.
Deposited on : 2019-12-20
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

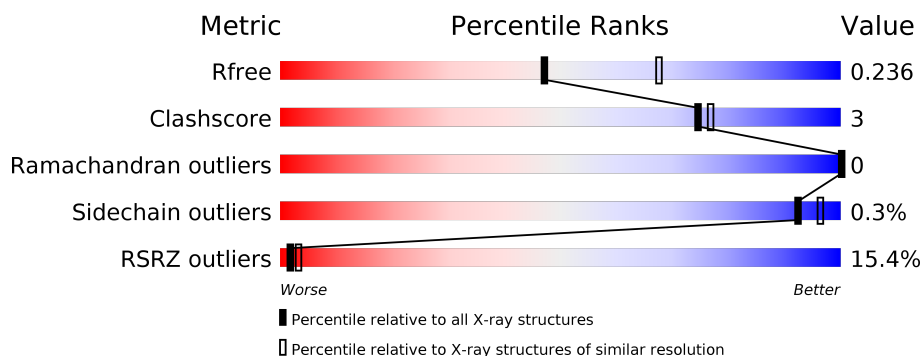
1 Overall quality at a glance

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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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 on 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	472	<div> <div>6%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	B	472	<div> <div>3%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	C	472	<div> <div>7%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	D	472	<div> <div>7%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	E	472	<div> <div>29%</div> <div>85%</div> <div>6%</div> <div>9%</div> </div>
1	F	472	<div> <div>35%</div> <div>84%</div> <div>7%</div> <div>9%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21835 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.

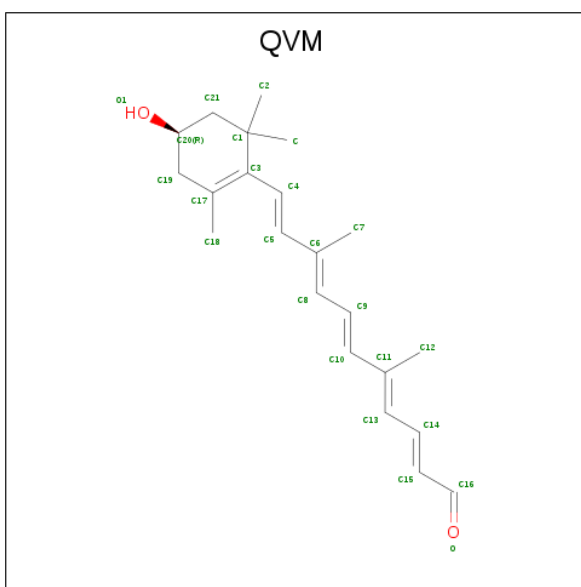
- Molecule 1 is a protein called carotenoid cleavage dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	1	0
			3619	2333	590	689	7			
1	B	453	Total	C	N	O	S	0	2	0
			3649	2353	596	693	7			
1	C	453	Total	C	N	O	S	0	1	0
			3612	2330	590	685	7			
1	D	452	Total	C	N	O	S	0	0	0
			3596	2321	587	681	7			
1	E	431	Total	C	N	O	S	0	0	0
			3431	2212	561	651	7			
1	F	430	Total	C	N	O	S	0	0	0
			3379	2185	554	633	7			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co) (labeled as "Ligand of Interest" by author).

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

- Molecule 3 is (2E,4E,6E,8E,10E)-11-[(4R)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-5,9-dimethylundeca-2,4,6,8,10-pentaenal (three-letter code: QVM) (formula: C₂₂H₃₀O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			24	22	2		
3	B	1	Total	C	O	0	0
			24	22	2		
3	C	1	Total	C	O	0	0
			24	22	2		
3	D	1	Total	C	O	0	0
			24	22	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		

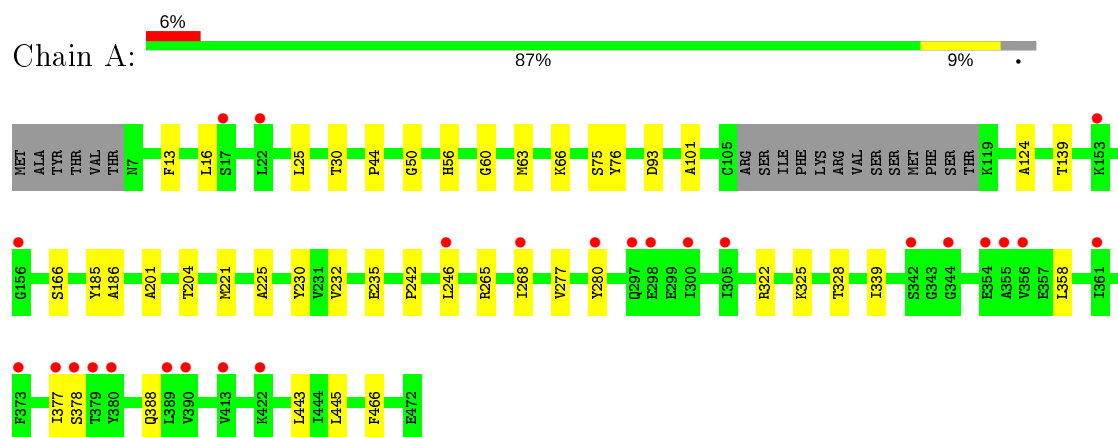
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	111	Total 111	O 111	0	0
6	B	120	Total 120	O 120	0	0
6	C	98	Total 98	O 98	0	0
6	D	80	Total 80	O 80	0	0
6	E	21	Total 21	O 21	0	0
6	F	13	Total 13	O 13	0	0

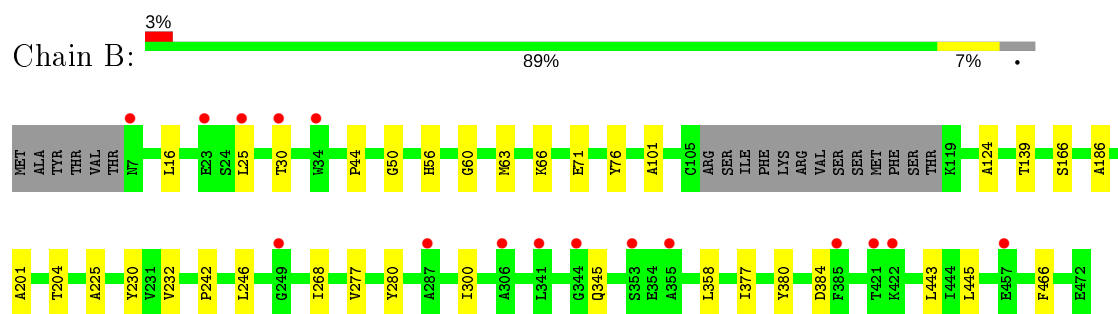
3 Residue-property plots [i](#)

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.

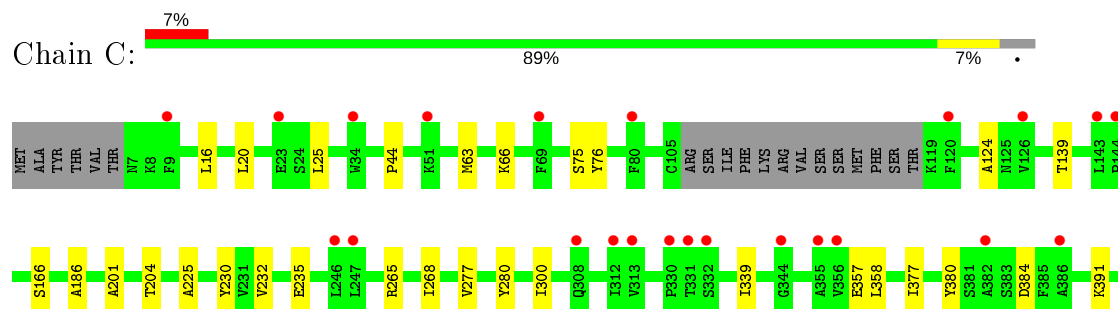
- Molecule 1: carotenoid cleavage dioxygenase

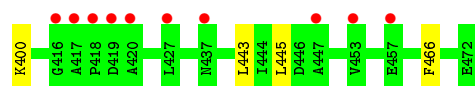


- Molecule 1: carotenoid cleavage dioxygenase

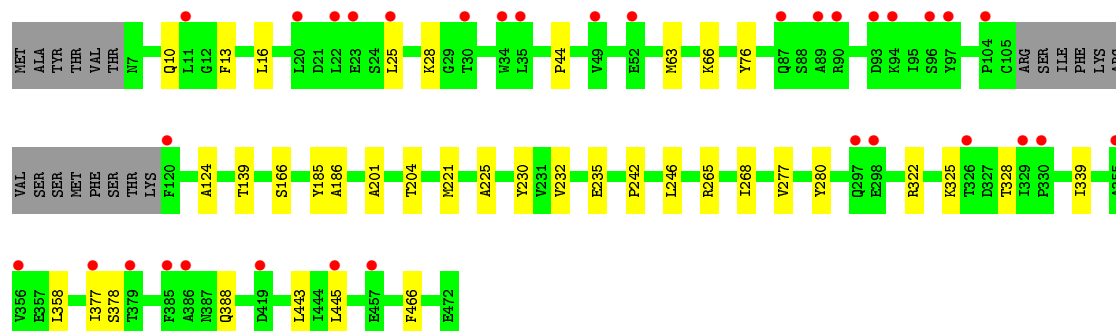
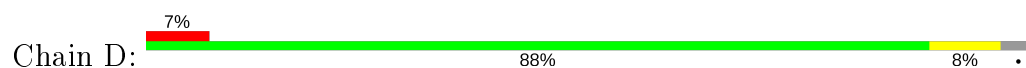


- Molecule 1: carotenoid cleavage dioxygenase

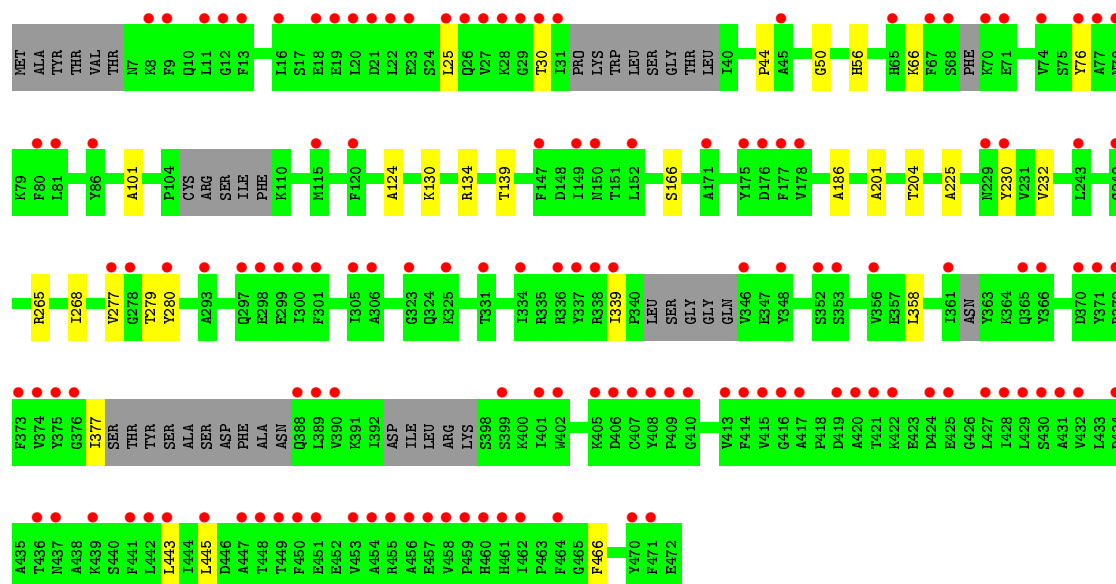
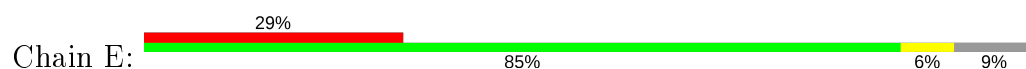




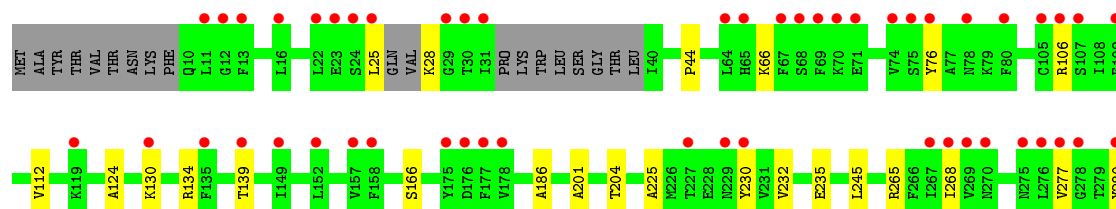
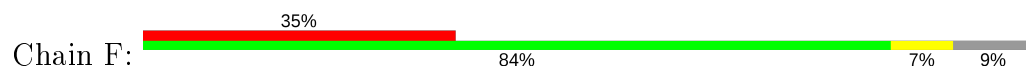
- Molecule 1: carotenoid cleavage dioxygenase

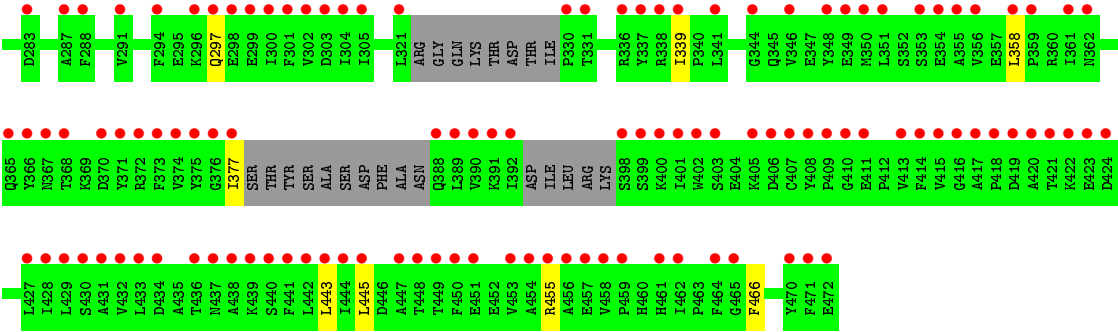


- Molecule 1: carotenoid cleavage dioxygenase



- Molecule 1: carotenoid cleavage dioxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	107.25Å 107.25Å 490.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.13 – 2.35 49.13 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.13-2.35) 99.9 (49.13-2.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.213 , 0.234 0.218 , 0.236	Depositor DCC
R_{free} test set	6518 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21835	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QVM, CL, CO, NA

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	0.64	0/3712	0.75	0/5041
1	B	0.63	0/3742	0.75	0/5074
1	C	0.63	0/3705	0.74	0/5030
1	D	0.64	0/3689	0.75	0/5011
1	E	0.65	0/3513	0.75	0/4761
1	F	0.64	0/3463	0.74	0/4699
All	All	0.64	0/21824	0.75	0/29616

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	3619	0	3468	32	0
1	B	3649	0	3531	24	0
1	C	3612	0	3465	20	0
1	D	3596	0	3449	23	0
1	E	3431	0	3267	28	0
1	F	3379	0	3205	20	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	24	0	0	0	0
3	B	24	0	0	1	0
3	C	24	0	0	0	0
3	D	24	0	0	0	0
4	A	1	0	0	0	0
4	E	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	111	0	0	0	0
6	B	120	0	0	1	0
6	C	98	0	0	1	0
6	D	80	0	0	0	0
6	E	21	0	0	0	0
6	F	13	0	0	1	0
All	All	21835	0	20385	135	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 (135) 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:358:LEU:HD12	1:C:377:ILE:HD12	1.46	0.98
1:B:358:LEU:HD12	1:B:377:ILE:HD12	1.46	0.97
1:F:358:LEU:HD12	1:F:377:ILE:HD12	1.48	0.93
1:E:358:LEU:HD12	1:E:377:ILE:HD12	1.50	0.91
1:D:358:LEU:HD12	1:D:377:ILE:HD12	1.52	0.88
1:A:358:LEU:HD12	1:A:377:ILE:HD12	1.53	0.88
1:C:166:SER:HB2	1:C:186:ALA:HB1	1.59	0.82
1:A:166:SER:HB2	1:A:186:ALA:HB1	1.62	0.82
1:D:166:SER:HB2	1:D:186:ALA:HB1	1.62	0.81
1:B:166:SER:HB2	1:B:186:ALA:HB1	1.63	0.81
1:B:30:THR:HG23	1:E:50:GLY:HA2	1.64	0.80
1:A:93:ASP:HB3	1:E:30:THR:HG21	1.61	0.80
1:E:166:SER:HB2	1:E:186:ALA:HB1	1.66	0.77
1:F:166:SER:HB2	1:F:186:ALA:HB1	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:THR:CG2	1:E:50:GLY:HA2	2.20	0.70
1:D:325:LYS:O	1:D:328:THR:HG22	1.94	0.68
1:D:13:PHE:O	1:D:322:ARG:NH1	2.28	0.66
1:A:13:PHE:O	1:A:322:ARG:NH1	2.28	0.66
1:A:93:ASP:CG	1:E:30:THR:HG22	2.16	0.66
1:A:325:LYS:O	1:A:328:THR:HG22	1.99	0.63
1:E:265:ARG:HG3	1:E:279:THR:HG23	1.81	0.63
1:A:50:GLY:HA2	1:E:30:THR:HG23	1.80	0.63
1:F:28:LYS:HE2	1:F:455:ARG:HD2	1.83	0.60
1:B:358:LEU:HD12	1:B:377:ILE:CD1	2.29	0.54
1:A:358:LEU:HD12	1:A:377:ILE:CD1	2.34	0.53
1:A:93:ASP:CG	1:E:30:THR:CG2	2.78	0.52
1:A:166:SER:CB	1:A:186:ALA:HB1	2.37	0.52
1:C:391:LYS:HD3	1:C:400:LYS:HE3	1.92	0.52
1:E:443:LEU:HD21	1:E:445:LEU:HD21	1.92	0.52
1:A:378:SER:HB3	1:A:388:GLN:HB2	1.91	0.51
1:D:166:SER:CB	1:D:186:ALA:HB1	2.37	0.51
1:C:166:SER:CB	1:C:186:ALA:HB1	2.35	0.51
1:A:66:LYS:O	1:A:76:TYR:HA	2.12	0.50
1:C:358:LEU:HD12	1:C:377:ILE:CD1	2.28	0.50
1:D:358:LEU:HD12	1:D:377:ILE:CD1	2.34	0.50
1:E:66:LYS:O	1:E:76:TYR:HA	2.12	0.50
1:F:443:LEU:HD21	1:F:445:LEU:HD21	1.94	0.50
1:E:44:PRO:HD3	1:E:466:PHE:CE2	2.47	0.49
1:B:66:LYS:O	1:B:76:TYR:HA	2.11	0.49
1:C:230:TYR:CE1	1:C:277:VAL:HG21	2.47	0.49
1:D:230:TYR:CE1	1:D:277:VAL:HG21	2.47	0.49
1:B:30:THR:HG23	1:E:50:GLY:CA	2.40	0.49
1:E:358:LEU:HD12	1:E:377:ILE:CD1	2.32	0.49
1:A:443:LEU:HD21	1:A:445:LEU:HD21	1.94	0.49
1:D:66:LYS:O	1:D:76:TYR:HA	2.12	0.49
1:F:358:LEU:HD12	1:F:377:ILE:CD1	2.31	0.49
1:C:66:LYS:O	1:C:76:TYR:HA	2.12	0.49
1:F:66:LYS:O	1:F:76:TYR:HA	2.11	0.49
1:D:443:LEU:HD21	1:D:445:LEU:HD21	1.94	0.49
1:F:166:SER:CB	1:F:186:ALA:HB1	2.39	0.49
1:E:166:SER:CB	1:E:186:ALA:HB1	2.41	0.49
1:B:30:THR:CG2	1:E:50:GLY:CA	2.90	0.48
1:B:44:PRO:HD3	1:B:466:PHE:CE2	2.48	0.48
1:B:230:TYR:CE1	1:B:277:VAL:HG21	2.48	0.48
1:C:443:LEU:HD21	1:C:445:LEU:HD21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PRO:HD3	1:A:466:PHE:CE2	2.49	0.48
1:F:44:PRO:HD3	1:F:466:PHE:CE2	2.48	0.48
1:B:443:LEU:HD21	1:B:445:LEU:HD21	1.95	0.48
1:E:230:TYR:CE1	1:E:277:VAL:HG21	2.48	0.48
1:F:124:ALA:HA	1:F:139:THR:HB	1.96	0.48
1:A:235:GLU:OE1	1:A:265:ARG:HD2	2.14	0.48
1:C:44:PRO:HD3	1:C:466:PHE:CE2	2.49	0.48
1:D:44:PRO:HD3	1:D:466:PHE:CE2	2.48	0.48
1:F:230:TYR:CE1	1:F:277:VAL:HG21	2.49	0.47
1:B:124:ALA:HA	1:B:139:THR:HB	1.97	0.47
1:A:230:TYR:CE1	1:A:277:VAL:HG21	2.49	0.47
1:D:124:ALA:HA	1:D:139:THR:HB	1.97	0.47
1:E:124:ALA:HA	1:E:139:THR:HB	1.96	0.47
1:D:378:SER:HB3	1:D:388:GLN:HB2	1.96	0.47
1:A:124:ALA:HA	1:A:139:THR:HB	1.97	0.46
1:C:124:ALA:HA	1:C:139:THR:HB	1.98	0.46
1:D:325:LYS:O	1:D:328:THR:CG2	2.64	0.46
1:B:166:SER:CB	1:B:186:ALA:HB1	2.37	0.46
1:B:225:ALA:HB3	1:B:232:VAL:HB	1.98	0.45
1:F:235:GLU:OE1	1:F:265:ARG:HD2	2.16	0.45
1:C:225:ALA:HB3	1:C:232:VAL:HB	1.98	0.45
1:D:225:ALA:HB3	1:D:232:VAL:HB	1.99	0.45
1:E:225:ALA:HB3	1:E:232:VAL:HB	1.98	0.45
1:D:235:GLU:OE1	1:D:265:ARG:HD2	2.17	0.45
1:D:28:LYS:HG2	1:F:297:GLN:HE22	1.81	0.44
1:F:112:VAL:HG23	6:F:1113:HOH:O	2.18	0.44
1:D:25:LEU:HD11	1:D:76:TYR:HB2	2.00	0.44
3:B:503:QVM:O	6:B:601:HOH:O	2.21	0.44
1:A:225:ALA:HB3	1:A:232:VAL:HB	2.00	0.44
1:E:268:ILE:HD11	1:E:339:ILE:HG21	2.00	0.44
1:F:225:ALA:HB3	1:F:232:VAL:HB	1.99	0.44
1:B:268:ILE:HD12	1:B:280:TYR:CE2	2.53	0.43
1:F:268:ILE:HD11	1:F:339:ILE:HG21	1.99	0.43
1:C:20:LEU:HB2	6:C:621:HOH:O	2.18	0.43
1:C:268:ILE:HD12	1:C:280:TYR:CE2	2.54	0.42
1:C:268:ILE:HD13	1:C:300:ILE:HD12	2.01	0.42
1:A:93:ASP:HB3	1:E:30:THR:CG2	2.42	0.42
1:C:201:ALA:O	1:C:204:THR:HG22	2.19	0.42
1:B:201:ALA:O	1:B:204:THR:HG22	2.19	0.42
1:A:93:ASP:CB	1:E:30:THR:HG21	2.39	0.42
1:D:201:ALA:O	1:D:204:THR:HG22	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LYS:O	1:A:328:THR:CG2	2.66	0.42
1:E:25:LEU:HD11	1:E:76:TYR:HB2	2.01	0.42
1:E:201:ALA:O	1:E:204:THR:HG22	2.20	0.42
1:C:380:TYR:HB3	1:C:384:ASP:OD2	2.19	0.42
1:A:30:THR:OG1	1:B:50:GLY:HA2	2.20	0.42
1:D:185:TYR:OH	1:D:221:MET:HB2	2.20	0.42
1:F:201:ALA:O	1:F:204:THR:HG22	2.20	0.42
1:A:201:ALA:O	1:A:204:THR:HG22	2.19	0.41
1:A:268:ILE:HD12	1:A:280:TYR:CE2	2.55	0.41
1:B:25:LEU:HD11	1:B:76:TYR:HB2	2.02	0.41
1:A:268:ILE:HD11	1:A:339:ILE:HG21	2.02	0.41
1:A:44:PRO:HB2	1:A:60:GLY:HA3	2.01	0.41
1:A:50:GLY:CA	1:E:30:THR:HG23	2.47	0.41
1:C:268:ILE:HD11	1:C:339:ILE:HG21	2.02	0.41
1:D:268:ILE:HD12	1:D:280:TYR:CE2	2.56	0.41
1:D:268:ILE:HD11	1:D:339:ILE:HG21	2.02	0.41
1:A:25:LEU:HD11	1:A:76:TYR:HB2	2.02	0.41
1:C:25:LEU:HD11	1:C:76:TYR:HB2	2.02	0.41
1:A:185:TYR:OH	1:A:221:MET:HB2	2.20	0.41
1:F:245:LEU:HA	1:F:245:LEU:HD12	1.95	0.41
1:C:16:LEU:HD23	1:C:63:MET:SD	2.60	0.41
1:B:16:LEU:HD23	1:B:63:MET:SD	2.61	0.41
1:C:235:GLU:OE1	1:C:265:ARG:HD2	2.21	0.41
1:E:268:ILE:HD12	1:E:280:TYR:CE2	2.56	0.41
1:F:130:LYS:HA	1:F:134:ARG:O	2.21	0.41
1:F:268:ILE:HD12	1:F:280:TYR:CE2	2.56	0.41
1:E:56:HIS:HB2	1:E:101:ALA:HB3	2.02	0.41
1:D:16:LEU:HD23	1:D:63:MET:SD	2.61	0.40
1:D:242:PRO:O	1:D:246:LEU:HG	2.21	0.40
1:A:16:LEU:HD23	1:A:63:MET:SD	2.62	0.40
1:B:242:PRO:O	1:B:246:LEU:HG	2.21	0.40
1:B:268:ILE:HD13	1:B:300:ILE:HD12	2.04	0.40
1:A:242:PRO:O	1:A:246:LEU:HG	2.21	0.40
1:B:44:PRO:HB2	1:B:60:GLY:HA3	2.04	0.40
1:A:56:HIS:HB2	1:A:101:ALA:HB3	2.04	0.40
1:B:380:TYR:HB3	1:B:384:ASP:OD2	2.21	0.40
1:B:56:HIS:HB2	1:B:101:ALA:HB3	2.04	0.40
1:E:130:LYS:HA	1:E:134:ARG:O	2.21	0.40
1:F:25:LEU:HD11	1:F:76:TYR:HB2	2.02	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	450/472 (95%)	434 (96%)	16 (4%)	0	100	100
1	B	451/472 (96%)	435 (96%)	16 (4%)	0	100	100
1	C	450/472 (95%)	434 (96%)	16 (4%)	0	100	100
1	D	448/472 (95%)	433 (97%)	15 (3%)	0	100	100
1	E	415/472 (88%)	403 (97%)	12 (3%)	0	100	100
1	F	418/472 (89%)	402 (96%)	16 (4%)	0	100	100
All	All	2632/2832 (93%)	2541 (96%)	91 (4%)	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	387/417 (93%)	386 (100%)	1 (0%)	92	96
1	B	394/417 (94%)	392 (100%)	2 (0%)	88	94
1	C	385/417 (92%)	383 (100%)	2 (0%)	88	94
1	D	383/417 (92%)	382 (100%)	1 (0%)	92	96
1	E	364/417 (87%)	364 (100%)	0	100	100
1	F	352/417 (84%)	351 (100%)	1 (0%)	92	96
All	All	2265/2502 (90%)	2258 (100%)	7 (0%)	92	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	B	71	GLU
1	B	345	GLN
1	C	75	SER
1	C	357	GLU
1	D	10	GLN
1	F	106	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	QVM	B	503	-	24,24,24	0.50	0	31,32,32	0.46	0
3	QVM	C	502	-	24,24,24	0.36	0	31,32,32	0.51	0
3	QVM	D	502	-	24,24,24	0.56	0	31,32,32	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	QVM	A	502	-	24,24,24	0.53	0	31,32,32	0.46	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	QVM	B	503	-	-	0/16/35/35	0/1/1/1
3	QVM	C	502	-	-	0/16/35/35	0/1/1/1
3	QVM	D	502	-	-	0/16/35/35	0/1/1/1
3	QVM	A	502	-	-	0/16/35/35	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

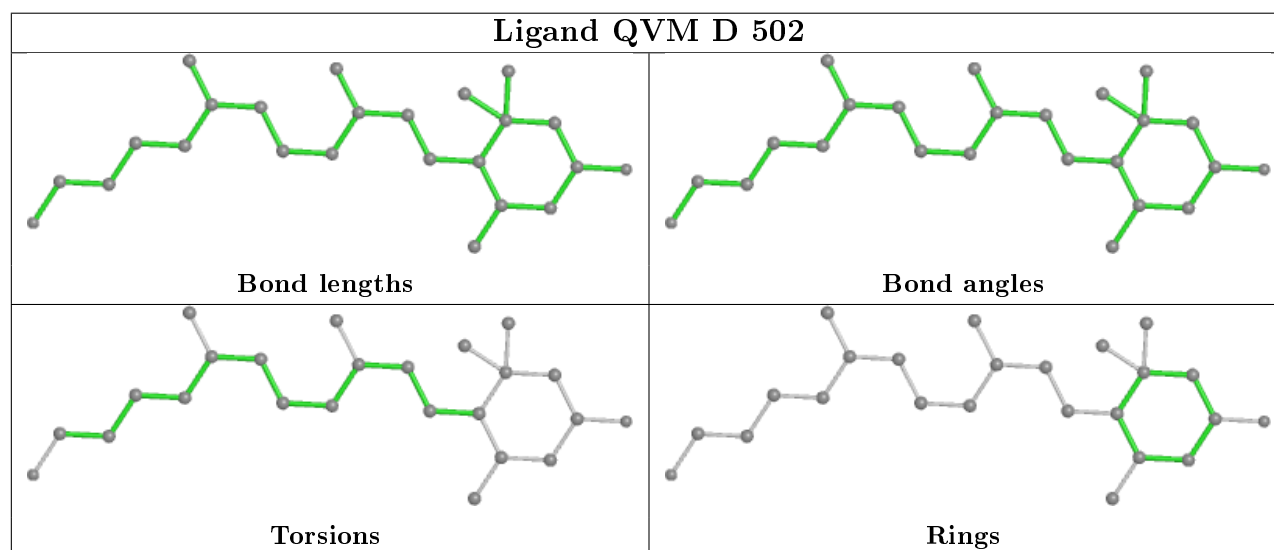
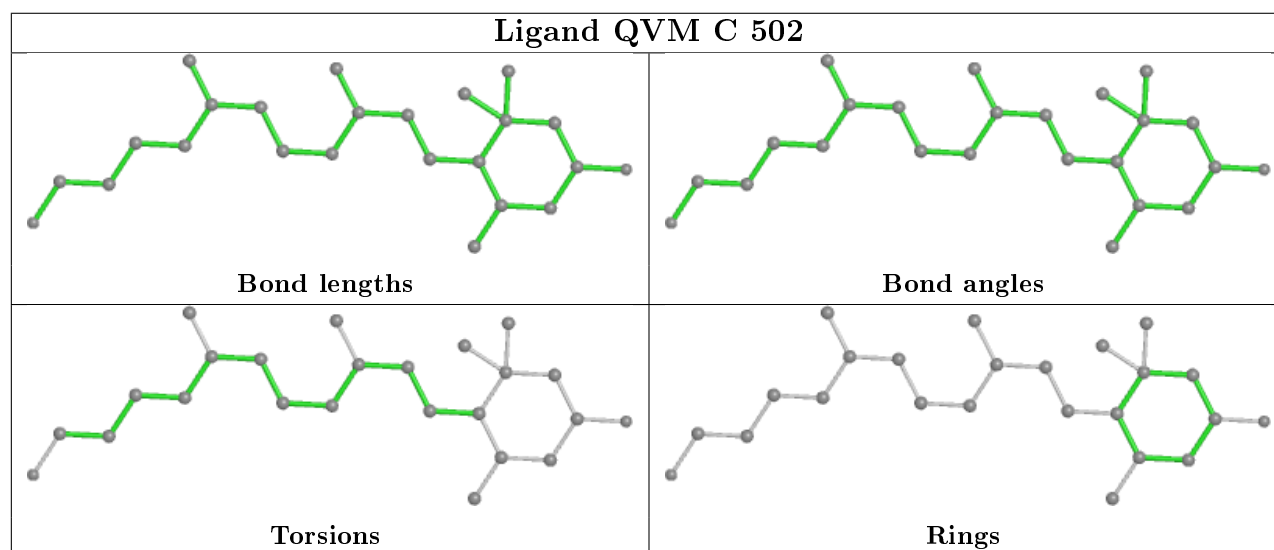
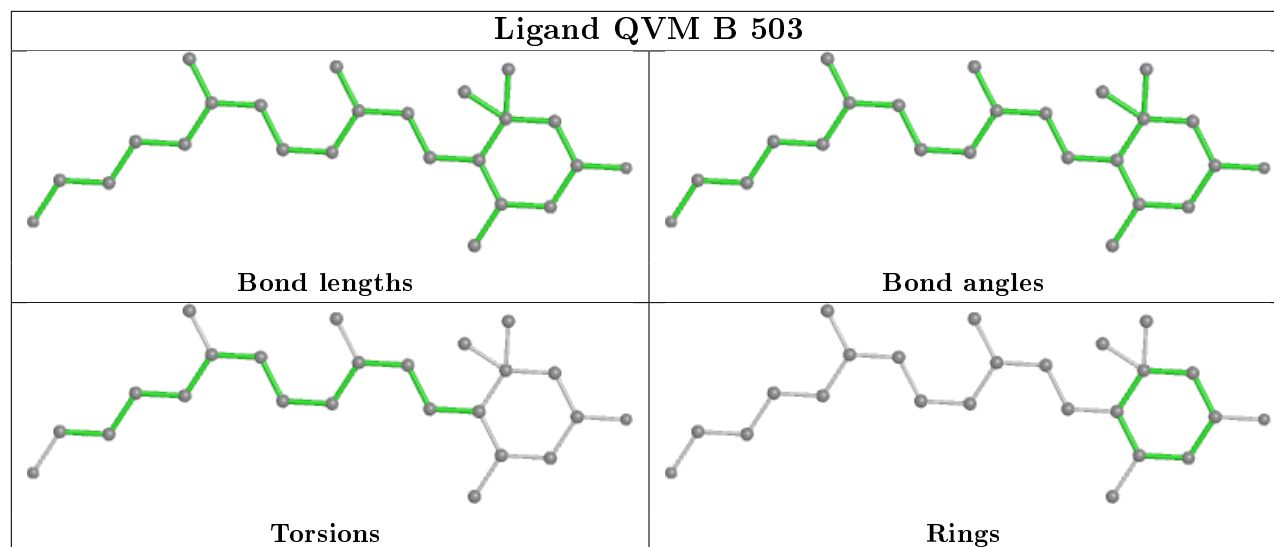
There are no torsion outliers.

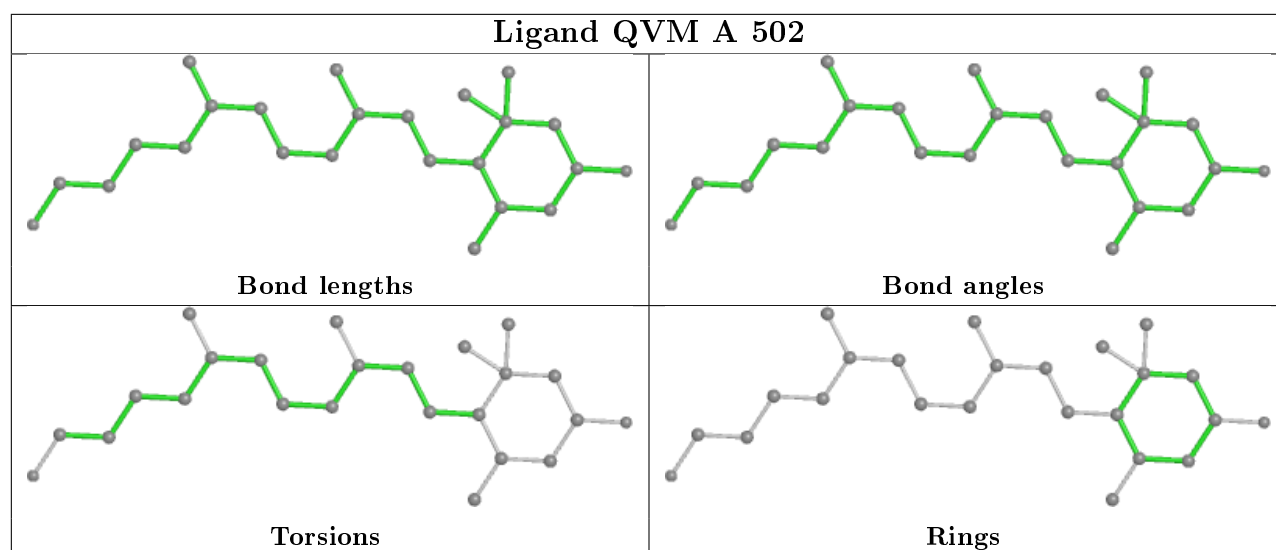
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	QVM	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

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	453/472 (95%)	0.39	26 (5%) 23 34	42, 68, 103, 123	0
1	B	453/472 (95%)	0.34	16 (3%) 44 56	36, 64, 105, 124	0
1	C	453/472 (95%)	0.52	33 (7%) 15 22	43, 71, 110, 127	0
1	D	452/472 (95%)	0.58	33 (7%) 15 22	44, 75, 118, 152	0
1	E	431/472 (91%)	1.50	136 (31%) 0 0	48, 98, 172, 206	0
1	F	430/472 (91%)	2.03	167 (38%) 0 0	57, 108, 189, 208	0
All	All	2672/2832 (94%)	0.88	411 (15%) 2 3	36, 77, 150, 208	0

All (411) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	31	ILE	14.2
1	F	374	VAL	12.5
1	F	25	LEU	11.3
1	E	30	THR	10.9
1	F	443	LEU	10.6
1	F	276	LEU	10.6
1	F	373	PHE	9.6
1	E	31	ILE	9.1
1	F	458	VAL	9.0
1	F	389	LEU	9.0
1	F	70	LYS	8.9
1	F	470	TYR	8.3
1	E	278	GLY	8.2
1	F	74	VAL	8.2
1	F	30	THR	8.1
1	F	375	TYR	7.6
1	F	351	LEU	7.5
1	E	427	LEU	7.4
1	F	436	THR	7.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	453	VAL	7.0
1	F	445	LEU	6.8
1	E	25	LEU	6.7
1	F	427	LEU	6.7
1	F	422	LYS	6.7
1	F	448	THR	6.6
1	F	441	PHE	6.5
1	F	67	PHE	6.5
1	F	392	ILE	6.5
1	F	417	ALA	6.5
1	F	456	ALA	6.4
1	F	457	GLU	6.4
1	F	428	ILE	6.2
1	F	424	ASP	6.2
1	F	454	ALA	6.2
1	E	447	ALA	6.1
1	F	440	SER	6.1
1	E	432	VAL	6.1
1	E	422	LYS	6.0
1	F	414	PHE	6.0
1	F	401	ILE	5.9
1	F	177	PHE	5.9
1	F	413	VAL	5.8
1	E	67	PHE	5.8
1	E	149	ILE	5.8
1	E	425	GLU	5.7
1	F	29	GLY	5.7
1	E	8	LYS	5.6
1	E	421	THR	5.6
1	F	415	VAL	5.5
1	E	457	GLU	5.5
1	D	89	ALA	5.5
1	F	291	VAL	5.4
1	E	76	TYR	5.4
1	E	443	LEU	5.4
1	F	278	GLY	5.3
1	F	390	VAL	5.3
1	F	450	PHE	5.3
1	F	403	SER	5.1
1	F	69	PHE	5.1
1	F	178	VAL	5.1
1	F	471	PHE	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	299	GLU	5.0
1	E	152	LEU	5.0
1	F	76	TYR	5.0
1	E	448	THR	5.0
1	F	388	GLN	5.0
1	E	74	VAL	5.0
1	E	374	VAL	4.9
1	F	277	VAL	4.9
1	E	407	CYS	4.9
1	F	464	PHE	4.9
1	E	453	VAL	4.9
1	F	405	LYS	4.9
1	F	432	VAL	4.9
1	E	417	ALA	4.9
1	F	339	ILE	4.8
1	D	25	LEU	4.8
1	F	341	LEU	4.8
1	F	376	GLY	4.8
1	E	375	TYR	4.7
1	E	424	ASP	4.7
1	F	442	LEU	4.7
1	F	451	GLU	4.7
1	F	407	CYS	4.7
1	C	417	ALA	4.7
1	F	419	ASP	4.7
1	F	105	CYS	4.7
1	F	408	TYR	4.6
1	E	20	LEU	4.6
1	F	447	ALA	4.5
1	F	400	LYS	4.5
1	D	20	LEU	4.5
1	F	24	SER	4.4
1	F	149	ILE	4.4
1	C	69	PHE	4.4
1	F	434	ASP	4.4
1	E	388	GLN	4.4
1	E	414	PHE	4.4
1	F	13	PHE	4.4
1	F	418	PRO	4.4
1	F	300	ILE	4.4
1	E	445	LEU	4.4
1	E	178	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	459	PRO	4.4
1	F	406	ASP	4.3
1	F	439	LYS	4.3
1	E	442	LEU	4.3
1	F	337	TYR	4.3
1	E	22	LEU	4.2
1	E	415	VAL	4.2
1	F	297	GLN	4.2
1	E	405	LYS	4.2
1	E	406	ASP	4.2
1	F	402	TRP	4.1
1	E	177	PHE	4.1
1	E	366	TYR	4.1
1	F	268	ILE	4.0
1	F	437	ASN	4.0
1	F	75	SER	4.0
1	A	297	GLN	4.0
1	E	436	THR	4.0
1	F	371	TYR	4.0
1	E	454	ALA	4.0
1	E	373	PHE	4.0
1	D	386	ALA	3.9
1	F	65	HIS	3.9
1	F	449	THR	3.9
1	E	441	PHE	3.9
1	F	462	ILE	3.9
1	F	420	ALA	3.9
1	F	461	HIS	3.9
1	F	107	SER	3.9
1	F	356	VAL	3.8
1	E	150	ASN	3.8
1	F	430	SER	3.8
1	A	373	PHE	3.8
1	E	389	LEU	3.8
1	E	371	TYR	3.8
1	F	416	GLY	3.8
1	E	460	HIS	3.8
1	E	458	VAL	3.7
1	F	361	ILE	3.7
1	F	410	GLY	3.7
1	F	444	ILE	3.7
1	F	294	PHE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	301	PHE	3.7
1	C	420	ALA	3.6
1	E	451	GLU	3.6
1	E	28	LYS	3.6
1	A	344	GLY	3.6
1	D	34	TRP	3.6
1	F	421	THR	3.6
1	F	22	LEU	3.5
1	E	470	TYR	3.5
1	E	346	VAL	3.5
1	D	419	ASP	3.5
1	A	356	VAL	3.5
1	F	175	TYR	3.4
1	F	304	ILE	3.4
1	B	355	ALA	3.4
1	D	93	ASP	3.4
1	F	438	ALA	3.4
1	E	298	GLU	3.4
1	F	230	TYR	3.4
1	E	297	GLN	3.3
1	E	23	GLU	3.3
1	E	277	VAL	3.3
1	F	330	PRO	3.3
1	F	348	TYR	3.3
1	E	428	ILE	3.3
1	E	464	PHE	3.3
1	F	301	PHE	3.3
1	E	416	GLY	3.3
1	E	26	GLN	3.2
1	F	353	SER	3.2
1	C	34	TRP	3.2
1	E	336	ARG	3.2
1	F	455	ARG	3.2
1	E	450	PHE	3.2
1	F	354	GLU	3.2
1	E	80	PHE	3.2
1	E	68	SER	3.2
1	A	377	ILE	3.2
1	E	12	GLY	3.2
1	E	21	ASP	3.2
1	F	109	PHE	3.2
1	E	420	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	456	ALA	3.2
1	F	429	LEU	3.2
1	E	230	TYR	3.2
1	B	422	LYS	3.1
1	E	78	ASN	3.1
1	A	156	GLY	3.1
1	E	339	ILE	3.1
1	F	336	ARG	3.1
1	D	90	ARG	3.1
1	F	16	LEU	3.1
1	F	372	ARG	3.1
1	E	462	ILE	3.1
1	F	267	ILE	3.1
1	E	419	ASP	3.1
1	D	355	ALA	3.0
1	F	472	GLU	3.0
1	C	51	LYS	3.0
1	E	45	ALA	3.0
1	F	355	ALA	3.0
1	F	229	ASN	3.0
1	E	376	GLY	3.0
1	F	299	GLU	3.0
1	E	334	ILE	3.0
1	C	418	PRO	3.0
1	C	246	LEU	3.0
1	E	65	HIS	3.0
1	C	386	ALA	3.0
1	E	431	ALA	3.0
1	E	300	ILE	3.0
1	E	361	ILE	3.0
1	F	365	GLN	2.9
1	C	419	ASP	2.9
1	F	366	TYR	2.9
1	F	346	VAL	2.9
1	F	368	THR	2.9
1	D	94	LYS	2.9
1	E	19	GLU	2.9
1	E	305	ILE	2.9
1	E	455	ARG	2.9
1	F	350	MET	2.9
1	B	7	ASN	2.9
1	F	302	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	23	GLU	2.9
1	D	23	GLU	2.9
1	E	11	LEU	2.9
1	F	280	TYR	2.9
1	F	409	PRO	2.8
1	E	280	TYR	2.8
1	E	337	TYR	2.8
1	B	249	GLY	2.8
1	D	104	PRO	2.8
1	E	325	LYS	2.8
1	F	269	VAL	2.8
1	E	409	PRO	2.7
1	D	379	THR	2.7
1	A	355	ALA	2.7
1	A	378	SER	2.7
1	D	96	SER	2.7
1	F	431	ALA	2.7
1	C	427	LEU	2.7
1	F	64	LEU	2.7
1	A	280	TYR	2.7
1	F	398	SER	2.7
1	C	331	THR	2.7
1	E	434	ASP	2.7
1	E	175	TYR	2.7
1	A	389	LEU	2.7
1	B	34	TRP	2.7
1	F	11	LEU	2.7
1	A	246	LEU	2.7
1	C	247	LEU	2.7
1	E	413	VAL	2.7
1	D	35	LEU	2.7
1	E	249	GLY	2.7
1	F	370	ASP	2.6
1	A	300	ILE	2.6
1	D	329	ILE	2.6
1	D	49	VAL	2.6
1	E	81	LEU	2.6
1	F	465	GLY	2.6
1	B	25	LEU	2.6
1	C	80	PHE	2.6
1	B	30	THR	2.6
1	E	353	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	437	ASN	2.6
1	E	18	GLU	2.6
1	C	416	GLY	2.6
1	E	29	GLY	2.6
1	F	12	GLY	2.6
1	E	408	TYR	2.5
1	F	71	GLU	2.5
1	F	68	SER	2.5
1	A	354[A]	GLU	2.5
1	F	298	GLU	2.5
1	E	70	LYS	2.5
1	E	461	HIS	2.5
1	D	97	TYR	2.5
1	E	71	GLU	2.5
1	F	106	ARG	2.5
1	E	410	GLY	2.5
1	E	115	MET	2.5
1	E	86	TYR	2.5
1	A	268	ILE	2.5
1	C	344	GLY	2.5
1	A	17	SER	2.5
1	E	27	VAL	2.5
1	E	147	PHE	2.5
1	D	52	GLU	2.5
1	A	422	LYS	2.4
1	C	330	PRO	2.4
1	F	338	ARG	2.4
1	D	22	LEU	2.4
1	F	23	GLU	2.4
1	F	433	LEU	2.4
1	E	437	ASN	2.4
1	C	23	GLU	2.4
1	A	379	THR	2.4
1	B	344	GLY	2.4
1	C	120	PHE	2.4
1	F	157	VAL	2.4
1	F	283	ASP	2.4
1	F	275	ASN	2.4
1	F	362	ASN	2.4
1	E	13	PHE	2.4
1	E	356	VAL	2.4
1	A	342	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	439	LYS	2.4
1	C	308[A]	GLN	2.4
1	E	229	ASN	2.4
1	E	370	ASP	2.4
1	C	332	SER	2.3
1	F	270	ASN	2.3
1	A	298	GLU	2.3
1	B	457	GLU	2.3
1	E	293	ALA	2.3
1	F	358	LEU	2.3
1	F	331	THR	2.3
1	E	176	ASP	2.3
1	E	430	SER	2.3
1	F	176	ASP	2.3
1	D	385	PHE	2.3
1	D	297	GLN	2.3
1	D	330	PRO	2.3
1	C	9	PHE	2.3
1	C	312	ILE	2.3
1	F	305	ILE	2.3
1	C	382	ALA	2.3
1	E	372	ARG	2.3
1	F	359	PRO	2.3
1	B	306	ALA	2.3
1	E	306	ALA	2.3
1	F	287	ALA	2.3
1	E	365	GLN	2.3
1	C	126	VAL	2.3
1	C	453	VAL	2.3
1	F	119	LYS	2.3
1	F	303	ASP	2.3
1	D	11	LEU	2.2
1	E	338	ARG	2.2
1	A	390	VAL	2.2
1	F	288	PHE	2.2
1	C	447	ALA	2.2
1	B	421	THR	2.2
1	B	341	LEU	2.2
1	A	413	VAL	2.2
1	C	144	PRO	2.2
1	A	153	LYS	2.2
1	D	30	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	16	LEU	2.2
1	E	348	TYR	2.2
1	D	87	GLN	2.2
1	D	445	LEU	2.2
1	E	243	LEU	2.2
1	E	471	PHE	2.2
1	F	135	PHE	2.2
1	F	344	GLY	2.2
1	D	457	GLU	2.2
1	A	22	LEU	2.2
1	C	356	VAL	2.2
1	D	356	VAL	2.2
1	E	390	VAL	2.2
1	F	158	PHE	2.2
1	F	130	LYS	2.2
1	E	449	THR	2.2
1	E	429	LEU	2.2
1	E	399	SER	2.2
1	F	78	ASN	2.1
1	F	80	PHE	2.1
1	F	139	THR	2.1
1	B	353	SER	2.1
1	C	313	VAL	2.1
1	F	349	GLU	2.1
1	D	326	THR	2.1
1	A	305	ILE	2.1
1	F	399	SER	2.1
1	F	411	GLU	2.1
1	A	380	TYR	2.1
1	D	120	PHE	2.1
1	F	423	GLU	2.1
1	A	361	ILE	2.1
1	F	152	LEU	2.1
1	C	355	ALA	2.1
1	E	331	THR	2.1
1	F	227	THR	2.1
1	B	385	PHE	2.1
1	E	9	PHE	2.1
1	E	120	PHE	2.1
1	E	323	GLY	2.1
1	D	377	ILE	2.1
1	E	401	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	352	SER	2.1
1	C	143	LEU	2.0
1	C	457	GLU	2.0
1	D	298	GLU	2.0
1	E	402	TRP	2.0
1	F	391	LYS	2.0
1	F	367	ASN	2.0
1	B	287	ALA	2.0
1	E	77	ALA	2.0
1	E	459	PRO	2.0
1	F	321	LEU	2.0
1	F	377	ILE	2.0
1	E	171	ALA	2.0
1	F	296	LYS	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 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.

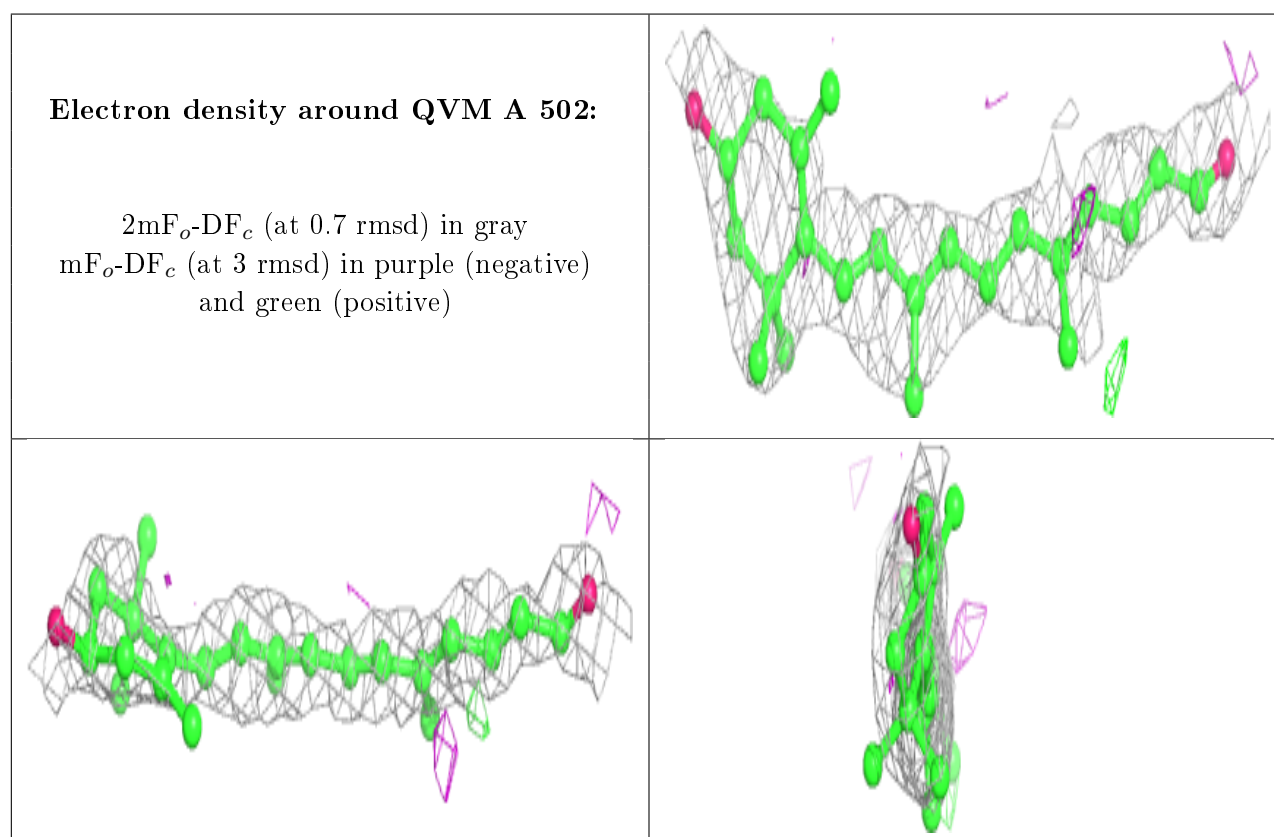
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	QVM	A	502	24/24	0.81	0.36	58,70,85,91	0
3	QVM	D	502	24/24	0.83	0.36	75,82,99,100	0
3	QVM	B	503	24/24	0.84	0.39	60,68,77,81	0
3	QVM	C	502	24/24	0.89	0.21	71,74,85,88	0
2	CO	F	1000	1/1	0.90	0.17	89,89,89,89	0
4	CL	A	503	1/1	0.92	0.17	80,80,80,80	0
4	CL	E	502	1/1	0.93	0.28	72,72,72,72	0
2	CO	E	501	1/1	0.95	0.19	72,72,72,72	0
5	NA	B	502	1/1	0.96	0.11	73,73,73,73	0

Continued on next page...

Continued from previous page...

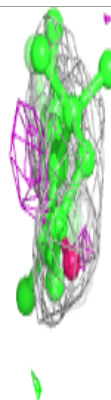
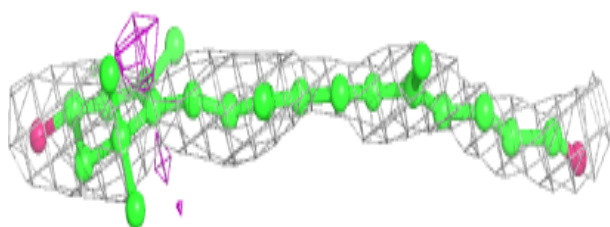
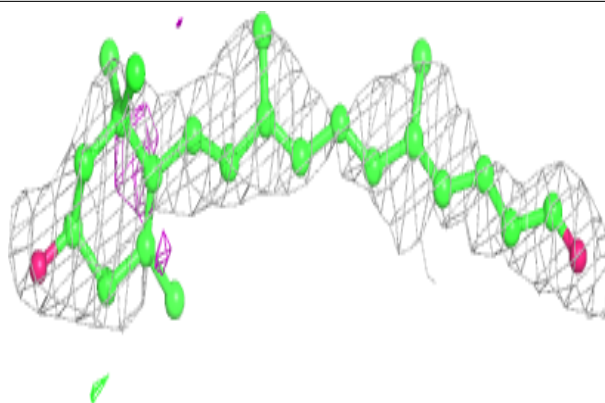
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NA	C	503	1/1	0.98	0.07	62,62,62,62	0
2	CO	A	501	1/1	0.99	0.16	47,47,47,47	0
2	CO	C	501	1/1	1.00	0.18	52,52,52,52	0
2	CO	D	501	1/1	1.00	0.18	55,55,55,55	0
2	CO	B	501	1/1	1.00	0.14	43,43,43,43	0

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.

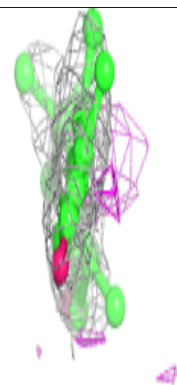
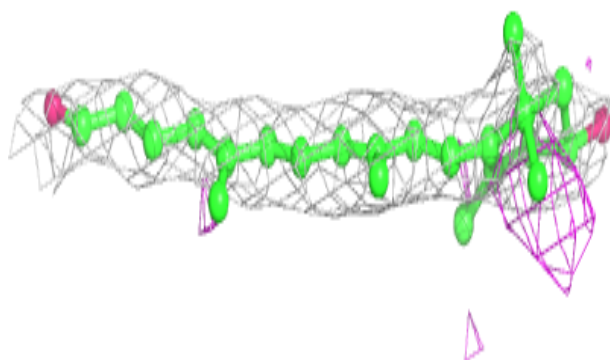
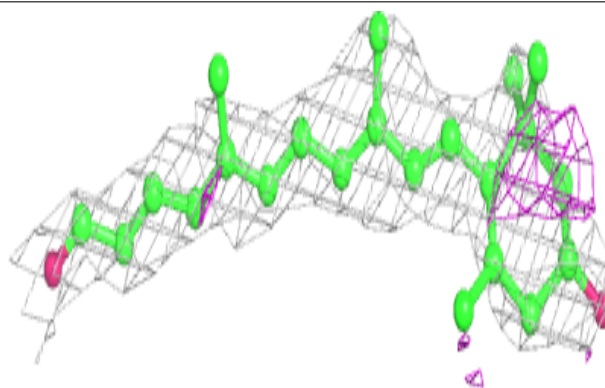


Electron density around QVM D 502:

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

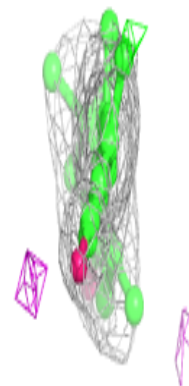
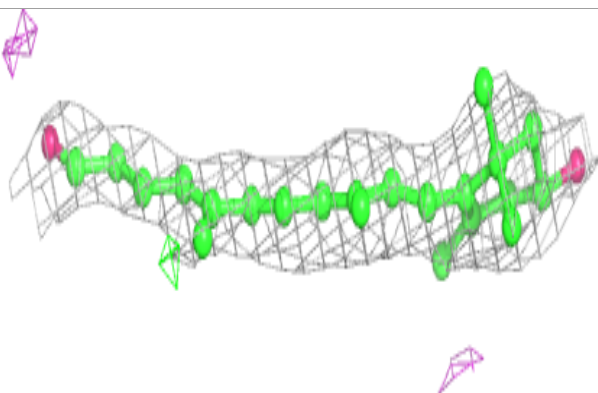
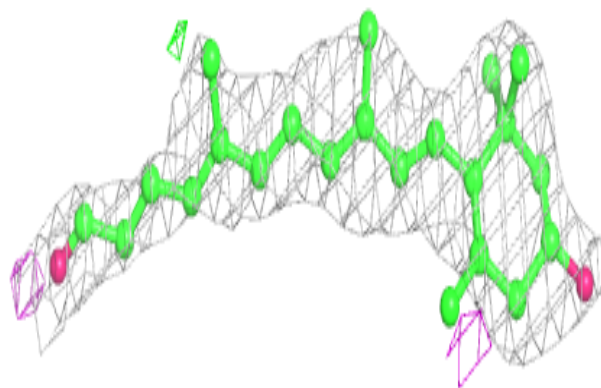
**Electron density around QVM B 503:**

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



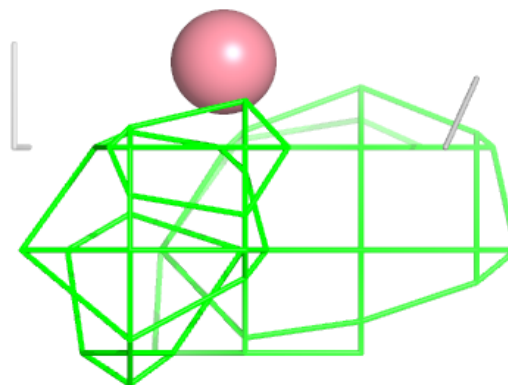
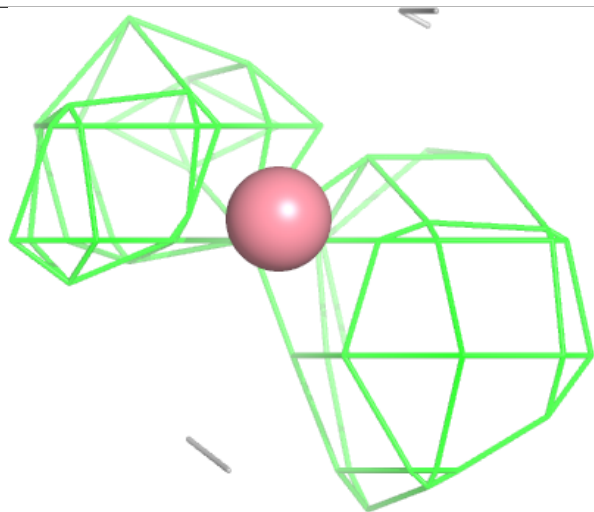
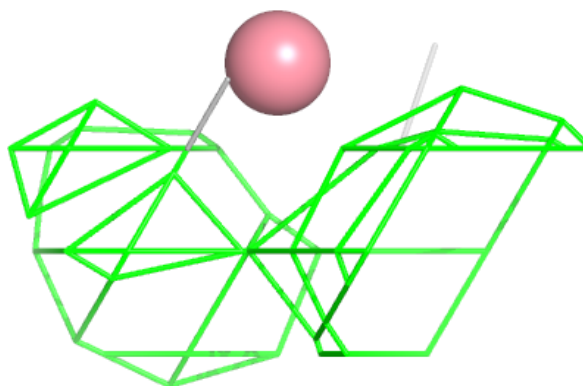
Electron density around QVM C 502:

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



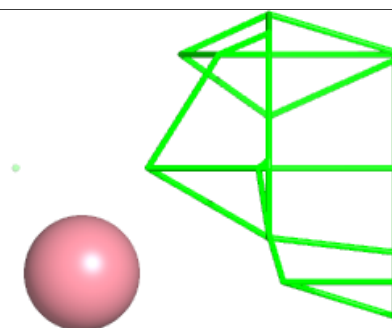
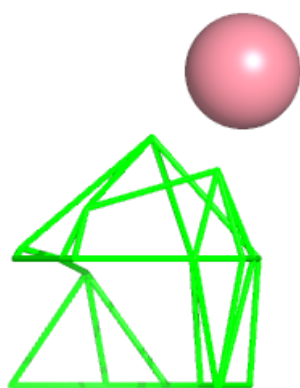
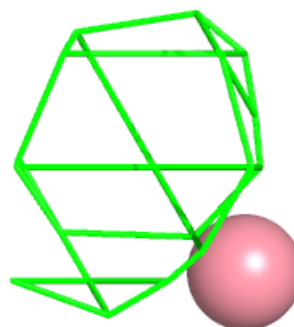
Electron density around CO F 1000:

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



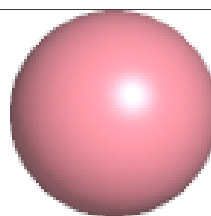
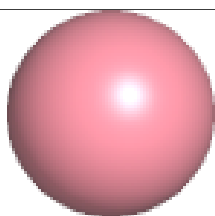
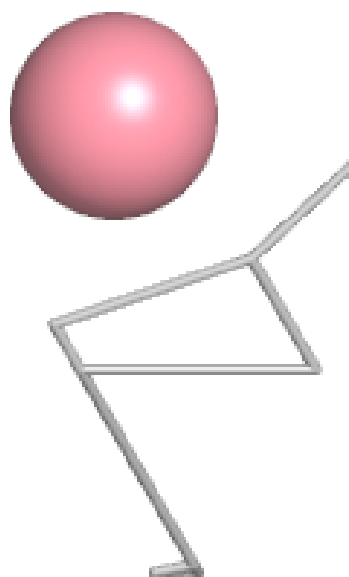
Electron density around CO E 501:

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



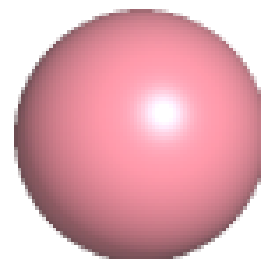
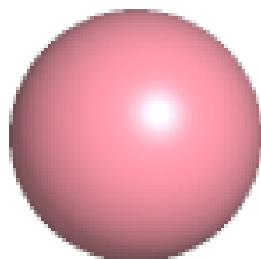
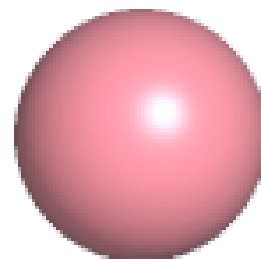
Electron density around CO A 501:

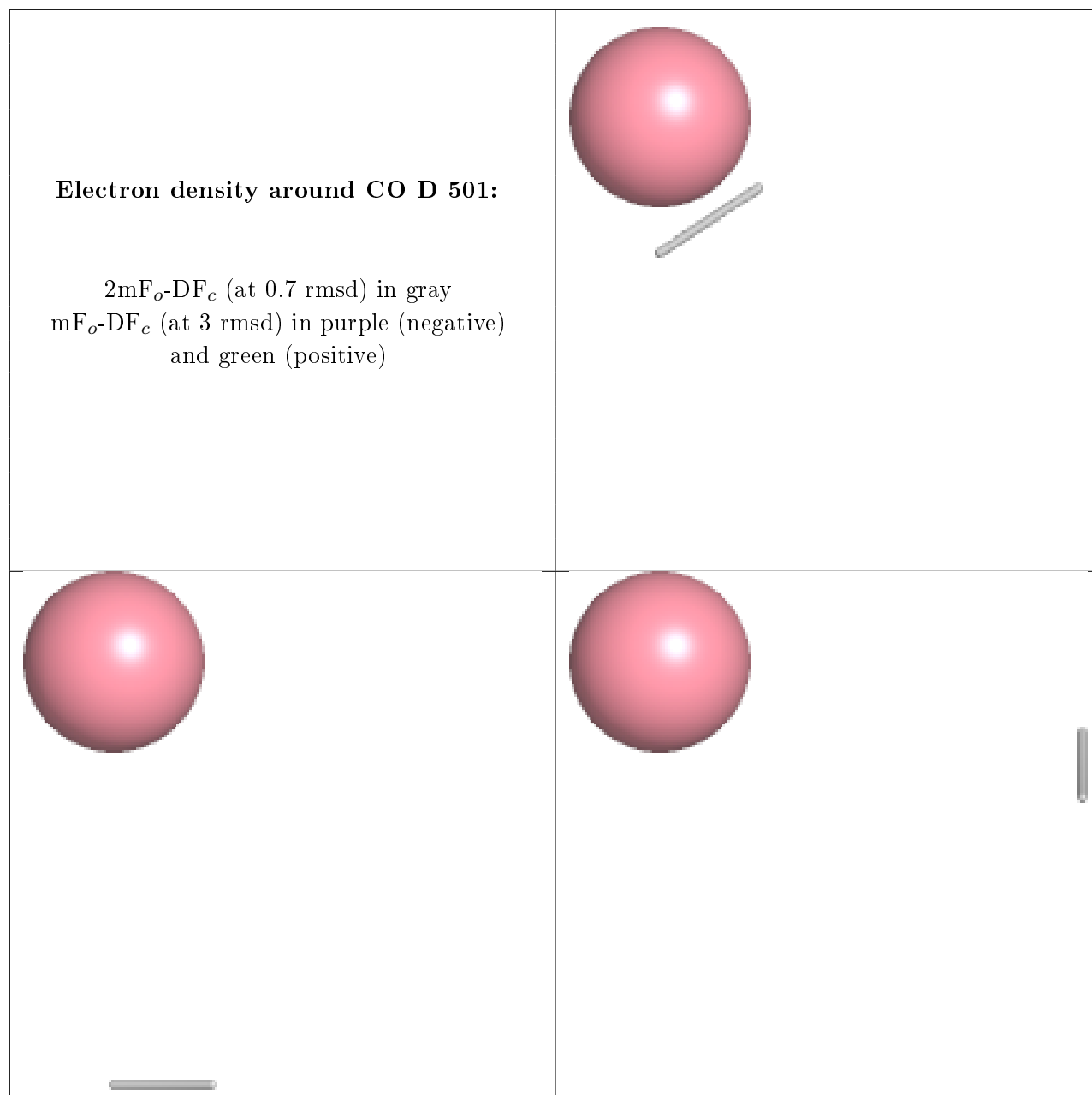
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

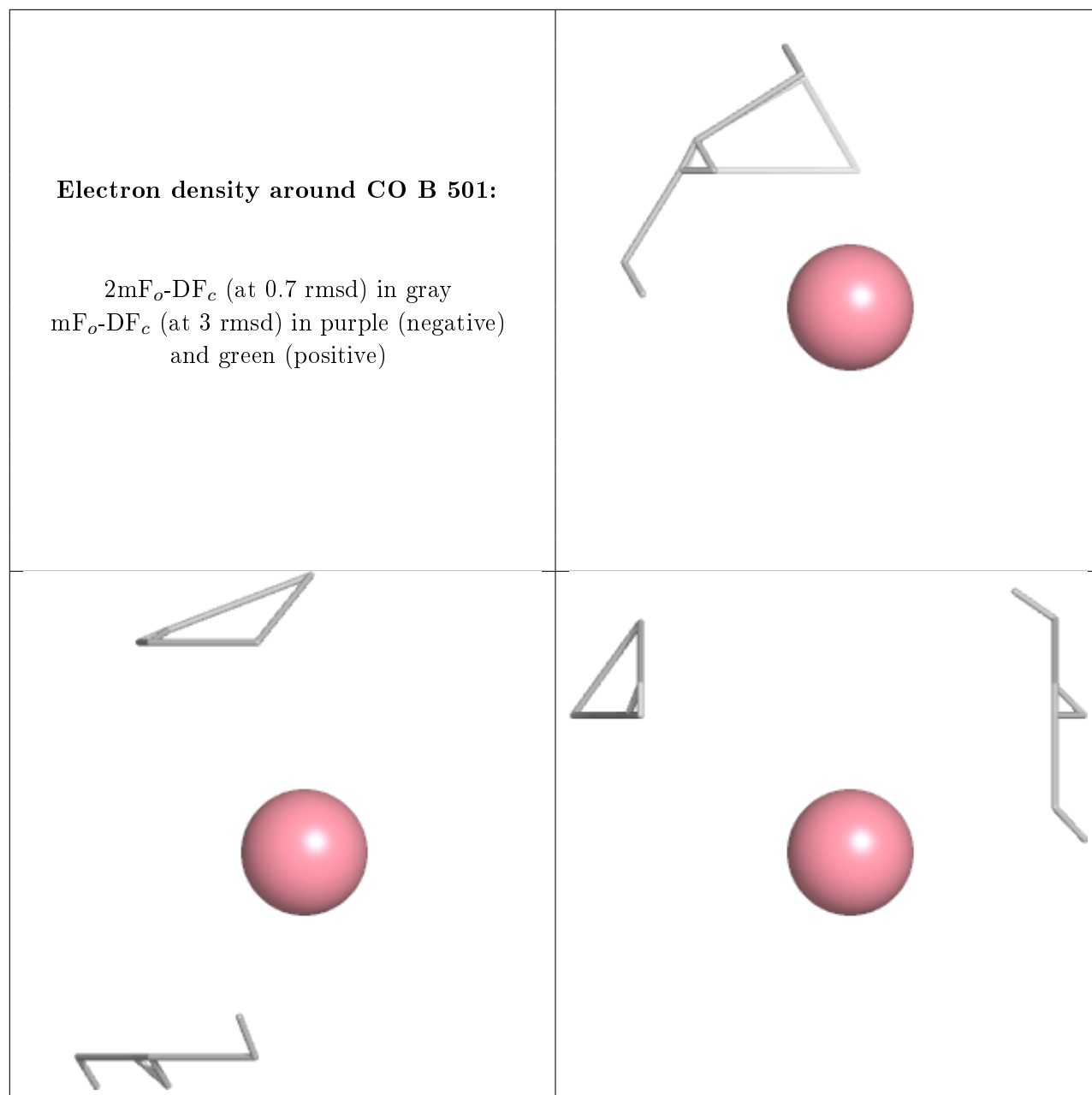


Electron density around CO C 501:

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







6.5 Other polymers ⓘ

There are no such residues in this entry.