



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:22 PM UTC

PDB ID : 4D06 / pdb_00004d06
Title : Bacterial chalcone isomerase complexed with naringenin
Authors : Thomsen, M.; Palm, G.J.; Hinrichs, W.
Deposited on : 2014-04-24
Resolution : 2.00 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

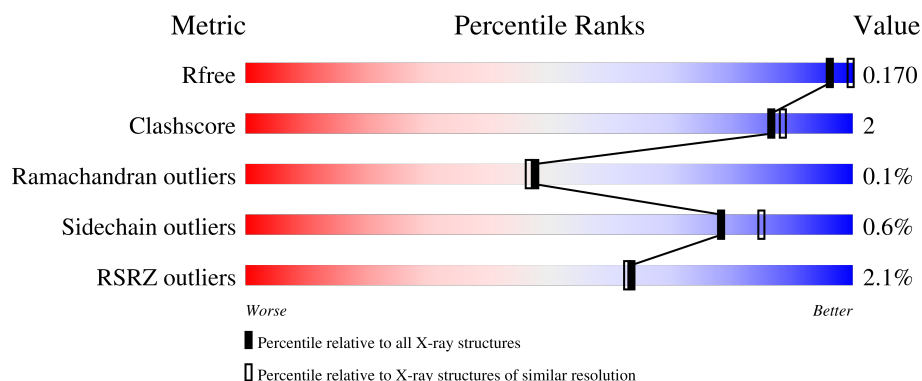
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	283	 3% 95% 5%
1	B	283	 % 84% 7% 8%
1	C	283	 2% 93% 6%
1	D	283	 % 86% 6% 8%
1	E	283	 4% 95% 5%

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Mol	Chain	Length	Quality of chain
1	F	283	%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	F	303	-	X	-	-

2 Entry composition [i](#)

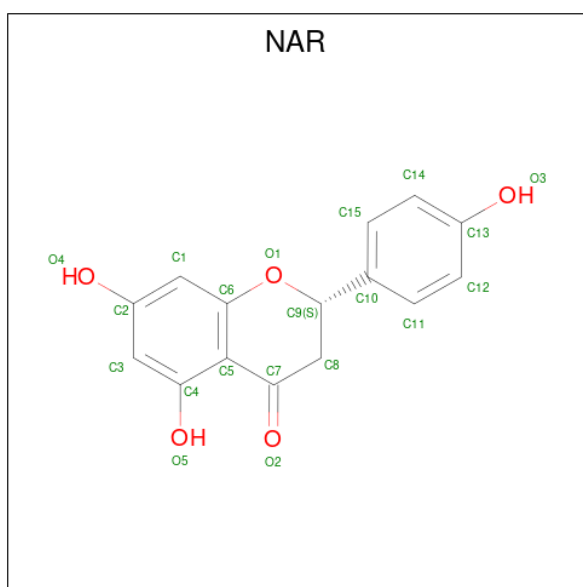
There are 6 unique types of molecules in this entry. The entry contains 15609 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CHALCONE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	5	0
			2312	1495	380	423	14			
1	B	259	Total	C	N	O	S	0	8	0
			2172	1421	349	387	15			
1	C	282	Total	C	N	O	S	0	7	0
			2326	1509	380	423	14			
1	D	259	Total	C	N	O	S	0	8	0
			2170	1422	349	384	15			
1	E	282	Total	C	N	O	S	0	8	0
			2331	1509	381	426	15			
1	F	259	Total	C	N	O	S	0	6	0
			2161	1417	348	382	14			

- Molecule 2 is NARINGENIN (CCD ID: NAR) (formula: C₁₅H₁₂O₅).

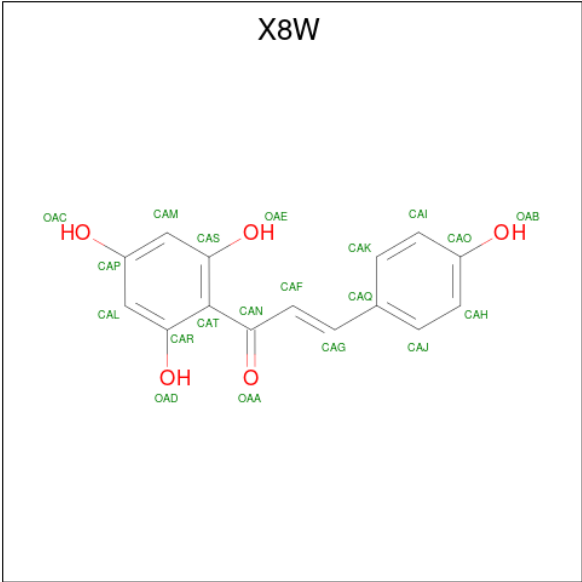


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	15	5		
2	C	1	Total	C	O	0	0
			20	15	5		
2	D	1	Total	C	O	0	0
			20	15	5		
2	D	1	Total	C	O	0	0
			20	15	5		
2	E	1	Total	C	O	0	0
			20	15	5		
2	F	1	Total	C	O	0	0
			20	15	5		
2	F	1	Total	C	O	0	1
			19	12	7		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

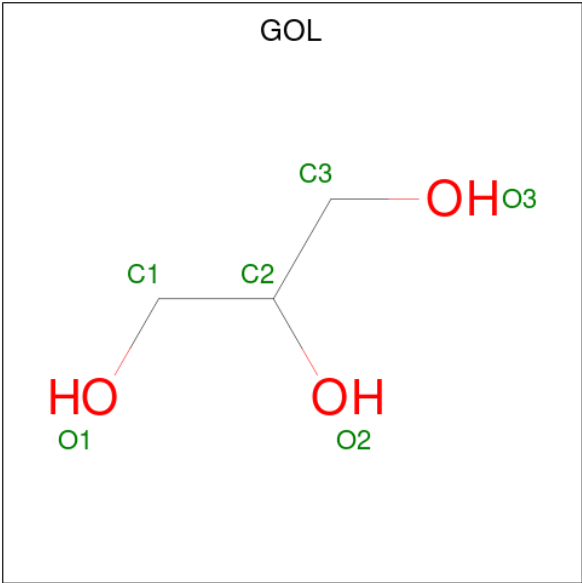
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	2	Total	Cl	0	0
			2	2		
3	C	3	Total	Cl	0	0
			3	3		
3	D	3	Total	Cl	0	0
			3	3		
3	E	4	Total	Cl	0	0
			4	4		
3	F	3	Total	Cl	0	0
			3	3		

- Molecule 4 is (2E)-3-(4-hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)prop-2-en-1-one (CCD ID: X8W) (formula: C₁₅H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			20	15	5		
4	D	1	Total	C	O	0	1
			36	26	10		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	357	Total 361	O 361	0	4
6	B	325	Total 329	O 329	0	4
6	C	345	Total 347	O 347	0	2
6	D	294	Total 297	O 297	0	3
6	E	310	Total 312	O 312	0	2
6	F	264	Total 267	O 267	0	3

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.

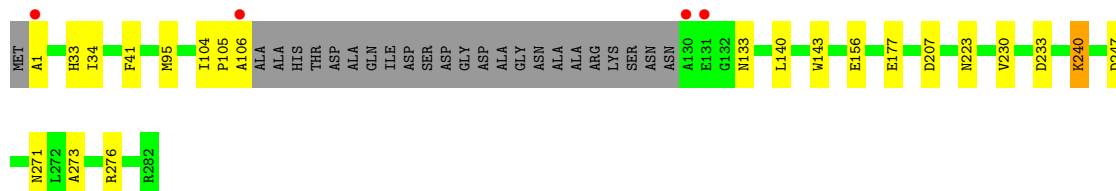
• Molecule 1: CHALCONE ISOMERASE

Chain A: 

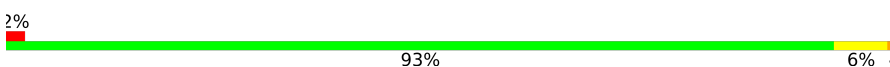


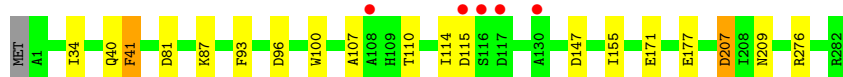
• Molecule 1: CHALCONE ISOMERASE

Chain B: 



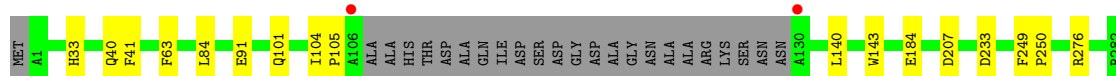
• Molecule 1: CHALCONE ISOMERASE

Chain C: 



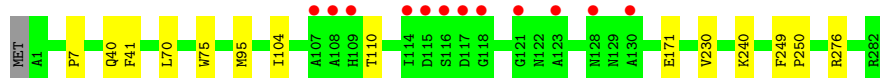
• Molecule 1: CHALCONE ISOMERASE

Chain D: 

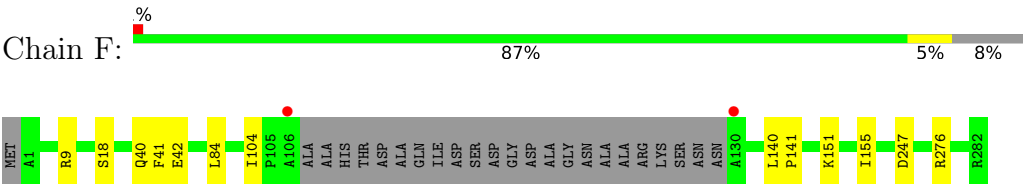


• Molecule 1: CHALCONE ISOMERASE

Chain E: 



● Molecule 1: CHALCONE ISOMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.16Å 187.99Å 196.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 2.00 49.18 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.18-2.00) 100.0 (49.18-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.140 , 0.163 0.151 , 0.170	Depositor DCC
R_{free} test set	11215 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15609	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: NAR, GOL, CL, X8W

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	1.11	0/2400	1.03	1/3262 (0.0%)
1	B	1.17	8/2265 (0.4%)	1.06	5/3078 (0.2%)
1	C	1.27	6/2421 (0.2%)	1.07	3/3291 (0.1%)
1	D	1.26	3/2266 (0.1%)	1.07	3/3077 (0.1%)
1	E	1.21	3/2425 (0.1%)	1.05	2/3295 (0.1%)
1	F	1.23	4/2254 (0.2%)	1.04	2/3064 (0.1%)
All	All	1.21	24/14031 (0.2%)	1.05	16/19067 (0.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207	ASP	CB-CG	6.70	1.68	1.52
1	C	110	THR	CA-C	6.66	1.61	1.52
1	F	18	SER	C-O	6.63	1.31	1.23
1	B	156	GLU	C-O	-5.84	1.16	1.24
1	C	147	ASP	C-O	-5.80	1.17	1.23
1	F	42	GLU	CA-C	5.80	1.60	1.52
1	B	207	ASP	CB-CG	5.79	1.66	1.52
1	E	104	ILE	C-O	-5.54	1.20	1.24
1	B	140	LEU	C-O	-5.45	1.19	1.24
1	B	106	ALA	N-CA	5.38	1.56	1.46
1	F	9	ARG	N-CA	5.37	1.52	1.46
1	C	107	ALA	N-CA	5.37	1.52	1.46
1	D	63	PHE	CA-CB	5.37	1.60	1.53
1	B	273	ALA	C-O	-5.36	1.17	1.24
1	B	223	ASN	CA-C	-5.32	1.46	1.52
1	D	207	ASP	C-O	-5.32	1.17	1.24
1	B	240	LYS	C-O	-5.25	1.17	1.24
1	B	34	ILE	CA-C	5.24	1.58	1.52
1	C	34	ILE	CA-CB	5.21	1.56	1.54
1	F	151	LYS	C-O	-5.17	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	184	GLU	C-O	-5.13	1.17	1.24
1	C	209	ASN	C-O	-5.05	1.18	1.24
1	E	70	LEU	CB-CG	-5.05	1.43	1.53
1	E	240	LYS	C-O	-5.01	1.17	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	233	ASP	N-CA-C	6.88	118.57	111.14
1	A	207	ASP	N-CA-C	5.79	119.87	112.34
1	B	271	ASN	N-CA-C	5.69	117.56	111.36
1	F	247	ASP	N-CA-C	5.67	118.40	111.82
1	B	233	ASP	N-CA-C	5.63	117.22	111.14
1	E	230	VAL	N-CA-C	5.50	116.15	110.82
1	B	133	ASN	CA-C-N	-5.36	115.07	120.21
1	B	133	ASN	C-N-CA	-5.36	115.07	120.21
1	C	41	PHE	N-CA-C	5.20	120.27	112.94
1	C	81	ASP	CA-C-N	-5.12	114.39	119.56
1	C	81	ASP	C-N-CA	-5.12	114.39	119.56
1	E	41	PHE	N-CA-C	5.05	120.06	112.94
1	D	140	LEU	CA-C-N	-5.04	115.05	120.03
1	D	140	LEU	C-N-CA	-5.04	115.05	120.03
1	F	40	GLN	N-CA-C	5.04	116.46	111.07
1	B	230	VAL	N-CA-C	5.00	116.11	111.45

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	2312	0	2229	9	0
1	B	2172	0	2113	12	0
1	C	2326	0	2251	6	0
1	D	2170	0	2123	10	0
1	E	2331	0	2254	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2161	0	2113	7	0
2	A	20	0	9	1	0
2	C	20	0	9	0	0
2	D	40	0	22	5	0
2	E	20	0	9	0	0
2	F	39	0	15	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	4	0	0	0	0
3	F	3	0	0	0	0
4	B	20	0	9	2	0
4	D	36	0	18	4	0
5	B	6	0	8	1	0
5	F	6	0	8	0	0
6	A	361	0	0	2	0
6	B	329	0	0	8	0
6	C	347	0	0	0	0
6	D	297	0	0	2	0
6	E	312	0	0	3	0
6	F	267	0	0	0	0
All	All	15609	0	13190	55	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 2.

All (55) 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:B:33[A]:HIS:NE2	6:B:2070[A]:HOH:O	1.58	0.93
4:B:301:X8W:HAM	5:B:302:GOL:O1	1.70	0.91
4:B:301:X8W:HAH	6:B:2182:HOH:O	1.83	0.77
1:C:93[B]:PHE:CD1	1:C:114:ILE:HD12	2.19	0.77
1:E:95[A]:MET:HE3	1:E:110:THR:HG22	1.71	0.72
1:B:177[A]:GLU:HG3	6:B:2230:HOH:O	1.91	0.69
1:C:171[A]:GLU:H	1:C:171[A]:GLU:CD	2.00	0.68
2:D:301:NAR:H81	6:D:2070:HOH:O	1.93	0.68
1:B:33[A]:HIS:CE1	6:B:2070[A]:HOH:O	2.19	0.65
1:E:95[A]:MET:HE2	1:E:110:THR:HA	1.82	0.61
1:E:171[A]:GLU:H	1:E:171[A]:GLU:CD	2.08	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ASN:ND2	1:A:131:GLU:H	2.04	0.55
1:B:240:LYS:NZ	1:B:247[A]:ASP:OD1	2.41	0.54
1:A:129:ASN:HD22	1:A:131:GLU:H	1.55	0.54
2:D:301:NAR:C15	4:D:303[A]:X8W:HAJ	2.38	0.54
1:F:104:ILE:HG12	2:F:301:NAR:C3	2.37	0.54
4:D:303[B]:X8W:OAB	6:D:2239:HOH:O	2.18	0.53
1:B:104[A]:ILE:HG22	1:B:105:PRO:O	2.08	0.53
6:A:2339:HOH:O	1:B:276:ARG:HD3	2.09	0.52
1:A:276:ARG:HD2	1:D:276:ARG:HD2	1.92	0.51
1:E:40[A]:GLN:NE2	6:E:2077:HOH:O	2.22	0.51
1:D:104:ILE:HG22	1:D:105:PRO:O	2.11	0.51
4:D:303[A]:X8W:CAT	4:D:303[A]:X8W:CAQ	2.90	0.50
1:B:1:ALA:HB2	6:B:2002:HOH:O	2.12	0.50
1:D:104:ILE:HG12	2:D:302:NAR:C3	2.42	0.49
1:D:249:PHE:CD1	1:D:250:PRO:HA	2.46	0.49
1:A:126:LYS:HE2	6:A:2197:HOH:O	2.12	0.49
1:C:276:ARG:HD2	1:F:276:ARG:HD2	1.96	0.48
1:B:1:ALA:CB	6:B:2004:HOH:O	2.61	0.48
1:F:104:ILE:HG12	2:F:301:NAR:C4	2.44	0.47
1:D:143:TRP:CE2	1:F:84:LEU:HG	2.49	0.47
1:D:101:GLN:OE1	2:D:301:NAR:O4	2.33	0.47
1:D:40:GLN:NE2	1:D:91[B]:GLU:HG3	2.30	0.46
1:E:7:PRO:HA	1:E:75:TRP:O	2.15	0.46
1:E:276:ARG:HD3	6:E:2299:HOH:O	2.16	0.46
1:A:103:GLN:HA	1:A:133:ASN:O	2.17	0.44
1:B:95[A]:MET:HE2	1:B:95[A]:MET:HB3	1.73	0.44
1:E:95[A]:MET:CE	1:E:110:THR:HA	2.48	0.43
1:D:33[B]:HIS:CE1	2:D:301:NAR:C7	3.02	0.43
1:A:36:ASP:O	1:A:40[A]:GLN:HG3	2.19	0.43
1:C:96:ASP:HB3	1:C:100:TRP:CZ2	2.54	0.43
1:B:177[A]:GLU:CG	6:B:2230:HOH:O	2.58	0.42
1:F:155:ILE:HD12	1:F:155:ILE:HA	1.95	0.42
1:C:40[A]:GLN:CD	1:C:87:LYS:HD3	2.44	0.42
1:D:40:GLN:HE22	1:D:91[B]:GLU:HG3	1.85	0.42
1:E:249:PHE:CD1	1:E:250:PRO:HA	2.55	0.42
1:A:126:LYS:O	1:A:127:SER:C	2.63	0.41
1:A:73:HIS:CE1	2:A:301:NAR:H82	2.55	0.41
1:F:140:LEU:HB3	1:F:141:PRO:HD2	2.03	0.41
1:A:249:PHE:CD1	1:A:250:PRO:HA	2.55	0.41
1:C:155:ILE:HD12	1:C:155:ILE:HA	1.95	0.41
1:B:143:TRP:CE2	1:D:84:LEU:HG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:ALA:HB3	6:B:2004:HOH:O	2.20	0.41
4:D:303[A]:X8W:CAQ	4:D:303[A]:X8W:CAN	2.98	0.41
6:E:2298:HOH:O	1:F:276:ARG:HD3	2.20	0.41

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	285/283 (101%)	280 (98%)	5 (2%)	0	100	100
1	B	263/283 (93%)	259 (98%)	4 (2%)	0	100	100
1	C	287/283 (101%)	281 (98%)	5 (2%)	1 (0%)	36	35
1	D	263/283 (93%)	260 (99%)	3 (1%)	0	100	100
1	E	288/283 (102%)	283 (98%)	5 (2%)	0	100	100
1	F	262/283 (93%)	259 (99%)	3 (1%)	0	100	100
All	All	1648/1698 (97%)	1622 (98%)	25 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	207	ASP

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	245/241 (102%)	242 (99%)	3 (1%)	63	70
1	B	233/241 (97%)	232 (100%)	1 (0%)	84	89
1	C	247/241 (102%)	244 (99%)	3 (1%)	63	70
1	D	233/241 (97%)	232 (100%)	1 (0%)	84	89
1	E	248/241 (103%)	248 (100%)	0	100	100
1	F	232/241 (96%)	231 (100%)	1 (0%)	84	89
All	All	1438/1446 (99%)	1429 (99%)	9 (1%)	78	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	171[A]	GLU
1	A	171[B]	GLU
1	B	41	PHE
1	C	41	PHE
1	C	115	ASP
1	C	177	GLU
1	D	41	PHE
1	F	41	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	109	HIS
1	A	129	ASN
1	A	224	GLN
1	A	257	ASN
1	B	224	GLN
1	C	101	GLN
1	C	224	GLN
1	D	101	GLN
1	D	224	GLN
1	D	257	ASN
1	E	101	GLN
1	E	224	GLN
1	E	274	ASN
1	F	40	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 ⓘ

Of 30 ligands modelled in this entry, 17 are monoatomic - leaving 13 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$
2	NAR	C	301	-	22,22,22	2.01	4 (18%)	32,32,32	2.32	12 (37%)
2	NAR	D	302	-	22,22,22	3.50	6 (27%)	32,32,32	5.88	13 (40%)
2	NAR	E	301	-	22,22,22	1.72	4 (18%)	32,32,32	2.57	12 (37%)
2	NAR	F	301	-	22,22,22	1.24	2 (9%)	32,32,32	2.32	7 (21%)
4	X8W	B	301	-	21,21,21	2.58	6 (28%)	29,29,29	1.51	6 (20%)
4	X8W	D	303[B]	-	18,18,21	1.12	2 (11%)	22,23,29	1.66	2 (9%)
4	X8W	D	303[A]	-	18,18,21	1.13	1 (5%)	22,23,29	1.22	3 (13%)
2	NAR	D	301	-	22,22,22	2.85	8 (36%)	32,32,32	2.57	11 (34%)
5	GOL	B	302	-	5,5,5	0.51	0	5,5,5	1.90	1 (20%)
5	GOL	F	303	-	5,5,5	1.09	0	5,5,5	1.97	2 (40%)
2	NAR	F	302[B]	-	9,9,22	3.37	3 (33%)	12,12,32	1.15	1 (8%)
2	NAR	A	301	-	22,22,22	1.60	3 (13%)	32,32,32	2.06	8 (25%)
2	NAR	F	302[A]	-	9,9,22	2.83	2 (22%)	12,12,32	1.19	1 (8%)

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	NAR	C	301	-	-	0/4/16/16	0/3/3/3
2	NAR	D	302	-	-	2/4/16/16	0/3/3/3
2	NAR	E	301	-	-	1/4/16/16	0/3/3/3
2	NAR	F	301	-	-	3/4/16/16	0/3/3/3
4	X8W	B	301	-	-	6/9/9/9	0/2/2/2
4	X8W	D	303[B]	-	-	2/2/2/9	0/2/2/2
4	X8W	D	303[A]	-	-	2/2/2/9	0/2/2/2
2	NAR	D	301	-	-	2/4/16/16	0/3/3/3
5	GOL	B	302	-	-	4/4/4/4	-
5	GOL	F	303	-	-	4/4/4/4	-
2	NAR	F	302[B]	-	-	-	0/1/1/3
2	NAR	A	301	-	-	0/4/16/16	0/3/3/3
2	NAR	F	302[A]	-	-	-	0/1/1/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	302	NAR	C14-C13	-11.53	1.17	1.39
2	D	302	NAR	C12-C13	8.83	1.55	1.39
4	B	301	X8W	CAF-CAG	7.82	1.52	1.33
2	D	301	NAR	C5-C4	7.65	1.53	1.41
2	F	302[B]	NAR	C1-C2	7.18	1.49	1.39
2	D	301	NAR	C5-C6	6.71	1.52	1.40
2	F	302[B]	NAR	C1-C6	6.51	1.48	1.39
4	B	301	X8W	CAF-CAN	6.44	1.58	1.47
2	F	302[A]	NAR	C1-C6	5.79	1.47	1.39
2	F	302[A]	NAR	C1-C2	5.62	1.47	1.39
2	C	301	NAR	C5-C4	5.29	1.49	1.41
2	C	301	NAR	C5-C6	4.77	1.49	1.40
2	E	301	NAR	C5-C4	4.64	1.48	1.41
2	A	301	NAR	C5-C6	4.20	1.48	1.40
2	D	301	NAR	O1-C6	4.16	1.43	1.38
2	D	301	NAR	O5-C4	3.97	1.44	1.36
2	E	301	NAR	C5-C6	3.94	1.47	1.40
2	D	302	NAR	C5-C6	3.93	1.47	1.40
2	C	301	NAR	O1-C9	3.69	1.53	1.44
4	D	303[A]	X8W	CAT-CAN	-3.67	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAR	C5-C7	3.65	1.55	1.46
2	C	301	NAR	O1-C6	3.63	1.42	1.38
2	D	302	NAR	C12-C11	3.59	1.44	1.38
2	A	301	NAR	C5-C4	3.39	1.46	1.41
4	B	301	X8W	CAQ-CAG	-3.35	1.38	1.47
2	E	301	NAR	O1-C9	3.10	1.51	1.44
2	F	301	NAR	C5-C4	3.10	1.46	1.41
2	A	301	NAR	O1-C9	3.05	1.51	1.44
2	F	301	NAR	C5-C6	2.94	1.45	1.40
2	D	302	NAR	C5-C4	2.85	1.46	1.41
2	D	302	NAR	C11-C10	2.82	1.43	1.39
4	B	301	X8W	CAT-CAN	-2.58	1.42	1.49
2	D	301	NAR	O2-C7	2.44	1.26	1.22
4	B	301	X8W	CAH-CAJ	2.41	1.42	1.38
4	B	301	X8W	OAC-CAP	-2.36	1.31	1.37
4	D	303[B]	X8W	CAL-CAR	2.32	1.42	1.38
4	D	303[B]	X8W	CAT-CAS	-2.26	1.38	1.41
2	D	301	NAR	C1-C2	2.25	1.42	1.39
2	D	301	NAR	C3-C4	2.16	1.42	1.38
2	F	302[B]	NAR	C3-C2	2.07	1.42	1.39
2	E	301	NAR	C5-C7	2.01	1.51	1.46

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302	NAR	C14-C15-C10	20.87	142.02	121.18
2	D	302	NAR	C15-C10-C11	-15.85	98.65	118.30
2	D	302	NAR	C15-C10-C9	13.36	150.78	120.63
2	D	302	NAR	O1-C6-C5	-7.82	113.80	121.64
2	F	301	NAR	O1-C6-C5	-7.30	114.32	121.64
2	E	301	NAR	O1-C6-C1	7.16	128.51	116.29
2	C	301	NAR	O1-C6-C1	6.53	127.45	116.29
2	D	302	NAR	O1-C6-C1	6.19	126.85	116.29
2	F	301	NAR	O1-C6-C1	6.12	126.75	116.29
2	A	301	NAR	O1-C6-C1	6.11	126.73	116.29
4	D	303[B]	X8W	CAR-CAT-CAN	5.93	124.50	120.09
2	E	301	NAR	O1-C6-C5	-5.86	115.76	121.64
2	D	302	NAR	C14-C13-C12	-5.86	110.45	119.77
2	D	301	NAR	C4-C5-C6	5.83	122.98	117.41
2	A	301	NAR	O1-C6-C5	-5.70	115.92	121.64
2	D	301	NAR	C6-C5-C7	-5.63	114.79	120.29
2	C	301	NAR	O1-C6-C5	-5.60	116.02	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAR	C3-C2-C1	5.53	128.06	120.47
2	D	301	NAR	C3-C4-C5	-5.38	114.89	120.92
2	D	301	NAR	O1-C9-C10	4.83	116.46	107.47
2	D	302	NAR	C11-C10-C9	-4.53	110.40	120.63
2	E	301	NAR	C3-C2-C1	4.43	126.55	120.47
2	D	301	NAR	O1-C6-C1	4.12	123.32	116.29
2	F	301	NAR	C6-O1-C9	4.06	122.64	115.54
2	C	301	NAR	C3-C2-C1	3.96	125.90	120.47
2	E	301	NAR	C4-C5-C6	3.95	121.17	117.41
2	E	301	NAR	C8-C7-C5	3.75	123.54	116.77
2	D	301	NAR	C1-C6-C5	-3.70	115.34	121.79
4	D	303[B]	X8W	CAS-CAT-CAN	-3.64	117.39	120.09
2	D	302	NAR	O1-C9-C10	-3.59	100.79	107.47
5	F	303	GOL	C3-C2-C1	-3.54	98.80	111.80
2	C	301	NAR	C4-C5-C6	3.50	120.75	117.41
2	E	301	NAR	C1-C6-C5	-3.49	115.72	121.79
2	C	301	NAR	C8-C7-C5	3.46	123.01	116.77
5	B	302	GOL	O1-C1-C2	-3.40	95.07	110.38
2	D	302	NAR	C12-C11-C10	3.27	124.45	121.18
4	D	303[A]	X8W	OAA-CAN-CAT	-3.20	117.21	124.80
2	F	301	NAR	C15-C10-C9	-3.12	113.58	120.63
2	E	301	NAR	O2-C7-C8	-3.03	115.87	120.81
2	A	301	NAR	O5-C4-C5	-3.03	115.55	121.14
2	C	301	NAR	C1-C6-C5	-3.02	116.52	121.79
2	D	302	NAR	O3-C13-C12	3.02	128.41	120.00
2	F	301	NAR	O5-C4-C5	-2.92	115.74	121.14
2	C	301	NAR	O2-C7-C8	-2.92	116.06	120.81
2	F	301	NAR	C11-C10-C9	2.88	127.13	120.63
2	E	301	NAR	C3-C4-C5	-2.80	117.78	120.92
4	B	301	X8W	CAJ-CAH-CAO	2.80	122.84	119.88
2	E	301	NAR	O2-C7-C5	-2.78	118.19	122.49
2	F	301	NAR	O1-C9-C10	2.75	112.59	107.47
2	C	301	NAR	C3-C4-C5	-2.73	117.86	120.92
4	D	303[A]	X8W	CAM-CAS-CAT	-2.69	118.24	120.87
2	F	302[A]	NAR	C5-C4-C3	2.67	124.13	120.47
2	D	302	NAR	C4-C3-C2	2.61	122.08	119.67
4	B	301	X8W	CAG-CAF-CAN	-2.61	117.36	121.61
2	A	301	NAR	C1-C6-C5	-2.57	117.31	121.79
2	D	302	NAR	C15-C14-C13	2.54	122.56	119.88
2	A	301	NAR	O2-C7-C5	-2.52	118.59	122.49
2	A	301	NAR	C8-C7-C5	2.49	121.26	116.77
2	D	301	NAR	C6-O1-C9	2.43	119.80	115.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAR	O1-C9-C10	2.42	111.97	107.47
4	D	303[A]	X8W	CAS-CAT-CAN	-2.40	118.31	120.09
4	B	301	X8W	CAR-CAL-CAP	-2.38	117.47	119.67
2	D	301	NAR	O2-C7-C5	-2.38	118.82	122.49
2	D	302	NAR	C6-C5-C7	2.34	122.56	120.29
4	B	301	X8W	OAA-CAN-CAF	-2.33	117.07	120.67
2	A	301	NAR	O1-C9-C10	2.32	111.79	107.47
2	E	301	NAR	C6-C5-C7	-2.31	118.03	120.29
2	F	302[B]	NAR	C4-C3-C2	2.29	122.09	119.26
2	D	301	NAR	O4-C2-C1	-2.26	113.94	119.85
5	F	303	GOL	O2-C2-C3	2.24	118.43	109.18
2	E	301	NAR	O4-C2-C3	-2.22	114.04	119.85
2	E	301	NAR	C6-O1-C9	2.22	119.42	115.54
4	B	301	X8W	CAI-CAO-CAH	-2.20	116.26	119.77
2	A	301	NAR	C3-C2-C1	2.19	123.48	120.47
4	B	301	X8W	OAB-CAO-CAH	2.16	126.00	120.00
2	C	301	NAR	O2-C7-C5	-2.15	119.16	122.49
2	C	301	NAR	C6-C5-C7	-2.10	118.25	120.29
2	C	301	NAR	O4-C2-C3	-2.04	114.52	119.85
2	D	301	NAR	C9-C8-C7	2.03	118.29	112.25

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	303[A]	X8W	OAA-CAN-CAT-CAR
4	D	303[A]	X8W	OAA-CAN-CAT-CAS
5	B	302	GOL	O1-C1-C2-C3
5	B	302	GOL	C1-C2-C3-O3
5	F	303	GOL	O1-C1-C2-C3
5	F	303	GOL	C1-C2-C3-O3
4	B	301	X8W	CAF-CAG-CAQ-CAK
4	B	301	X8W	CAF-CAG-CAQ-CAJ
5	B	302	GOL	O2-C2-C3-O3
5	F	303	GOL	O1-C1-C2-O2
4	B	301	X8W	OAA-CAN-CAT-CAS
4	D	303[B]	X8W	OAA-CAN-CAT-CAR
4	D	303[B]	X8W	OAA-CAN-CAT-CAS
5	B	302	GOL	O1-C1-C2-O2
4	B	301	X8W	CAF-CAN-CAT-CAS
4	B	301	X8W	OAA-CAN-CAT-CAR
5	F	303	GOL	O2-C2-C3-O3

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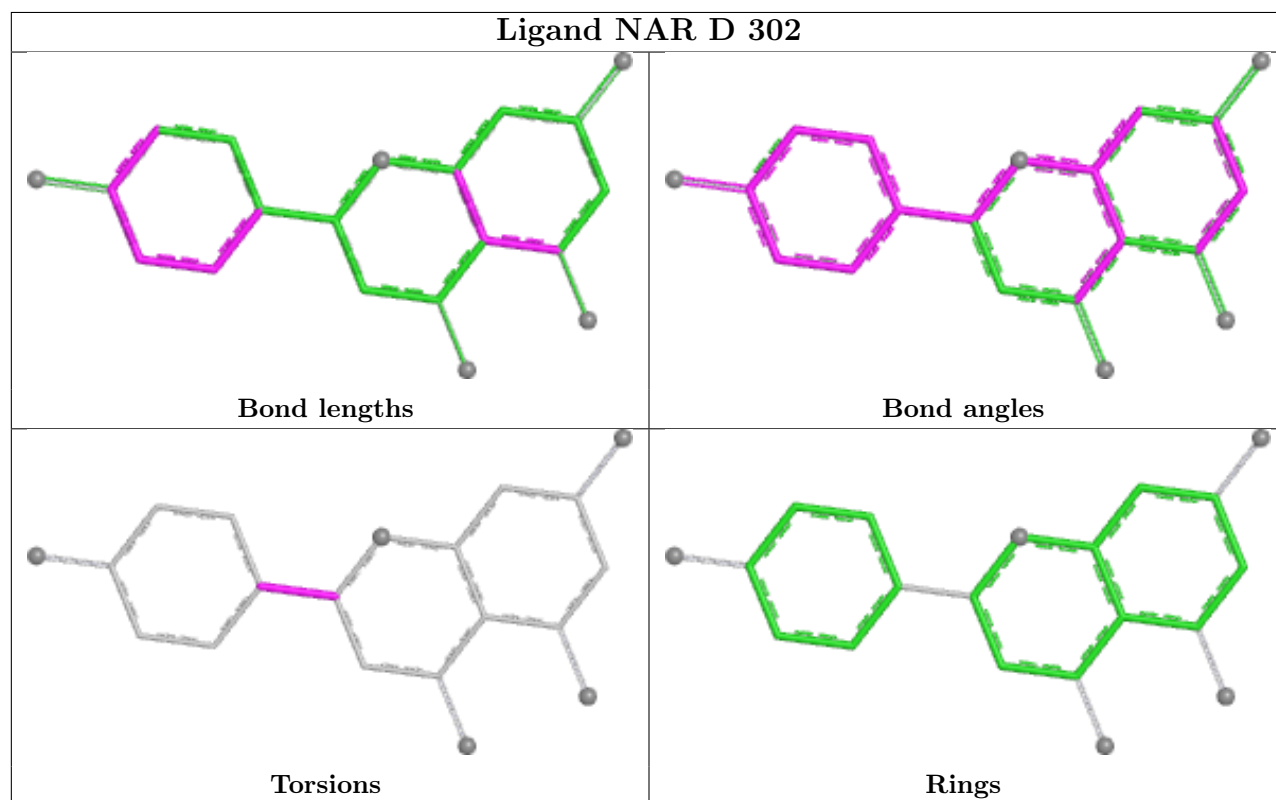
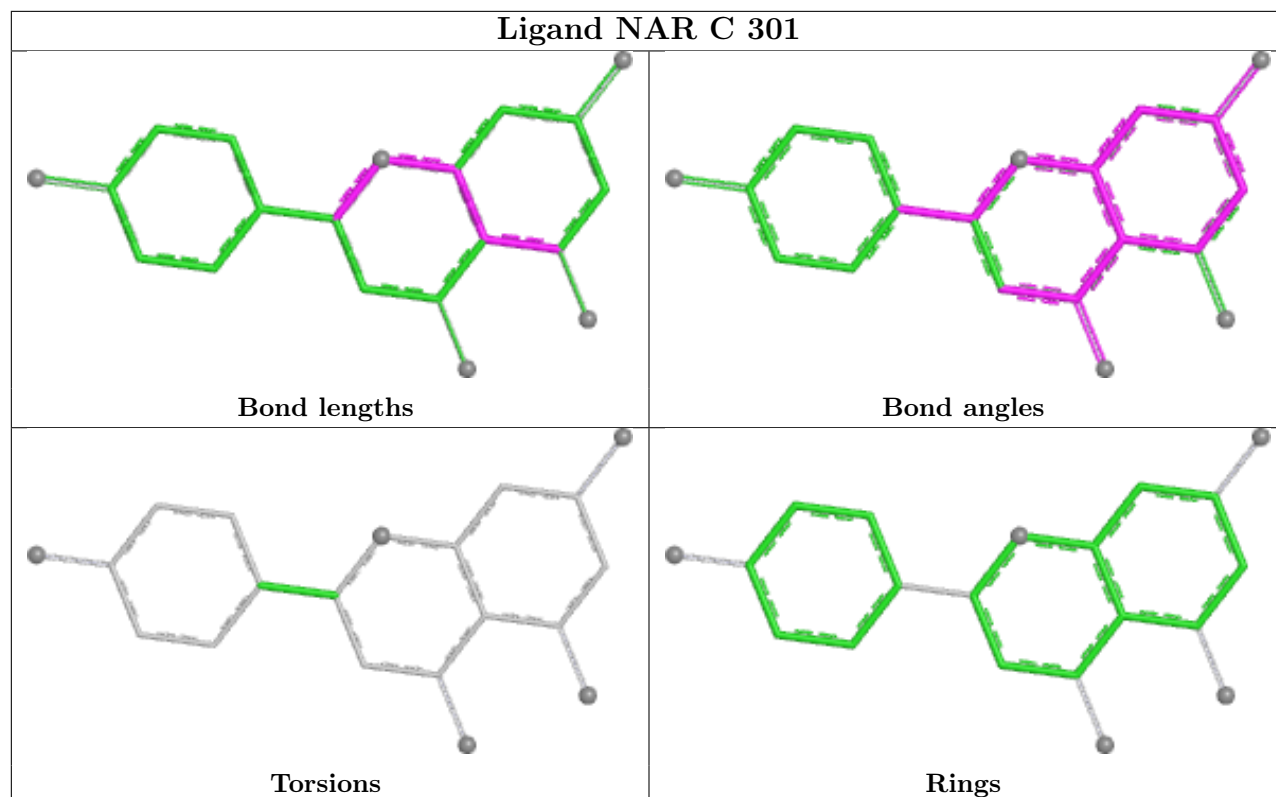
Mol	Chain	Res	Type	Atoms
2	F	301	NAR	C11-C10-C9-C8
2	D	302	NAR	C11-C10-C9-C8
2	F	301	NAR	C15-C10-C9-C8
2	D	302	NAR	C15-C10-C9-C8
2	E	301	NAR	C11-C10-C9-O1
2	D	301	NAR	C15-C10-C9-O1
4	B	301	X8W	CAF-CAN-CAT-CAR
2	D	301	NAR	C11-C10-C9-O1
2	F	301	NAR	C15-C10-C9-O1

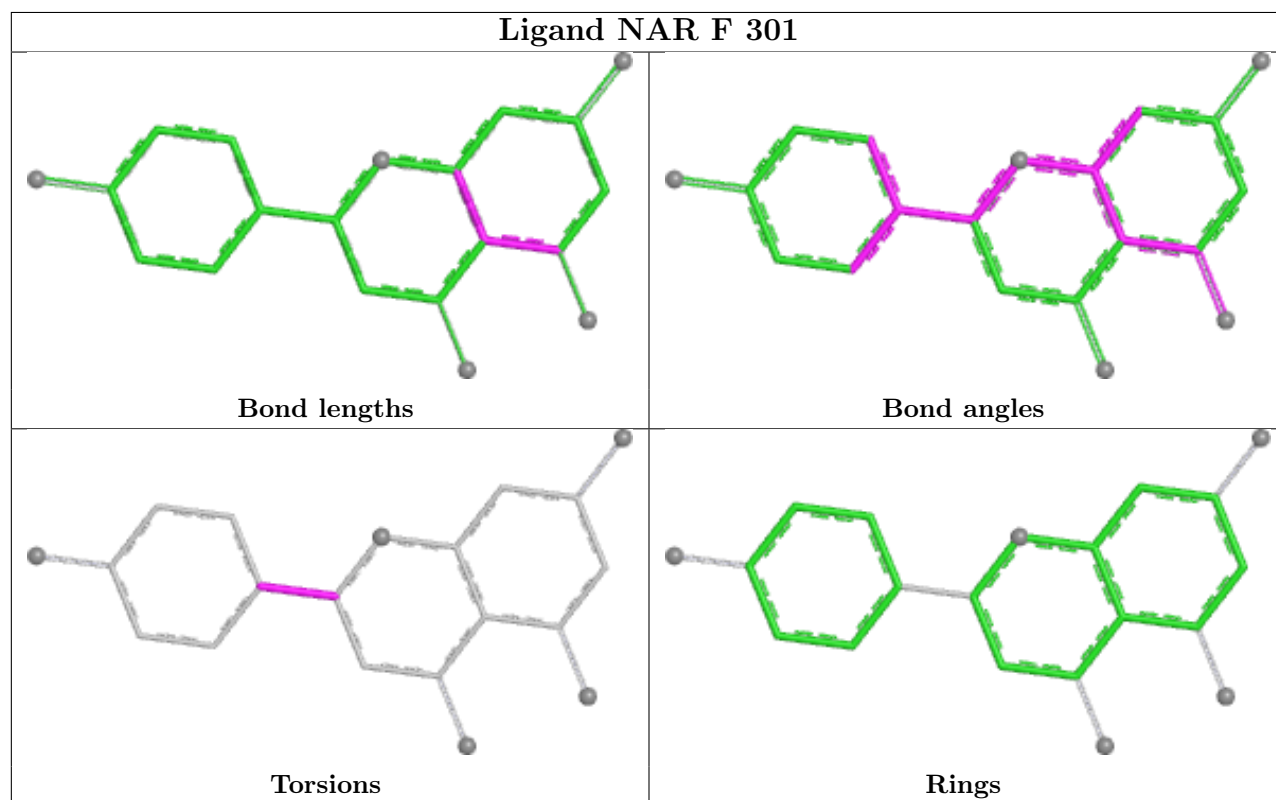
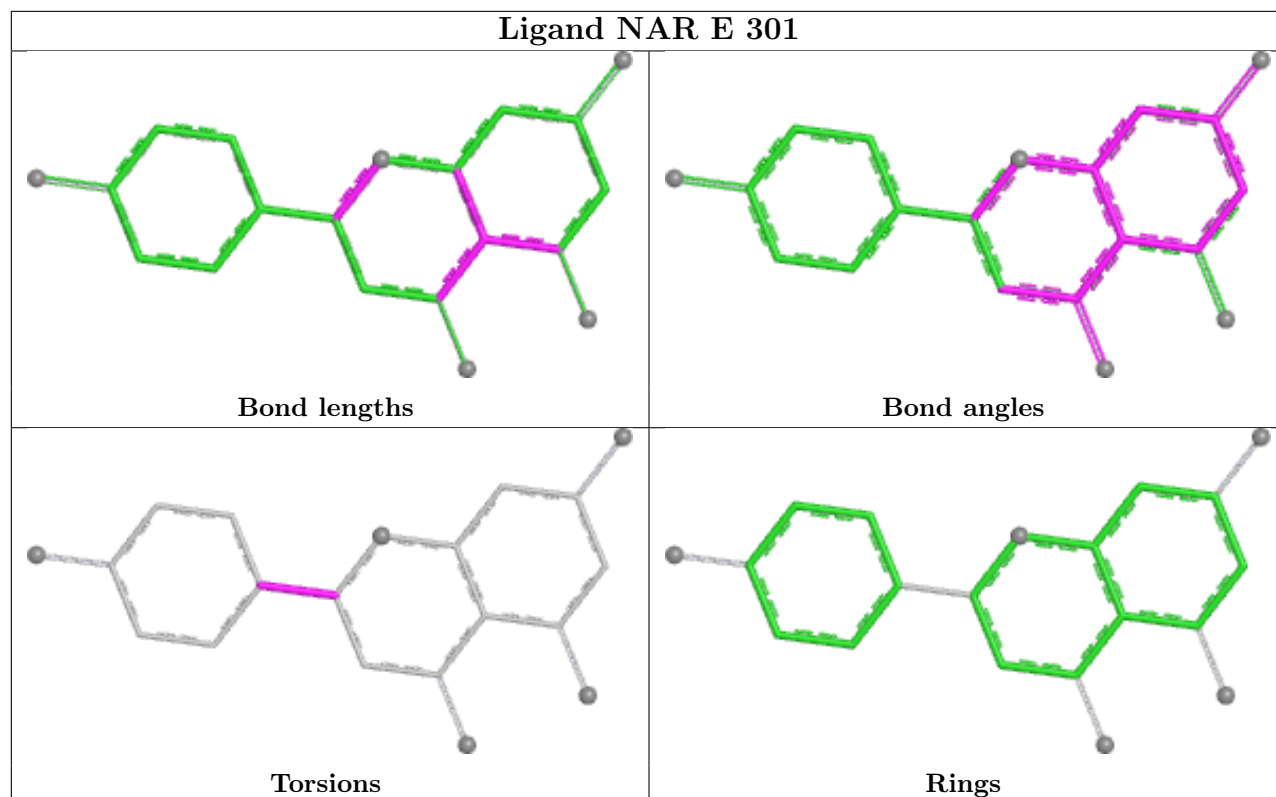
There are no ring outliers.

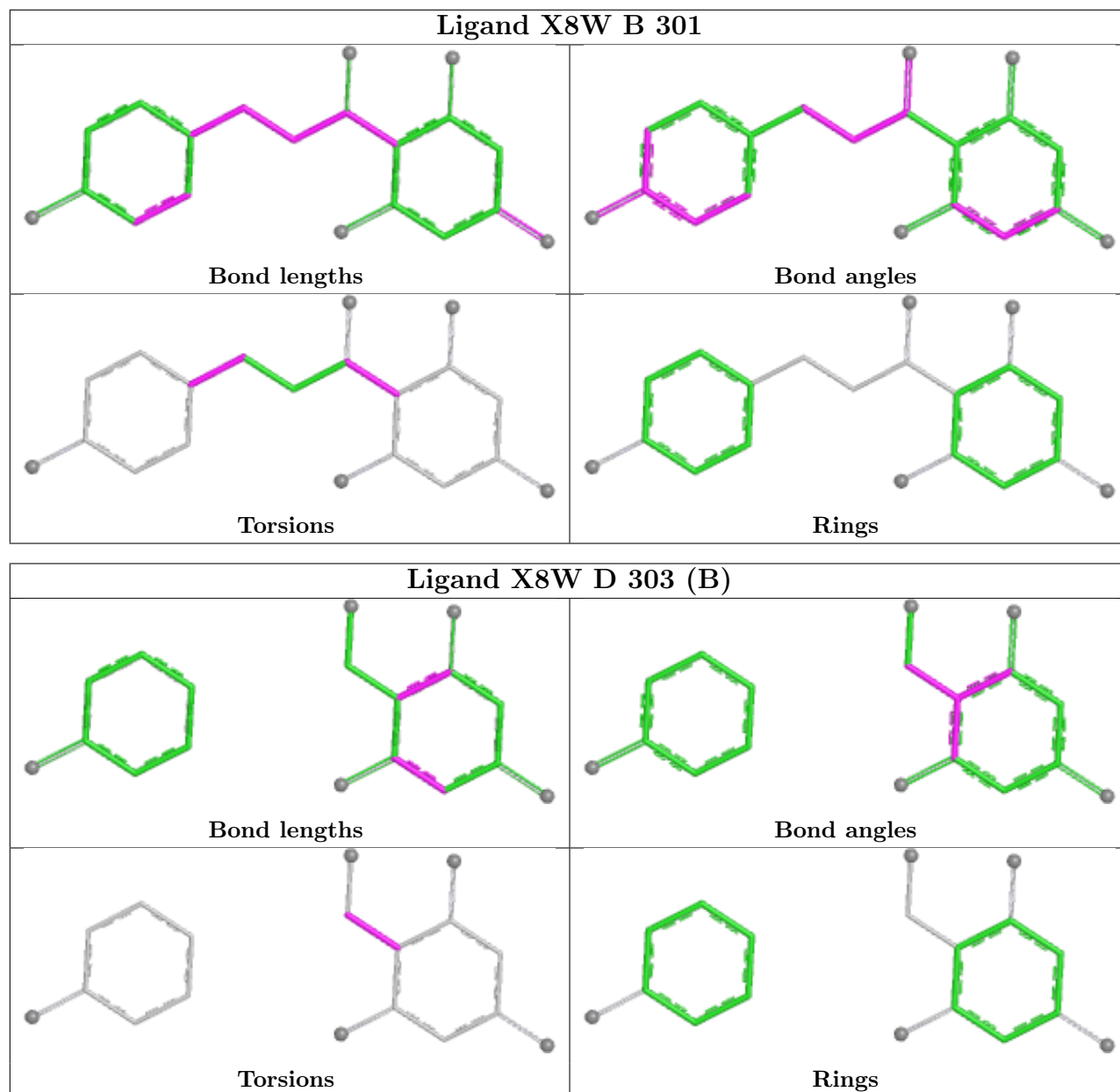
8 monomers are involved in 13 short contacts:

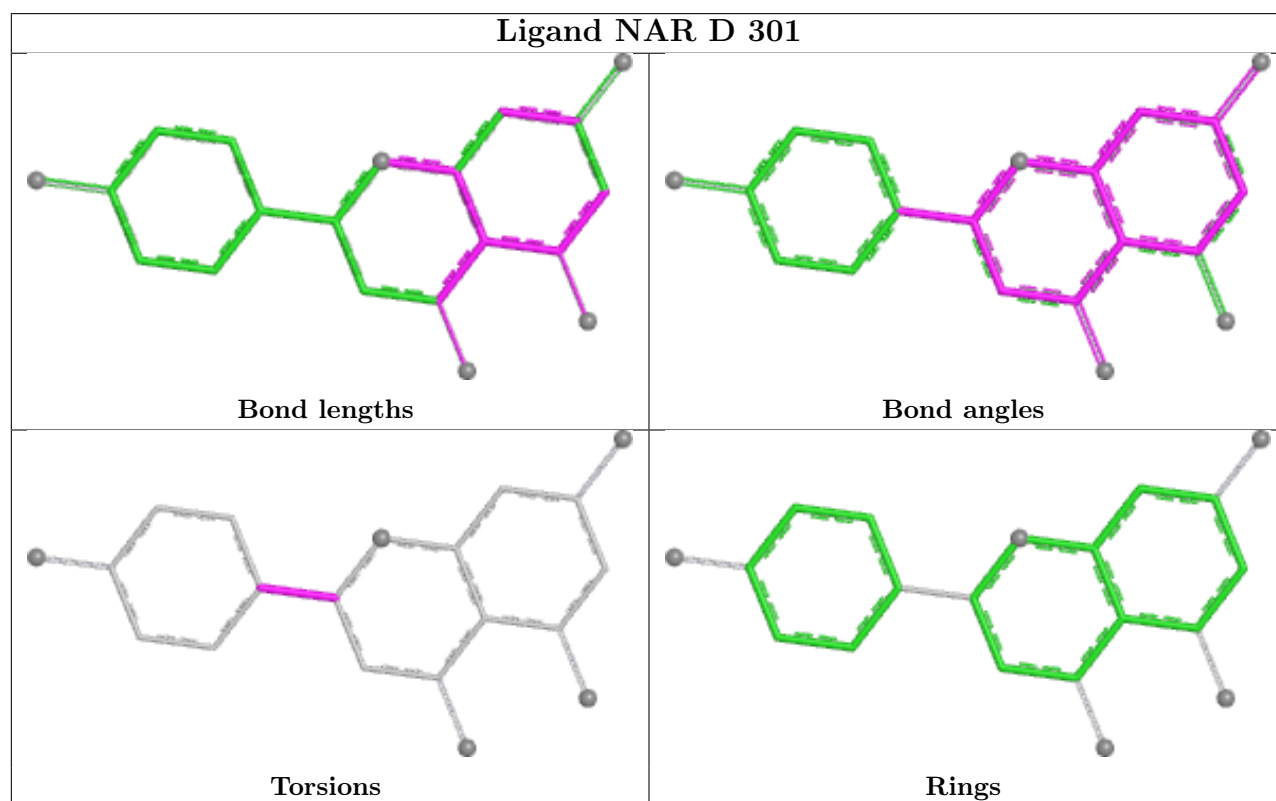
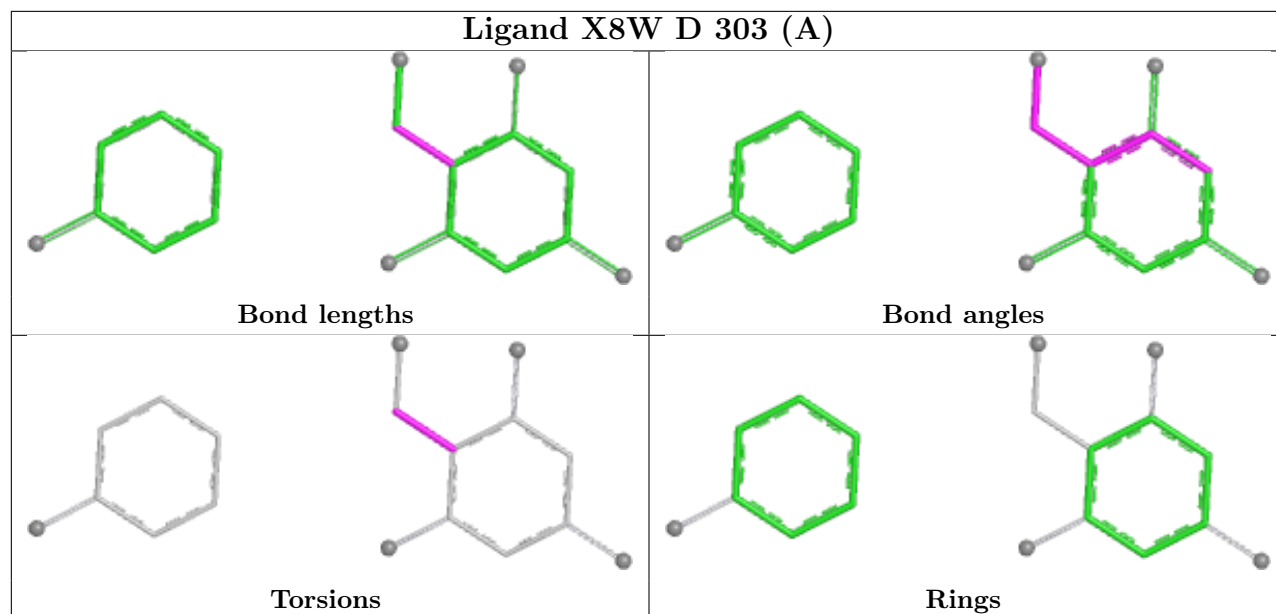
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	302	NAR	1	0
2	F	301	NAR	2	0
4	B	301	X8W	2	0
4	D	303[B]	X8W	1	0
4	D	303[A]	X8W	3	0
2	D	301	NAR	4	0
5	B	302	GOL	1	0
2	A	301	NAR	1	0

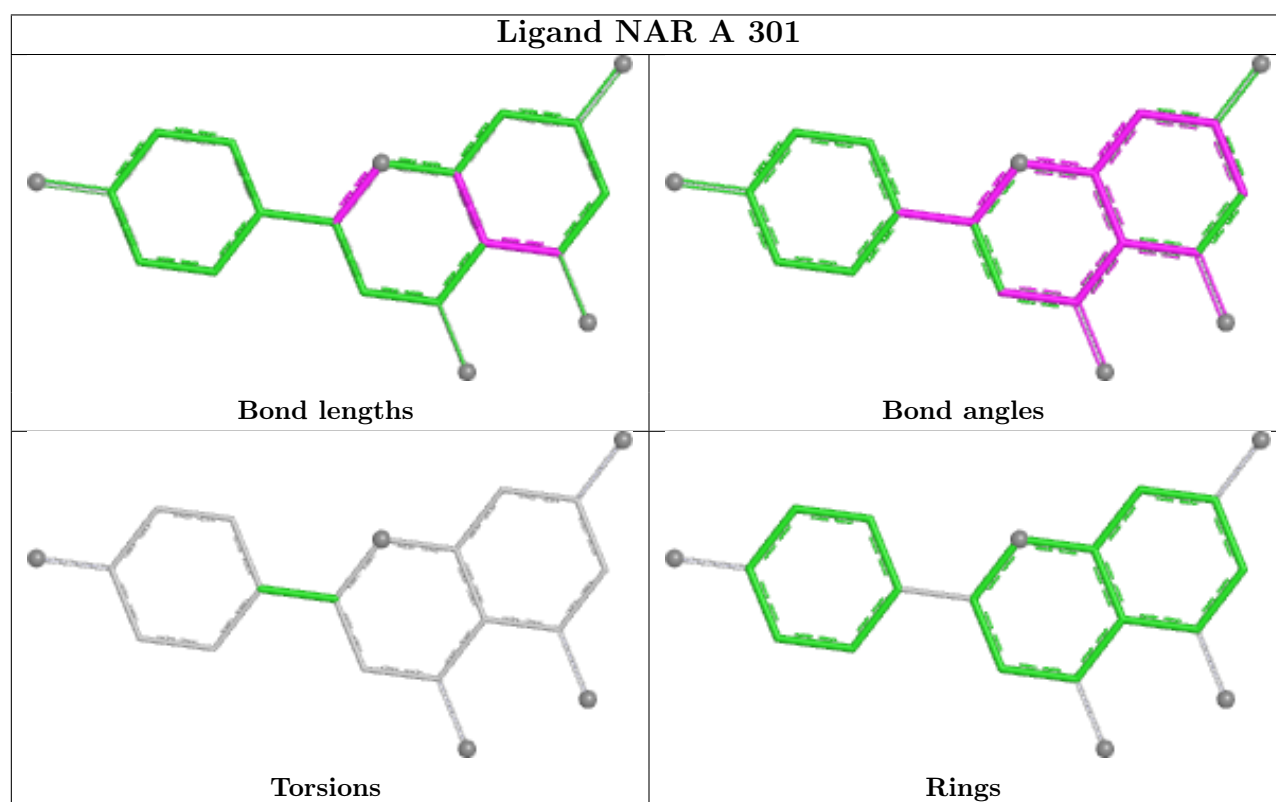
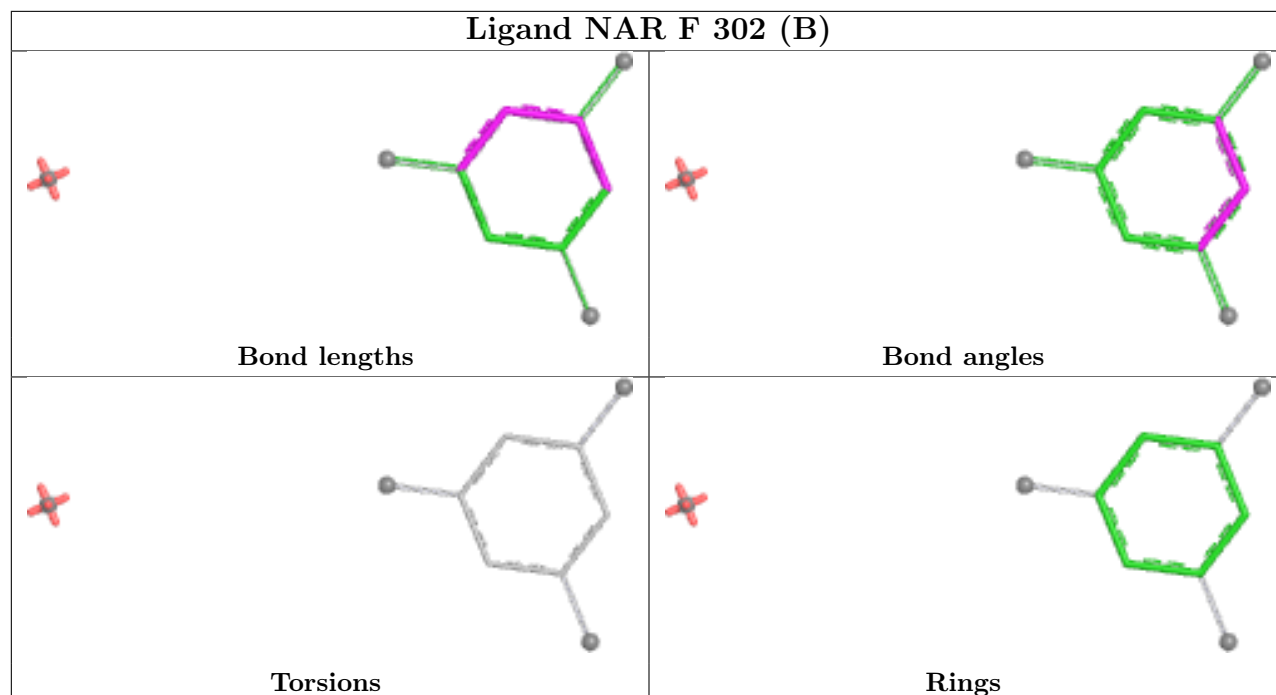
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

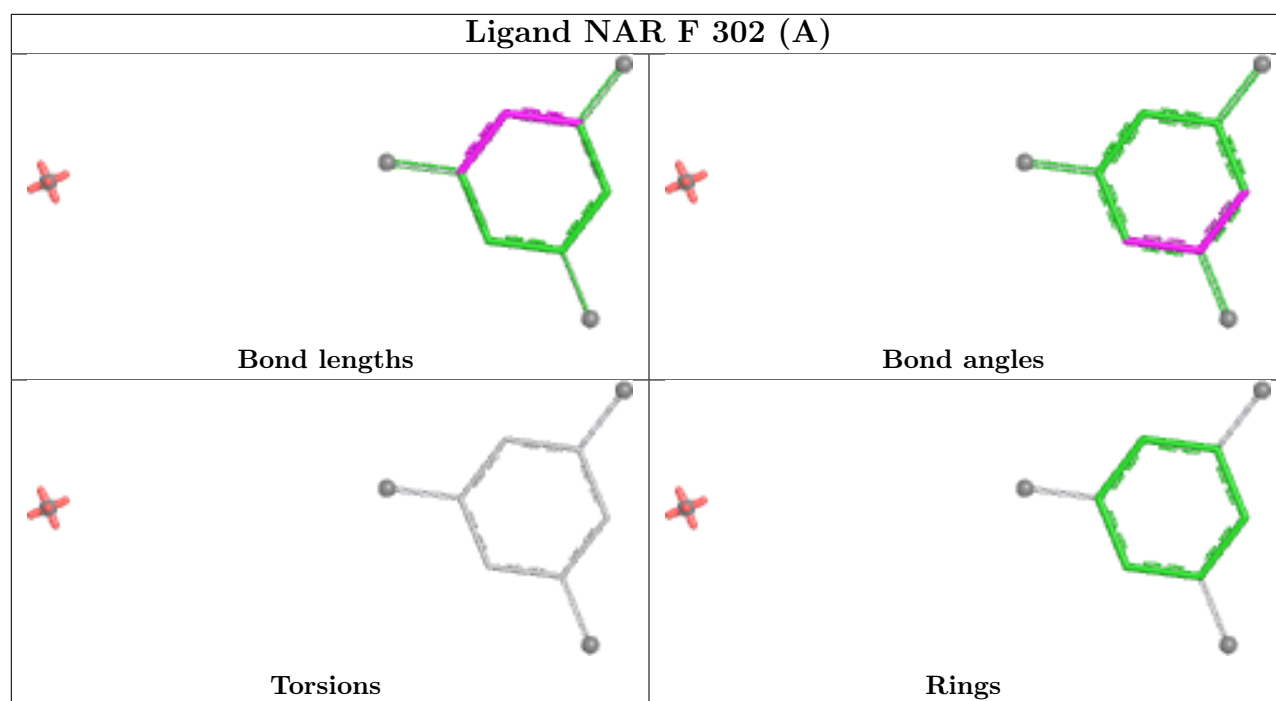












5.7 Other polymers [i](#)

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	282/283 (99%)	-0.45	9 (3%)	50	49	11, 24, 46, 70	5 (1%)
1	B	259/283 (91%)	-0.74	4 (1%)	72	71	12, 21, 32, 77	8 (3%)
1	C	282/283 (99%)	-0.58	5 (1%)	67	67	12, 22, 40, 64	7 (2%)
1	D	259/283 (91%)	-0.79	2 (0%)	82	82	11, 20, 29, 59	8 (3%)
1	E	282/283 (99%)	-0.53	12 (4%)	40	39	12, 22, 46, 69	8 (2%)
1	F	259/283 (91%)	-0.74	2 (0%)	82	82	10, 20, 33, 62	6 (2%)
All	All	1623/1698 (95%)	-0.63	34 (2%)	63	63	10, 21, 41, 77	42 (2%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	106	ALA	8.3
1	B	130	ALA	5.2
1	B	106	ALA	5.0
1	D	106	ALA	4.1
1	A	108	ALA	3.6
1	A	107	ALA	3.6
1	B	131	GLU	3.4
1	D	130	ALA	3.3
1	E	115	ASP	3.1
1	A	114	ILE	3.1
1	A	130	ALA	3.0
1	E	107	ALA	3.0
1	E	108	ALA	3.0
1	F	130	ALA	2.9
1	E	130	ALA	2.9
1	C	130	ALA	2.9
1	E	128	ASN	2.7
1	A	109	HIS	2.7
1	C	115	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	121	GLY	2.5
1	A	117	ASP	2.4
1	C	108	ALA	2.3
1	E	114	ILE	2.3
1	E	123	ALA	2.3
1	E	109	HIS	2.2
1	B	1	ALA	2.2
1	E	118	GLY	2.1
1	A	116	SER	2.1
1	C	116	SER	2.1
1	A	128	ASN	2.1
1	E	117	ASP	2.1
1	E	116	SER	2.1
1	C	117	ASP	2.1
1	E	121	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	X8W	B	301	20/20	0.77	0.24	49,58,69,78	8
2	NAR	D	301	20/20	0.81	0.23	35,49,61,62	11
2	NAR	F	302[B]	10/20	0.85	0.26	44,54,59,74	9
2	NAR	F	302[A]	10/20	0.85	0.26	47,57,59,74	9
3	CL	E	404	1/1	0.87	0.18	60,60,60,60	0
3	CL	C	403	1/1	0.87	0.16	54,54,54,54	0
3	CL	B	402	1/1	0.88	0.14	54,54,54,54	0
3	CL	A	402	1/1	0.88	0.19	53,53,53,53	0

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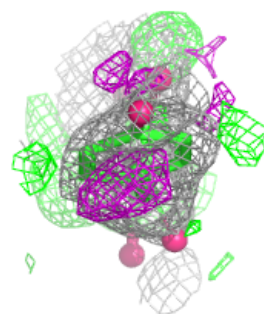
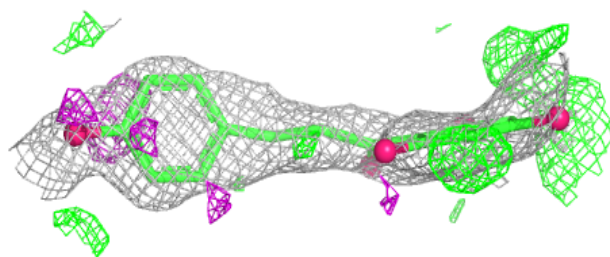
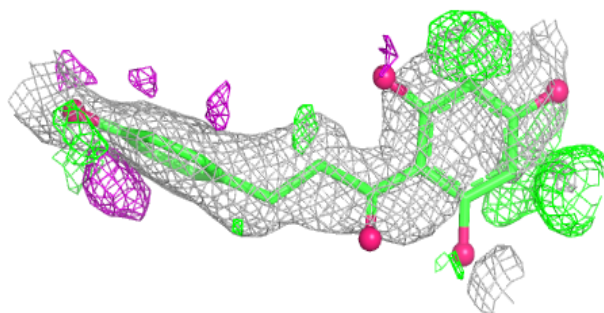
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	C	402	1/1	0.89	0.13	60,60,60,60	0
3	CL	D	403	1/1	0.90	0.13	49,49,49,49	0
4	X8W	D	303[A]	18/20	0.90	0.19	36,62,67,70	18
4	X8W	D	303[B]	18/20	0.90	0.19	37,39,76,77	18
3	CL	F	401	1/1	0.91	0.12	48,48,48,48	0
3	CL	E	402	1/1	0.92	0.13	59,59,59,59	0
5	GOL	B	302	6/6	0.93	0.14	26,27,27,27	6
5	GOL	F	303	6/6	0.93	0.11	34,36,39,44	0
3	CL	C	401	1/1	0.94	0.10	52,52,52,52	0
2	NAR	C	301	20/20	0.94	0.09	26,30,32,32	20
2	NAR	E	301	20/20	0.94	0.10	27,32,36,36	20
3	CL	A	401	1/1	0.95	0.12	59,59,59,59	0
2	NAR	F	301	20/20	0.95	0.09	28,30,32,32	20
3	CL	D	402	1/1	0.95	0.09	56,56,56,56	0
3	CL	B	401	1/1	0.95	0.10	53,53,53,53	0
2	NAR	D	302	20/20	0.95	0.09	26,28,35,44	20
2	NAR	A	301	20/20	0.95	0.09	26,30,33,33	20
3	CL	F	402	1/1	0.96	0.11	51,51,51,51	0
3	CL	E	403	1/1	0.96	0.12	63,63,63,63	1
3	CL	F	403	1/1	0.97	0.07	45,45,45,45	0
3	CL	E	401	1/1	0.97	0.07	50,50,50,50	0
3	CL	D	401	1/1	0.97	0.06	48,48,48,48	0

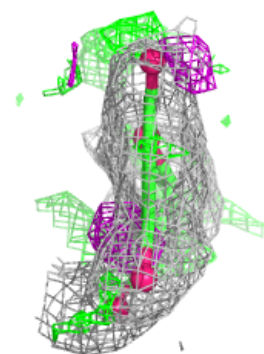
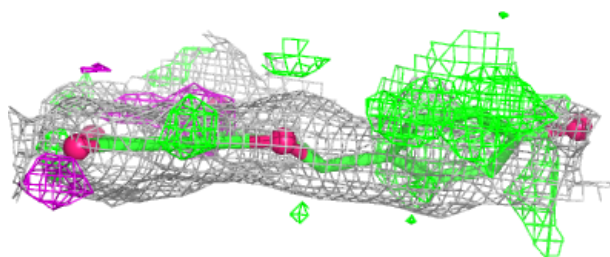
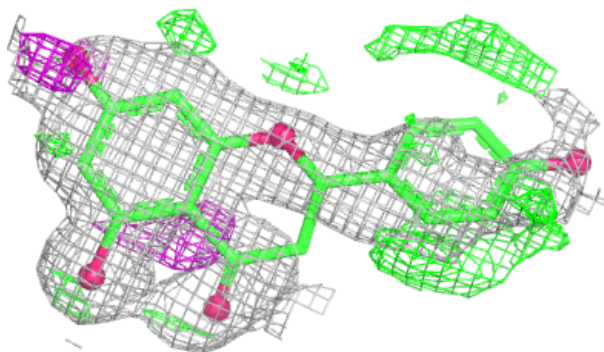
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around X8W B 301:

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

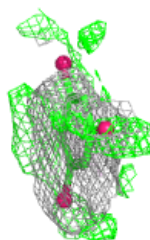
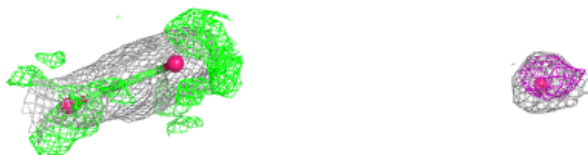
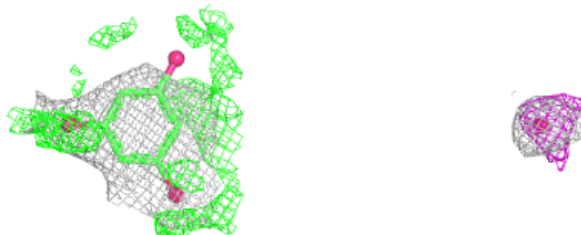
**Electron density around NAR D 301:**

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

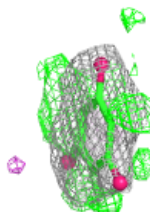
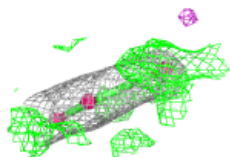
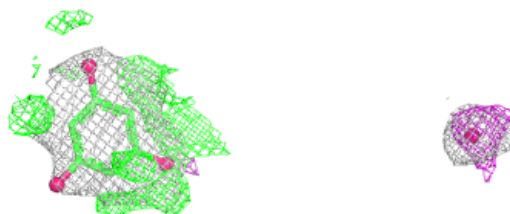


Electron density around NAR F 302 (B):

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

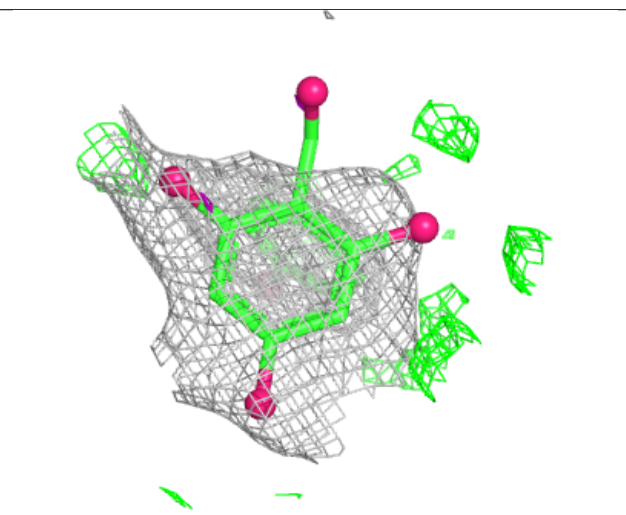
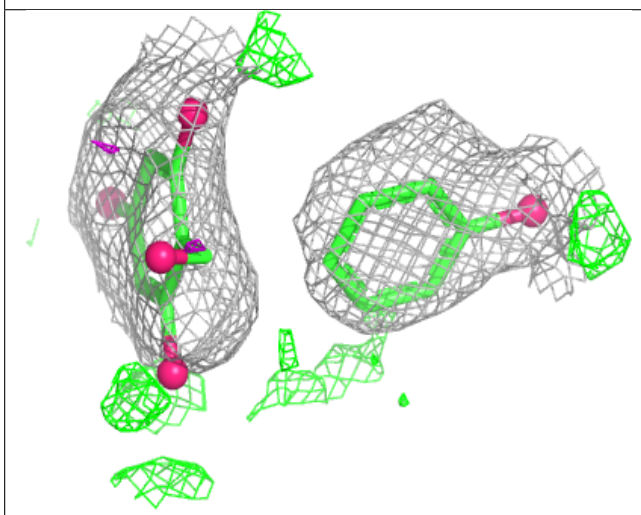
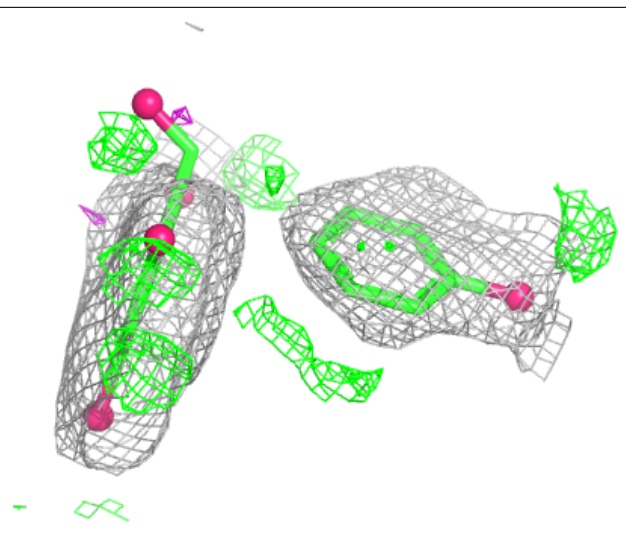
**Electron density around NAR F 302 (A):**

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and green (positive)



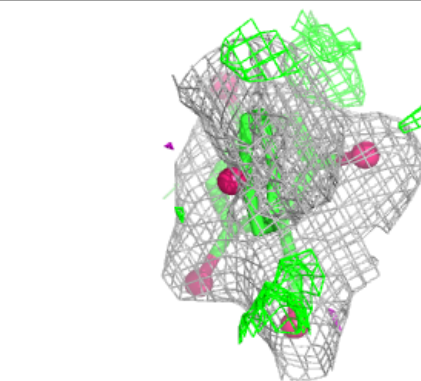
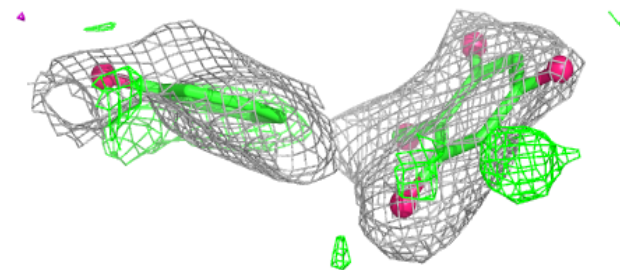
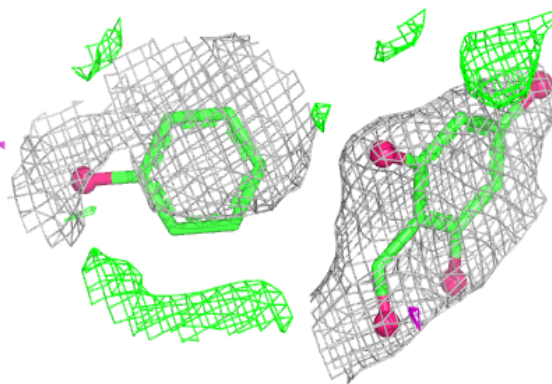
Electron density around X8W D 303 (A):

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

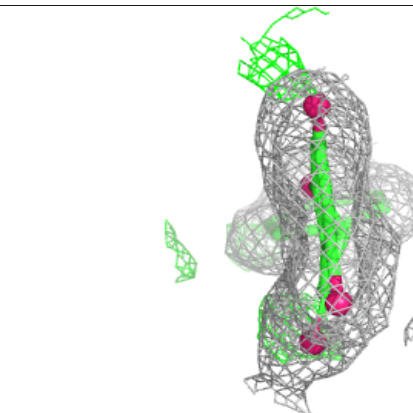
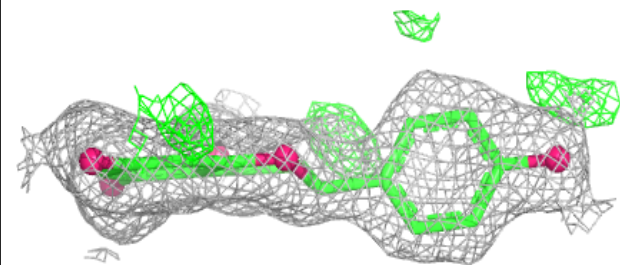
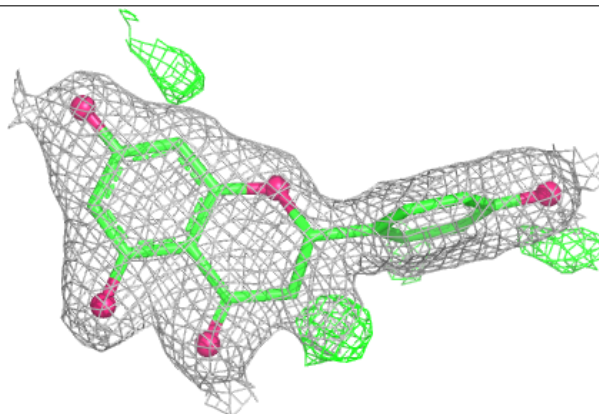


Electron density around X8W D 303 (B):

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and green (positive)

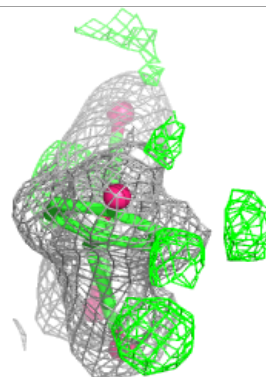
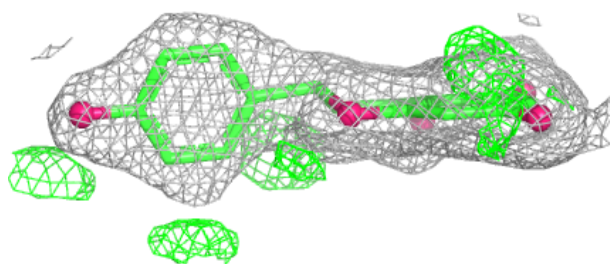
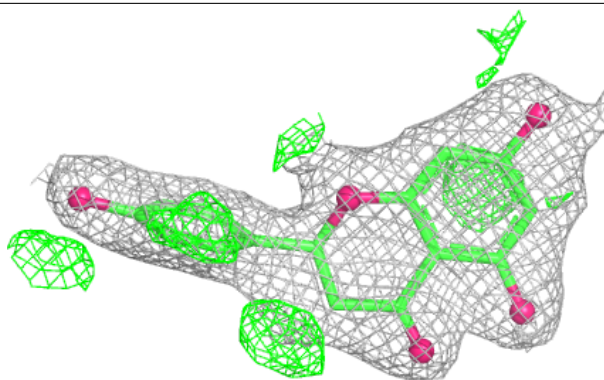
**Electron density around NAR C 301:**

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

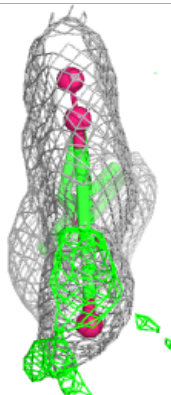
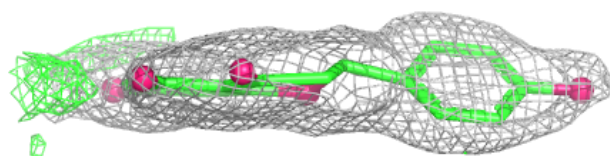
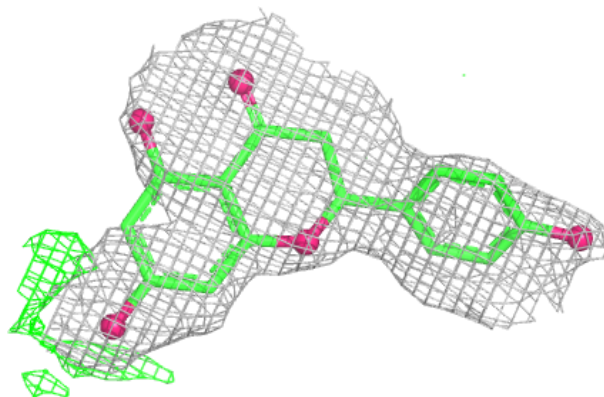


Electron density around NAR E 301:

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

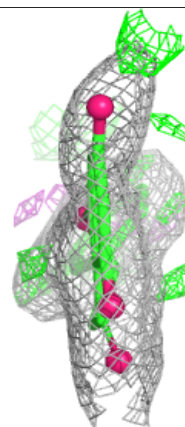
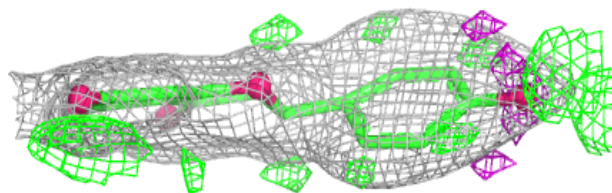
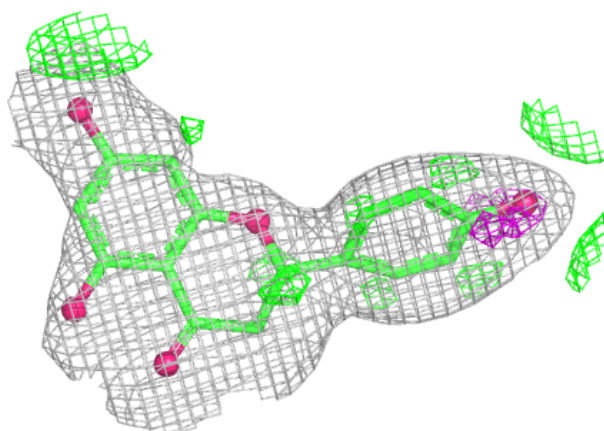
**Electron density around NAR F 301:**

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

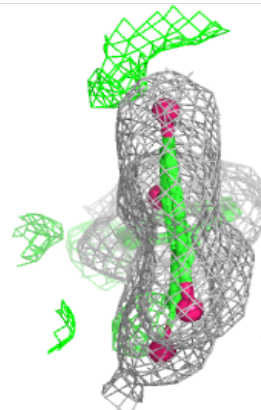
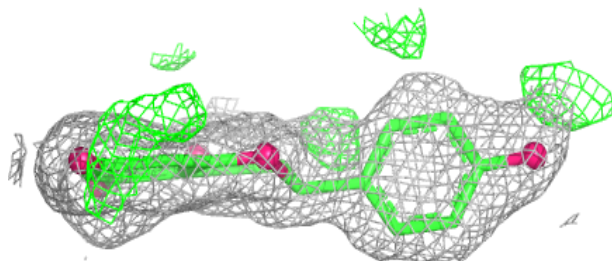
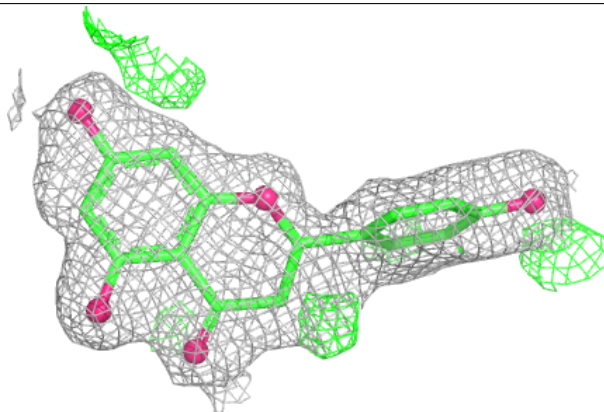


Electron density around NAR D 302:

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

**Electron density around NAR A 301:**

$2mF_o-DF_c$ (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.