Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:41 AM UTC

PDB ID	:	7TTZ / pdb_00007ttz
Title	:	Heterodimeric IgA Fc in complex with Staphylococcus aureus protein SSL7
Authors	:	Boulanger, M.J.; Verstraete, M.; Heinkel, F.; Escobar, E.; Dixit, S.; Von Kreudenstein, T.S.
Deposited on	:	2022-02-02
Resolution	:	2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

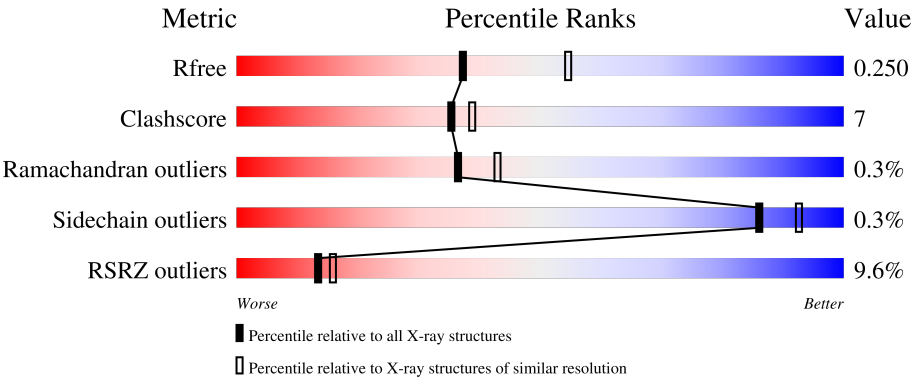
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	220	17% 76% 17% 6%
2	B	220	5% 81% 14% 5%
3	C	201	9% 79% 15% 5%
3	D	201	3% 82% 12% 6%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12875 atoms, of which 6363 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 IgA Fc.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	207	3156	1007	1562	276	303	8	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ARG	-	expression tag	UNP Q6MZV6
A	311	SER	CYS	engineered mutation	UNP Q6MZV6
A	337	THR	ASN	engineered mutation	UNP Q6MZV6
A	338	LEU	ILE	engineered mutation	UNP Q6MZV6
A	339	SER	THR	engineered mutation	UNP Q6MZV6
A	412	PHE	ALA	engineered mutation	UNP Q6MZV6
A	414	TYR	THR	engineered mutation	UNP Q6MZV6

- Molecule 2 is a protein called IgA Fc.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	210	3172	1002	1576	278	308	8	0	0	0

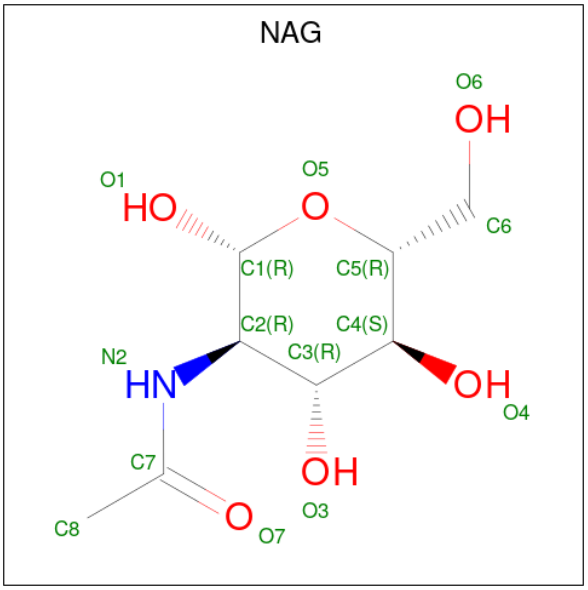
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	234	ARG	-	expression tag	UNP Q6MZV6
B	311	SER	CYS	engineered mutation	UNP Q6MZV6
B	337	THR	ASN	engineered mutation	UNP Q6MZV6
B	338	LEU	ILE	engineered mutation	UNP Q6MZV6
B	339	SER	THR	engineered mutation	UNP Q6MZV6
B	396	VAL	LEU	engineered mutation	UNP Q6MZV6
B	398	THR	TRP	engineered mutation	UNP Q6MZV6
B	416	LEU	ILE	engineered mutation	UNP Q6MZV6

- Molecule 3 is a protein called Superantigen-like protein SSL7.

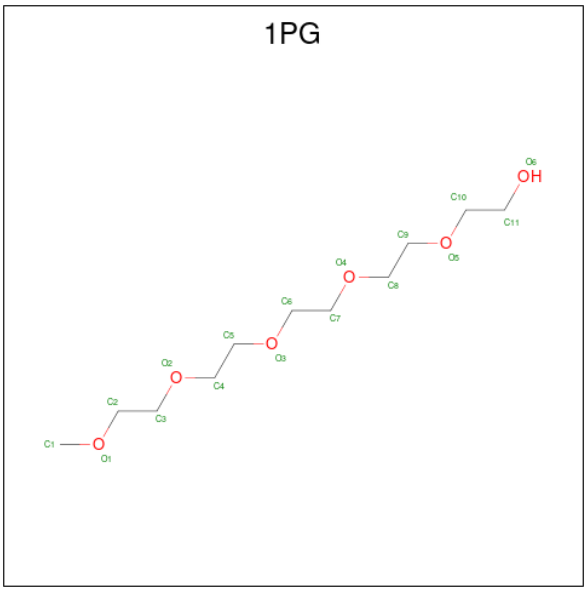
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	190	Total	C	H	N	O	S	0	0	0
			3070	966	1542	263	298	1			
3	D	188	Total	C	H	N	O	S	0	0	0
			3055	960	1536	263	295	1			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



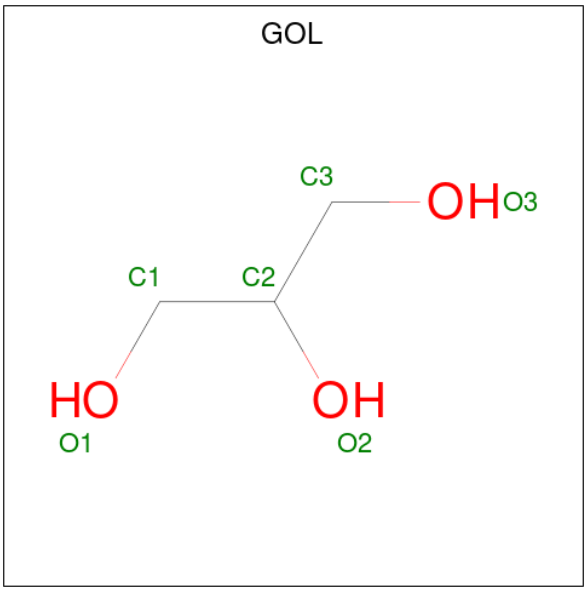
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 5 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (CCD ID: 1PG) (formula: $C_{11}H_{24}O_6$) (labeled as "Ligand of Interest" by depositor).



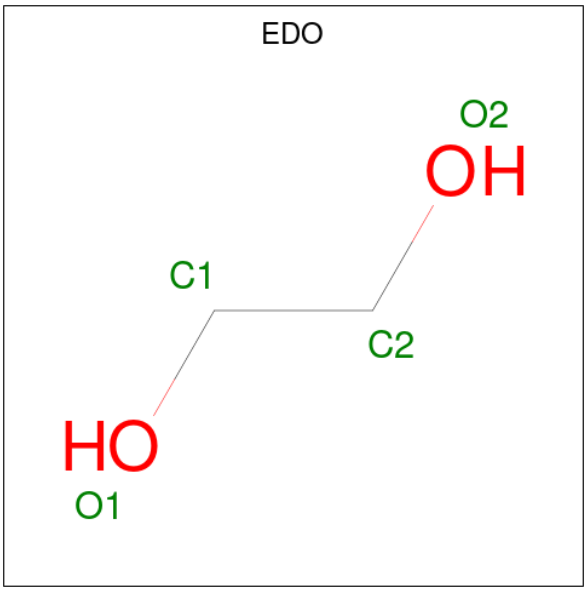
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 26 7 15 4	0	0
5	A	1	Total C H O 26 7 15 4	0	0
5	A	1	Total C H O 26 7 15 4	0	0
5	B	1	Total C H O 18 5 10 3	0	0
5	B	1	Total C H O 18 5 10 3	0	0
5	C	1	Total C H O 26 7 15 4	0	0
5	D	1	Total C H O 26 7 15 4	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 14 3 8 3	0	0
6	C	1	Total C H O 13 3 7 3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C H O 10 2 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C H O 10 2 6 2	0	0
7	D	1	Total C H O 10 2 6 2	0	0
7	D	1	Total C H O 10 2 6 2	0	0

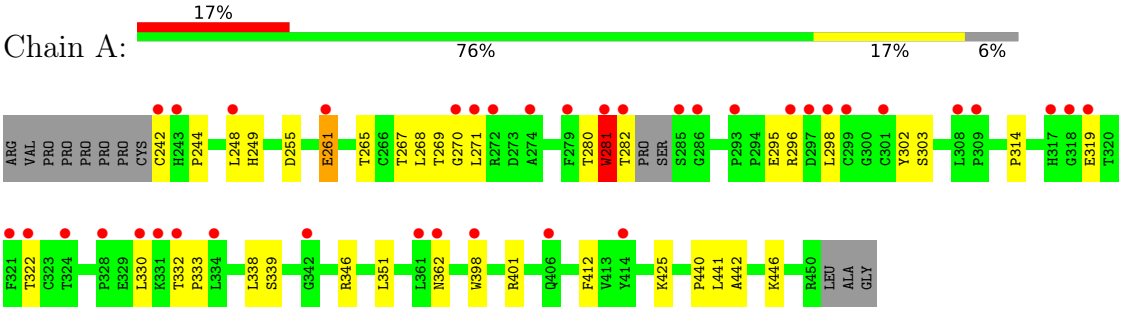
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	31	Total O 31 31	0	0
8	B	61	Total O 61 61	0	0
8	C	29	Total O 29 29	0	0
8	D	41	Total O 41 41	0	0

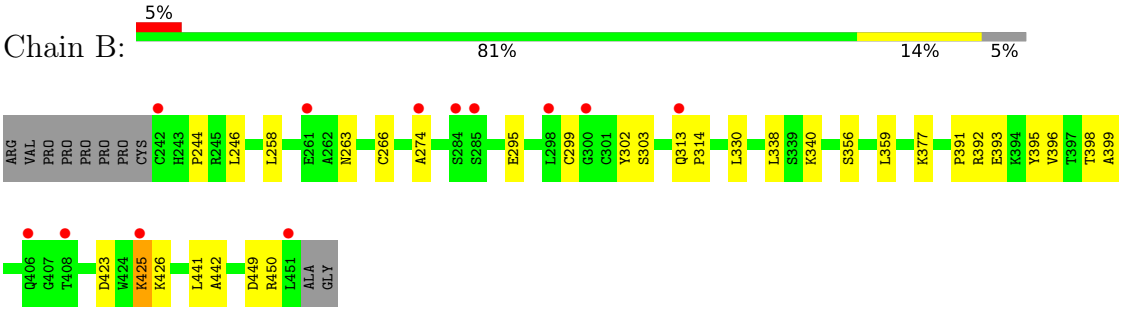
3 Residue-property plots (i)

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.

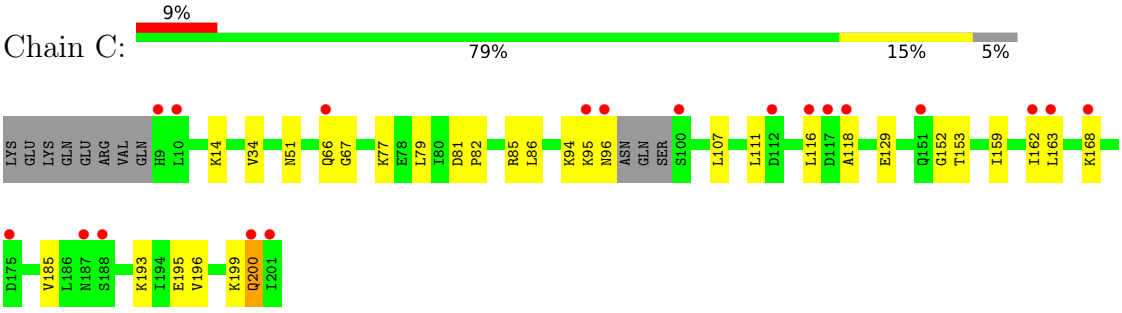
• Molecule 1: IgA Fc



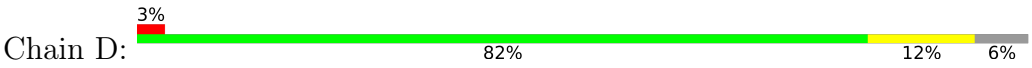
• Molecule 2: IgA Fc

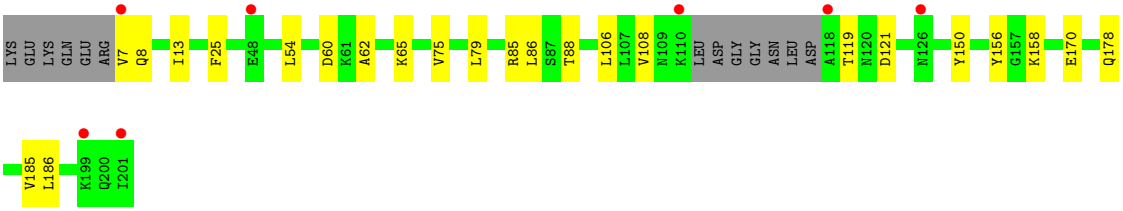


• Molecule 3: Superantigen-like protein SSL7



• Molecule 3: Superantigen-like protein SSL7




LYS GLU LYS GLN GLU ARG V7 Q8 I13 F25 E43 L54 D60 K61 A62 K65 V75 L79 R85 L86 S87 T88 L106 L107 V108 N109 K110 LEU ASP GLY GLY ASN LEU ASP A118 T119 N120 D121 N126 Y150 Y156 G157 K158 E170 Q178
V185 L186 K199 Q200 I201

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	135.50Å 165.45Å 46.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 2.35 39.56 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.4 (39.56-2.35) 92.6 (39.56-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.76 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.200 , 0.247 0.204 , 0.250	Depositor DCC
R_{free} test set	1997 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12875	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 1PG, NAG, EDO

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	0.38	1/1635 (0.1%)	0.65	5/2230 (0.2%)
2	B	0.26	0/1635	0.51	2/2233 (0.1%)
3	C	0.38	2/1547 (0.1%)	0.59	2/2070 (0.1%)
3	D	0.29	0/1538	0.50	0/2058
All	All	0.33	3/6355 (0.0%)	0.57	9/8591 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	200	GLN	CD-OE1	6.75	1.36	1.23
3	C	199	LYS	C-N	5.45	1.41	1.33
1	A	261	GLU	CD-OE2	5.42	1.35	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	199	LYS	CA-C-N	7.07	131.84	122.30
3	C	199	LYS	C-N-CA	7.07	131.84	122.30
1	A	280	THR	CA-C-N	-6.87	111.12	122.39
1	A	280	THR	C-N-CA	-6.87	111.12	122.39
2	B	425	LYS	CA-CB-CG	6.23	126.56	114.10
1	A	261	GLU	CA-CB-CG	5.79	125.69	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	281	TRP	CA-CB-CG	5.27	123.61	113.60
1	A	261	GLU	CG-CD-OE1	-5.09	106.69	118.40
2	B	377	LYS	CG-CD-CE	5.03	122.86	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	200	GLN	Sidechain

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	1594	1562	1562	34	1
2	B	1596	1576	1576	23	0
3	C	1528	1542	1542	29	1
3	D	1519	1536	1536	14	0
4	A	14	13	13	0	0
5	A	33	45	39	0	0
5	B	16	20	16	0	0
5	C	11	15	13	2	0
5	D	11	15	13	1	0
6	A	6	8	8	0	0
6	C	6	7	8	0	0
7	B	8	12	12	1	0
7	D	8	12	12	0	0
8	A	31	0	0	2	0
8	B	61	0	0	2	0
8	C	29	0	0	2	0
8	D	41	0	0	0	0
All	All	6512	6363	6350	94	1

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 7.

All (94) 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:362:ASN:OD1	1:A:425:LYS:NZ	2.07	0.86
2:B:359:LEU:O	2:B:425:LYS:NZ	2.12	0.81
1:A:398:TRP:HB3	2:B:398:THR:HG21	1.67	0.74
2:B:274:ALA:HB2	2:B:302:TYR:HB3	1.69	0.73
1:A:282:THR:OG1	1:A:322:THR:OG1	2.04	0.73
3:C:94:LYS:HG2	3:C:96:ASN:H	1.57	0.69
3:C:195:GLU:OE2	8:C:401:HOH:O	2.11	0.68
2:B:449:ASP:OD1	3:C:14:LYS:NZ	2.25	0.68
3:C:94:LYS:HE3	3:C:96:ASN:OD1	1.94	0.66
1:A:281:TRP:HB3	1:A:322:THR:O	1.97	0.65
2:B:423:ASP:HA	2:B:426:LYS:HE3	1.80	0.63
3:C:111:LEU:HD13	3:C:116:LEU:HD22	1.81	0.63
3:D:25:PHE:HB2	3:D:75:VAL:HG22	1.80	0.61
2:B:263:ASN:ND2	8:B:603:HOH:O	2.33	0.61
3:C:34:VAL:HG23	3:C:67:GLY:HA2	1.82	0.60
1:A:298:LEU:HD12	1:A:298:LEU:N	2.19	0.58
2:B:246:LEU:HD11	2:B:266:CYS:SG	2.43	0.58
1:A:401:ARG:NH2	8:A:602:HOH:O	2.26	0.58
1:A:261:GLU:OE1	1:A:261:GLU:C	2.47	0.58
2:B:295:GLU:O	2:B:303:SER:N	2.34	0.58
1:A:242:CYS:HB3	1:A:270:GLY:O	2.04	0.56
1:A:338:LEU:HD12	1:A:339:SER:H	1.71	0.56
3:D:185:VAL:C	3:D:186:LEU:HD12	2.31	0.56
1:A:398:TRP:CB	2:B:398:THR:HG21	2.34	0.56
3:C:129:GLU:HG3	3:C:185:VAL:CG2	2.38	0.54
1:A:338:LEU:HD12	1:A:339:SER:N	2.24	0.53
1:A:255:ASP:HB3	1:A:261:GLU:O	2.09	0.52
3:D:108:VAL:HB	3:D:119:THR:HG23	1.91	0.52
3:C:34:VAL:HG23	3:C:67:GLY:CA	2.40	0.52
1:A:296:ARG:HA	1:A:302:TYR:HA	1.92	0.52
3:C:111:LEU:CD1	3:C:116:LEU:HD22	2.39	0.52
1:A:244:PRO:HD3	1:A:270:GLY:O	2.10	0.51
3:D:106:LEU:HD23	3:D:121:ASP:HB3	1.91	0.51
3:D:54:LEU:HD12	3:D:88:THR:HG23	1.93	0.50
2:B:356:SER:HA	2:B:359:LEU:HD12	1.94	0.49
2:B:425:LYS:HA	2:B:450:ARG:HD2	1.94	0.49
3:C:153:THR:HG22	3:C:153:THR:O	2.12	0.49
2:B:441:LEU:O	2:B:442:ALA:HB3	2.12	0.49
3:C:162:ILE:HG13	3:C:168:LYS:HD2	1.95	0.49
2:B:258:LEU:HD21	3:C:82:PRO:HD2	1.95	0.48
1:A:412:PHE:CE1	2:B:396:VAL:HG11	2.48	0.48
3:D:13:ILE:HD11	3:D:150:TYR:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:PRO:O	1:A:319:GLU:HB2	2.14	0.48
3:D:79:LEU:C	3:D:79:LEU:HD12	2.39	0.47
3:C:129:GLU:CG	3:C:185:VAL:HG21	2.43	0.47
3:C:107:LEU:HD11	3:C:118:ALA:HB1	1.96	0.47
3:C:153:THR:O	3:C:153:THR:CG2	2.62	0.47
3:C:159:ILE:HG12	3:C:196:VAL:HG22	1.96	0.47
1:A:441:LEU:O	1:A:442:ALA:HB3	2.14	0.47
1:A:346:ARG:NH1	1:A:440:PRO:HG3	2.29	0.47
1:A:267:THR:CG2	1:A:269:THR:HG23	2.44	0.47
8:A:602:HOH:O	2:B:398:THR:HG22	2.16	0.46
3:D:7:VAL:HG12	3:D:7:VAL:O	2.15	0.46
3:C:77:LYS:HA	3:C:86:LEU:HD21	1.97	0.46
3:C:81:ASP:HB2	3:C:82:PRO:CD	2.46	0.46
3:C:162:ILE:HD13	3:C:193:LYS:HB2	1.98	0.46
3:C:85:ARG:HH12	5:C:301:1PG:H92	1.80	0.46
1:A:295:GLU:HA	1:A:295:GLU:OE1	2.17	0.45
1:A:244:PRO:HA	1:A:269:THR:O	2.17	0.45
1:A:295:GLU:O	1:A:303:SER:N	2.50	0.45
3:C:129:GLU:HG3	3:C:185:VAL:HG21	1.99	0.45
3:D:62:ALA:O	3:D:65:LYS:HG3	2.16	0.44
1:A:398:TRP:CG	2:B:398:THR:HG21	2.52	0.44
3:C:162:ILE:HG13	3:C:168:LYS:CD	2.47	0.44
1:A:248:LEU:HD12	1:A:265:THR:O	2.18	0.43
1:A:332:THR:O	1:A:333:PRO:C	2.60	0.43
1:A:351:LEU:H	1:A:446:LYS:NZ	2.16	0.43
1:A:330:LEU:HD12	1:A:330:LEU:O	2.17	0.43
3:C:129:GLU:HG3	3:C:185:VAL:HG22	1.99	0.43
3:D:86:LEU:C	3:D:86:LEU:HD23	2.43	0.43
3:C:79:LEU:HD12	3:C:79:LEU:C	2.43	0.43
2:B:391:PRO:HB2	2:B:393:GLU:OE1	2.19	0.43
3:C:162:ILE:O	3:C:163:LEU:HD12	2.18	0.43
3:D:8:GLN:HB2	3:D:156:TYR:CZ	2.54	0.43
2:B:338:LEU:HD21	7:B:503:EDO:H12	2.00	0.43
2:B:398:THR:HG22	2:B:399:ALA:N	2.33	0.43
1:A:248:LEU:HD12	1:A:249:HIS:H	1.83	0.43
2:B:340:LYS:NZ	8:B:605:HOH:O	2.52	0.43
3:D:85:ARG:HH12	5:D:301:1PG:H61	1.83	0.42
1:A:281:TRP:N	1:A:281:TRP:CD1	2.88	0.42
1:A:298:LEU:N	1:A:298:LEU:CD1	2.82	0.42
1:A:268:LEU:HG	1:A:271:LEU:HD11	2.01	0.42
2:B:313:GLN:HB2	2:B:314:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:PRO:HB2	2:B:330:LEU:HD21	2.02	0.41
3:C:51:ASN:ND2	8:C:405:HOH:O	2.49	0.41
3:C:94:LYS:CG	3:C:95:LYS:N	2.83	0.41
1:A:268:LEU:HD23	1:A:271:LEU:HD21	2.03	0.41
3:D:60:ASP:OD1	3:D:60:ASP:N	2.54	0.41
1:A:267:THR:HG22	1:A:269:THR:HG23	2.02	0.41
3:C:81:ASP:OD1	5:C:301:1PG:C5	2.69	0.41
3:D:158:LYS:HD2	3:D:170:GLU:OE1	2.21	0.41
2:B:392:ARG:HA	2:B:395:TYR:CE1	2.55	0.41
1:A:261:GLU:OE1	1:A:261:GLU:O	2.40	0.40
3:C:86:LEU:C	3:C:86:LEU:HD23	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLU:OE2	3:C:66:GLN:NE2[4_455]	2.19	0.01

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	203/220 (92%)	195 (96%)	8 (4%)	0	100	100
2	B	208/220 (94%)	198 (95%)	9 (4%)	1 (0%)	24	27
3	C	186/201 (92%)	175 (94%)	10 (5%)	1 (0%)	24	27
3	D	184/201 (92%)	179 (97%)	5 (3%)	0	100	100
All	All	781/842 (93%)	747 (96%)	32 (4%)	2 (0%)	36	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	299	CYS
3	C	152	GLY

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	177/188 (94%)	176 (99%)	1 (1%)	78 87
2	B	179/187 (96%)	179 (100%)	0	100 100
3	C	171/182 (94%)	171 (100%)	0	100 100
3	D	171/182 (94%)	170 (99%)	1 (1%)	78 87
All	All	698/739 (94%)	696 (100%)	2 (0%)	86 92

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

Mol	Chain	Res	Type
1	A	281	TRP
3	D	178	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	GLN
2	B	350	HIS
2	B	402	GLN
3	C	46	ASN
3	C	47	GLN
3	C	51	ASN
3	C	105	HIS
3	C	109	ASN
3	D	17	HIS
3	D	36	ASN
3	D	41	ASN

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

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	1PG	B	501	-	7,7,16	0.49	0	6,6,15	0.21	0
5	1PG	A	503	-	10,10,16	0.51	0	9,9,15	0.27	0
7	EDO	B	503	-	3,3,3	0.44	0	2,2,2	0.40	0
6	GOL	C	302	-	5,5,5	1.02	0	5,5,5	1.33	1 (20%)
4	NAG	A	501	1	14,14,15	0.39	0	17,19,21	0.39	0
5	1PG	B	502	-	7,7,16	0.46	0	6,6,15	0.28	0
5	1PG	A	502	-	10,10,16	0.52	0	9,9,15	0.32	0
6	GOL	A	505	-	5,5,5	0.81	0	5,5,5	1.23	1 (20%)
7	EDO	D	302	-	3,3,3	0.45	0	2,2,2	0.35	0
7	EDO	B	504	-	3,3,3	0.41	0	2,2,2	0.46	0
5	1PG	A	504	-	10,10,16	0.52	0	9,9,15	0.22	0
7	EDO	D	303	-	3,3,3	0.44	0	2,2,2	0.38	0
5	1PG	C	301	-	10,10,16	0.50	0	9,9,15	0.29	0
5	1PG	D	301	-	10,10,16	0.52	0	9,9,15	0.33	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
5	1PG	B	501	-	-	2/5/5/14	-
5	1PG	A	503	-	-	4/8/8/14	-
7	EDO	B	503	-	-	1/1/1/1	-
6	GOL	C	302	-	-	0/4/4/4	-
4	NAG	A	501	1	-	2/6/23/26	0/1/1/1
5	1PG	B	502	-	-	3/5/5/14	-
5	1PG	A	502	-	-	4/8/8/14	-
6	GOL	A	505	-	-	2/4/4/4	-
7	EDO	D	302	-	-	0/1/1/1	-
7	EDO	B	504	-	-	1/1/1/1	-
5	1PG	A	504	-	-	2/8/8/14	-
7	EDO	D	303	-	-	0/1/1/1	-
5	1PG	C	301	-	-	5/8/8/14	-
5	1PG	D	301	-	-	4/8/8/14	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	302	GOL	C3-C2-C1	-2.59	102.30	111.80
6	A	505	GOL	C3-C2-C1	-2.36	103.13	111.80

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	NAG	O5-C5-C6-O6
5	B	502	1PG	O3-C6-C7-O4
5	A	502	1PG	O5-C10-C11-O6
5	D	301	1PG	O5-C10-C11-O6
5	A	504	1PG	O3-C6-C7-O4
5	A	502	1PG	O4-C8-C9-O5
5	D	301	1PG	O4-C8-C9-O5
5	B	502	1PG	O4-C8-C9-O5
4	A	501	NAG	C4-C5-C6-O6
5	C	301	1PG	O3-C6-C7-O4
7	B	504	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	503	1PG	O3-C6-C7-O4
7	B	503	EDO	O1-C1-C2-O2
5	B	501	1PG	C6-C7-O4-C8
5	B	502	1PG	C7-C6-O3-C5
6	A	505	GOL	C1-C2-C3-O3
5	B	501	1PG	O4-C8-C9-O5
5	A	504	1PG	O5-C10-C11-O6
5	D	301	1PG	O3-C6-C7-O4
5	A	502	1PG	C7-C6-O3-C5
5	A	503	1PG	C7-C6-O3-C5
5	C	301	1PG	C8-C9-O5-C10
5	C	301	1PG	O5-C10-C11-O6
5	A	503	1PG	C11-C10-O5-C9
5	D	301	1PG	C6-C7-O4-C8
5	A	503	1PG	O4-C8-C9-O5
5	A	502	1PG	C9-C8-O4-C7
5	C	301	1PG	O4-C8-C9-O5
6	A	505	GOL	O2-C2-C3-O3
5	C	301	1PG	C11-C10-O5-C9

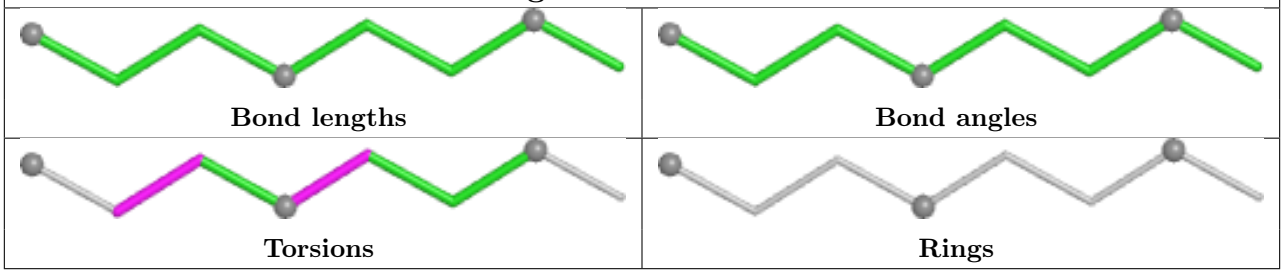
There are no ring outliers.

3 monomers are involved in 4 short contacts:

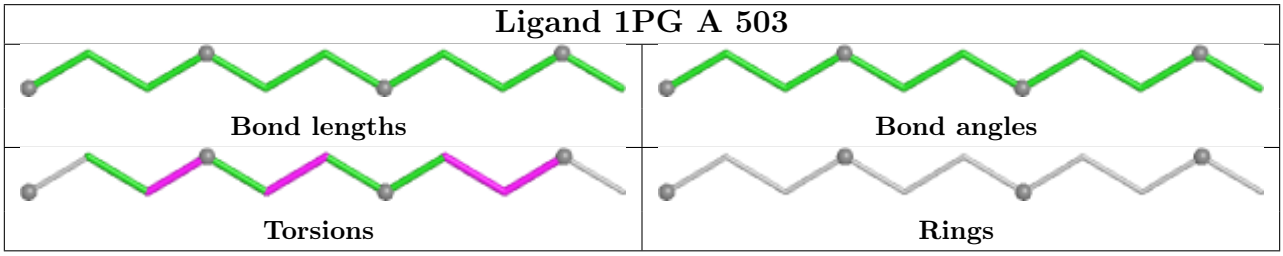
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	503	EDO	1	0
5	C	301	1PG	2	0
5	D	301	1PG	1	0

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 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.

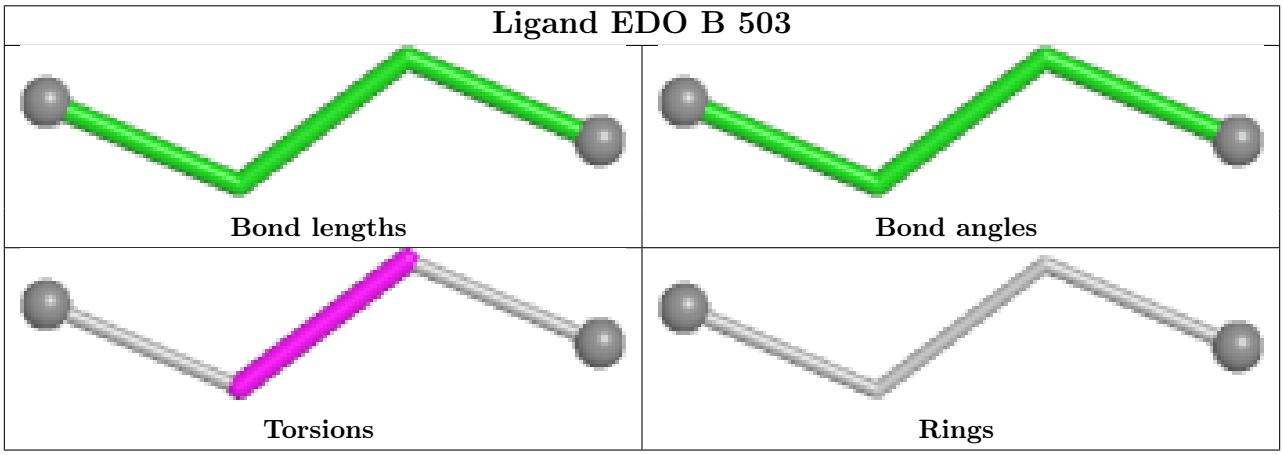
Ligand 1PG B 501



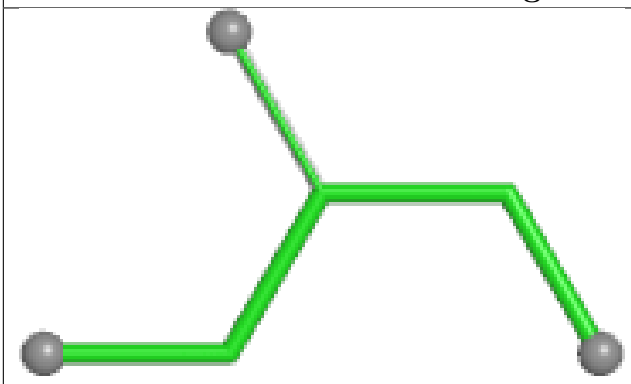
Ligand 1PG A 503



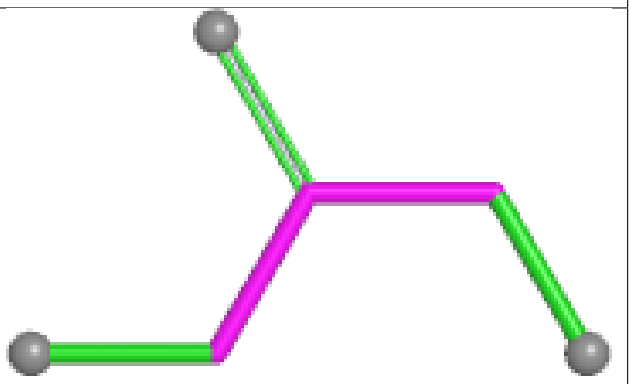
Ligand EDO B 503



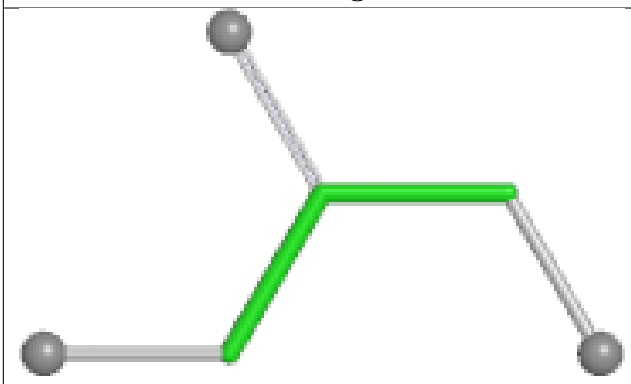
Ligand GOL C 302



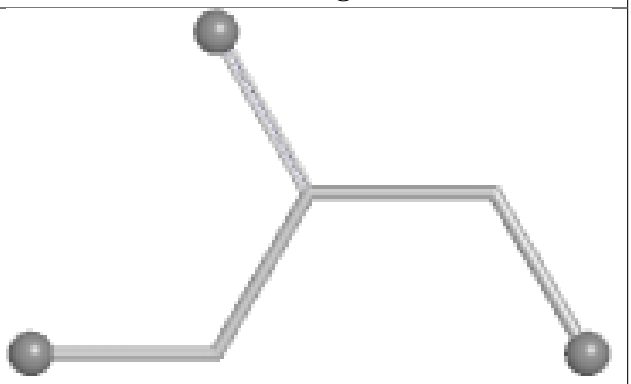
Bond lengths



Bond angles

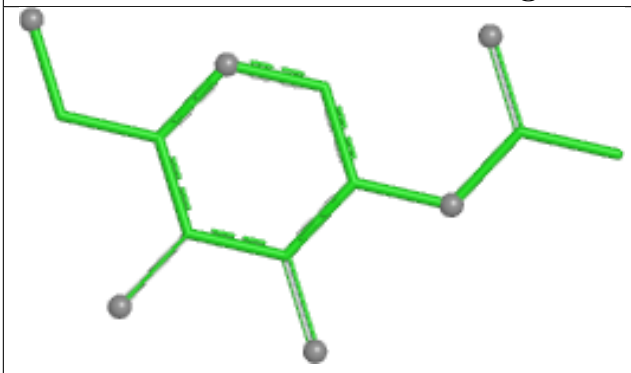


Torsions

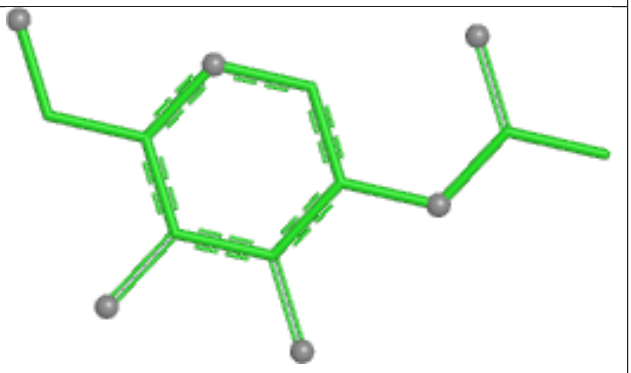


Rings

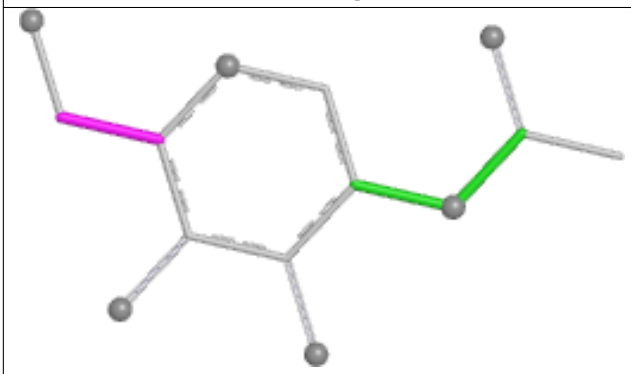
Ligand NAG A 501



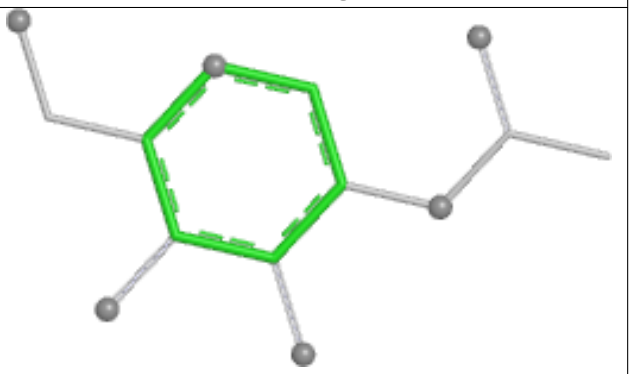
Bond lengths



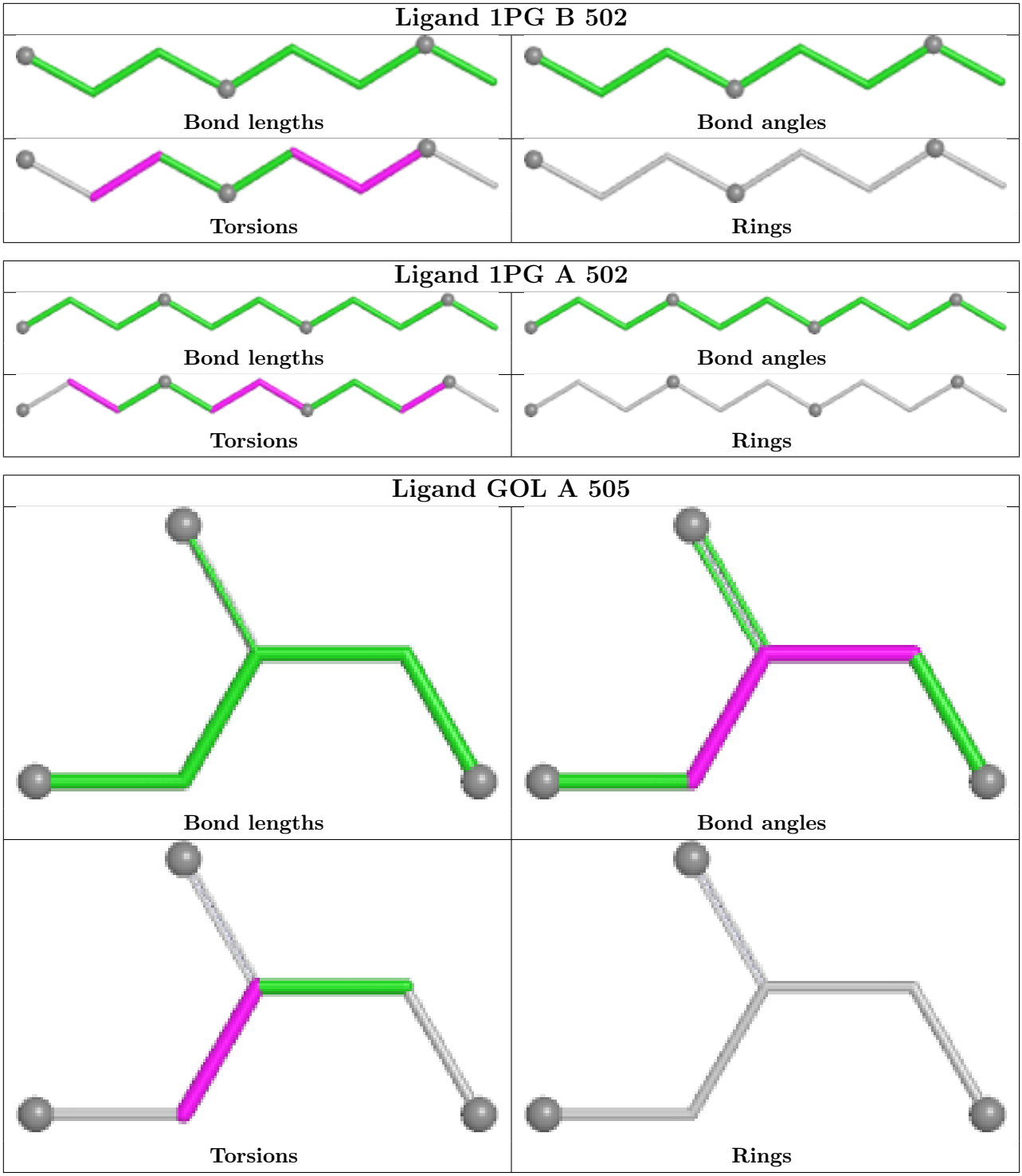
Bond angles



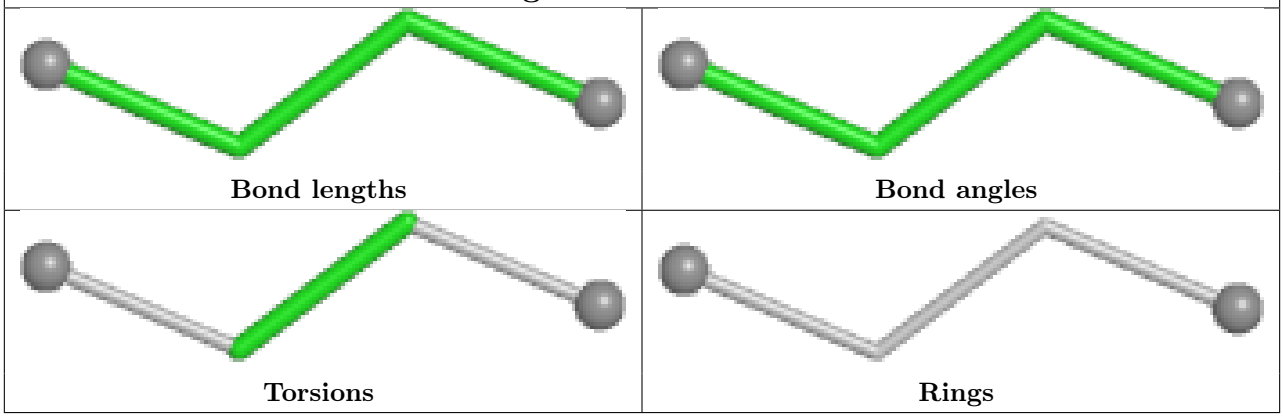
Torsions



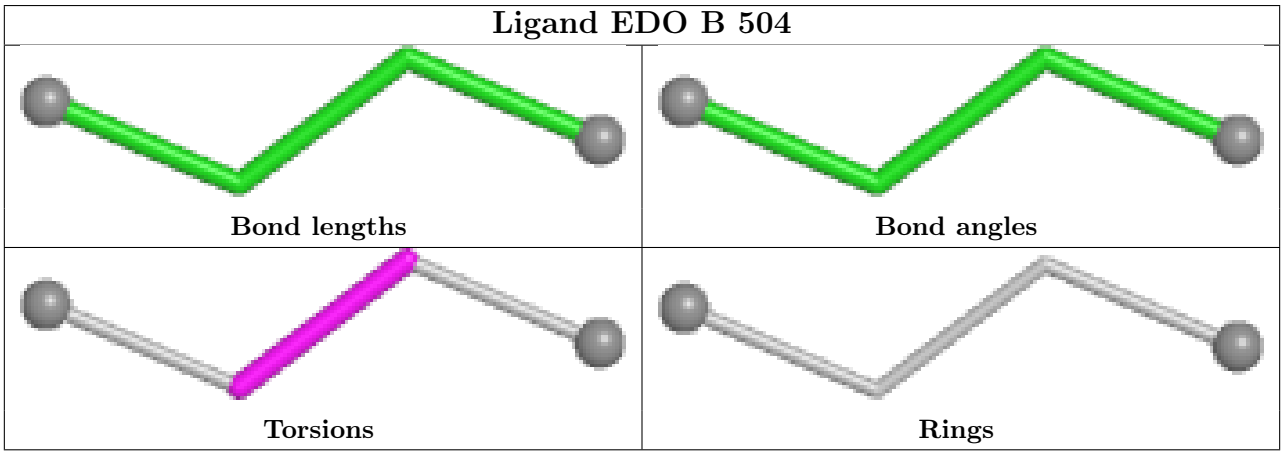
Rings


Ligand 1PG B 502
Bond lengths
Bond angles
Torsions
Rings
Ligand 1PG A 502
Bond lengths
Bond angles
Torsions
Rings
Ligand GOL A 505
Bond lengths
Bond angles
Torsions
Rings

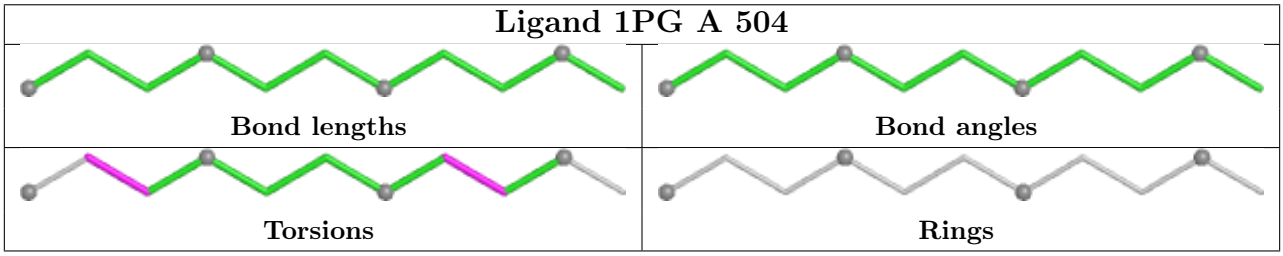
Ligand EDO D 302



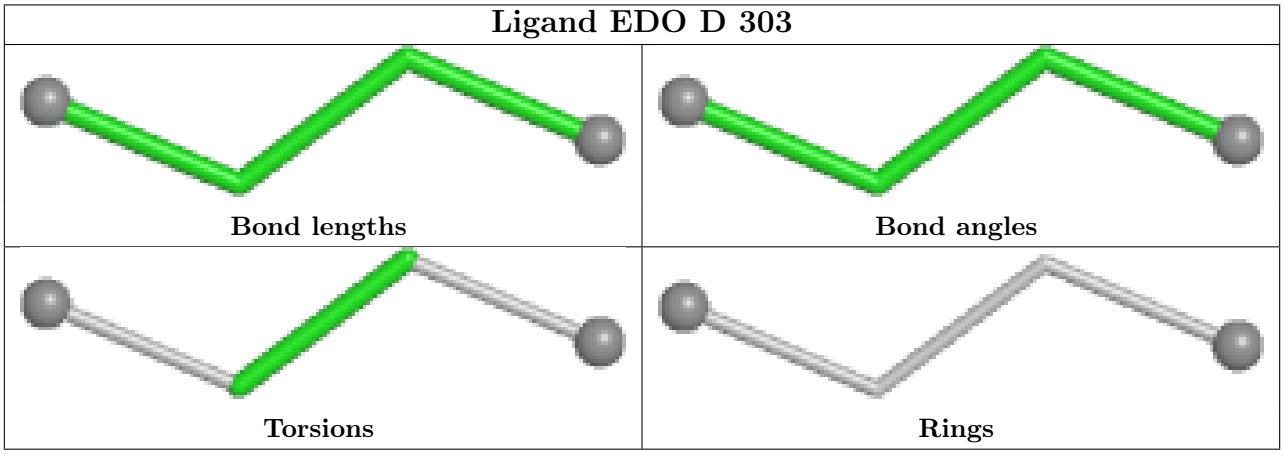
Ligand EDO B 504

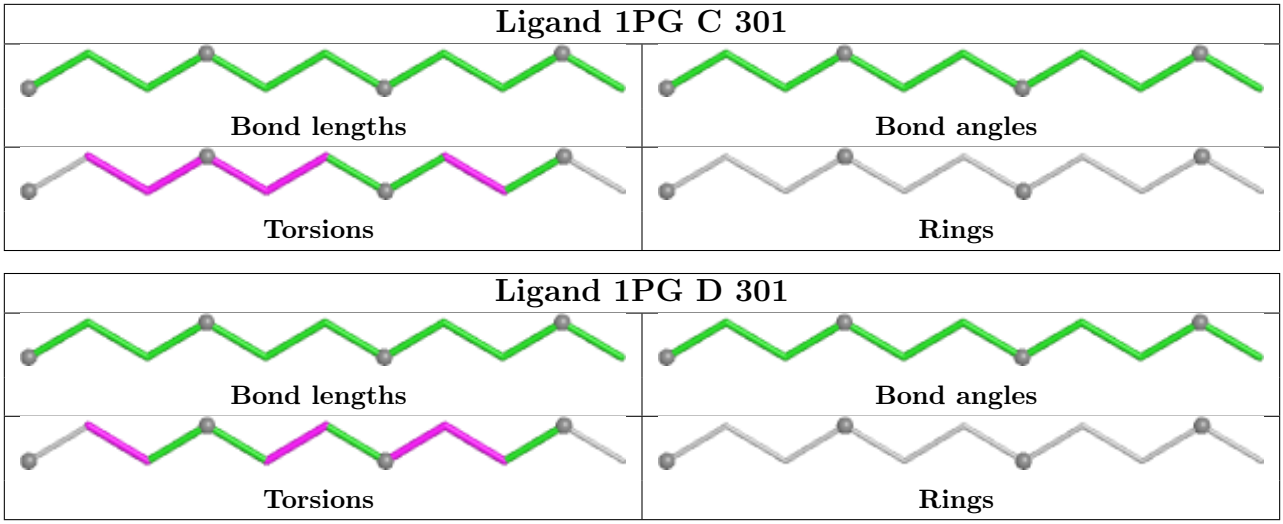


Ligand 1PG A 504



Ligand EDO D 303





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	207/220 (94%)	1.04	38 (18%) 3 3	39, 69, 119, 141	0
2	B	210/220 (95%)	0.58	12 (5%) 29 34	33, 57, 91, 120	0
3	C	190/201 (94%)	0.73	19 (10%) 12 14	39, 67, 99, 124	0
3	D	188/201 (93%)	0.45	7 (3%) 45 51	41, 57, 82, 100	0
All	All	795/842 (94%)	0.71	76 (9%) 13 16	33, 61, 109, 141	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	7	VAL	5.1
1	A	406	GLN	4.4
1	A	282	THR	4.2
1	A	271	LEU	4.2
3	C	96	ASN	4.1
3	C	100	SER	4.0
1	A	361	LEU	3.8
1	A	328	PRO	3.8
3	C	201	ILE	3.7
1	A	248	LEU	3.6
2	B	451	LEU	3.5
3	C	200	GLN	3.5
1	A	242	CYS	3.5
2	B	285	SER	3.4
1	A	272	ARG	3.4
1	A	270	GLY	3.3
3	D	126	ASN	3.3
3	D	201	ILE	3.3
1	A	324	THR	3.2
1	A	297	ASP	3.2
1	A	293	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	406	GLN	3.1
3	D	199	LYS	3.1
3	D	118	ALA	2.9
2	B	261	GLU	2.9
3	C	117	ASP	2.9
3	C	118	ALA	2.9
1	A	286	GLY	2.8
3	C	9	HIS	2.7
3	C	162	ILE	2.7
2	B	242	CYS	2.7
1	A	322	THR	2.6
1	A	331	LYS	2.6
1	A	274	ALA	2.6
1	A	279	PHE	2.6
1	A	298	LEU	2.6
1	A	334	LEU	2.6
3	C	95	LYS	2.6
1	A	296	ARG	2.6
1	A	261	GLU	2.5
1	A	301	CYS	2.5
3	C	66	GLN	2.5
1	A	243	HIS	2.5
1	A	285	SER	2.5
3	C	10	LEU	2.5
3	C	116	LEU	2.5
2	B	313	GLN	2.5
1	A	281	TRP	2.4
3	C	168	LYS	2.4
2	B	408	THR	2.4
1	A	309	PRO	2.4
1	A	342	GLY	2.3
2	B	284	SER	2.3
3	C	163	LEU	2.3
3	C	175	ASP	2.3
2	B	300	GLY	2.3
1	A	332	THR	2.3
3	C	151	GLN	2.3
1	A	330	LEU	2.3
2	B	298	LEU	2.3
1	A	414	TYR	2.3
1	A	362	ASN	2.2
1	A	308	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	299	CYS	2.2
1	A	319	GLU	2.2
2	B	274	ALA	2.2
1	A	318	GLY	2.2
3	C	187	ASN	2.1
3	D	48	GLU	2.1
3	D	110	LYS	2.1
1	A	317	HIS	2.1
1	A	321	PHE	2.1
3	C	112	ASP	2.1
1	A	398	TRP	2.1
2	B	425	LYS	2.0
3	C	188	SER	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
7	EDO	D	302	4/4	0.64	0.21	68,82,93,93	0
5	1PG	B	502	8/17	0.65	0.23	39,67,80,80	0
4	NAG	A	501	14/15	0.71	0.16	97,110,129,135	0
7	EDO	D	303	4/4	0.73	0.24	62,74,80,83	0
5	1PG	A	504	11/17	0.77	0.19	59,74,80,82	0
5	1PG	A	503	11/17	0.77	0.17	55,80,92,96	0
5	1PG	D	301	11/17	0.79	0.17	44,67,74,87	0
6	GOL	C	302	6/6	0.85	0.13	69,81,97,97	0
7	EDO	B	503	4/4	0.85	0.17	55,66,72,73	0
5	1PG	B	501	8/17	0.85	0.15	54,73,88,88	0

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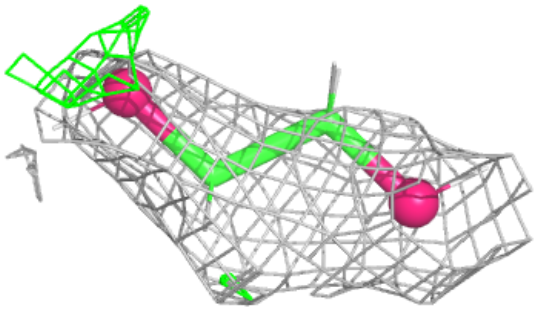
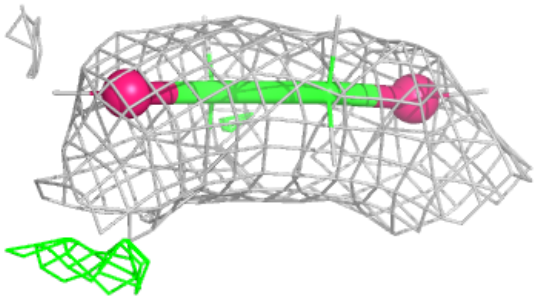
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	A	505	6/6	0.85	0.15	63,79,96,101	0
7	EDO	B	504	4/4	0.88	0.12	55,66,80,80	0
5	1PG	A	502	11/17	0.90	0.12	42,63,74,76	0
5	1PG	C	301	11/17	0.92	0.12	41,54,72,80	0

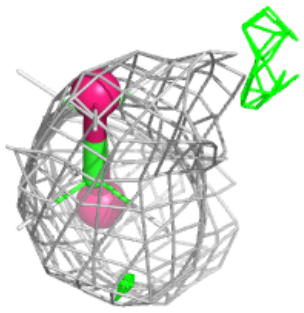
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EDO 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)

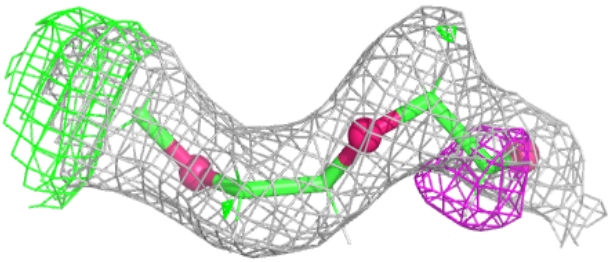


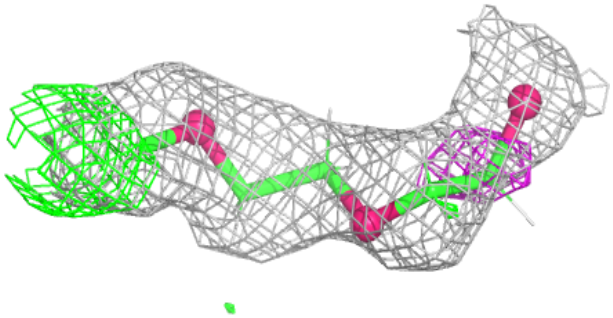


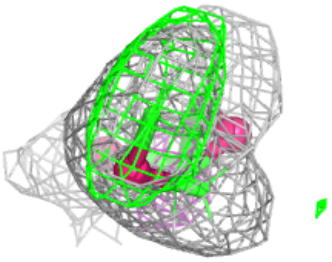


Electron density around 1PG B 502:

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

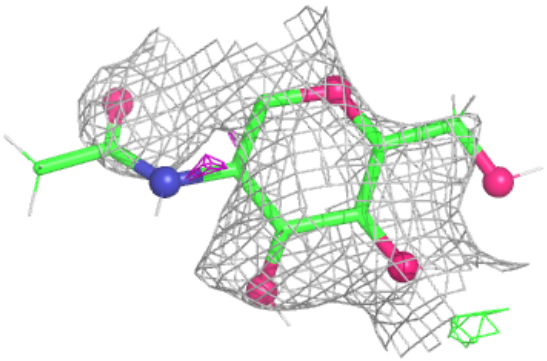


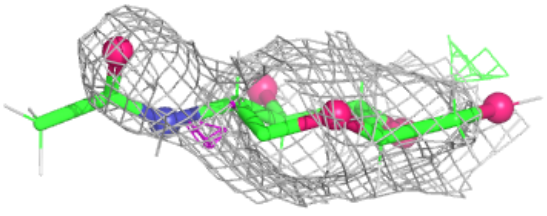


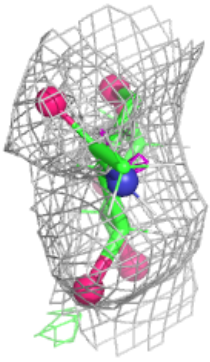


Electron density around NAG A 501:

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

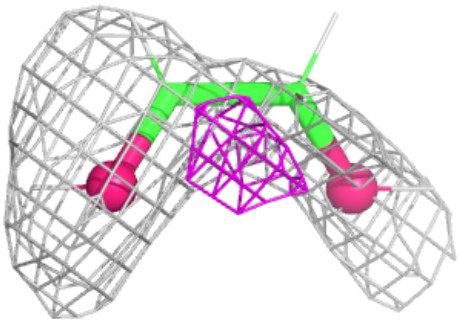


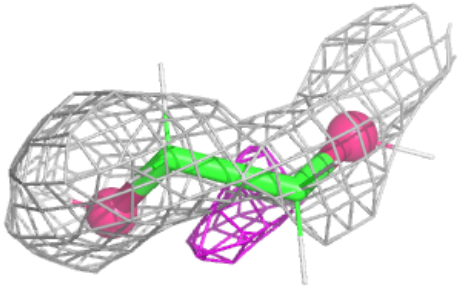


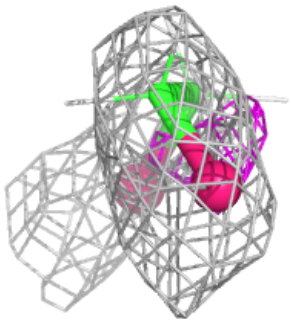


Electron density around EDO D 303:

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

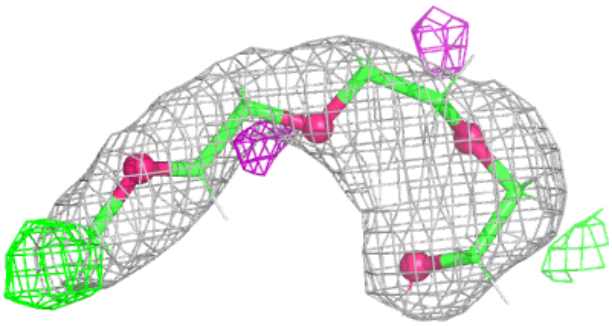


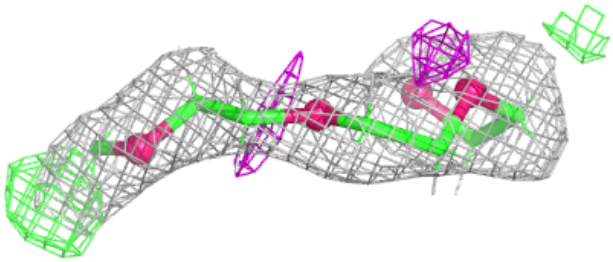


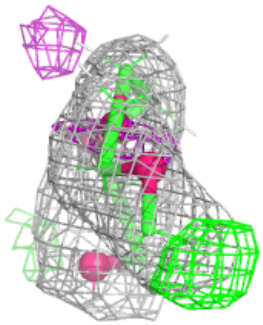


Electron density around 1PG A 504:

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

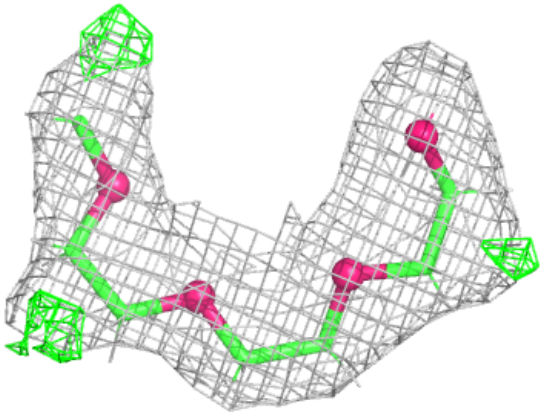


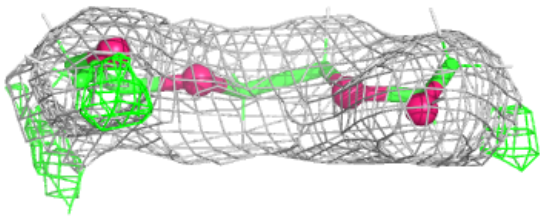


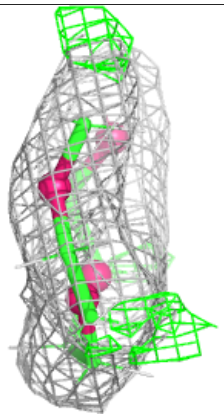


Electron density around 1PG A 503:

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

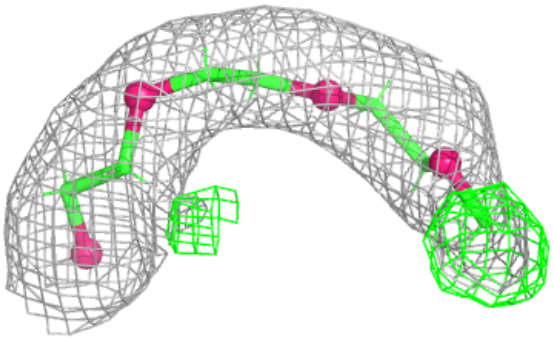


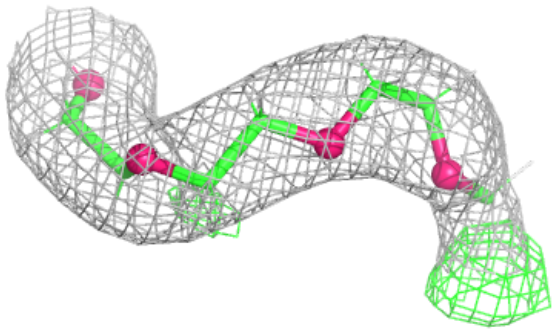


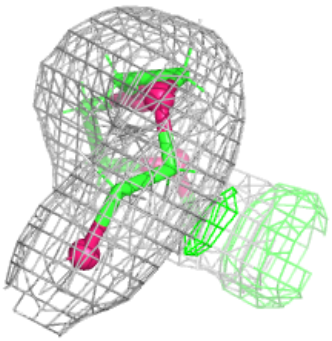


Electron density around 1PG D 301:

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

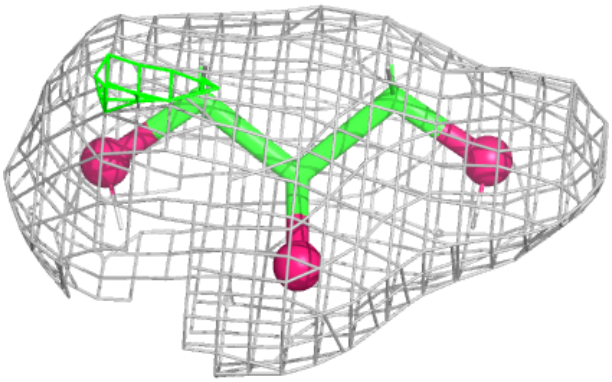


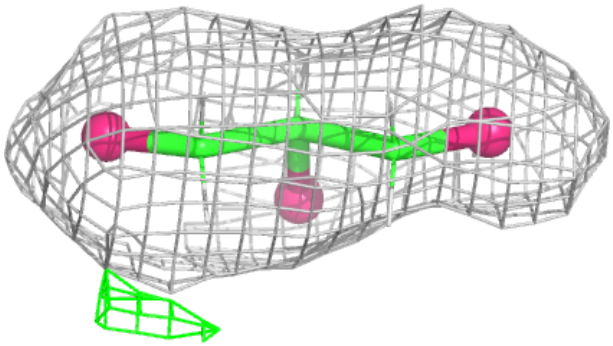


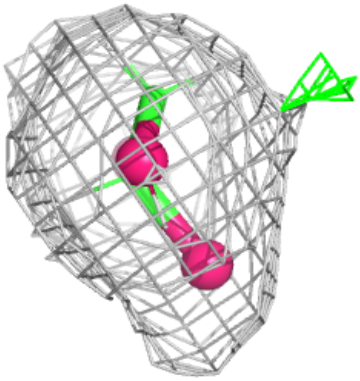


Electron density around GOL C 302:

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

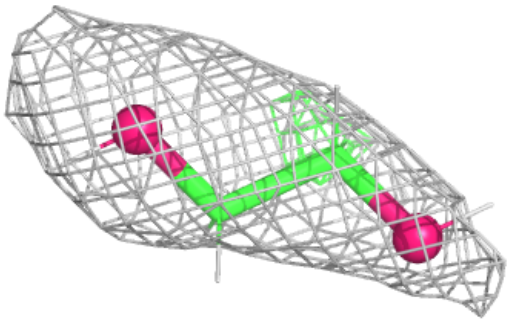


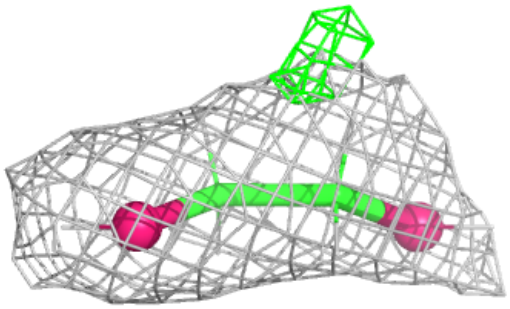


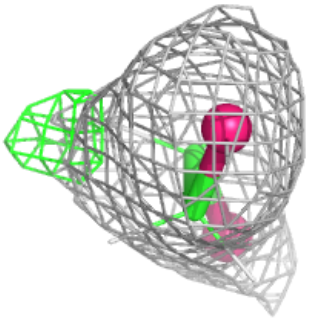


Electron density around EDO B 503:

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

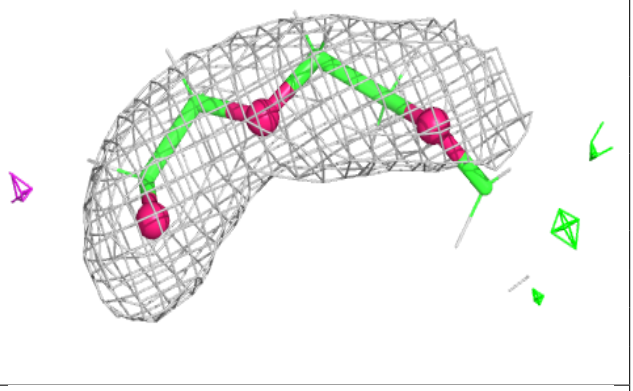


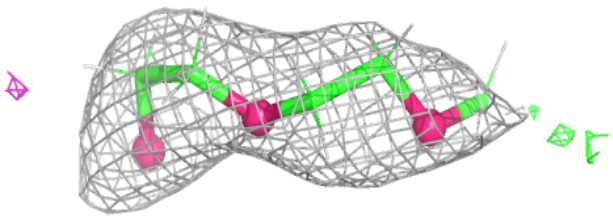


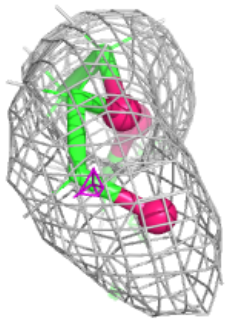


Electron density around 1PG B 501:

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

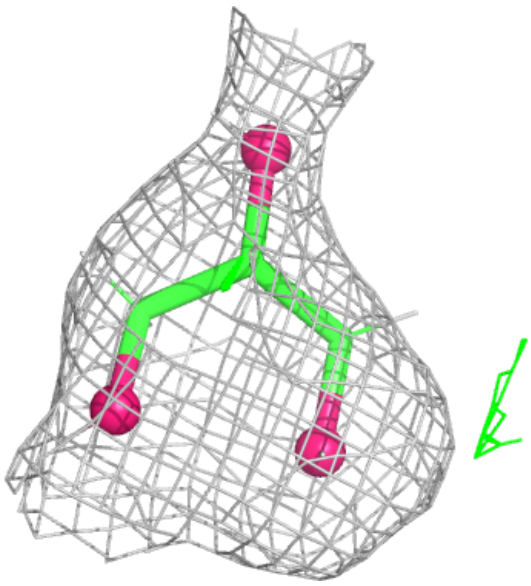


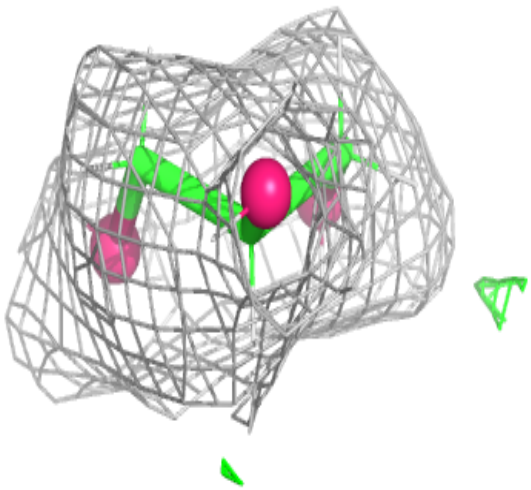


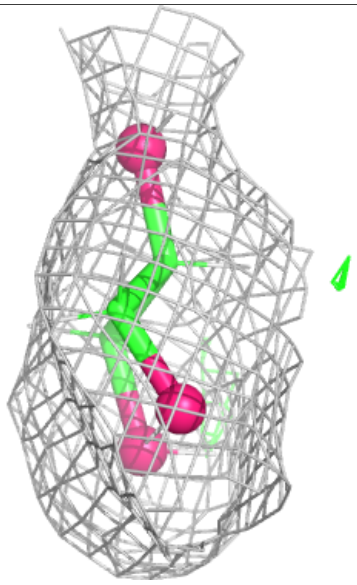


Electron density around GOL A 505:

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

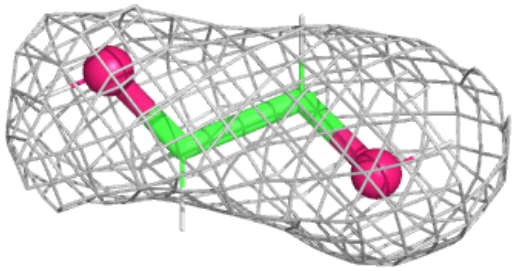


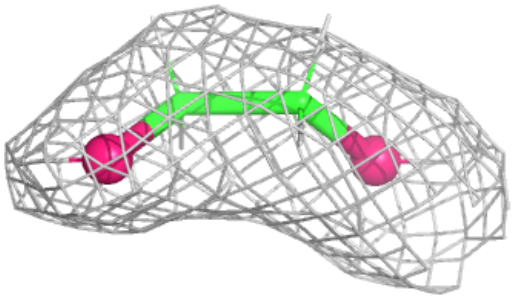


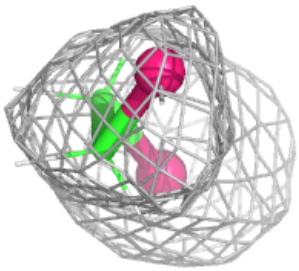


Electron density around EDO B 504:

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

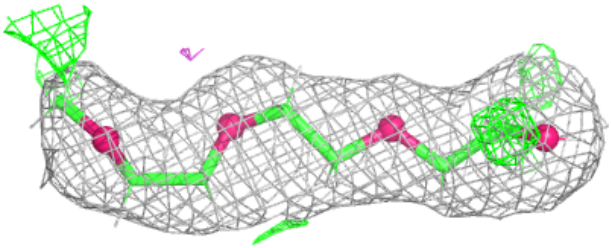


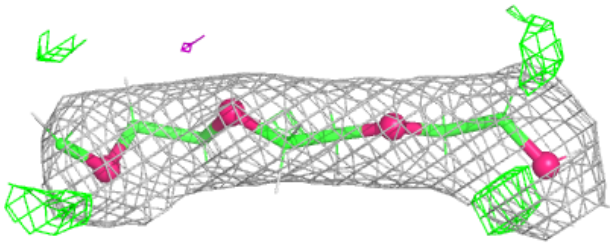


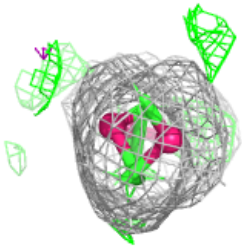


Electron density around 1PG A 502:

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

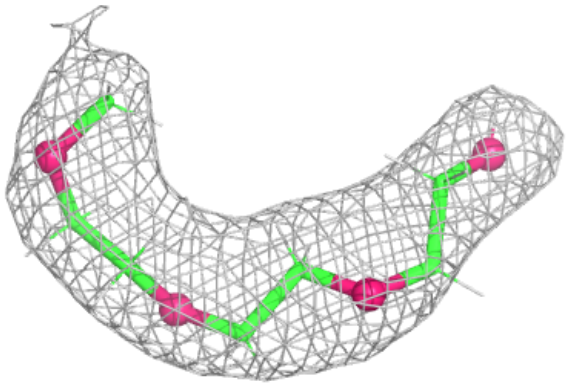


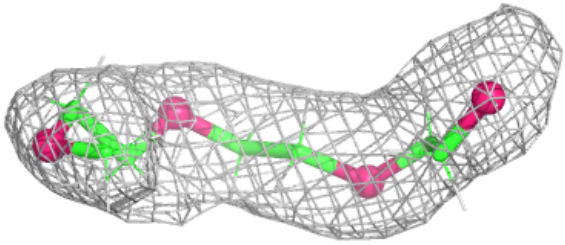


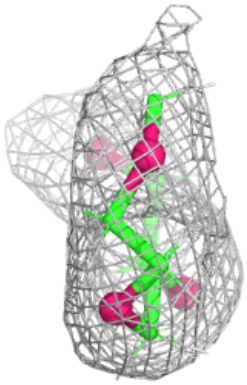


Electron density around 1PG C 301:

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







6.5 Other polymers

There are no such residues in this entry.