Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 05:52 pm GMT

PDB ID	:	6GHV
Title	:	Structure of a DC-SIGN CRD in complex with high affinity glycomimetic.
Authors	:	Thepaut, M.; Achilli, S.; Medve, L.; Bernardi, A.; Fieschi, F.
Deposited on	:	2018-05-09
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

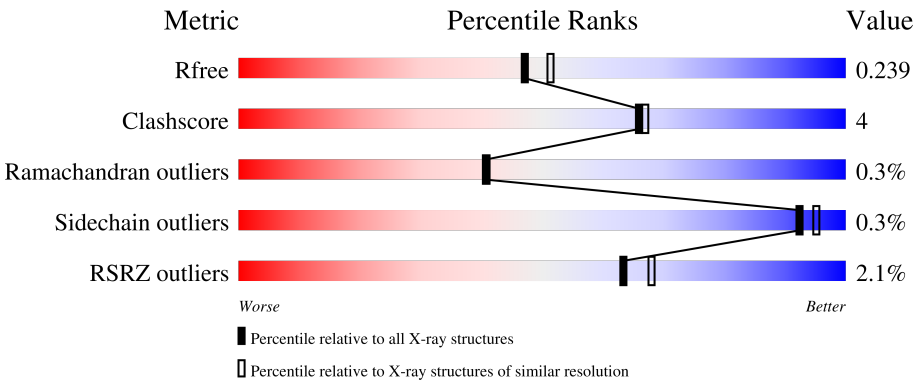
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	155	2%, 74%, 11%, 15%
1	B	155	%, 76%, 8%, •, 15%
1	C	155	%, 81%, 5%, 14%
1	D	155	3%, 77%, 8%, 14%
1	E	155	2%, 78%, 8%, 14%

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Mol	Chain	Length	Quality of chain
1	F	155	2% 76% 9% 15%

2 Entry composition (i)

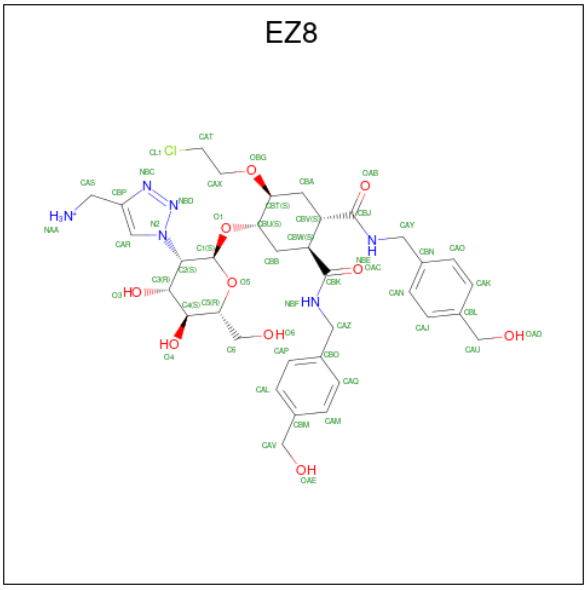
There are 5 unique types of molecules in this entry. The entry contains 7569 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CD209 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	132	1092	687	188	207	10	0	4	0
1	B	132	1092	687	188	207	10	0	4	0
1	C	133	1094	689	188	207	10	0	3	0
1	D	133	1104	695	190	209	10	0	5	0
1	E	133	1084	683	186	205	10	0	1	0
1	F	132	1088	685	188	205	10	0	3	0

- Molecule 2 is [1-[(2 {S},3 {S},4 {R},5 {S},6 {R})-2-[(1 {S},2 {S},4 {S},5 {S})-2-(2-chloroethyloxy)-4,5-bis[[4-(hydroxymethyl)phenyl]methylcarbamoyl]cyclohexyl]oxy-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-3-yl]-1,2,3-triazol-4-yl]methylazanium (three-letter code: EZ8) (formula: $C_{35}H_{48}ClN_6O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	52	35	1	6	10	0	0
2	B	1	52	35	1	6	10	0	0
2	C	1	52	35	1	6	10	0	0
2	D	1	52	35	1	6	10	0	0
2	E	1	52	35	1	6	10	0	0
2	F	1	52	35	1	6	10	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	3	3	3	0	0
3	B	3	3	3	0	0
3	C	3	3	3	0	0
3	D	3	3	3	0	0
3	E	3	3	3	0	0
3	F	3	3	3	0	0

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

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

- Molecule 5 is water.

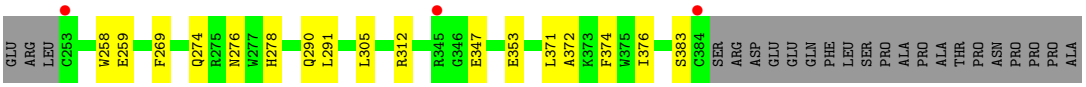
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	95	97	97	0	2
			Total	O		
5	B	125	127	127	0	2
			Total	O		
5	C	135	137	137	0	2
			Total	O		
5	D	99	101	101	0	2
			Total	O		
5	E	112	114	114	0	2
			Total	O		
5	F	94	95	95	0	1

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: CD209 antigen

Chain A:

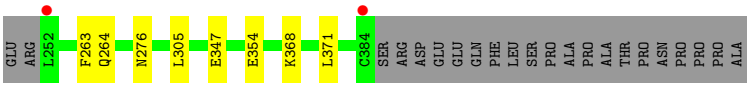


- Molecule 1: CD209 antigen

Chain B:

- Molecule 1: CD209 antigen

Chain C:



- Molecule 1: CD209 antigen

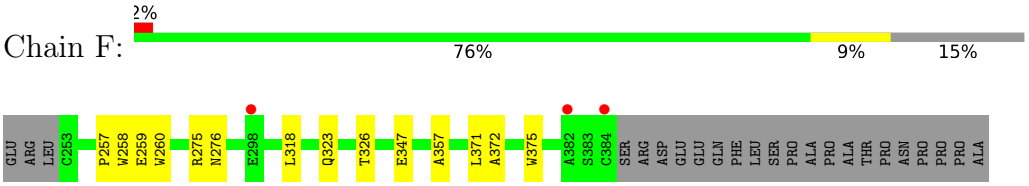
Chain D:

- Molecule 1: CD209 antigen

Chain E:

- Molecule 1: CD209 antigen

Chain F:


2%
76%
9%
15%
GLU
ARG
LEU
C253
P257
W258
E259
W260
R275
N276
E298
L318
Q323
T326
E347
A357
L371
A372
W375
A382
S383
C384
SER
ARG
ASP
GLU
GLU
GLN
PHE
LEU
SER
PRO
ALA
PRO
ALA
THR
PRO
ASN
PRO
PRO
PRO
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.61Å 57.51Å 107.25Å 90.00° 118.67° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 39.47 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (40.00-2.10) 98.6 (39.47-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.176 , 0.234 0.184 , 0.239	Depositor DCC
R_{free} test set	3261 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h-l,k,h 0.015 for l,k,-h-l 0.018 for h,-k,-h-l 0.021 for -h-l,-k,l 0.024 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7569	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, CA, EZ8

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	0.73	0/1138	0.75	0/1544
1	B	0.78	0/1138	0.79	0/1544
1	C	0.77	0/1137	0.76	0/1543
1	D	0.76	0/1153	0.77	0/1565
1	E	0.74	0/1121	0.77	0/1521
1	F	0.70	0/1132	0.77	0/1536
All	All	0.75	0/6819	0.77	0/9253

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 (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	1092	0	990	11	0
1	B	1092	0	990	12	0
1	C	1094	0	993	6	0
1	D	1104	0	1005	8	0
1	E	1084	0	981	8	0
1	F	1088	0	983	10	0
2	A	52	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	52	0	0	0	0
2	C	52	0	0	2	0
2	D	52	0	0	0	0
2	E	52	0	0	1	0
2	F	52	0	0	2	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
5	A	97	0	0	1	0
5	B	127	0	0	4	0
5	C	137	0	0	1	0
5	D	101	0	0	0	0
5	E	114	0	0	2	0
5	F	95	0	0	0	0
All	All	7569	0	5942	51	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 (51) 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:A:372:ALA:H	1:D:274:GLN:HE22	1.18	0.91
1:A:274:GLN:HE22	1:D:372:ALA:H	1.14	0.89
1:A:278:HIS:ND1	5:A:1101:HOH:O	2.24	0.69
1:F:275:ARG:HD2	1:F:375:TRP:CH2	2.31	0.65
1:E:274:GLN:HE22	1:F:372:ALA:H	1.47	0.61
1:B:300:GLN:HE22	1:B:364:TRP:HE1	1.49	0.59
1:E:337:PRO:HA	1:E:340:LYS:HD2	1.86	0.56
1:E:311:ASN:HB3	5:E:696:HOH:O	2.05	0.55
1:A:258:TRP:O	1:A:259:GLU:HB2	2.07	0.54
1:B:276:ASN:HA	1:B:371:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:TRP:O	1:F:259:GLU:HB2	2.09	0.52
1:F:276:ASN:HA	1:F:371:LEU:O	2.09	0.52
1:C:276:ASN:HA	1:C:371:LEU:O	2.10	0.51
1:A:276:ASN:HA	1:A:371:LEU:O	2.11	0.51
1:E:347:GLU:OE2	2:E:503:EZ8:O4	2.27	0.51
1:D:276:ASN:HA	1:D:371:LEU:O	2.11	0.51
1:D:352:GLY:O	1:D:353:GLU:HB2	2.12	0.50
1:E:368:LYS:HE3	5:E:615:HOH:O	2.13	0.48
1:B:258:TRP:O	1:B:259:GLU:HB2	2.13	0.48
1:B:290[A]:GLN:HG3	5:B:1201:HOH:O	2.14	0.48
1:C:354:GLU:OE2	2:C:1001:EZ8:O3	2.33	0.47
1:F:257:PRO:HB2	1:F:260:TRP:CD1	2.50	0.47
1:A:269:PHE:O	1:A:376:ILE:HA	2.15	0.46
1:B:290[B]:GLN:HG2	1:B:291:LEU:O	2.16	0.46
1:F:258:TRP:O	1:F:259:GLU:CB	2.62	0.46
1:B:320:ASP:OD1	1:B:355:ASP:HA	2.16	0.46
1:F:275:ARG:HD2	1:F:375:TRP:CZ3	2.50	0.45
1:E:275:ARG:HD2	1:E:375:TRP:CH2	2.51	0.45
2:A:1001:EZ8:CAL	1:D:312:ARG:HG3	2.47	0.45
1:A:258:TRP:O	1:A:259:GLU:CB	2.65	0.44
1:A:305:LEU:HD21	1:C:305:LEU:CD2	2.48	0.44
1:C:263:PHE:CE1	1:C:264:GLN:HG3	2.53	0.44
1:B:300:GLN:NE2	1:B:364:TRP:HE1	2.15	0.44
1:D:320:ASP:OD1	1:D:355:ASP:HA	2.18	0.43
1:A:312:ARG:HD2	1:A:374:PHE:CE2	2.54	0.43
1:E:258:TRP:O	1:E:259:GLU:HB2	2.18	0.43
1:B:281:ILE:HG22	1:B:285:LYS:HE2	2.00	0.42
1:A:347:GLU:OE2	2:A:1001:EZ8:O4	2.37	0.42
1:B:368:LYS:HE3	5:B:1125:HOH:O	2.19	0.42
1:D:275:ARG:HD2	1:D:375:TRP:CZ3	2.55	0.42
1:F:323:GLN:NE2	1:F:326:THR:OG1	2.43	0.42
1:F:347:GLU:OE2	2:F:502:EZ8:O4	2.38	0.42
1:B:285:LYS:HE3	5:B:1168:HOH:O	2.19	0.42
1:A:290[B]:GLN:HG2	1:A:291:LEU:O	2.19	0.41
1:F:318:LEU:HB3	1:F:357:ALA:HB3	2.03	0.41
1:C:368:LYS:NZ	5:C:1108:HOH:O	2.53	0.41
1:B:272[B]:ASN:ND2	5:B:1104:HOH:O	2.49	0.41
1:B:258:TRP:O	1:B:259:GLU:CB	2.68	0.41
1:D:258:TRP:O	1:D:259:GLU:HB2	2.21	0.40
1:E:309:ARG:HG2	2:F:502:EZ8:CAT	2.51	0.40
1:C:347:GLU:OE2	2:C:1001:EZ8:O4	2.40	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	134/155 (86%)	132 (98%)	1 (1%)	1 (1%)	22	18
1	B	134/155 (86%)	131 (98%)	3 (2%)	0	100	100
1	C	134/155 (86%)	132 (98%)	2 (2%)	0	100	100
1	D	136/155 (88%)	131 (96%)	5 (4%)	0	100	100
1	E	132/155 (85%)	128 (97%)	3 (2%)	1 (1%)	19	15
1	F	133/155 (86%)	131 (98%)	2 (2%)	0	100	100
All	All	803/930 (86%)	785 (98%)	16 (2%)	2 (0%)	41	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	353	GLU
1	A	353	GLU

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	120/136 (88%)	119 (99%)	1 (1%)	81	86
1	B	120/136 (88%)	119 (99%)	1 (1%)	81	86
1	C	120/136 (88%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	122/136 (90%)	122 (100%)	0	100	100
1	E	118/136 (87%)	118 (100%)	0	100	100
1	F	119/136 (88%)	119 (100%)	0	100	100
All	All	719/816 (88%)	717 (100%)	2 (0%)	92	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	383	SER
1	B	300	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	GLN
1	B	300	GLN
1	B	304	GLN
1	B	328	GLN
1	C	362	ASN
1	D	274	GLN
1	D	362	ASN
1	E	264	GLN
1	E	274	GLN
1	F	323	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 32 are monoatomic - leaving 6 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	EZ8	A	1001	3	56,56,56	2.12	16 (28%)	67,77,77	1.67	7 (10%)
2	EZ8	D	502	3	56,56,56	1.97	14 (25%)	67,77,77	1.29	9 (13%)
2	EZ8	E	503	3	56,56,56	2.44	15 (26%)	67,77,77	1.50	13 (19%)
2	EZ8	B	1001	3	56,56,56	1.82	12 (21%)	67,77,77	1.32	9 (13%)
2	EZ8	C	1001	3	56,56,56	2.40	13 (23%)	67,77,77	1.23	7 (10%)
2	EZ8	F	502	3	56,56,56	2.07	12 (21%)	67,77,77	1.42	13 (19%)

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	EZ8	A	1001	3	-	5/32/74/74	0/5/5/5
2	EZ8	D	502	3	-	5/32/74/74	0/5/5/5
2	EZ8	E	503	3	-	8/32/74/74	0/5/5/5
2	EZ8	B	1001	3	-	5/32/74/74	0/5/5/5
2	EZ8	C	1001	3	-	5/32/74/74	0/5/5/5
2	EZ8	F	502	3	-	6/32/74/74	0/5/5/5

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	EZ8	NBC-NBD	-9.09	1.18	1.34
2	F	502	EZ8	NBC-NBD	-8.64	1.18	1.34
2	E	503	EZ8	NBD-N2	-8.05	1.20	1.34
2	E	503	EZ8	NBC-NBD	-6.84	1.22	1.34
2	C	1001	EZ8	CBA-CBV	-6.58	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	EZ8	C2-N2	-6.27	1.40	1.49
2	C	1001	EZ8	CBB-CBW	-5.79	1.45	1.53
2	D	502	EZ8	CBB-CBW	-5.77	1.45	1.53
2	A	1001	EZ8	CAZ-CBO	-5.71	1.39	1.51
2	F	502	EZ8	CBA-CBV	-5.64	1.45	1.53
2	E	503	EZ8	CAR-CBP	-5.59	1.27	1.36
2	E	503	EZ8	CBB-CBW	-5.51	1.45	1.53
2	B	1001	EZ8	CAZ-CBO	-5.34	1.39	1.51
2	D	502	EZ8	CBA-CBV	-5.32	1.45	1.53
2	D	502	EZ8	CAY-CBN	-5.19	1.40	1.51
2	A	1001	EZ8	CBA-CBV	-5.01	1.46	1.53
2	A	1001	EZ8	CBB-CBW	-4.89	1.46	1.53
2	E	503	EZ8	CAZ-CBO	-4.87	1.40	1.51
2	C	1001	EZ8	CAU-CBL	-4.71	1.35	1.51
2	B	1001	EZ8	CBB-CBW	-4.69	1.46	1.53
2	D	502	EZ8	CAZ-CBO	-4.68	1.41	1.51
2	E	503	EZ8	CAY-CBN	-4.51	1.41	1.51
2	F	502	EZ8	NBD-N2	-4.45	1.26	1.34
2	C	1001	EZ8	CAZ-CBO	-4.38	1.41	1.51
2	B	1001	EZ8	CAU-CBL	-4.38	1.36	1.51
2	C	1001	EZ8	C2-N2	-4.34	1.42	1.49
2	B	1001	EZ8	CAY-CBN	-4.30	1.42	1.51
2	A	1001	EZ8	CAY-CBN	-4.26	1.42	1.51
2	D	502	EZ8	CAU-CBL	-4.15	1.37	1.51
2	E	503	EZ8	CAU-CBL	-3.95	1.37	1.51
2	E	503	EZ8	CAV-CBM	-3.86	1.38	1.51
2	B	1001	EZ8	CAV-CBM	-3.75	1.38	1.51
2	C	1001	EZ8	CAY-CBN	-3.67	1.43	1.51
2	E	503	EZ8	CBA-CBV	-3.54	1.48	1.53
2	A	1001	EZ8	CAV-CBM	-3.46	1.39	1.51
2	E	503	EZ8	O5-C1	3.43	1.50	1.41
2	D	502	EZ8	CAV-CBM	-3.38	1.39	1.51
2	A	1001	EZ8	CAR-N2	-3.34	1.32	1.35
2	A	1001	EZ8	C1-C2	-3.34	1.49	1.52
2	F	502	EZ8	CAU-CBL	-3.33	1.40	1.51
2	C	1001	EZ8	CAV-CBM	-3.31	1.40	1.51
2	F	502	EZ8	CAY-CBN	-3.27	1.44	1.51
2	F	502	EZ8	C1-C2	-3.19	1.49	1.52
2	D	502	EZ8	CBU-CBT	3.18	1.57	1.52
2	C	1001	EZ8	C1-C2	3.16	1.55	1.52
2	A	1001	EZ8	CBU-CBT	3.02	1.57	1.52
2	A	1001	EZ8	CAU-CBL	-3.01	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	502	EZ8	CBB-CBW	-2.98	1.49	1.53
2	D	502	EZ8	O1-CBU	-2.96	1.39	1.44
2	C	1001	EZ8	C3-C4	-2.94	1.44	1.52
2	F	502	EZ8	CAZ-CBO	-2.92	1.45	1.51
2	F	502	EZ8	CAR-CBP	-2.90	1.31	1.36
2	B	1001	EZ8	CAZ-NBF	2.88	1.51	1.46
2	C	1001	EZ8	CAR-N2	-2.81	1.32	1.35
2	E	503	EZ8	CBB-CBU	2.71	1.57	1.52
2	F	502	EZ8	CAV-CBM	-2.66	1.42	1.51
2	A	1001	EZ8	OBG-CBT	2.63	1.48	1.43
2	E	503	EZ8	CAS-CBP	-2.62	1.48	1.51
2	F	502	EZ8	CAZ-NBF	2.59	1.51	1.46
2	B	1001	EZ8	CAS-CBP	-2.57	1.48	1.51
2	D	502	EZ8	OBG-CBT	2.57	1.48	1.43
2	C	1001	EZ8	CBW-CBK	2.51	1.55	1.51
2	B	1001	EZ8	CAR-CBP	-2.50	1.32	1.36
2	B	1001	EZ8	C2-N2	-2.48	1.45	1.49
2	B	1001	EZ8	CAY-NBE	2.48	1.50	1.46
2	D	502	EZ8	CAR-CBP	-2.46	1.32	1.36
2	E	503	EZ8	CBU-CBT	2.45	1.56	1.52
2	D	502	EZ8	O4-C4	2.33	1.48	1.43
2	A	1001	EZ8	CBW-CBK	2.29	1.55	1.51
2	D	502	EZ8	O5-C5	2.26	1.49	1.44
2	A	1001	EZ8	CAR-CBP	-2.20	1.32	1.36
2	E	503	EZ8	C4-C5	-2.19	1.48	1.53
2	A	1001	EZ8	O1-C1	2.17	1.47	1.41
2	C	1001	EZ8	CAY-NBE	2.17	1.50	1.46
2	F	502	EZ8	CBA-CBT	2.16	1.56	1.52
2	D	502	EZ8	CAR-N2	-2.16	1.33	1.35
2	D	502	EZ8	CBB-CBU	-2.12	1.48	1.52
2	A	1001	EZ8	CAY-NBE	2.09	1.50	1.46
2	E	503	EZ8	CBW-CBK	2.09	1.55	1.51
2	A	1001	EZ8	O3-C3	-2.06	1.38	1.43
2	B	1001	EZ8	CBV-CBJ	2.05	1.55	1.51
2	B	1001	EZ8	CBA-CBV	-2.03	1.50	1.53

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	EZ8	CAR-N2-C2	-10.17	116.47	125.48
2	B	1001	EZ8	CBV-CBW-CBK	4.73	117.90	111.24
2	E	503	EZ8	CAR-N2-C2	-4.43	121.56	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1001	EZ8	OAC-CBK-CBW	-3.98	116.94	121.73
2	E	503	EZ8	O5-C5-C6	3.59	115.37	106.44
2	F	502	EZ8	O5-C5-C6	3.17	114.31	106.44
2	D	502	EZ8	OAC-CBK-CBW	-3.06	118.04	121.73
2	C	1001	EZ8	C1-O5-C5	-3.04	107.71	113.69
2	F	502	EZ8	C3-C4-C5	-3.03	104.84	110.24
2	A	1001	EZ8	CAZ-NBF-CBK	3.02	126.67	122.34
2	B	1001	EZ8	CBW-CBB-CBU	-2.99	105.47	111.74
2	E	503	EZ8	C3-C4-C5	-2.90	105.07	110.24
2	D	502	EZ8	O5-C5-C6	-2.84	99.38	106.44
2	E	503	EZ8	CAR-CBP-NBC	-2.83	107.14	111.34
2	E	503	EZ8	CBV-CBW-CBK	2.80	115.18	111.24
2	C	1001	EZ8	CAY-NBE-CBJ	2.78	126.34	122.34
2	A	1001	EZ8	OAB-CBJ-CBV	-2.77	118.39	121.73
2	C	1001	EZ8	O5-C5-C6	2.73	113.23	106.44
2	C	1001	EZ8	C6-C5-C4	-2.71	106.67	113.00
2	D	502	EZ8	CBW-CBB-CBU	-2.70	106.08	111.74
2	B	1001	EZ8	O1-C1-O5	2.68	118.17	110.67
2	F	502	EZ8	CAR-CBP-NBC	-2.68	107.36	111.34
2	A	1001	EZ8	CAS-CBP-CAR	-2.67	122.10	127.60
2	A	1001	EZ8	C6-C5-C4	-2.65	106.80	113.00
2	C	1001	EZ8	CBP-CAR-N2	-2.62	103.30	107.35
2	D	502	EZ8	CAY-CBN-CAO	-2.62	115.47	120.91
2	D	502	EZ8	CAY-CBN-CAN	2.61	126.34	120.91
2	F	502	EZ8	CAY-CBN-CAN	-2.61	115.50	120.91
2	E	503	EZ8	C1-O5-C5	-2.54	108.71	113.69
2	F	502	EZ8	OAC-CBK-CBW	-2.53	118.68	121.73
2	F	502	EZ8	CAR-N2-C2	-2.46	123.30	125.48
2	E	503	EZ8	CBP-CAR-N2	-2.44	103.58	107.35
2	F	502	EZ8	O5-C5-C4	-2.44	105.27	109.69
2	A	1001	EZ8	O6-C6-C5	-2.43	102.96	111.29
2	F	502	EZ8	CBW-CBK-NBF	2.42	120.16	116.24
2	D	502	EZ8	C1-O5-C5	2.37	118.34	113.69
2	F	502	EZ8	C1-O5-C5	-2.37	109.03	113.69
2	F	502	EZ8	CAY-CBN-CAO	2.30	125.69	120.91
2	E	503	EZ8	CAY-CBN-CAO	2.29	125.66	120.91
2	B	1001	EZ8	O6-C6-C5	-2.28	103.48	111.29
2	C	1001	EZ8	OAC-CBK-CBW	-2.26	119.00	121.73
2	E	503	EZ8	OBG-CAX-CAT	-2.24	103.42	109.80
2	D	502	EZ8	CBW-CBV-CBJ	-2.21	108.13	111.24
2	E	503	EZ8	CAY-CBN-CAN	-2.18	116.40	120.91
2	B	1001	EZ8	CBB-CBW-CBV	2.16	113.87	110.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	503	EZ8	OAC-CBK-CBW	-2.16	119.13	121.73
2	A	1001	EZ8	CBV-CBJ-NBE	2.15	119.70	116.24
2	F	502	EZ8	O5-C1-C2	2.15	112.61	109.09
2	E	503	EZ8	O5-C5-C4	-2.14	105.81	109.69
2	B	1001	EZ8	CBV-CBA-CBT	-2.14	107.26	111.74
2	C	1001	EZ8	O1-CBU-CBB	2.14	113.75	109.62
2	B	1001	EZ8	CBW-CBK-NBF	2.13	119.68	116.24
2	D	502	EZ8	CBA-CBT-CBU	-2.11	108.00	110.85
2	E	503	EZ8	CAX-OBG-CBT	2.09	118.71	113.87
2	F	502	EZ8	CBP-CAR-N2	-2.08	104.13	107.35
2	F	502	EZ8	CBV-CBJ-NBE	-2.05	112.92	116.24
2	B	1001	EZ8	CBA-CBV-CBW	-2.01	107.90	110.78
2	D	502	EZ8	O5-C1-C2	2.01	112.38	109.09

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	EZ8	NBF-CBK-CBW-CBV
2	B	1001	EZ8	NBF-CBK-CBW-CBV
2	B	1001	EZ8	OAC-CBK-CBW-CBV
2	C	1001	EZ8	NBF-CBK-CBW-CBV
2	C	1001	EZ8	OAC-CBK-CBW-CBV
2	D	502	EZ8	NBF-CBK-CBW-CBV
2	D	502	EZ8	OAC-CBK-CBW-CBV
2	E	503	EZ8	NBF-CBK-CBW-CBV
2	E	503	EZ8	OAC-CBK-CBW-CBV
2	F	502	EZ8	NBF-CBK-CBW-CBV
2	F	502	EZ8	OAC-CBK-CBW-CBV
2	D	502	EZ8	C4-C5-C6-O6
2	E	503	EZ8	O5-C5-C6-O6
2	D	502	EZ8	O5-C5-C6-O6
2	E	503	EZ8	C4-C5-C6-O6
2	F	502	EZ8	O5-C5-C6-O6
2	F	502	EZ8	C4-C5-C6-O6
2	C	1001	EZ8	CL1-CAT-CAX-OBG
2	A	1001	EZ8	OAC-CBK-CBW-CBV
2	E	503	EZ8	CL1-CAT-CAX-OBG
2	F	502	EZ8	CL1-CAT-CAX-OBG
2	E	503	EZ8	CBA-CBT-OBG-CAX
2	E	503	EZ8	CBU-CBT-OBG-CAX
2	E	503	EZ8	CAT-CAX-OBG-CBT

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Mol	Chain	Res	Type	Atoms
2	F	502	EZ8	CAT-CAX-OBG-CBT
2	A	1001	EZ8	CL1-CAT-CAX-OBG
2	C	1001	EZ8	O5-C5-C6-O6
2	A	1001	EZ8	OAC-CBK-CBW-CBB
2	B	1001	EZ8	OAD-CAU-CBL-CAJ
2	B	1001	EZ8	CL1-CAT-CAX-OBG
2	A	1001	EZ8	NBF-CBK-CBW-CBB
2	B	1001	EZ8	NBF-CBK-CBW-CBB
2	D	502	EZ8	NBF-CBK-CBW-CBB
2	C	1001	EZ8	OAE-CAV-CBM-CAM

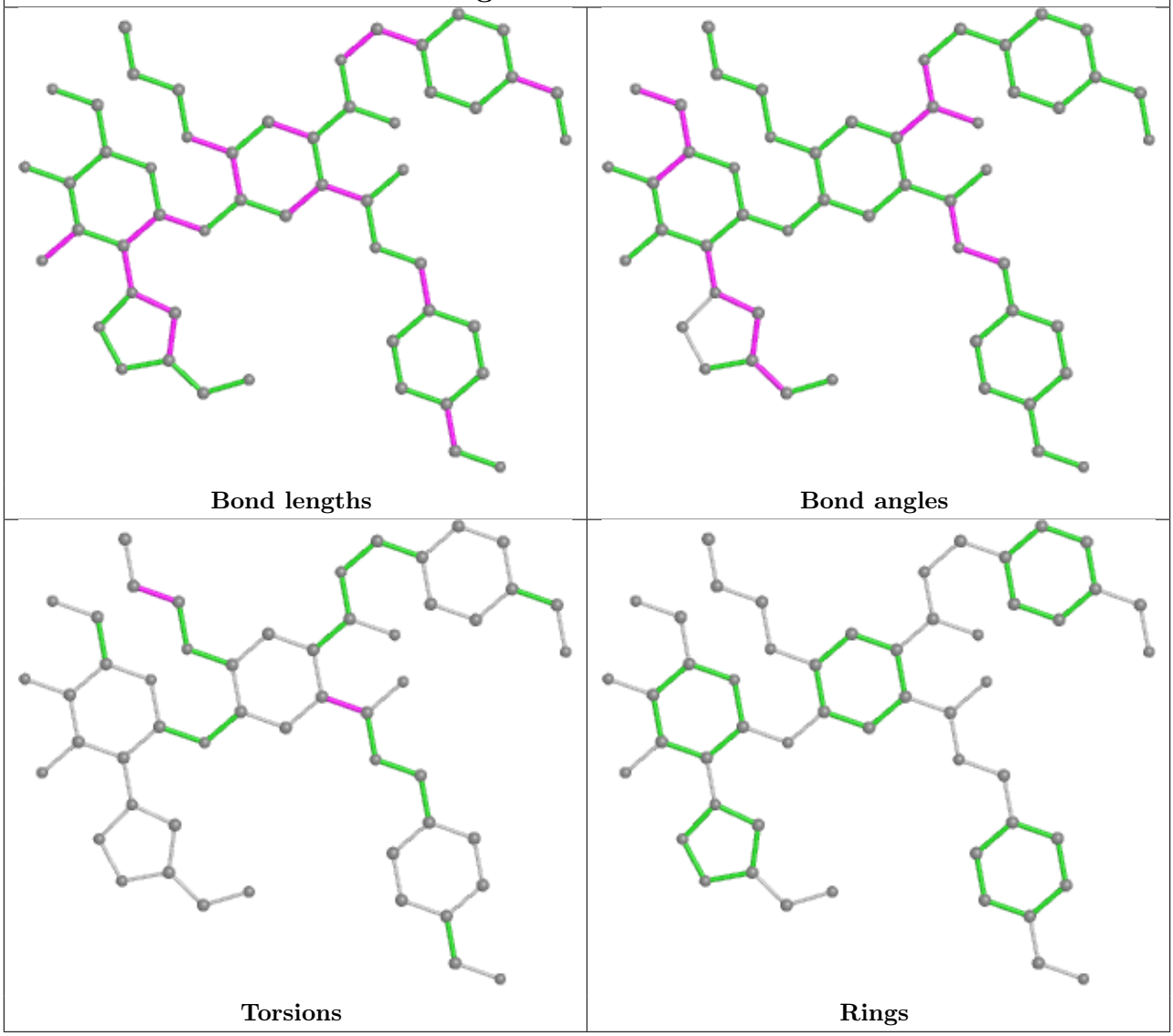
There are no ring outliers.

4 monomers are involved in 7 short contacts:

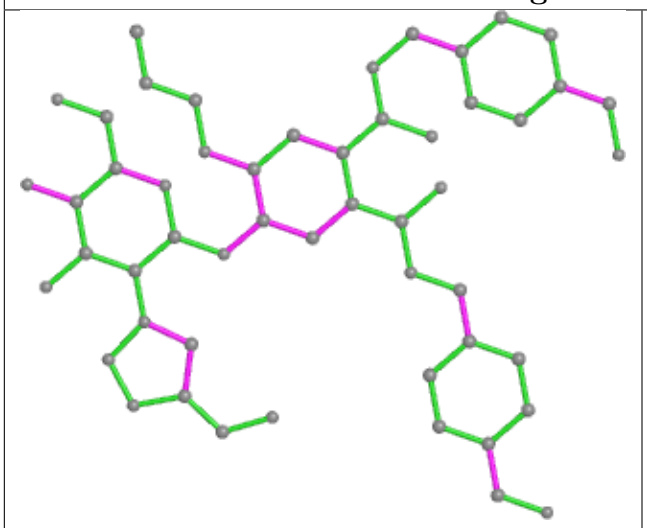
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	EZ8	2	0
2	E	503	EZ8	1	0
2	C	1001	EZ8	2	0
2	F	502	EZ8	2	0

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 then 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.

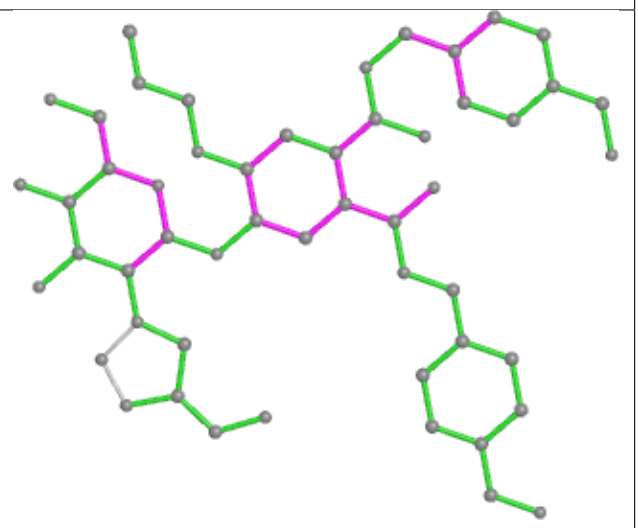
Ligand EZ8 A 1001



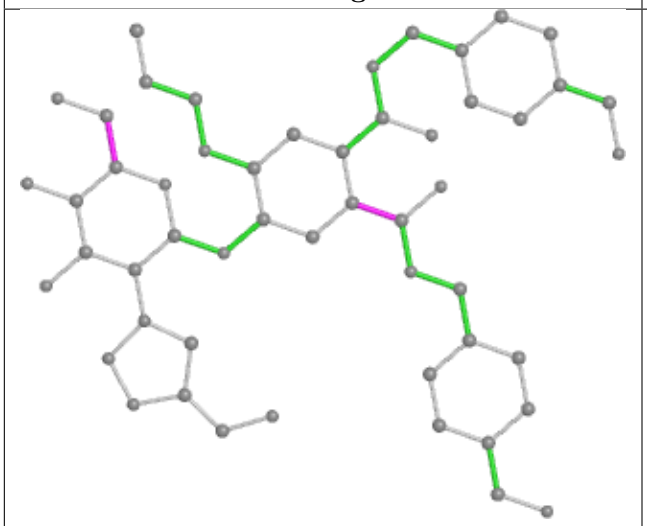
Ligand EZ8 D 502



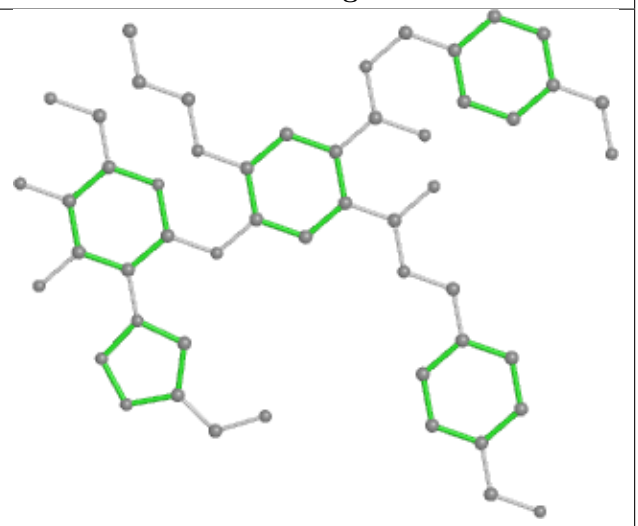
Bond lengths



Bond angles

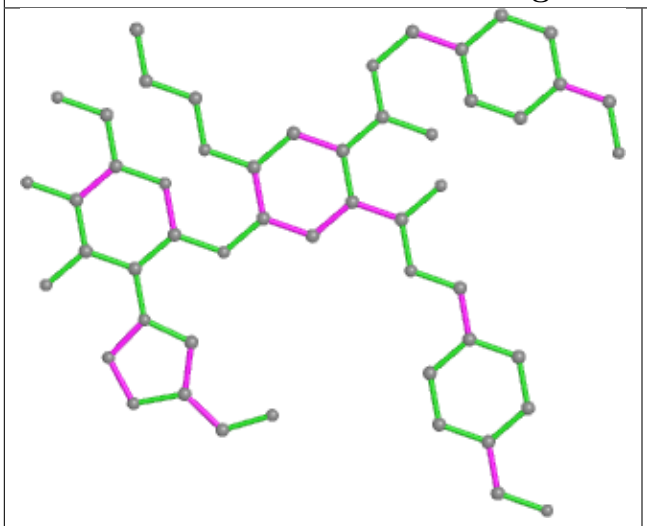


Torsions



Rings

Ligand EZ8 E 503



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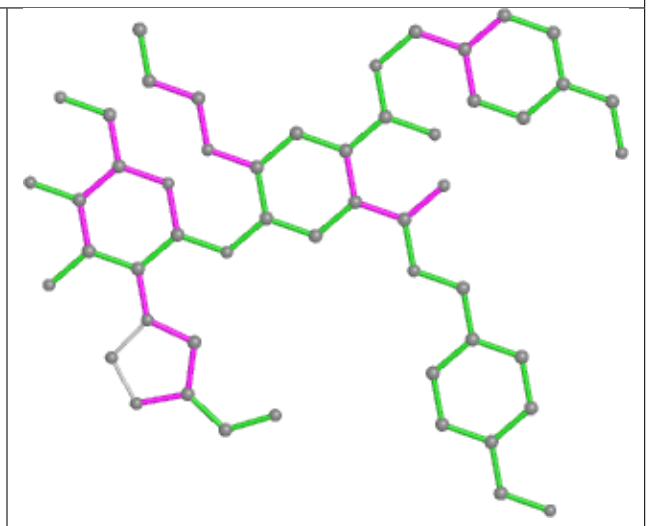

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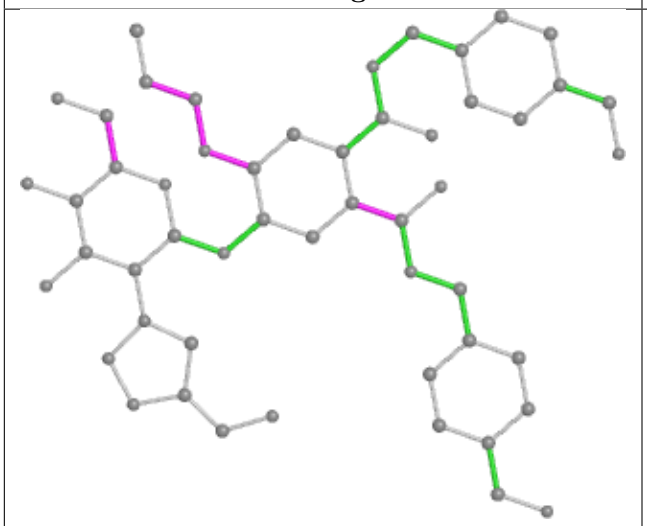

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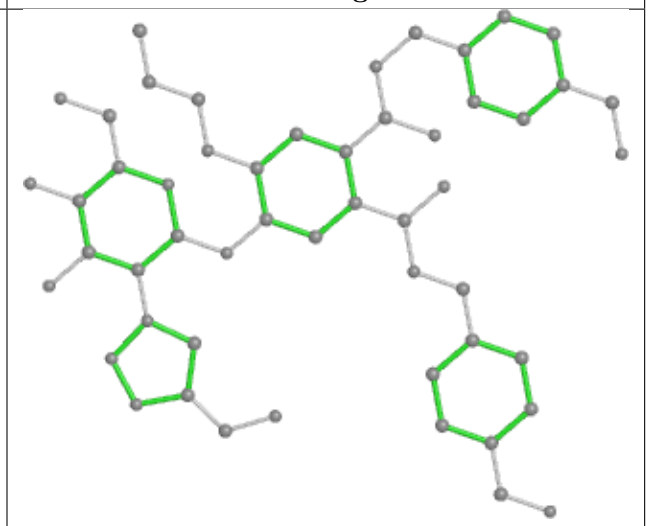
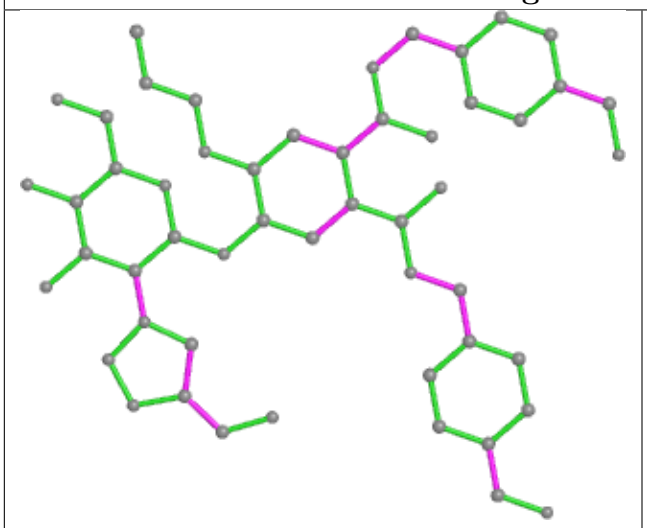
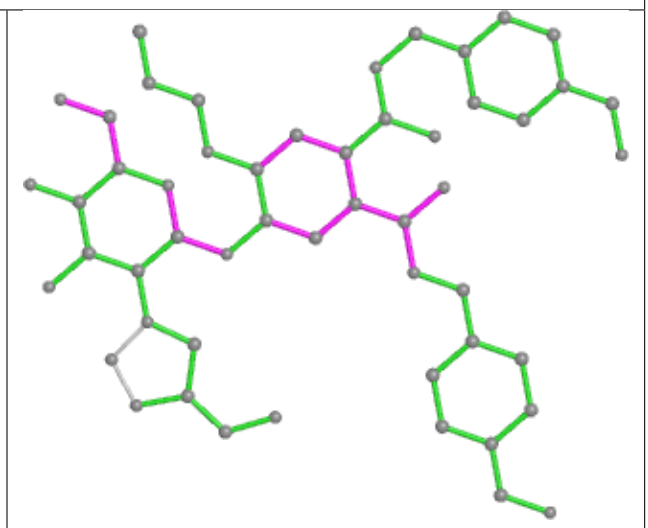


Rings

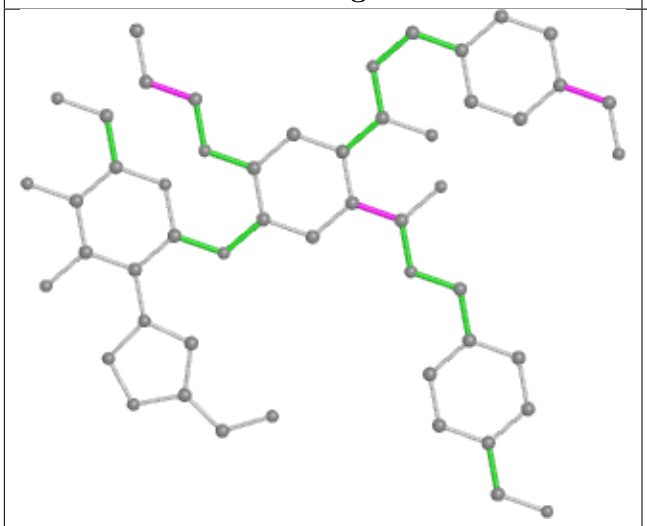
Ligand EZ8 B 1001



Bond lengths



Bond angles



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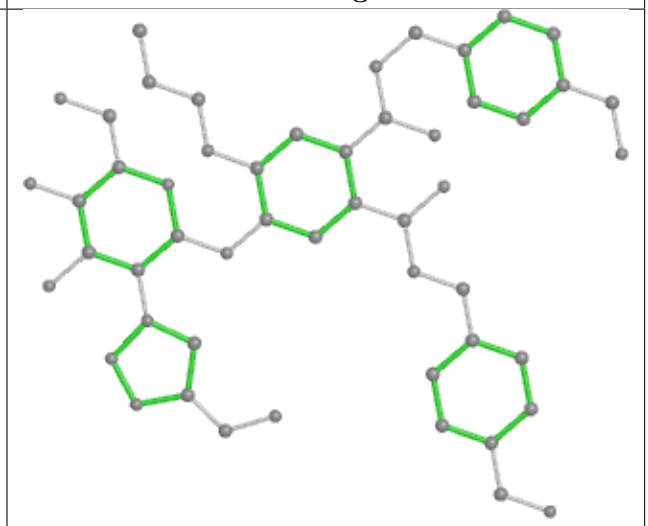
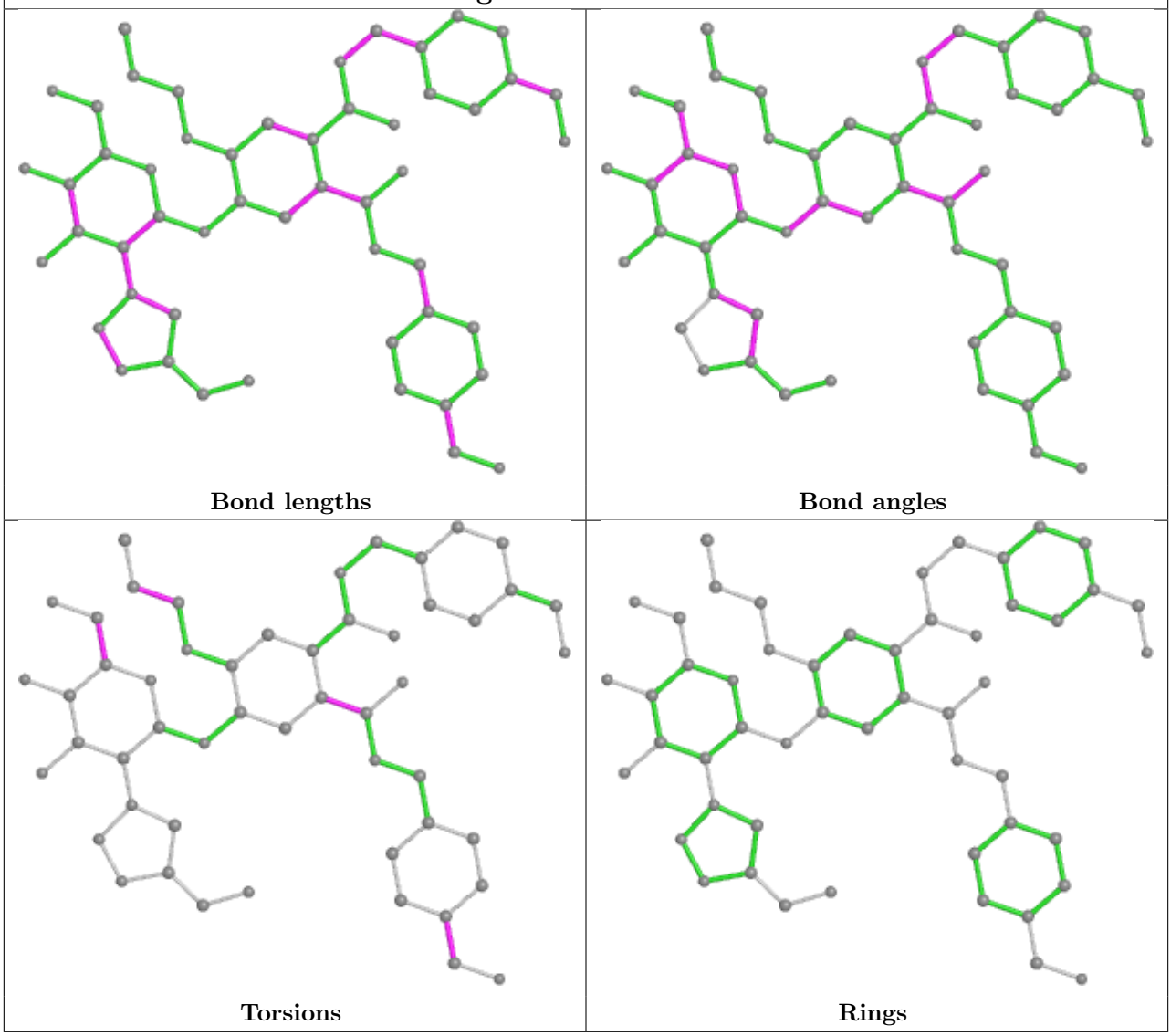
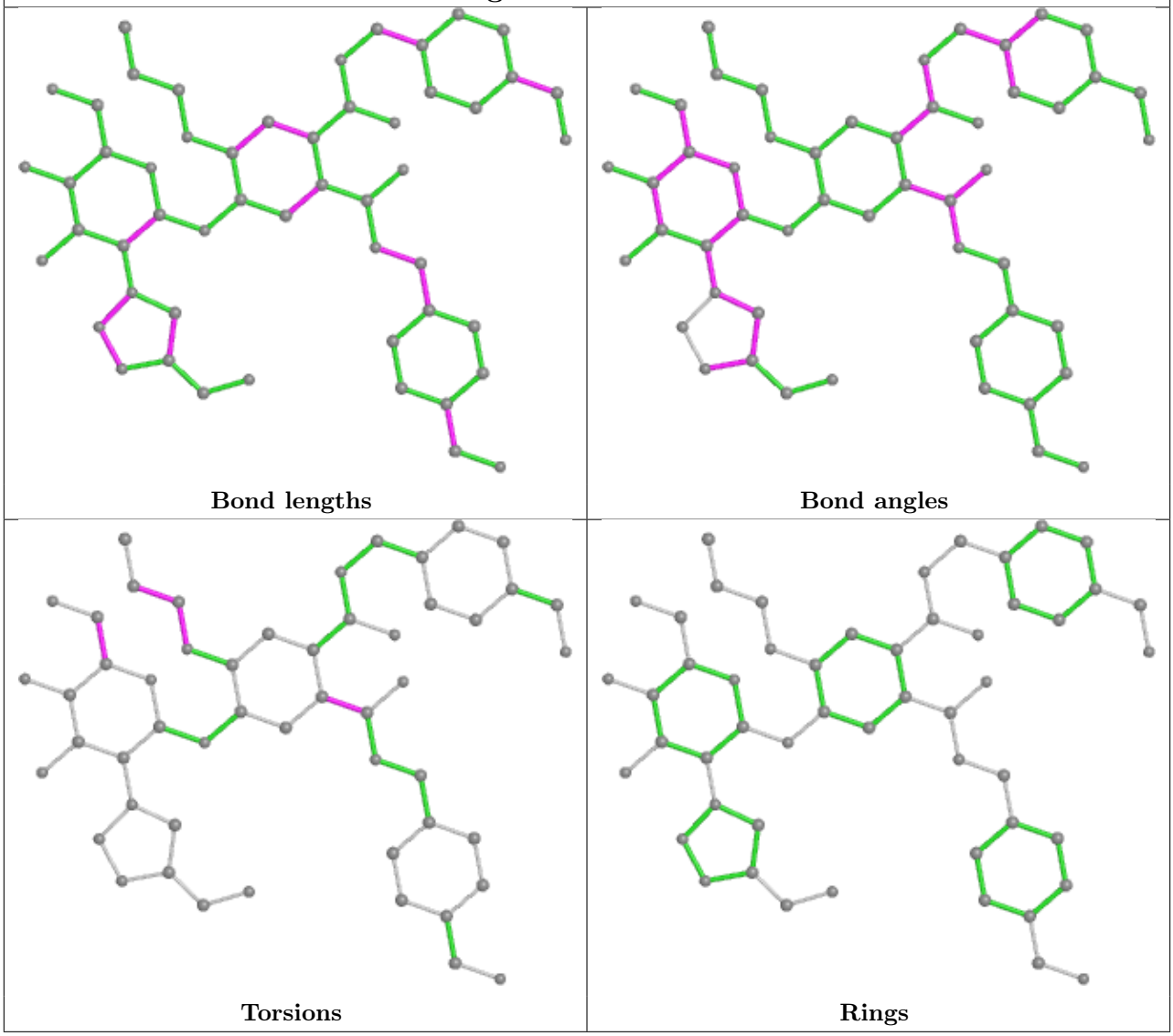


Rings

Ligand EZ8 C 1001



Ligand EZ8 F 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	132/155 (85%)	-0.24	3 (2%)	60	65	23, 33, 47, 93	0
1	B	132/155 (85%)	-0.21	2 (1%)	73	77	20, 29, 43, 97	0
1	C	133/155 (85%)	-0.25	2 (1%)	73	77	21, 29, 44, 68	0
1	D	133/155 (85%)	-0.16	4 (3%)	50	56	24, 33, 53, 100	0
1	E	133/155 (85%)	-0.22	3 (2%)	60	65	23, 33, 49, 69	0
1	F	132/155 (85%)	-0.22	3 (2%)	60	65	24, 36, 49, 84	0
All	All	795/930 (85%)	-0.22	17 (2%)	63	68	20, 32, 49, 100	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	384	CYS	6.9
1	B	384	CYS	6.1
1	D	252	LEU	6.1
1	E	252	LEU	5.5
1	A	253	CYS	5.0
1	C	252	LEU	4.2
1	D	383	SER	4.1
1	B	383	SER	4.0
1	E	253	CYS	2.9
1	A	384	CYS	2.7
1	E	345	ARG	2.6
1	D	253	CYS	2.3
1	A	345	ARG	2.2
1	F	382	ALA	2.1
1	F	384	CYS	2.1
1	C	384	CYS	2.1
1	F	298[A]	GLU	2.1

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(Å^2)	Q<0.9
4	CL	A	1007	1/1	0.79	0.25	65,65,65,65	0
3	CA	A	1004	1/1	0.86	0.06	49,49,49,49	0
4	CL	A	1006	1/1	0.87	0.16	64,64,64,64	0
3	CA	D	505	1/1	0.90	0.09	62,62,62,62	0
4	CL	E	501	1/1	0.90	0.12	72,72,72,72	0
4	CL	D	501	1/1	0.92	0.08	59,59,59,59	0
2	EZ8	D	502	52/52	0.93	0.11	24,31,61,68	0
3	CA	E	506	1/1	0.93	0.11	53,53,53,53	0
4	CL	D	506	1/1	0.93	0.08	56,56,56,56	0
3	CA	C	1004	1/1	0.93	0.07	51,51,51,51	0
4	CL	B	1006	1/1	0.94	0.25	63,63,63,63	0
3	CA	B	1004	1/1	0.94	0.06	54,54,54,54	0
2	EZ8	E	503	52/52	0.94	0.12	23,36,56,77	0
2	EZ8	A	1001	52/52	0.94	0.12	26,35,58,61	0
2	EZ8	C	1001	52/52	0.95	0.11	23,30,47,53	0
4	CL	C	1005	1/1	0.95	0.09	60,60,60,60	0
4	CL	C	1006	1/1	0.95	0.18	58,58,58,58	0
2	EZ8	F	502	52/52	0.95	0.11	27,31,45,52	0
2	EZ8	B	1001	52/52	0.95	0.11	22,29,47,54	0
4	CL	B	1005	1/1	0.95	0.07	66,66,66,66	0
4	CL	A	1005	1/1	0.96	0.09	64,64,64,64	0
4	CL	E	502	1/1	0.96	0.10	54,54,54,54	0
3	CA	F	505	1/1	0.97	0.04	50,50,50,50	0
4	CL	E	507	1/1	0.97	0.14	59,59,59,59	0
4	CL	F	501	1/1	0.97	0.07	51,51,51,51	0
4	CL	F	506	1/1	0.97	0.07	61,61,61,61	0
3	CA	A	1002	1/1	0.99	0.09	30,30,30,30	0

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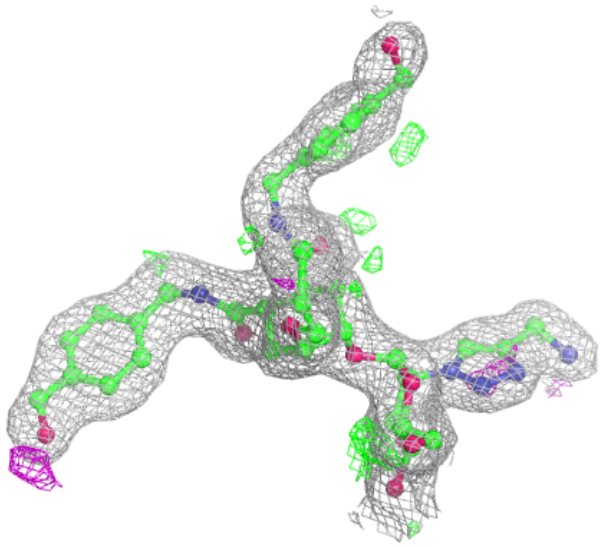
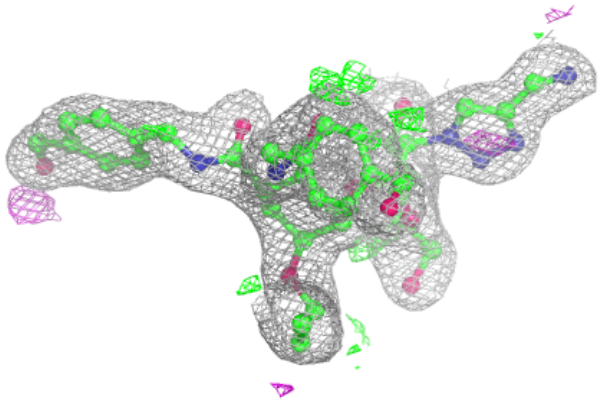
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	D	504	1/1	0.99	0.06	27,27,27,27	0
3	CA	B	1002	1/1	0.99	0.11	22,22,22,22	0
3	CA	A	1003	1/1	0.99	0.07	29,29,29,29	0
3	CA	F	503	1/1	0.99	0.08	28,28,28,28	0
3	CA	F	504	1/1	0.99	0.08	26,26,26,26	0
3	CA	C	1003	1/1	0.99	0.06	27,27,27,27	0
3	CA	E	504	1/1	1.00	0.07	29,29,29,29	0
3	CA	E	505	1/1	1.00	0.06	26,26,26,26	0
3	CA	D	503	1/1	1.00	0.06	26,26,26,26	0
3	CA	B	1003	1/1	1.00	0.10	25,25,25,25	0
3	CA	C	1002	1/1	1.00	0.07	25,25,25,25	0

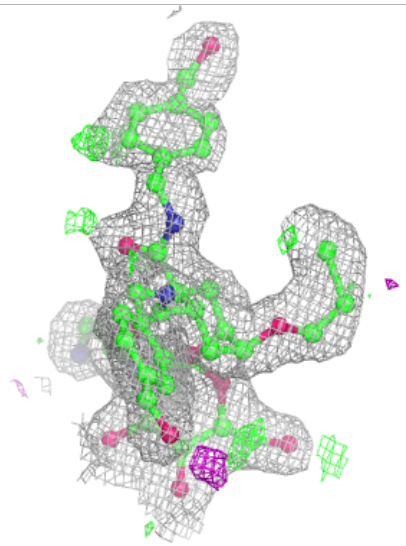
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EZ8 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)

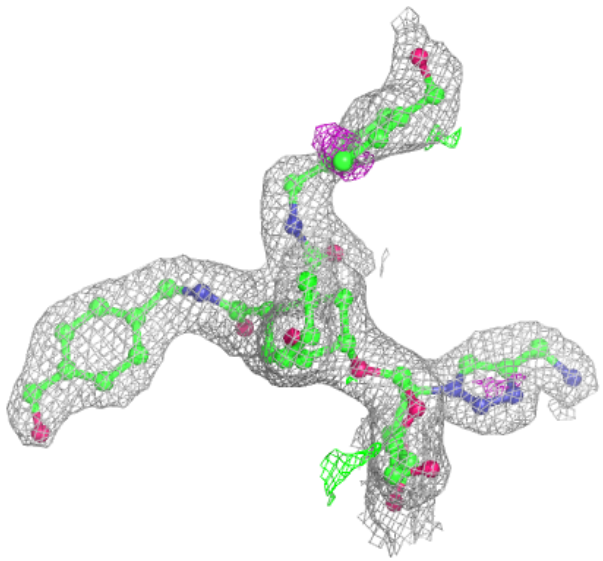


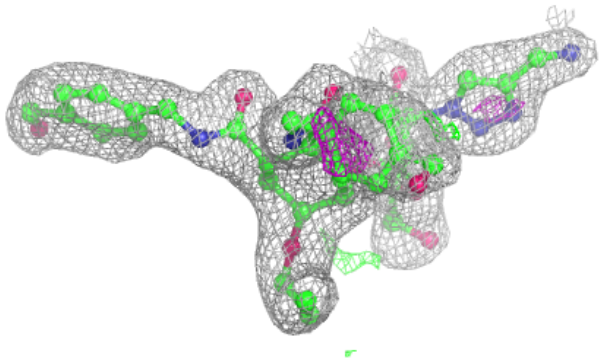




Electron density around EZ8 E 503:

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





Electron density around EZ8 A 1001:

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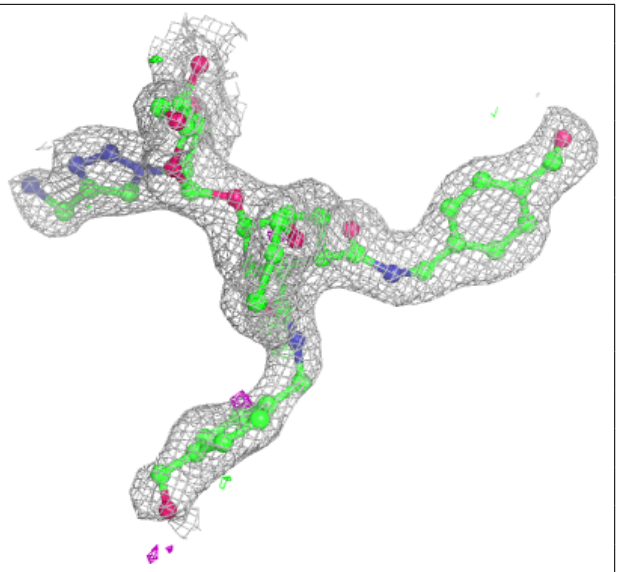
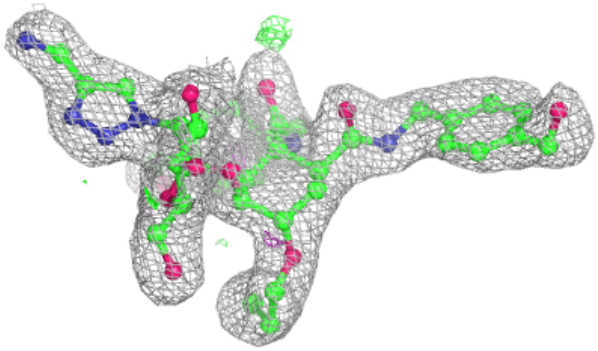
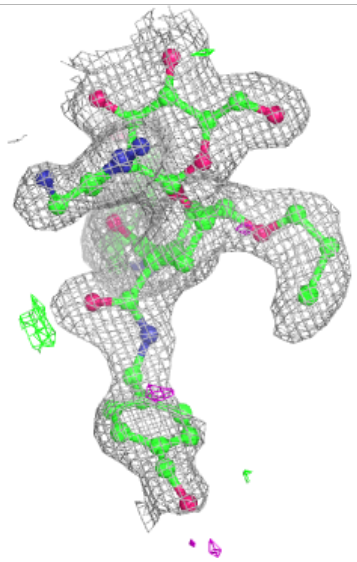
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

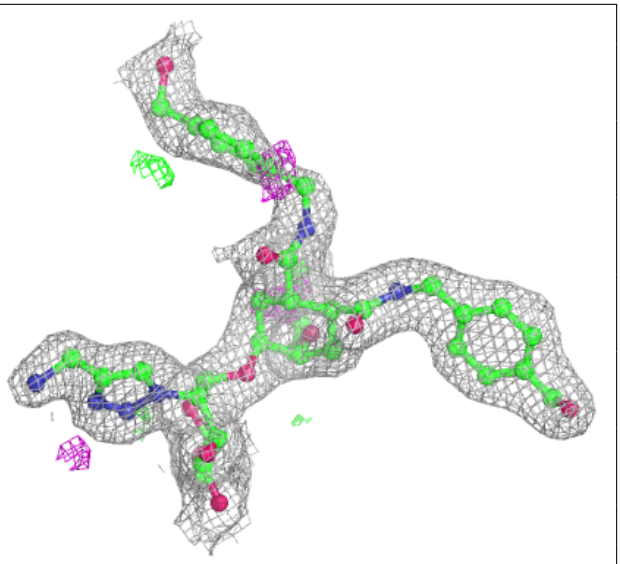


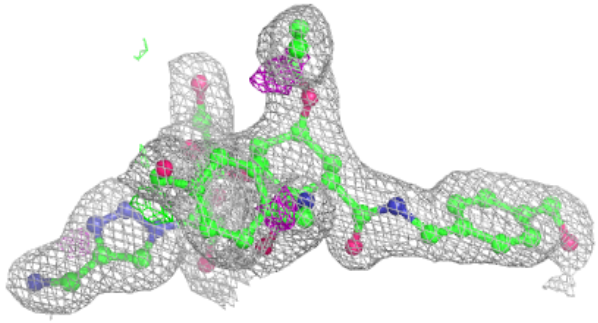


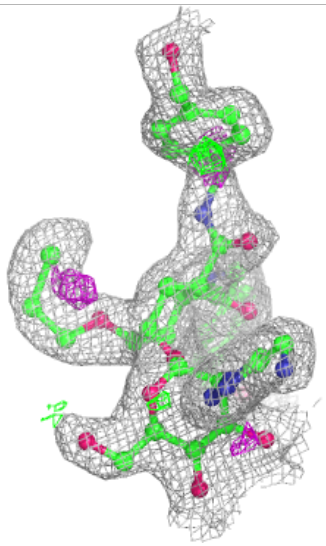


Electron density around EZ8 C 1001:

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

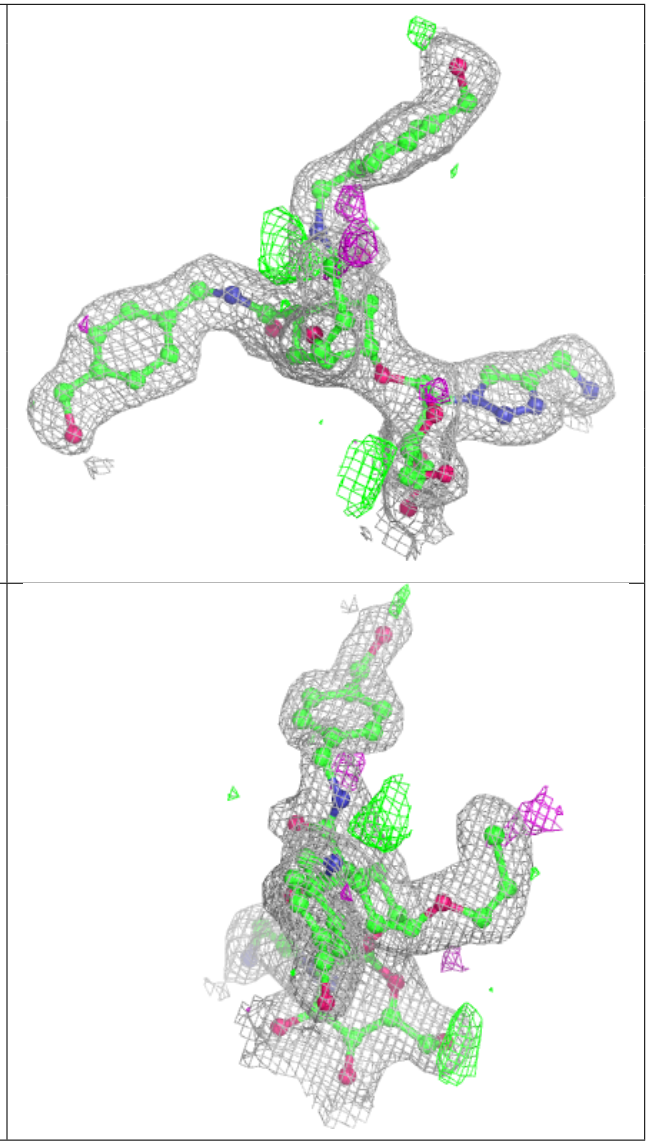






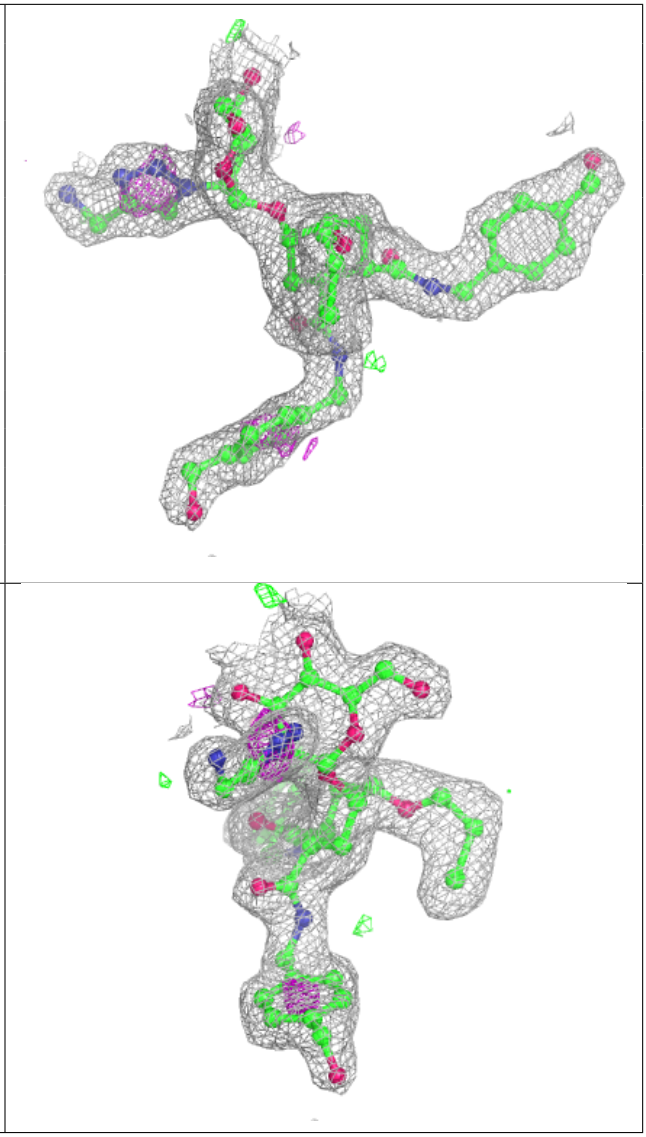
Electron density around EZ8 F 502:

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



Electron density around EZ8 B 1001:

$2mF_o$-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.