



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2022 – 02:14 PM EDT

PDB ID : 6MN5
Title : Crystal structure of aminoglycoside acetyltransferase AAC(3)-IVa, H154A mutant, in complex with gentamicin C1A
Authors : Stogios, P.J.; Evdokimova, E.; Kim, Y.; Di Leo, R.; Savchenko, A.; Joachimiak, A.; Satchell, K.J.; Center for Structural Genomics of Infectious Diseases (CS-GID)
Deposited on : 2018-10-01
Resolution : 2.58 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
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)	:	2.27

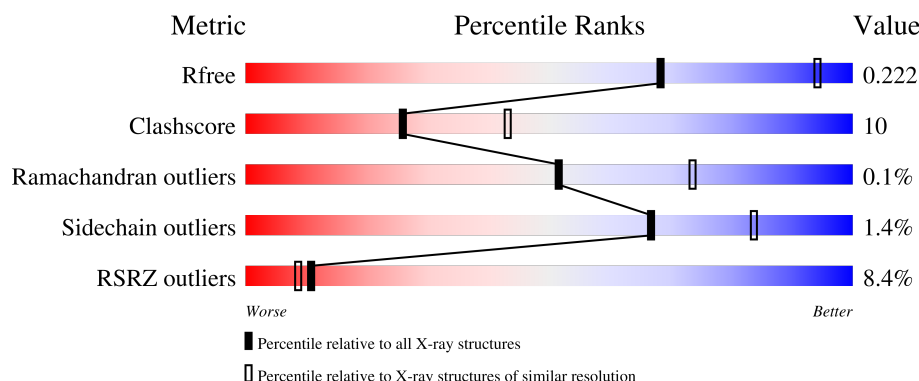
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	262	
1	B	262	
1	C	262	
1	D	262	
1	E	262	

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Mol	Chain	Length	Quality of chain
1	F	262	<div> <div>21%</div> <div>65%</div> <div>33%</div> <div>..</div> </div>

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
3	ZN	E	302	-	-	X	-
6	EDO	C	314	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12951 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 Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	2	0
			1981	1258	351	364	8			
1	B	259	Total	C	N	O	S	0	0	0
			1970	1251	350	361	8			
1	C	259	Total	C	N	O	S	0	0	0
			1970	1251	350	361	8			
1	D	260	Total	C	N	O	S	0	0	0
			1975	1253	351	363	8			
1	E	259	Total	C	N	O	S	0	0	0
			1964	1248	347	361	8			
1	F	259	Total	C	N	O	S	0	0	0
			1964	1248	347	361	8			

There are 30 discrepancies between the modelled and reference sequences:

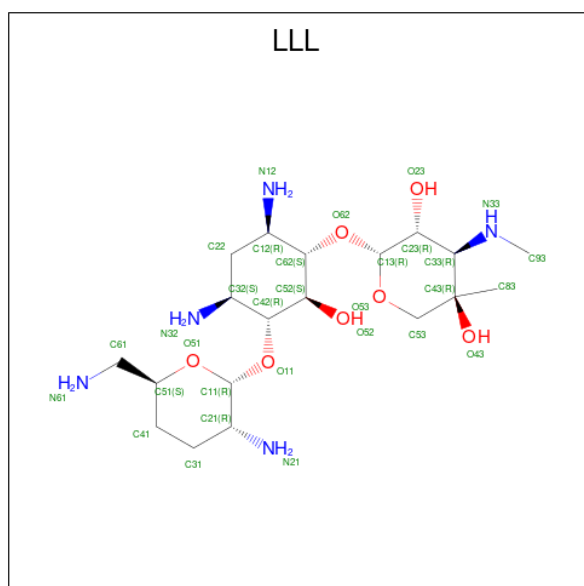
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q306W4
A	-2	GLN	-	expression tag	UNP Q306W4
A	-1	GLN	-	expression tag	UNP Q306W4
A	0	MET	-	expression tag	UNP Q306W4
A	154	ALA	HIS	engineered mutation	UNP Q306W4
B	-3	GLY	-	expression tag	UNP Q306W4
B	-2	GLN	-	expression tag	UNP Q306W4
B	-1	GLN	-	expression tag	UNP Q306W4
B	0	MET	-	expression tag	UNP Q306W4
B	154	ALA	HIS	engineered mutation	UNP Q306W4
C	-3	GLY	-	expression tag	UNP Q306W4
C	-2	GLN	-	expression tag	UNP Q306W4
C	-1	GLN	-	expression tag	UNP Q306W4
C	0	MET	-	expression tag	UNP Q306W4
C	154	ALA	HIS	engineered mutation	UNP Q306W4
D	-3	GLY	-	expression tag	UNP Q306W4
D	-2	GLN	-	expression tag	UNP Q306W4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLN	-	expression tag	UNP Q306W4
D	0	MET	-	expression tag	UNP Q306W4
D	154	ALA	HIS	engineered mutation	UNP Q306W4
E	-3	GLY	-	expression tag	UNP Q306W4
E	-2	GLN	-	expression tag	UNP Q306W4
E	-1	GLN	-	expression tag	UNP Q306W4
E	0	MET	-	expression tag	UNP Q306W4
E	154	ALA	HIS	engineered mutation	UNP Q306W4
F	-3	GLY	-	expression tag	UNP Q306W4
F	-2	GLN	-	expression tag	UNP Q306W4
F	-1	GLN	-	expression tag	UNP Q306W4
F	0	MET	-	expression tag	UNP Q306W4
F	154	ALA	HIS	engineered mutation	UNP Q306W4

- Molecule 2 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C₁₉H₃₉N₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	19	5	7		
2	B	1	Total	C	N	O	0	0
			31	19	5	7		
2	C	1	Total	C	N	O	0	0
			31	19	5	7		

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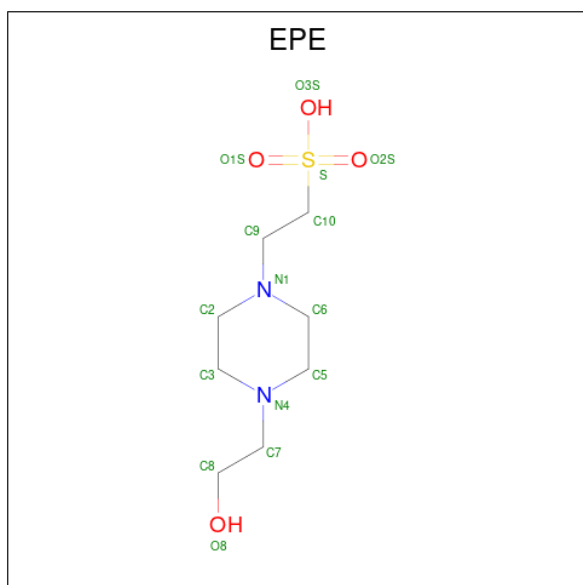
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			31	19	5	7		
2	E	1	Total	C	N	O	0	0
			31	19	5	7		
2	F	1	Total	C	N	O	0	0
			31	19	5	7		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

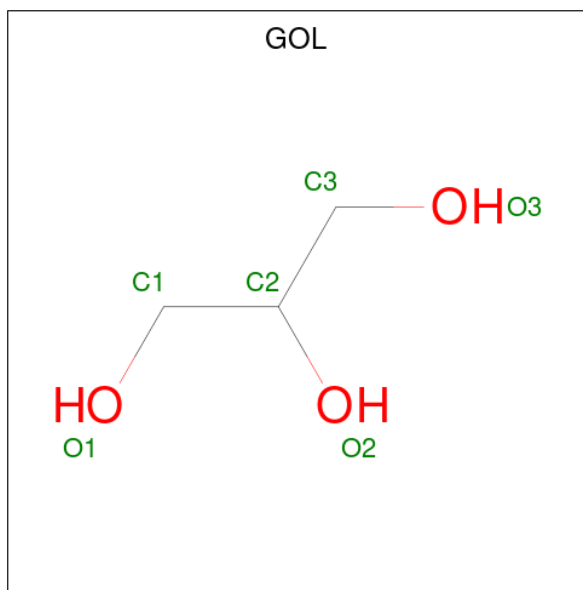
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



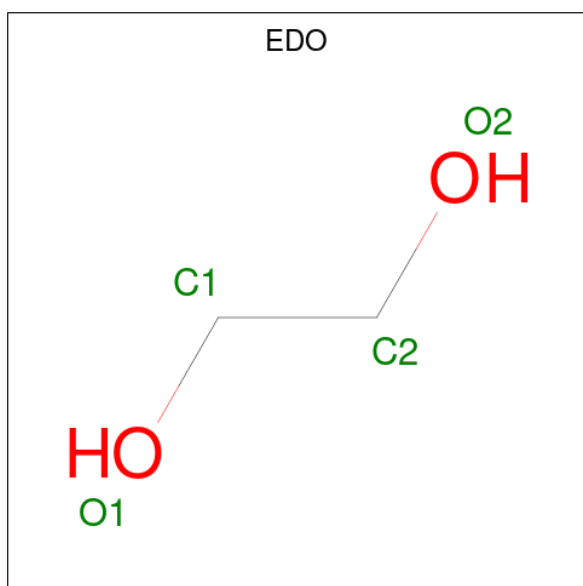
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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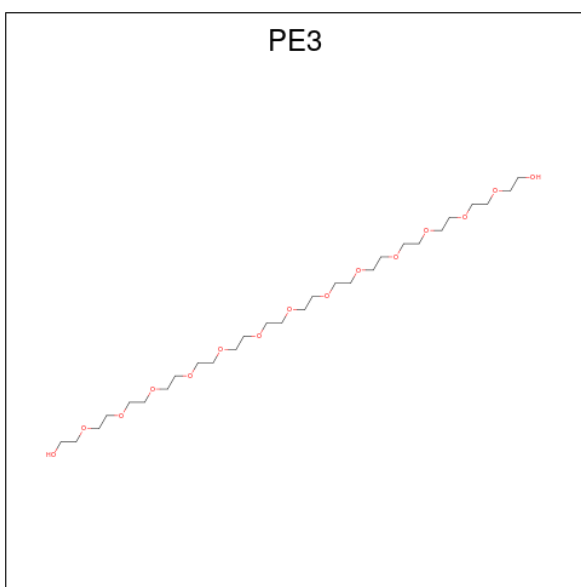
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0

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

- Molecule 7 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1,41-DIOL (three-letter code: PE3) (formula: C₂₈H₅₈O₁₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			16	10	6		
7	C	1	Total	C	O	0	0
			10	6	4		
7	D	1	Total	C	O	0	0
			16	10	6		

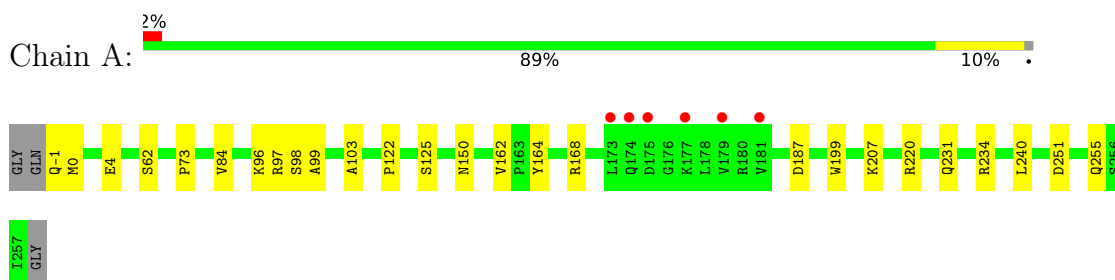
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	161	Total	O	0	3
			164	164		
8	B	120	Total	O	0	4
			124	124		
8	C	97	Total	O	0	1
			98	98		
8	D	76	Total	O	0	1
			77	77		
8	E	25	Total	O	0	0
			25	25		
8	F	30	Total	O	0	1
			31	31		

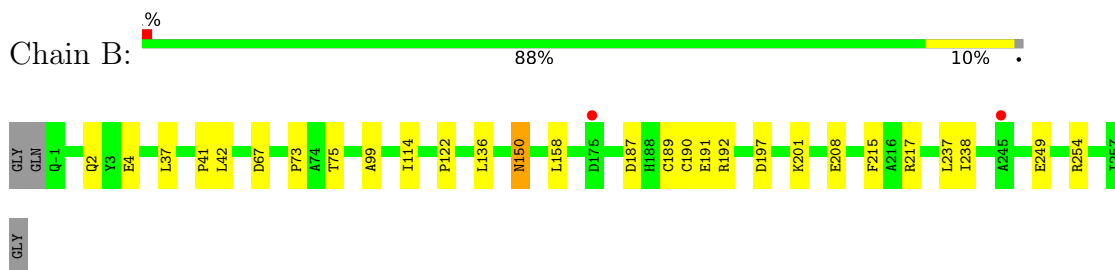
3 Residue-property plots [i](#)

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.

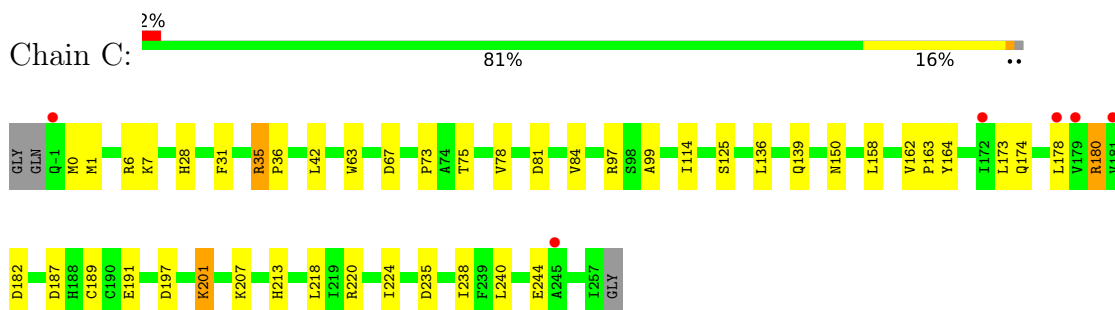
- Molecule 1: Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa



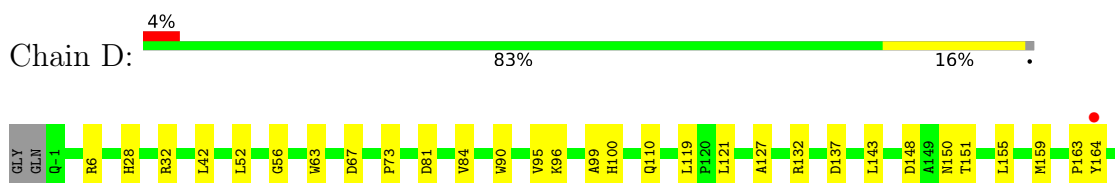
- Molecule 1: Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa



- Molecule 1: Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa

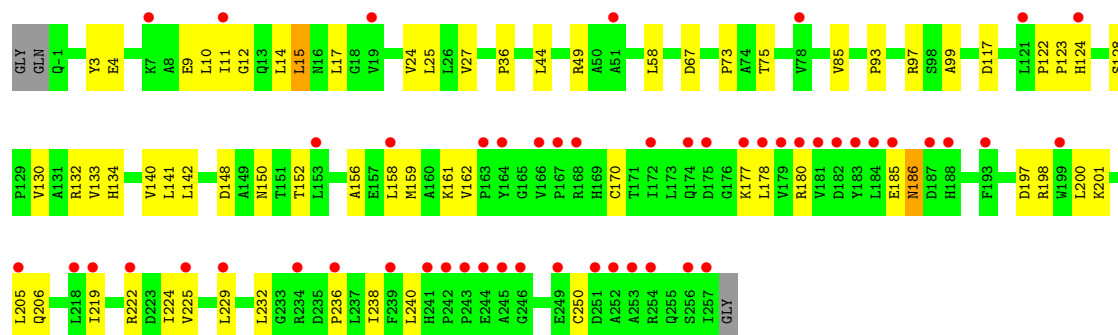
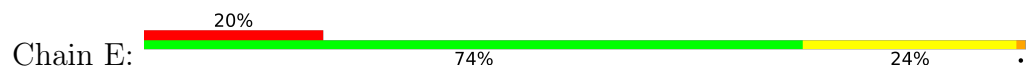


- Molecule 1: Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa

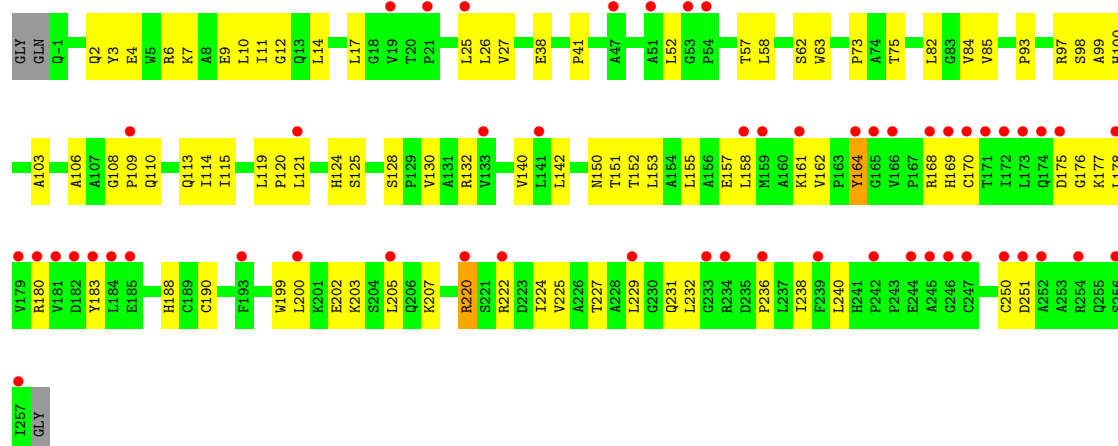




- Molecule 1: Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa



- Molecule 1: Aminoglycoside N(3)-acetyltransferase, AAC(3)-IVa



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.61Å 131.88Å 266.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.40 – 2.58 39.41 – 2.58	Depositor EDS
% Data completeness (in resolution range)	95.6 (38.40-2.58) 89.8 (39.41-2.58)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.58Å)	Xtriage
Refinement program	PHENIX (dev_3026: ???)	Depositor
R, R_{free}	0.187 , 0.221 0.186 , 0.222	Depositor DCC
R_{free} test set	2000 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12951	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: ZN, LLL, GOL, PE3, EPE, 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	0.25	0/2038	0.44	0/2781
1	B	0.25	0/2021	0.43	0/2758
1	C	0.32	0/2021	0.46	0/2758
1	D	0.27	0/2026	0.46	0/2763
1	E	0.27	0/2015	0.50	0/2751
1	F	0.30	0/2015	0.51	0/2751
All	All	0.28	0/12136	0.47	0/16562

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	1981	0	1975	18	0
1	B	1970	0	1963	29	0
1	C	1970	0	1963	42	0
1	D	1975	0	1966	29	0
1	E	1964	0	1954	46	0
1	F	1964	0	1953	78	0
2	A	31	0	39	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	39	9	0
2	C	31	0	39	5	0
2	D	31	0	39	5	0
2	E	31	0	39	6	0
2	F	31	0	39	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	2	0
3	F	1	0	0	0	0
4	A	30	0	36	1	0
4	B	30	0	36	3	0
4	C	30	0	36	5	0
4	D	30	0	36	1	0
4	E	30	0	36	1	0
4	F	30	0	36	2	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	12	0	16	1	0
6	A	44	0	66	5	0
6	B	32	0	48	2	0
6	C	36	0	54	6	0
6	D	32	0	48	2	0
6	E	16	0	24	1	0
6	F	4	0	6	0	0
7	B	16	0	20	4	0
7	C	10	0	13	0	0
7	D	16	0	20	1	0
8	A	164	0	0	3	0
8	B	124	0	0	2	0
8	C	98	0	0	3	0
8	D	77	0	0	3	0
8	E	25	0	0	0	0
8	F	31	0	0	2	0
All	All	12951	0	12563	262	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 10.

All (262) 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:F:125:SER:HA	1:F:158:LEU:HD13	1.40	1.03
2:D:301:LLL:N32	2:D:301:LLL:O51	2.09	0.85
2:F:301:LLL:H933	2:F:301:LLL:H832	1.58	0.83
1:F:125:SER:HA	1:F:158:LEU:CD1	2.09	0.82
1:C:173:LEU:HD23	1:C:178:LEU:HD23	1.61	0.82
1:C:28:HIS:HD2	8:C:437:HOH:O	1.61	0.82
1:F:142:LEU:HD21	1:F:150:ASN:HB2	1.61	0.82
1:C:28:HIS:CD2	8:C:437:HOH:O	2.33	0.81
1:B:201:LYS:HE2	7:B:314:PE3:H361	1.65	0.78
1:D:163:PRO:HB2	1:D:257:ILE:HG23	1.67	0.77
1:E:142:LEU:HD21	1:E:150:ASN:HB2	1.66	0.76
1:E:250:CYS:SG	3:E:302:ZN:ZN	1.73	0.75
1:D:127:ALA:HA	1:D:132:ARG:HH21	1.51	0.75
1:F:177:LYS:HE3	1:F:178:LEU:HD12	1.69	0.74
1:B:254:ARG:HH22	6:B:307:EDO:H21	1.52	0.74
2:C:301:LLL:O52	2:C:301:LLL:O53	2.06	0.73
2:A:301:LLL:O53	2:A:301:LLL:O52	2.06	0.73
2:E:301:LLL:O53	2:E:301:LLL:O52	2.06	0.71
1:D:248:GLU:O	1:D:251:ASP:N	2.24	0.71
2:D:301:LLL:H322	2:D:301:LLL:C51	2.04	0.71
1:F:11:ILE:HD12	1:F:12:GLY:N	2.05	0.71
1:D:201:LYS:HE2	7:D:315:PE3:H302	1.71	0.71
1:B:201:LYS:CE	7:B:314:PE3:H361	2.21	0.70
2:F:301:LLL:H933	2:F:301:LLL:C83	2.22	0.70
2:B:301:LLL:O53	2:B:301:LLL:O52	2.05	0.69
2:D:301:LLL:O53	2:D:301:LLL:O52	2.10	0.69
2:F:301:LLL:C13	2:F:301:LLL:H3	2.05	0.69
1:C:35:ARG:NH1	4:C:304:EPE:O3S	2.23	0.69
2:F:301:LLL:O52	2:F:301:LLL:O53	2.09	0.69
1:F:62:SER:HG	1:F:97:ARG:HH11	1.40	0.68
1:F:200:LEU:HD11	1:F:205:LEU:HD12	1.74	0.67
1:C:220:ARG:HG3	6:C:314:EDO:H12	1.77	0.67
1:F:153:LEU:HD21	1:F:224:ILE:HB	1.76	0.67
1:B:2:GLN:NE2	1:C:213:HIS:O	2.27	0.67
1:B:201:LYS:NZ	7:B:314:PE3:H361	2.10	0.66
1:F:232:LEU:HG	1:F:238:ILE:HD11	1.75	0.66
1:C:244:GLU:OE2	1:C:244:GLU:N	2.29	0.66
1:E:250:CYS:HG	3:E:302:ZN:ZN	1.05	0.65
6:A:306:EDO:H21	1:B:42:LEU:HB2	1.77	0.65
1:F:41:PRO:HB3	1:F:85:VAL:HG12	1.78	0.64
1:A:220:ARG:HG3	6:A:316:EDO:H12	1.78	0.64
1:E:156:ALA:HB2	1:E:225:VAL:HG12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:ILE:HD12	1:F:12:GLY:H	1.61	0.64
2:F:301:LLL:H322	2:F:301:LLL:H11A	1.46	0.64
6:A:306:EDO:H12	1:B:41:PRO:HD2	1.81	0.63
1:F:57:THR:HG22	1:F:108:GLY:HA3	1.81	0.63
1:C:150:ASN:HD21	1:C:224:ILE:HD13	1.64	0.63
1:E:25:LEU:HD11	1:E:141:LEU:HB3	1.81	0.63
1:F:121:LEU:HD22	1:F:183:TYR:HB3	1.81	0.63
2:E:301:LLL:O51	2:E:301:LLL:N32	2.29	0.62
1:F:190:CYS:SG	2:F:301:LLL:N32	2.69	0.62
1:F:124:HIS:HB3	1:F:130:VAL:HG11	1.80	0.61
1:F:224:ILE:HD12	1:F:225:VAL:N	2.16	0.61
1:C:173:LEU:CD2	1:C:178:LEU:HD23	2.30	0.61
1:E:97:ARG:H	6:E:305:EDO:H22	1.65	0.61
1:C:201:LYS:NZ	8:C:401:HOH:O	2.33	0.60
1:C:31:PHE:O	1:C:35:ARG:HG2	2.00	0.60
1:D:100:HIS:HB2	1:D:119:LEU:HD12	1.83	0.60
1:C:180:ARG:NH1	1:C:182:ASP:OD2	2.34	0.60
1:F:178:LEU:HD12	1:F:178:LEU:H	1.65	0.59
1:C:81:ASP:HA	4:C:303:EPE:H32	1.83	0.59
1:F:222:ARG:HA	1:F:225:VAL:HG22	1.84	0.59
1:F:240:LEU:HD12	1:F:250:CYS:HB3	1.85	0.59
1:A:97:ARG:H	6:A:310:EDO:H22	1.68	0.58
2:B:301:LLL:N21	8:B:401:HOH:O	2.32	0.58
1:C:73:PRO:HG3	1:C:99:ALA:HA	1.86	0.58
1:E:124:HIS:HB3	1:E:130:VAL:HG21	1.86	0.58
1:F:10:LEU:O	1:F:14:LEU:HD12	2.03	0.57
1:F:205:LEU:O	1:F:220:ARG:NH2	2.37	0.57
1:F:17:LEU:CD2	1:F:207:LYS:HB2	2.35	0.57
1:F:199:TRP:HH2	1:F:238:ILE:HD12	1.69	0.57
1:E:162:VAL:HG21	1:E:186:ASN:ND2	2.20	0.57
1:B:67:ASP:OD2	2:B:301:LLL:O43	2.20	0.56
1:F:251:ASP:OD2	1:F:251:ASP:N	2.36	0.56
1:B:2:GLN:HE21	1:B:2:GLN:HA	1.70	0.56
1:F:169:HIS:CG	1:F:180:ARG:HE	2.24	0.56
1:E:232:LEU:HD23	1:E:238:ILE:HG22	1.87	0.55
1:B:187:ASP:OD2	2:B:301:LLL:H222	2.06	0.55
1:E:122:PRO:HG2	1:E:158:LEU:HD11	1.88	0.55
1:F:17:LEU:HD23	1:F:207:LYS:HB2	1.89	0.55
1:F:113:GLN:OE1	1:F:132:ARG:NH2	2.40	0.55
1:E:11:ILE:O	1:E:15:LEU:HG	2.07	0.55
1:D:28:HIS:HD2	8:D:421:HOH:O	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:LEU:HD23	1:D:121:LEU:HD11	1.88	0.54
1:F:164:TYR:CE1	1:F:188:HIS:HE1	2.25	0.54
1:E:134:HIS:CE1	1:E:222:ARG:HG2	2.42	0.54
1:F:26:LEU:HB3	1:F:140:VAL:HG22	1.89	0.54
1:F:224:ILE:HD12	1:F:225:VAL:HG13	1.89	0.54
1:B:67:ASP:OD1	2:B:301:LLL:N33	2.41	0.54
1:F:199:TRP:CH2	1:F:238:ILE:HD12	2.43	0.54
1:F:114:ILE:HG23	1:F:132:ARG:HB2	1.89	0.54
1:A:62:SER:HB3	1:A:97:ARG:HE	1.73	0.54
1:B:73:PRO:HG3	1:B:99:ALA:HA	1.90	0.54
1:C:139:GLN:HE21	6:C:314:EDO:H11	1.72	0.53
1:F:202:GLU:HB2	1:F:203:LYS:HD2	1.91	0.53
1:F:125:SER:O	1:F:128:SER:HB3	2.09	0.53
1:B:122:PRO:HG2	1:B:158:LEU:HD11	1.91	0.52
1:A:207:LYS:HG3	6:A:316:EDO:H22	1.91	0.52
1:C:67:ASP:OD2	2:C:301:LLL:O43	2.24	0.52
1:E:197:ASP:O	1:E:201:LYS:HG2	2.09	0.52
1:F:231:GLN:OE1	1:F:238:ILE:HD13	2.09	0.52
2:B:301:LLL:H3	2:B:301:LLL:C13	2.18	0.52
1:E:73:PRO:HG3	1:E:99:ALA:HA	1.90	0.52
1:E:200:LEU:HD21	1:E:205:LEU:HB2	1.92	0.52
1:B:192:ARG:NH2	1:B:238:ILE:O	2.35	0.52
1:E:128:SER:OG	1:E:130:VAL:HG22	2.10	0.52
1:E:123:PRO:HD2	1:E:185:GLU:HG3	1.92	0.51
1:E:240:LEU:HD11	1:E:250:CYS:HA	1.91	0.51
1:D:150:ASN:HD21	1:D:224:ILE:HD13	1.75	0.51
2:D:301:LLL:N32	2:D:301:LLL:C11	2.73	0.51
1:E:3:TYR:OH	1:E:9:GLU:OE1	2.26	0.51
1:F:168:ARG:HB2	1:F:183:TYR:CE2	2.45	0.51
1:C:75:THR:HG22	1:F:84:VAL:HG11	1.92	0.51
1:F:109:PRO:HG2	1:F:110:GLN:NE2	2.25	0.51
1:D:148:ASP:OD1	1:D:148:ASP:N	2.44	0.51
2:E:301:LLL:N32	2:E:301:LLL:C11	2.73	0.51
1:A:73:PRO:HG3	1:A:99:ALA:HA	1.93	0.51
1:D:90:TRP:HA	1:D:95:VAL:HG11	1.93	0.51
1:C:63:TRP:HE1	6:C:313:EDO:H22	1.77	0.50
1:E:224:ILE:HD12	1:E:224:ILE:H	1.76	0.50
1:C:42:LEU:HD21	1:F:93:PRO:HG3	1.94	0.50
1:C:84:VAL:HG21	1:F:75:THR:HA	1.93	0.50
1:D:6:ARG:NH2	8:D:404:HOH:O	2.43	0.50
1:E:49:ARG:HG3	1:E:58:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:GLU:OE2	4:B:303:EPE:H81	2.12	0.49
1:E:232:LEU:HD22	1:E:236:PRO:HA	1.93	0.49
1:D:42:LEU:HD21	1:E:93:PRO:HG3	1.94	0.49
1:E:150:ASN:OD1	1:E:152:THR:HB	2.13	0.49
1:C:35:ARG:NE	4:C:304:EPE:O3S	2.46	0.49
1:F:98:SER:N	1:F:115:ILE:HD11	2.28	0.49
1:A:234:ARG:NH2	8:A:407:HOH:O	2.46	0.49
1:A:251:ASP:O	1:A:255[A]:GLN:HG2	2.12	0.49
1:D:155:LEU:O	1:D:159:MET:HG3	2.12	0.49
1:A:164:TYR:CD2	1:A:240:LEU:HD11	2.48	0.48
1:F:240:LEU:HB2	1:F:250:CYS:SG	2.53	0.48
1:E:185:GLU:HG2	1:E:186:ASN:H	1.78	0.48
1:A:98:SER:OG	1:A:103:ALA:HA	2.14	0.48
1:C:125:SER:HA	1:C:158:LEU:HD23	1.95	0.48
1:E:10:LEU:O	1:E:14:LEU:HD12	2.13	0.48
1:F:73:PRO:HG3	1:F:99:ALA:HA	1.95	0.48
1:F:4:GLU:OE1	4:F:303:EPE:H21	2.14	0.48
1:C:75:THR:HA	1:F:84:VAL:HG21	1.95	0.48
1:A:187:ASP:OD2	2:A:301:LLL:H222	2.14	0.47
1:F:200:LEU:HD13	1:F:227:THR:OG1	2.13	0.47
1:A:162:VAL:HG11	1:A:164:TYR:CZ	2.50	0.47
4:E:304:EPE:H82	4:E:304:EPE:H31	1.54	0.47
1:A:4:GLU:OE1	4:A:303:EPE:H21	2.14	0.47
1:B:150:ASN:ND2	8:B:404:HOH:O	2.46	0.47
1:E:177:LYS:HG2	1:E:178:LEU:H	1.80	0.47
1:F:200:LEU:HG	1:F:200:LEU:O	2.15	0.47
1:A:168:ARG:NH2	8:A:410:HOH:O	2.48	0.47
2:A:301:LLL:O51	2:A:301:LLL:N32	2.43	0.47
1:C:67:ASP:OD2	2:C:301:LLL:N33	2.49	0.46
1:F:62:SER:OG	1:F:97:ARG:HD2	2.15	0.46
1:F:225:VAL:O	1:F:229:LEU:HG	2.15	0.46
1:B:114:ILE:HD11	1:B:136:LEU:HD12	1.96	0.46
1:D:73:PRO:HG3	1:D:99:ALA:HA	1.98	0.46
1:F:17:LEU:HD21	1:F:207:LYS:O	2.15	0.46
1:F:98:SER:HB2	1:F:103:ALA:HA	1.97	0.46
2:F:301:LLL:C83	2:F:301:LLL:C93	2.93	0.46
2:A:301:LLL:H322	2:A:301:LLL:H11A	1.63	0.46
1:F:169:HIS:CD2	1:F:180:ARG:HE	2.33	0.46
1:E:4:GLU:HG2	1:E:36:PRO:HB2	1.97	0.46
1:C:197:ASP:O	1:C:201:LYS:HG3	2.16	0.46
1:F:6:ARG:HH11	1:F:38:GLU:CD	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:HIS:HB2	1:F:190:CYS:H	1.81	0.46
4:F:304:EPE:H81	4:F:304:EPE:H31	1.77	0.46
1:B:67:ASP:OD1	2:B:301:LLL:C93	2.64	0.45
1:D:110:GLN:NE2	8:D:407:HOH:O	2.47	0.45
1:A:199:TRP:CD2	1:A:231:GLN:HG3	2.51	0.45
1:F:200:LEU:HD21	1:F:205:LEU:HB2	1.97	0.45
2:A:301:LLL:H3	2:A:301:LLL:C13	2.26	0.45
1:F:2:GLN:NE2	8:F:401:HOH:O	2.36	0.45
1:D:202:GLU:OE2	6:D:314:EDO:O2	2.35	0.45
1:E:162:VAL:HG21	1:E:186:ASN:HD22	1.80	0.45
1:B:249:GLU:H	1:B:249:GLU:HG2	1.57	0.45
1:C:218:LEU:HG	6:C:314:EDO:O1	2.15	0.45
2:F:301:LLL:H832	2:F:301:LLL:C93	2.37	0.45
1:B:197:ASP:OD2	1:B:217:ARG:NH1	2.50	0.44
1:B:249:GLU:OE1	2:B:301:LLL:H21	2.17	0.44
1:C:114:ILE:HD11	1:C:136:LEU:HD12	1.99	0.44
1:C:164:TYR:CD2	1:C:240:LEU:HD11	2.52	0.44
1:D:63:TRP:HH2	1:D:151:THR:HG21	1.82	0.44
1:E:12:GLY:HA2	1:E:15:LEU:HD11	1.99	0.44
1:D:137:ASP:OD1	1:D:220:ARG:NH1	2.50	0.44
1:F:157:GLU:O	1:F:162:VAL:HG23	2.17	0.44
1:D:52:LEU:HB3	1:D:56:GLY:HA3	1.99	0.44
1:F:7:LYS:O	1:F:11:ILE:HG13	2.16	0.44
1:D:202:GLU:CD	6:D:314:EDO:HO2	2.21	0.44
1:B:2:GLN:HE22	1:C:213:HIS:HB3	1.82	0.44
1:A:84:VAL:HG21	1:B:75:THR:HA	2.00	0.44
1:A:122:PRO:HD2	1:A:125:SER:HB3	1.99	0.44
1:B:208:GLU:HB3	1:B:215:PHE:HE1	1.83	0.44
1:E:27:VAL:HA	1:E:141:LEU:O	2.18	0.44
1:E:67:ASP:OD1	2:E:301:LLL:N33	2.50	0.44
1:E:140:VAL:HG12	1:E:142:LEU:HD11	1.99	0.44
1:F:26:LEU:HD23	1:F:27:VAL:N	2.33	0.44
1:C:189:CYS:SG	1:C:191:GLU:HB2	2.59	0.43
2:E:301:LLL:C11	2:E:301:LLL:H322	2.28	0.43
1:C:162:VAL:HG22	1:C:163:PRO:HD2	2.01	0.43
1:D:67:ASP:OD1	2:D:301:LLL:C93	2.66	0.43
1:F:7:LYS:NZ	8:F:402:HOH:O	2.51	0.43
1:C:78:VAL:HG12	1:C:97:ARG:HH21	1.84	0.43
1:D:96:LYS:HA	5:D:305:GOL:H2	1.99	0.43
1:F:100:HIS:HB2	1:F:119:LEU:HD12	2.00	0.43
1:F:232:LEU:HB3	1:F:236:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LYS:HD2	6:C:314:EDO:H21	2.00	0.43
1:D:171:THR:HG23	1:D:178:LEU:HB3	2.01	0.43
1:C:235:ASP:HB3	1:C:238:ILE:HB	2.00	0.43
1:E:148:ASP:OD1	1:E:148:ASP:N	2.51	0.43
1:B:37:LEU:O	4:B:303:EPE:H101	2.18	0.43
1:E:117:ASP:OD1	1:E:132:ARG:NH1	2.52	0.43
1:E:198:ARG:HD3	1:E:198:ARG:HA	1.74	0.43
1:E:44:LEU:HD23	1:E:85:VAL:HG21	2.01	0.43
1:E:14:LEU:O	1:E:17:LEU:HB3	2.19	0.43
1:E:240:LEU:HD12	1:E:240:LEU:HA	1.53	0.43
1:F:162:VAL:HG11	1:F:164:TYR:CZ	2.54	0.43
1:B:189:CYS:SG	1:B:191:GLU:HB2	2.59	0.42
7:B:314:PE3:H382	7:B:314:PE3:H352	1.66	0.42
1:C:35:ARG:HB2	1:C:36:PRO:HA	2.01	0.42
1:F:6:ARG:HD2	1:F:38:GLU:CD	2.39	0.42
1:B:190:CYS:SG	2:B:301:LLL:N32	2.75	0.42
1:C:187:ASP:OD1	2:C:301:LLL:H62	2.19	0.42
1:E:140:VAL:HG12	1:E:142:LEU:CD1	2.49	0.42
1:F:25:LEU:HB3	1:F:52:LEU:HD11	2.01	0.42
2:C:301:LLL:H322	2:C:301:LLL:C51	2.32	0.42
1:C:1:MET:HE2	1:C:1:MET:HB3	1.91	0.42
1:C:35:ARG:HH11	4:C:304:EPE:HOS3	1.59	0.42
1:D:143:LEU:HD12	1:D:143:LEU:HA	1.80	0.42
1:B:2:GLN:NE2	1:C:213:HIS:HB3	2.35	0.42
1:F:63:TRP:NE1	1:F:82:LEU:HD11	2.34	0.42
1:A:96:LYS:NZ	8:A:409:HOH:O	2.46	0.42
1:E:159:MET:HB2	1:E:229:LEU:HD21	2.00	0.42
2:A:301:LLL:N32	2:A:301:LLL:C11	2.83	0.41
1:D:164:TYR:CD1	1:D:240:LEU:HD11	2.55	0.41
1:F:119:LEU:HA	1:F:120:PRO:HD3	1.86	0.41
1:F:130:VAL:HG22	1:F:155:LEU:HD22	2.02	0.41
1:A:-1:GLN:N	1:D:32:ARG:HG2	2.34	0.41
1:F:3:TYR:OH	1:F:9:GLU:OE1	2.24	0.41
1:F:153:LEU:N	1:F:153:LEU:HD23	2.34	0.41
1:C:6:ARG:HG2	1:C:6:ARG:HH11	1.85	0.41
1:D:81:ASP:HA	4:D:304:EPE:H32	2.02	0.41
1:C:7:LYS:NZ	6:C:309:EDO:H12	2.35	0.41
2:E:301:LLL:H3	2:E:301:LLL:C13	2.31	0.41
1:F:124:HIS:CE1	1:F:151:THR:HG21	2.56	0.41
1:B:237:LEU:O	6:B:307:EDO:H22	2.21	0.41
4:B:303:EPE:H81	4:B:303:EPE:H52	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:GLU:OE1	1:D:252:ALA:HB2	2.21	0.41
1:F:52:LEU:HD23	1:F:52:LEU:HA	1.90	0.41
1:F:58:LEU:O	1:F:106:ALA:HA	2.21	0.41
1:E:186:ASN:N	1:E:186:ASN:OD1	2.54	0.41
1:F:63:TRP:CZ2	1:F:82:LEU:HD21	2.56	0.41
1:C:6:ARG:HG2	1:C:6:ARG:NH1	2.36	0.40
1:E:24:VAL:HG22	1:E:133:VAL:HG23	2.03	0.40
1:F:62:SER:OG	1:F:62:SER:O	2.33	0.40
1:F:115:ILE:HD12	1:F:115:ILE:HA	1.84	0.40
1:F:176:GLY:O	1:F:177:LYS:HD2	2.22	0.40
4:C:304:EPE:H81	4:C:304:EPE:H52	1.54	0.40
1:E:200:LEU:CD1	1:E:206:GLN:HB2	2.51	0.40
1:D:84:VAL:HG11	1:E:75:THR:HG22	2.03	0.40
1:E:140:VAL:O	1:E:219:ILE:HG22	2.21	0.40
1:F:152:THR:O	1:F:155:LEU:HB3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/262 (99%)	249 (96%)	9 (4%)	1 (0%)	34	55
1	B	257/262 (98%)	250 (97%)	7 (3%)	0	100	100
1	C	257/262 (98%)	246 (96%)	10 (4%)	1 (0%)	34	55
1	D	258/262 (98%)	243 (94%)	15 (6%)	0	100	100
1	E	257/262 (98%)	241 (94%)	16 (6%)	0	100	100
1	F	257/262 (98%)	235 (91%)	22 (9%)	0	100	100
All	All	1545/1572 (98%)	1464 (95%)	79 (5%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	0	MET
1	A	0	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/212 (100%)	211 (100%)	1 (0%)	88	96
1	B	210/212 (99%)	209 (100%)	1 (0%)	88	96
1	C	210/212 (99%)	206 (98%)	4 (2%)	57	77
1	D	210/212 (99%)	209 (100%)	1 (0%)	88	96
1	E	209/212 (99%)	204 (98%)	5 (2%)	49	72
1	F	209/212 (99%)	204 (98%)	5 (2%)	49	72
All	All	1260/1272 (99%)	1243 (99%)	17 (1%)	67	85

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	B	150	ASN
1	C	35	ARG
1	C	174	GLN
1	C	180	ARG
1	C	201	LYS
1	D	177	LYS
1	E	15	LEU
1	E	161	LYS
1	E	170	CYS
1	E	180	ARG
1	E	186	ASN
1	F	161	LYS
1	F	164	TYR
1	F	170	CYS
1	F	175	ASP
1	F	220	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2	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 73 ligands modelled in this entry, 6 are monoatomic - leaving 67 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	$\# Z > 2$
6	EDO	A	315	-	3,3,3	0.47	0	2,2,2	0.27	0
2	LLL	A	301	-	29,33,33	0.48	0	34,49,49	1.27	4 (11%)
4	EPE	C	304	-	15,15,15	2.03	1 (6%)	18,20,20	1.12	3 (16%)
6	EDO	B	313	-	3,3,3	0.45	0	2,2,2	0.36	0
6	EDO	A	307	-	3,3,3	0.47	0	2,2,2	0.28	0
6	EDO	E	305	-	3,3,3	0.46	0	2,2,2	0.32	0
7	PE3	B	314	-	15,15,42	0.40	0	14,14,41	0.82	0
5	GOL	B	305	-	5,5,5	0.97	0	5,5,5	1.01	0
4	EPE	E	304	-	15,15,15	2.03	1 (6%)	18,20,20	1.09	3 (16%)
4	EPE	F	304	-	15,15,15	2.03	1 (6%)	18,20,20	1.10	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LLL	D	301	-	29,33,33	0.48	0	34,49,49	1.26	4 (11%)
6	EDO	B	311	-	3,3,3	0.47	0	2,2,2	0.31	0
6	EDO	A	306	-	3,3,3	0.46	0	2,2,2	0.31	0
6	EDO	D	307	-	3,3,3	0.48	0	2,2,2	0.27	0
6	EDO	C	310	-	3,3,3	0.36	0	2,2,2	0.21	0
6	EDO	C	314	-	3,3,3	0.41	0	2,2,2	0.44	0
6	EDO	D	309	-	3,3,3	0.48	0	2,2,2	0.31	0
6	EDO	B	312	-	3,3,3	0.46	0	2,2,2	0.31	0
4	EPE	A	304	-	15,15,15	2.04	1 (6%)	18,20,20	1.10	3 (16%)
6	EDO	A	309	-	3,3,3	0.46	0	2,2,2	0.31	0
6	EDO	A	310	-	3,3,3	0.49	0	2,2,2	0.31	0
6	EDO	C	309	-	3,3,3	0.47	0	2,2,2	0.32	0
6	EDO	A	314	-	3,3,3	0.45	0	2,2,2	0.39	0
6	EDO	D	308	-	3,3,3	0.48	0	2,2,2	0.32	0
6	EDO	A	312	-	3,3,3	0.31	0	2,2,2	0.51	0
5	GOL	C	305	-	5,5,5	0.90	0	5,5,5	0.99	0
2	LLL	F	301	-	29,33,33	0.43	0	34,49,49	1.28	4 (11%)
4	EPE	A	303	-	15,15,15	2.04	1 (6%)	18,20,20	1.10	3 (16%)
4	EPE	C	303	-	15,15,15	2.03	1 (6%)	18,20,20	1.09	3 (16%)
2	LLL	B	301	-	29,33,33	0.48	0	34,49,49	1.27	4 (11%)
6	EDO	C	307	-	3,3,3	0.44	0	2,2,2	0.49	0
6	EDO	D	314	-	3,3,3	0.43	0	2,2,2	0.11	0
6	EDO	E	306	-	3,3,3	0.48	0	2,2,2	0.31	0
6	EDO	B	307	-	3,3,3	0.46	0	2,2,2	0.33	0
6	EDO	D	311	-	3,3,3	0.46	0	2,2,2	0.37	0
6	EDO	B	306	-	3,3,3	0.46	0	2,2,2	0.33	0
6	EDO	E	307	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EPE	D	304	-	15,15,15	2.04	1 (6%)	18,20,20	1.10	3 (16%)
6	EDO	D	310	-	3,3,3	0.47	0	2,2,2	0.34	0
6	EDO	C	312	-	3,3,3	0.45	0	2,2,2	0.38	0
6	EDO	D	312	-	3,3,3	0.46	0	2,2,2	0.35	0
5	GOL	A	305	-	5,5,5	0.90	0	5,5,5	0.99	0
6	EDO	A	313	-	3,3,3	0.46	0	2,2,2	0.36	0
4	EPE	E	303	-	15,15,15	2.02	1 (6%)	18,20,20	1.10	3 (16%)
6	EDO	C	308	-	3,3,3	0.45	0	2,2,2	0.37	0
6	EDO	F	305	-	3,3,3	0.48	0	2,2,2	0.30	0
4	EPE	D	303	-	15,15,15	2.04	1 (6%)	18,20,20	1.10	3 (16%)
6	EDO	B	308	-	3,3,3	0.47	0	2,2,2	0.32	0
6	EDO	E	308	-	3,3,3	0.44	0	2,2,2	0.43	0
7	PE3	D	315	-	15,15,42	0.53	0	14,14,41	0.90	0
4	EPE	B	304	-	15,15,15	2.03	1 (6%)	18,20,20	1.10	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PE3	C	315	-	9,9,42	0.35	0	8,8,41	1.01	0
6	EDO	A	311	-	3,3,3	0.45	0	2,2,2	0.39	0
6	EDO	B	310	-	3,3,3	0.47	0	2,2,2	0.30	0
5	GOL	D	305	-	5,5,5	0.91	0	5,5,5	1.01	0
4	EPE	F	303	-	15,15,15	2.04	1 (6%)	18,20,20	1.10	3 (16%)
6	EDO	C	311	-	3,3,3	0.45	0	2,2,2	0.36	0
2	LLL	C	301	-	29,33,33	0.47	0	34,49,49	1.26	4 (11%)
2	LLL	E	301	-	29,33,33	0.47	0	34,49,49	1.26	4 (11%)
4	EPE	B	303	-	15,15,15	2.04	1 (6%)	18,20,20	1.10	3 (16%)
6	EDO	D	313	-	3,3,3	0.47	0	2,2,2	0.33	0
6	EDO	B	309	-	3,3,3	0.46	0	2,2,2	0.29	0
6	EDO	A	308	-	3,3,3	0.49	0	2,2,2	0.20	0
6	EDO	A	316	-	3,3,3	0.44	0	2,2,2	0.36	0
6	EDO	C	306	-	3,3,3	0.46	0	2,2,2	0.32	0
5	GOL	D	306	-	5,5,5	0.89	0	5,5,5	0.99	0
6	EDO	C	313	-	3,3,3	0.46	0	2,2,2	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
6	EDO	A	315	-	-	0/1/1/1	-
2	LLL	A	301	-	-	3/11/65/65	0/3/3/3
4	EPE	C	304	-	-	4/9/19/19	0/1/1/1
6	EDO	B	313	-	-	0/1/1/1	-
6	EDO	A	307	-	-	0/1/1/1	-
6	EDO	E	305	-	-	0/1/1/1	-
7	PE3	B	314	-	-	8/13/13/40	-
5	GOL	B	305	-	-	0/4/4/4	-
4	EPE	E	304	-	-	4/9/19/19	0/1/1/1
4	EPE	F	304	-	-	3/9/19/19	0/1/1/1
2	LLL	D	301	-	-	4/11/65/65	0/3/3/3
6	EDO	B	311	-	-	0/1/1/1	-
6	EDO	A	306	-	-	0/1/1/1	-
6	EDO	D	307	-	-	0/1/1/1	-
6	EDO	C	310	-	-	1/1/1/1	-
6	EDO	C	314	-	-	0/1/1/1	-
6	EDO	D	309	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	312	-	-	0/1/1/1	-
4	EPE	A	304	-	-	4/9/19/19	0/1/1/1
6	EDO	A	309	-	-	0/1/1/1	-
6	EDO	A	310	-	-	0/1/1/1	-
6	EDO	C	309	-	-	1/1/1/1	-
6	EDO	A	314	-	-	0/1/1/1	-
6	EDO	D	308	-	-	1/1/1/1	-
6	EDO	A	312	-	-	1/1/1/1	-
5	GOL	C	305	-	-	2/4/4/4	-
2	LLL	F	301	-	-	2/11/65/65	0/3/3/3
4	EPE	A	303	-	-	7/9/19/19	0/1/1/1
4	EPE	C	303	-	-	5/9/19/19	0/1/1/1
2	LLL	B	301	-	-	3/11/65/65	0/3/3/3
6	EDO	C	307	-	-	0/1/1/1	-
6	EDO	D	314	-	-	0/1/1/1	-
6	EDO	E	306	-	-	0/1/1/1	-
6	EDO	B	307	-	-	0/1/1/1	-
6	EDO	D	311	-	-	0/1/1/1	-
6	EDO	B	306	-	-	0/1/1/1	-
6	EDO	E	307	-	-	0/1/1/1	-
4	EPE	D	304	-	-	4/9/19/19	0/1/1/1
6	EDO	D	310	-	-	0/1/1/1	-
6	EDO	C	312	-	-	0/1/1/1	-
6	EDO	D	312	-	-	0/1/1/1	-
5	GOL	A	305	-	-	0/4/4/4	-
6	EDO	A	313	-	-	0/1/1/1	-
4	EPE	E	303	-	-	7/9/19/19	0/1/1/1
6	EDO	C	308	-	-	0/1/1/1	-
6	EDO	F	305	-	-	0/1/1/1	-
4	EPE	D	303	-	-	5/9/19/19	0/1/1/1
6	EDO	B	308	-	-	0/1/1/1	-
6	EDO	E	308	-	-	0/1/1/1	-
7	PE3	D	315	-	-	5/13/13/40	-
4	EPE	B	304	-	-	3/9/19/19	0/1/1/1
7	PE3	C	315	-	-	1/7/7/40	-
6	EDO	A	311	-	-	0/1/1/1	-
6	EDO	B	310	-	-	0/1/1/1	-
5	GOL	D	305	-	-	0/4/4/4	-
4	EPE	F	303	-	-	3/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	C	311	-	-	0/1/1/1	-
2	LLL	C	301	-	-	3/11/65/65	0/3/3/3
2	LLL	E	301	-	-	3/11/65/65	0/3/3/3
4	EPE	B	303	-	-	4/9/19/19	0/1/1/1
6	EDO	D	313	-	-	1/1/1/1	-
6	EDO	B	309	-	-	0/1/1/1	-
6	EDO	A	308	-	-	0/1/1/1	-
6	EDO	A	316	-	-	0/1/1/1	-
6	EDO	C	306	-	-	0/1/1/1	-
5	GOL	D	306	-	-	0/4/4/4	-
6	EDO	C	313	-	-	0/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	303	EPE	C10-S	-7.70	1.66	1.77
4	D	304	EPE	C10-S	-7.69	1.66	1.77
4	D	303	EPE	C10-S	-7.69	1.66	1.77
4	A	303	EPE	C10-S	-7.69	1.66	1.77
4	A	304	EPE	C10-S	-7.67	1.66	1.77
4	F	303	EPE	C10-S	-7.67	1.66	1.77
4	C	303	EPE	C10-S	-7.66	1.66	1.77
4	F	304	EPE	C10-S	-7.66	1.66	1.77
4	E	304	EPE	C10-S	-7.65	1.66	1.77
4	B	304	EPE	C10-S	-7.65	1.66	1.77
4	C	304	EPE	C10-S	-7.64	1.66	1.77
4	E	303	EPE	C10-S	-7.62	1.66	1.77

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	LLL	C11-O11-C42	-3.43	109.48	117.96
2	F	301	LLL	C11-O11-C42	-3.43	109.48	117.96
2	C	301	LLL	C11-O11-C42	-3.42	109.50	117.96
2	D	301	LLL	C13-O62-C62	-3.42	109.50	117.96
2	B	301	LLL	C13-O62-C62	-3.42	109.51	117.96
2	A	301	LLL	C13-O62-C62	-3.41	109.52	117.96
2	A	301	LLL	C11-O11-C42	-3.41	109.53	117.96
2	E	301	LLL	C11-O11-C42	-3.41	109.53	117.96
2	C	301	LLL	C13-O62-C62	-3.41	109.53	117.96
2	C	301	LLL	C93-N33-C33	-3.40	109.43	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	LLL	C13-O62-C62	-3.40	109.55	117.96
2	F	301	LLL	C13-O62-C62	-3.39	109.58	117.96
2	D	301	LLL	C11-O11-C42	-3.39	109.58	117.96
2	A	301	LLL	C93-N33-C33	-3.38	109.46	114.38
2	F	301	LLL	C93-N33-C33	-3.36	109.49	114.38
2	D	301	LLL	C93-N33-C33	-3.36	109.50	114.38
2	B	301	LLL	C93-N33-C33	-3.35	109.50	114.38
2	E	301	LLL	C93-N33-C33	-3.34	109.52	114.38
2	E	301	LLL	C11-O51-C51	-3.33	109.44	113.13
2	B	301	LLL	C11-O51-C51	-3.32	109.46	113.13
2	D	301	LLL	C11-O51-C51	-3.31	109.46	113.13
2	F	301	LLL	C11-O51-C51	-3.29	109.49	113.13
2	A	301	LLL	C11-O51-C51	-3.28	109.50	113.13
2	C	301	LLL	C11-O51-C51	-3.27	109.51	113.13
4	B	304	EPE	O3S-S-C10	2.31	109.51	105.77
4	F	303	EPE	O3S-S-C10	2.31	109.50	105.77
4	A	303	EPE	O3S-S-C10	2.30	109.49	105.77
4	A	304	EPE	O3S-S-C10	2.30	109.49	105.77
4	E	303	EPE	O3S-S-C10	2.29	109.48	105.77
4	D	303	EPE	O3S-S-C10	2.29	109.47	105.77
4	B	303	EPE	O3S-S-C10	2.29	109.47	105.77
4	D	304	EPE	O3S-S-C10	2.28	109.46	105.77
4	C	303	EPE	O3S-S-C10	2.28	109.46	105.77
4	C	304	EPE	O3S-S-C10	2.27	109.45	105.77
4	E	304	EPE	O3S-S-C10	2.27	109.44	105.77
4	F	304	EPE	O3S-S-C10	2.26	109.42	105.77
4	E	303	EPE	O2S-S-C10	2.15	109.51	106.92
4	A	303	EPE	O1S-S-C10	2.14	109.50	106.92
4	D	304	EPE	O2S-S-C10	2.14	109.49	106.92
4	F	304	EPE	O1S-S-C10	2.14	109.49	106.92
4	B	303	EPE	O1S-S-C10	2.13	109.48	106.92
4	F	304	EPE	O2S-S-C10	2.13	109.48	106.92
4	B	304	EPE	O1S-S-C10	2.13	109.48	106.92
4	A	304	EPE	O2S-S-C10	2.13	109.48	106.92
4	D	304	EPE	O1S-S-C10	2.13	109.48	106.92
4	F	303	EPE	O1S-S-C10	2.13	109.48	106.92
4	A	304	EPE	O1S-S-C10	2.13	109.47	106.92
4	B	303	EPE	O2S-S-C10	2.12	109.47	106.92
4	A	303	EPE	O2S-S-C10	2.12	109.47	106.92
4	C	303	EPE	O2S-S-C10	2.11	109.46	106.92
4	B	304	EPE	O2S-S-C10	2.11	109.46	106.92
4	D	303	EPE	O2S-S-C10	2.11	109.46	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	304	EPE	O1S-S-C10	2.11	109.46	106.92
4	E	303	EPE	O1S-S-C10	2.11	109.46	106.92
4	C	304	EPE	O2S-S-C10	2.11	109.45	106.92
4	E	304	EPE	O2S-S-C10	2.11	109.45	106.92
4	D	303	EPE	O1S-S-C10	2.11	109.45	106.92
4	C	303	EPE	O1S-S-C10	2.10	109.44	106.92
4	E	304	EPE	O1S-S-C10	2.10	109.44	106.92
4	F	303	EPE	O2S-S-C10	2.09	109.44	106.92

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	LLL	C23-C33-N33-C93
2	B	301	LLL	C21-C11-O11-C42
2	B	301	LLL	C23-C33-N33-C93
2	C	301	LLL	O51-C51-C61-N61
2	C	301	LLL	C23-C33-N33-C93
2	D	301	LLL	O51-C51-C61-N61
2	D	301	LLL	C23-C33-N33-C93
2	E	301	LLL	C23-C33-N33-C93
4	A	303	EPE	C10-C9-N1-C6
4	A	303	EPE	S-C10-C9-N1
4	A	303	EPE	C9-C10-S-O2S
4	A	303	EPE	C9-C10-S-O3S
4	B	303	EPE	C9-C10-S-O1S
4	B	303	EPE	C9-C10-S-O2S
4	B	303	EPE	C9-C10-S-O3S
4	B	304	EPE	N4-C7-C8-O8
4	C	303	EPE	C9-C10-S-O1S
4	C	303	EPE	C9-C10-S-O2S
4	D	303	EPE	C10-C9-N1-C2
4	D	303	EPE	C10-C9-N1-C6
4	D	304	EPE	C9-C10-S-O1S
4	D	304	EPE	C9-C10-S-O3S
4	E	303	EPE	C9-C10-S-O1S
4	E	304	EPE	C8-C7-N4-C3
4	F	303	EPE	C10-C9-N1-C2
4	F	303	EPE	C10-C9-N1-C6
4	F	303	EPE	C8-C7-N4-C3
4	B	303	EPE	N4-C7-C8-O8
4	E	304	EPE	N4-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
4	D	304	EPE	N4-C7-C8-O8
4	C	304	EPE	N4-C7-C8-O8
4	D	303	EPE	N4-C7-C8-O8
4	E	303	EPE	C9-C10-S-O3S
7	B	314	PE3	O25-C26-C27-O28
7	B	314	PE3	O34-C35-C36-O37
5	C	305	GOL	C1-C2-C3-O3
7	B	314	PE3	C35-C36-O37-C38
6	D	313	EDO	O1-C1-C2-O2
4	A	303	EPE	N4-C7-C8-O8
4	C	303	EPE	C9-C10-S-O3S
7	D	315	PE3	C32-C33-O34-C35
6	C	309	EDO	O1-C1-C2-O2
4	A	303	EPE	C10-C9-N1-C2
4	A	304	EPE	C10-C9-N1-C2
4	A	304	EPE	C10-C9-N1-C6
4	C	303	EPE	C10-C9-N1-C2
4	C	304	EPE	C10-C9-N1-C6
4	E	303	EPE	C10-C9-N1-C2
4	E	303	EPE	C10-C9-N1-C6
4	E	304	EPE	C10-C9-N1-C2
4	E	304	EPE	C10-C9-N1-C6
4	F	304	EPE	C10-C9-N1-C6
7	D	315	PE3	C30-C29-O28-C27
6	C	310	EDO	O1-C1-C2-O2
4	E	303	EPE	C8-C7-N4-C3
4	E	303	EPE	C8-C7-N4-C5
7	B	314	PE3	C36-C35-O34-C33
4	F	304	EPE	N4-C7-C8-O8
4	A	303	EPE	C9-C10-S-O1S
4	D	304	EPE	C9-C10-S-O2S
4	E	303	EPE	C9-C10-S-O2S
7	B	314	PE3	O37-C38-C39-O40
2	D	301	LLL	C52-C42-O11-C11
4	A	304	EPE	N4-C7-C8-O8
2	E	301	LLL	C52-C42-O11-C11
2	A	301	LLL	C52-C62-O62-C13
2	E	301	LLL	C52-C62-O62-C13
6	D	308	EDO	O1-C1-C2-O2
2	D	301	LLL	C52-C62-O62-C13
2	B	301	LLL	C52-C62-O62-C13
7	B	314	PE3	C33-C32-O31-C30

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Mol	Chain	Res	Type	Atoms
4	B	304	EPE	C10-C9-N1-C2
4	C	303	EPE	C10-C9-N1-C6
4	C	304	EPE	C10-C9-N1-C2
4	F	304	EPE	C10-C9-N1-C2
7	B	314	PE3	O28-C29-C30-O31
4	D	303	EPE	C8-C7-N4-C3
2	F	301	LLL	C52-C62-O62-C13
2	C	301	LLL	C52-C62-O62-C13
7	C	315	PE3	O37-C38-C39-O40
7	D	315	PE3	O31-C32-C33-O34
4	D	303	EPE	C8-C7-N4-C5
2	F	301	LLL	C23-C33-N33-C93
5	C	305	GOL	O2-C2-C3-O3
7	D	315	PE3	O34-C35-C36-O37
7	B	314	PE3	C26-C27-O28-C29
7	D	315	PE3	O28-C29-C30-O31
2	A	301	LLL	C52-C42-O11-C11
4	C	304	EPE	S-C10-C9-N1
6	A	312	EDO	O1-C1-C2-O2
4	A	304	EPE	C9-C10-S-O2S
4	B	304	EPE	C10-C9-N1-C6

There are no ring outliers.

26 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	LLL	6	0
4	C	304	EPE	4	0
6	E	305	EDO	1	0
7	B	314	PE3	4	0
4	E	304	EPE	1	0
4	F	304	EPE	1	0
2	D	301	LLL	5	0
6	A	306	EDO	2	0
6	C	314	EDO	4	0
6	A	310	EDO	1	0
6	C	309	EDO	1	0
2	F	301	LLL	8	0
4	A	303	EPE	1	0
4	C	303	EPE	1	0
2	B	301	LLL	9	0
6	D	314	EDO	2	0

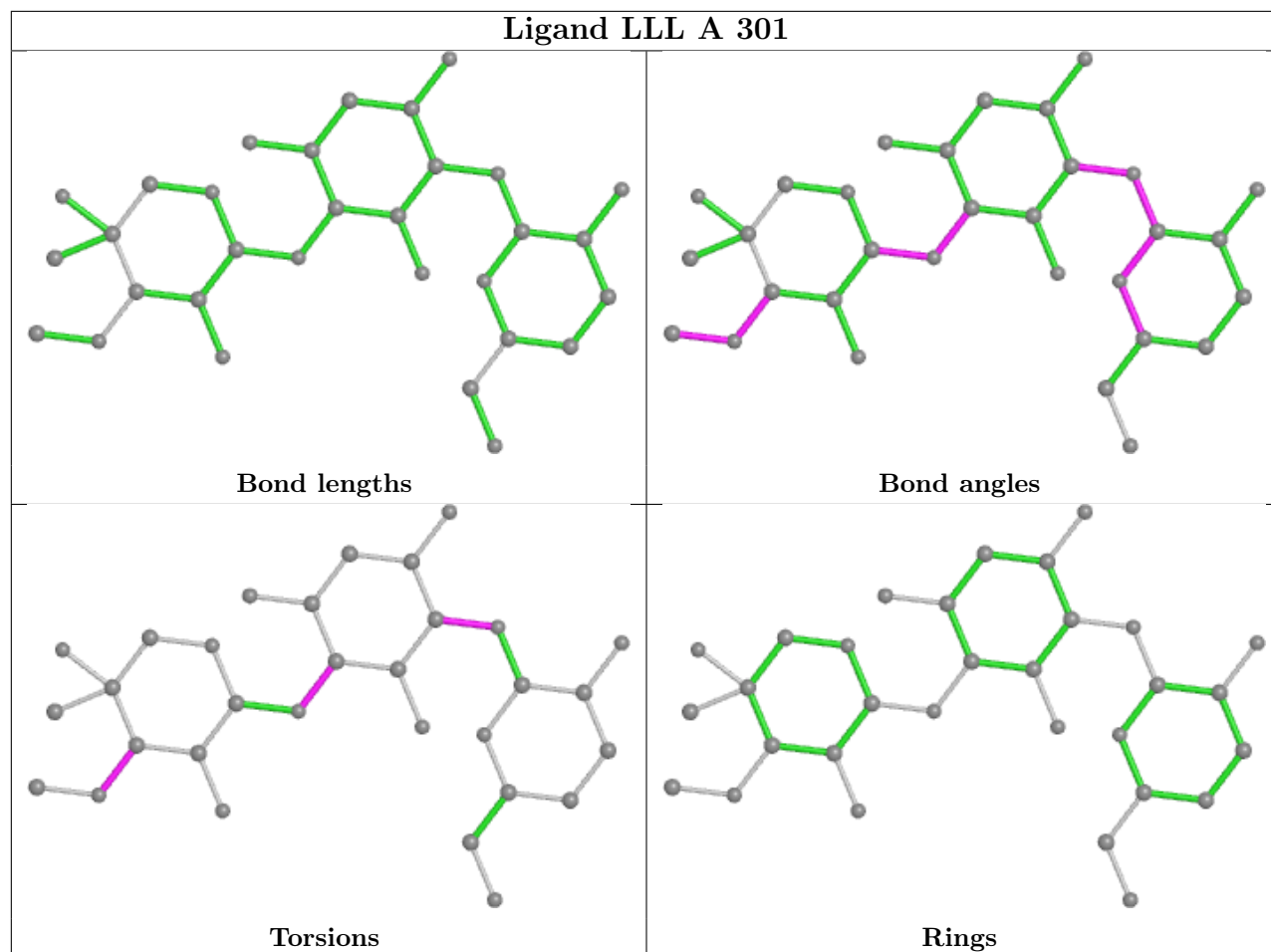
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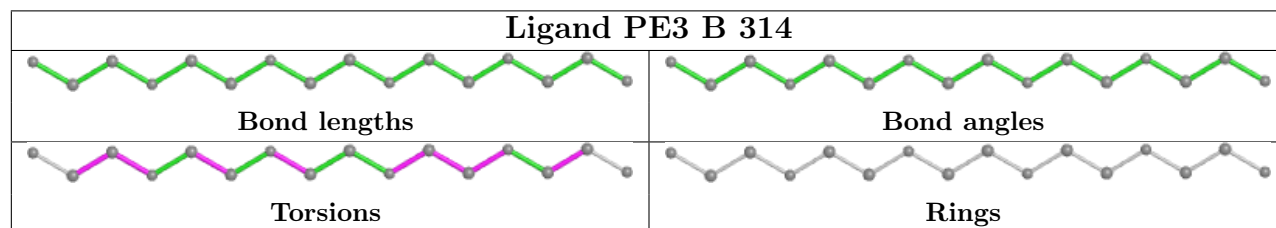
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	307	EDO	2	0
4	D	304	EPE	1	0
7	D	315	PE3	1	0
5	D	305	GOL	1	0
4	F	303	EPE	1	0
2	C	301	LLL	5	0
2	E	301	LLL	6	0
4	B	303	EPE	3	0
6	A	316	EDO	2	0
6	C	313	EDO	1	0

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.

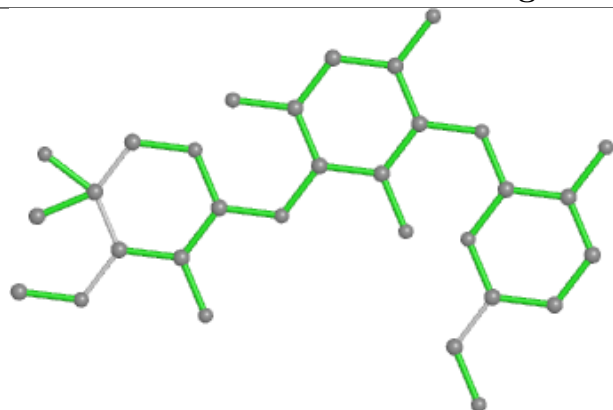
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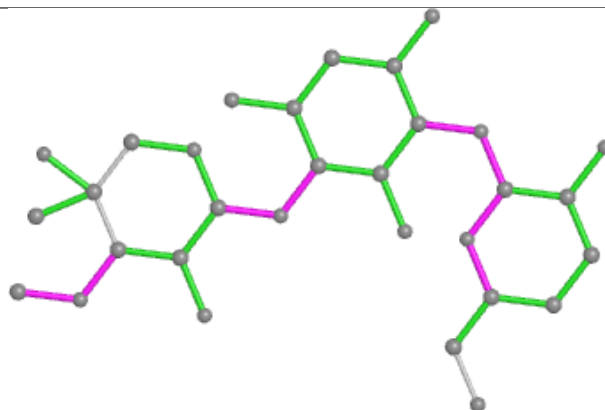
Ligand PE3 B 314



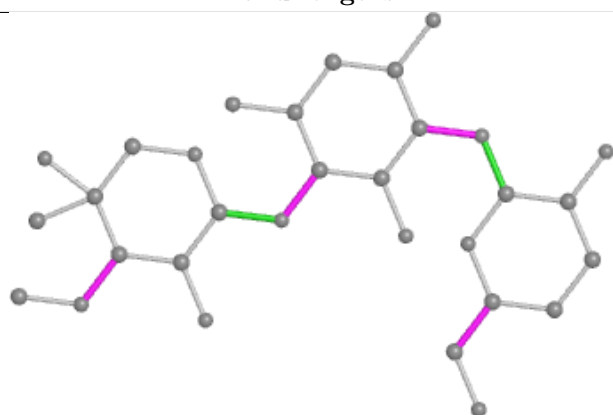
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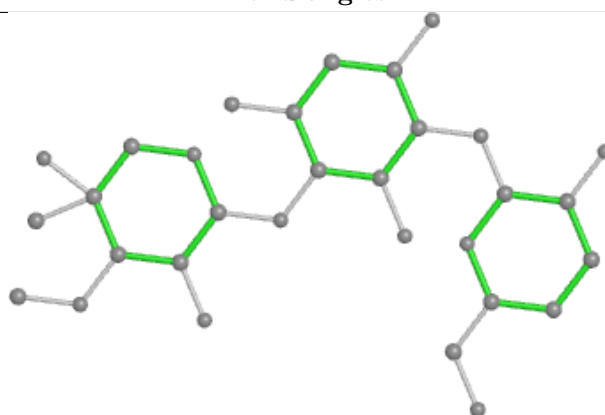
Bond lengths



Bond angles

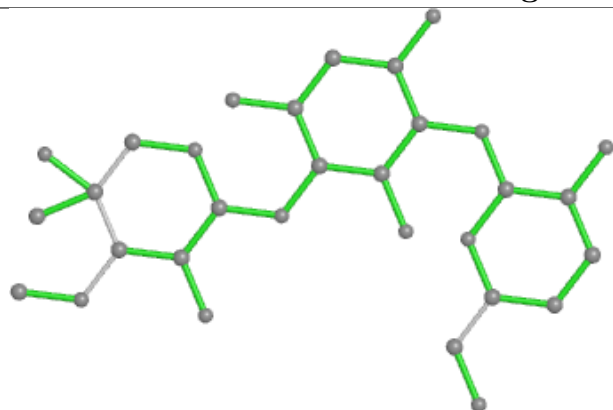


Torsions

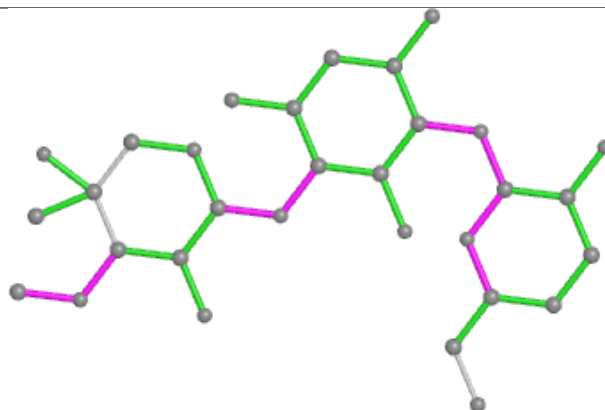


Rings

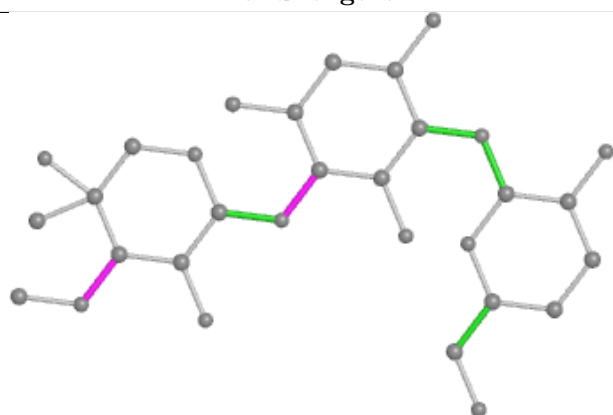
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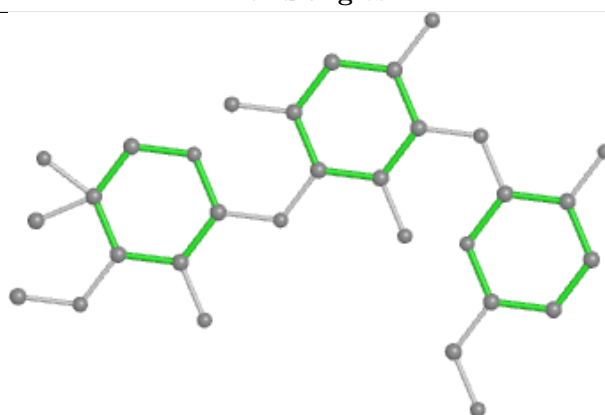
Bond lengths



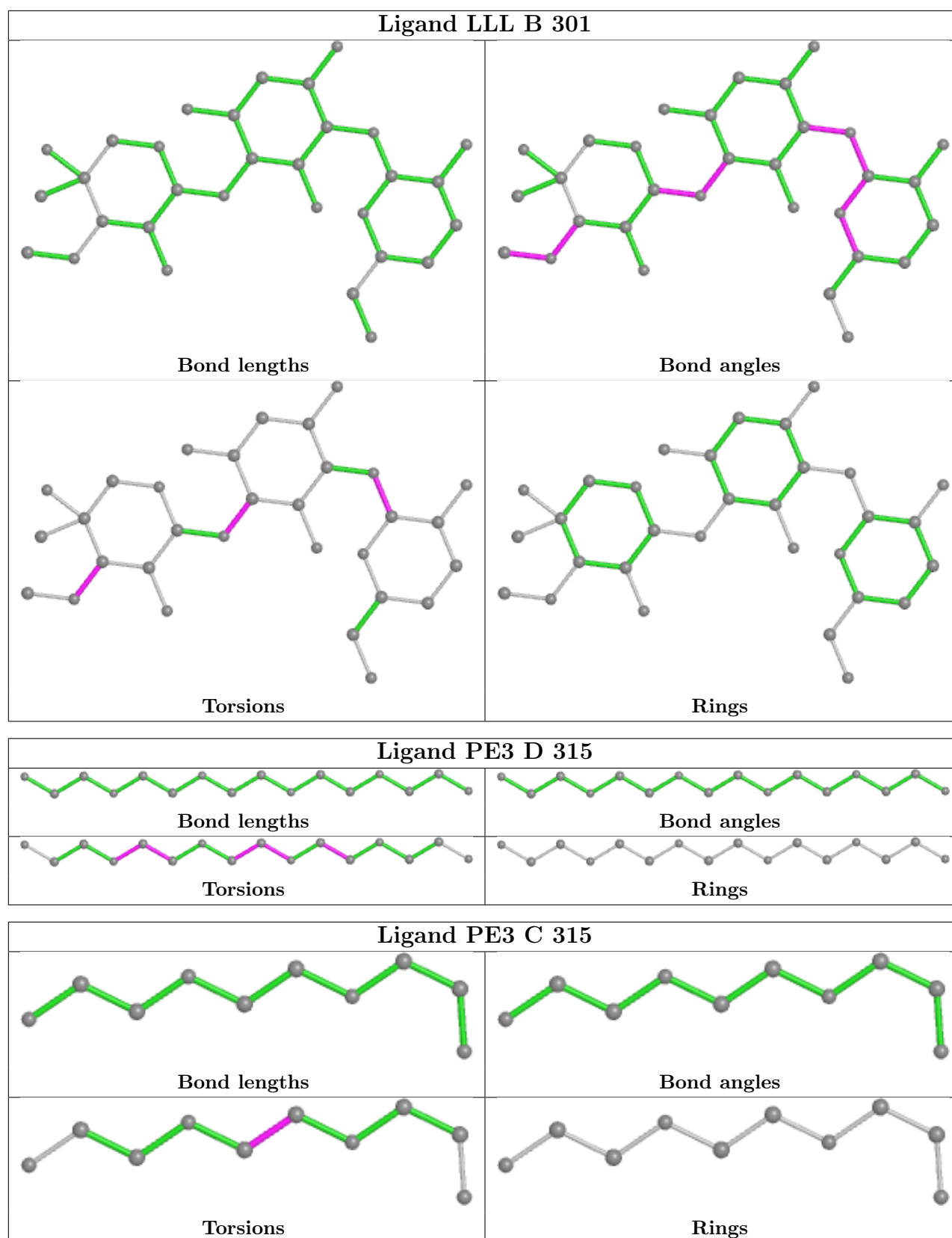
Bond angles



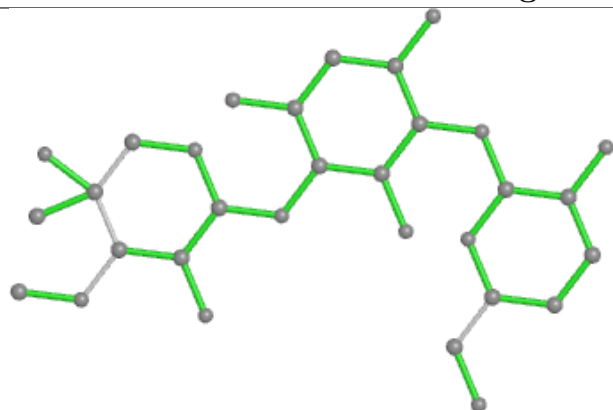
Torsions



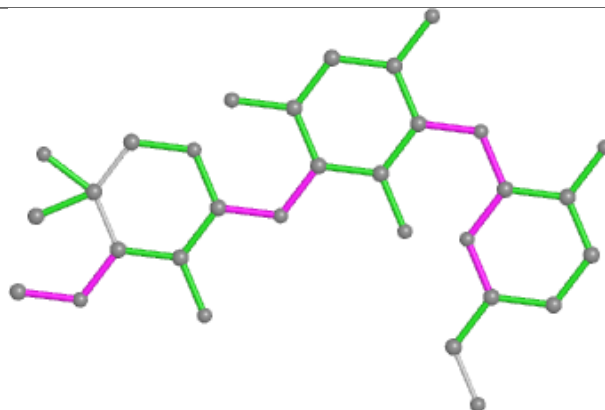
Rings



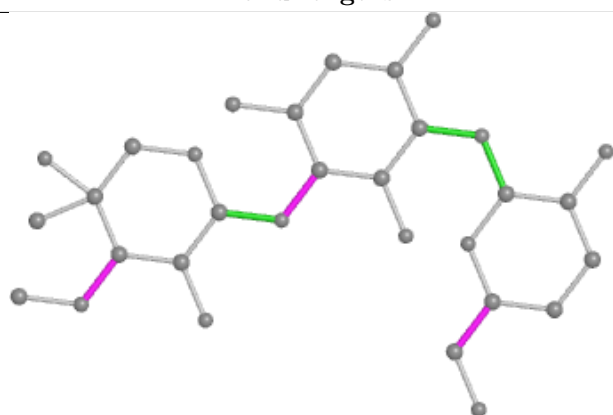
Ligand LLL C 301



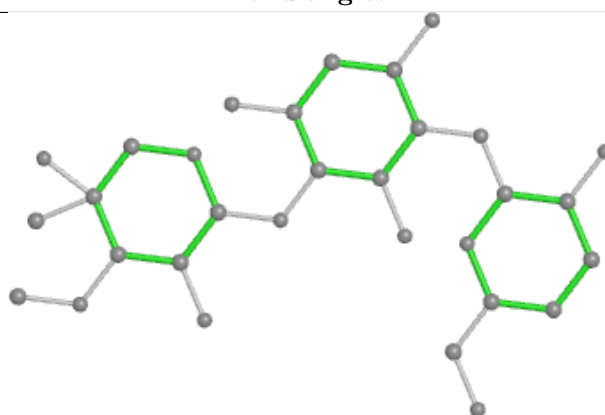
Bond lengths



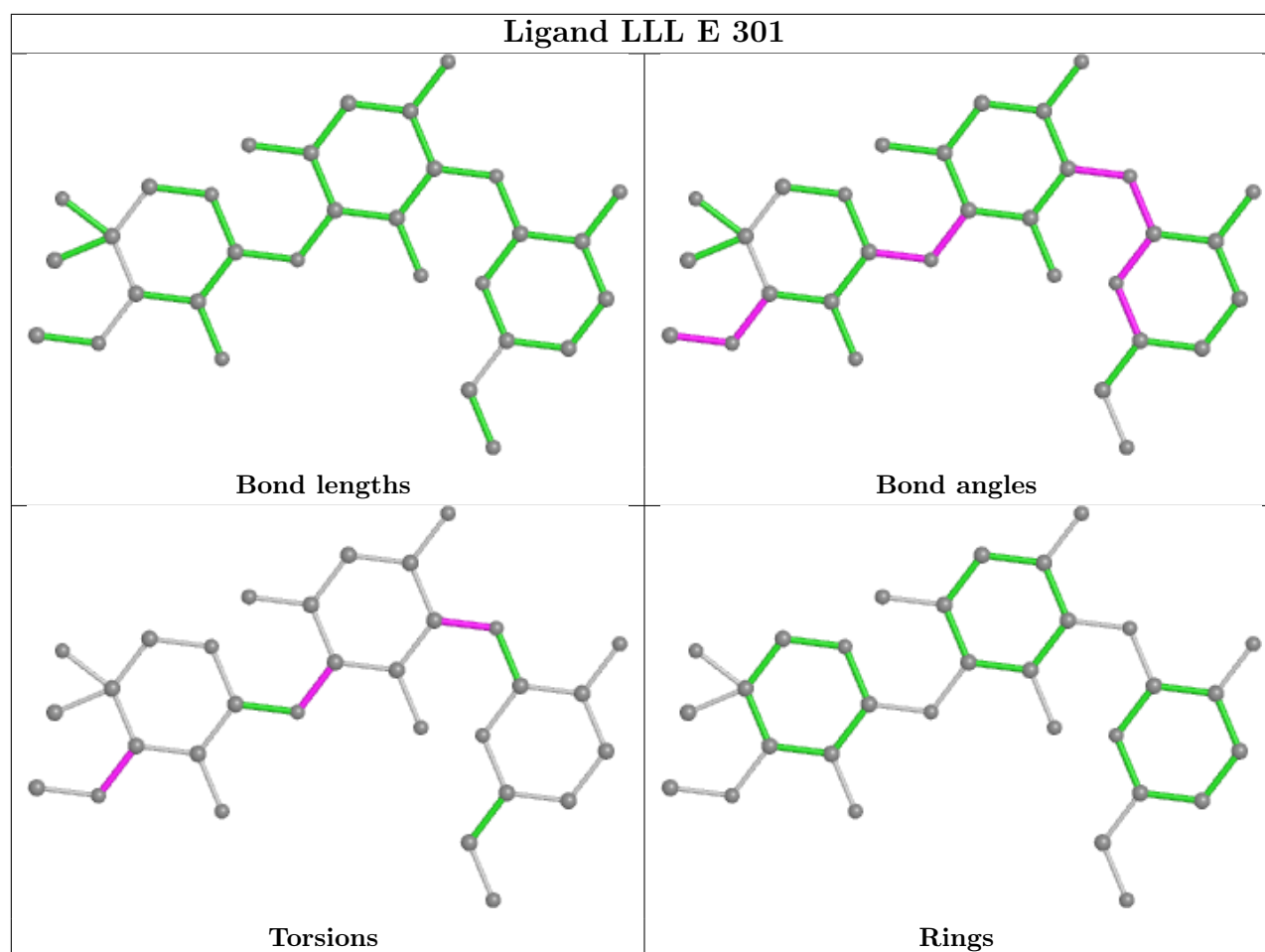
Bond angles



Torsions



Rings



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	259/262 (98%)	-0.06	6 (2%) 60 57	40, 57, 88, 129	0
1	B	259/262 (98%)	-0.13	2 (0%) 86 85	38, 59, 99, 148	0
1	C	259/262 (98%)	0.11	6 (2%) 60 57	45, 66, 113, 148	0
1	D	260/262 (99%)	0.09	11 (4%) 36 32	43, 76, 125, 169	0
1	E	259/262 (98%)	1.04	52 (20%) 1 0	55, 121, 188, 218	0
1	F	259/262 (98%)	1.13	54 (20%) 1 0	61, 140, 213, 242	0
All	All	1555/1572 (98%)	0.36	131 (8%) 11 9	38, 77, 181, 242	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	233	GLY	9.5
1	F	245	ALA	8.8
1	F	184	LEU	8.6
1	E	245	ALA	8.0
1	F	19	VAL	7.5
1	E	167	PRO	7.4
1	E	179	VAL	7.1
1	E	244	GLU	6.8
1	E	239	PHE	6.8
1	F	181	VAL	6.6
1	F	179	VAL	6.3
1	E	229	LEU	6.0
1	E	205	LEU	5.7
1	D	174	GLN	5.7
1	F	166	VAL	5.7
1	F	239	PHE	5.7
1	E	184	LEU	5.7
1	E	181	VAL	5.6
1	E	251	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	193	PHE	5.2
1	F	121	LEU	5.2
1	E	164	TYR	4.9
1	E	193	PHE	4.9
1	F	158	LEU	4.8
1	E	178	LEU	4.7
1	F	173	LEU	4.7
1	E	246	GLY	4.6
1	F	168	ARG	4.6
1	E	121	LEU	4.5
1	F	185	GLU	4.5
1	F	170	CYS	4.4
1	F	174	GLN	4.4
1	F	257	ILE	4.3
1	E	19	VAL	4.3
1	B	245	ALA	4.2
1	F	205	LEU	4.1
1	F	172	ILE	4.0
1	E	242	PRO	4.0
1	F	183	TYR	4.0
1	E	166	VAL	3.8
1	D	180	ARG	3.7
1	F	254	ARG	3.7
1	E	174	GLN	3.6
1	F	182	ASP	3.6
1	B	175	ASP	3.6
1	F	164	TYR	3.6
1	E	243	PRO	3.6
1	E	172	ILE	3.6
1	E	180	ARG	3.6
1	F	251	ASP	3.6
1	A	173	LEU	3.5
1	E	124	HIS	3.5
1	E	254	ARG	3.5
1	E	175	ASP	3.4
1	E	182	ASP	3.4
1	E	241	HIS	3.3
1	E	183	TYR	3.3
1	F	161	LYS	3.3
1	F	242	PRO	3.2
1	F	244	GLU	3.2
1	E	257	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	252	ALA	3.1
1	E	188	HIS	3.1
1	E	177	LYS	3.1
1	C	181	VAL	3.1
1	D	245	ALA	3.1
1	E	236	PRO	3.1
1	C	179	VAL	3.1
1	F	178	LEU	3.0
1	F	246	GLY	3.0
1	E	168	ARG	2.9
1	E	218	LEU	2.9
1	F	53	GLY	2.9
1	A	177	LYS	2.9
1	E	153	LEU	2.9
1	F	175	ASP	2.8
1	F	165	GLY	2.8
1	F	229	LEU	2.8
1	A	174	GLN	2.8
1	E	234	ARG	2.8
1	A	181	VAL	2.8
1	E	253	ALA	2.8
1	F	200	LEU	2.7
1	F	252	ALA	2.7
1	E	219	ILE	2.7
1	F	51	ALA	2.7
1	F	250	CYS	2.7
1	E	51	ALA	2.6
1	F	180	ARG	2.6
1	D	178	LEU	2.6
1	E	163	PRO	2.6
1	F	256	SER	2.6
1	D	254	ARG	2.6
1	F	234	ARG	2.6
1	E	185	GLU	2.6
1	F	54	PRO	2.5
1	F	220	ARG	2.5
1	E	225	VAL	2.5
1	C	-1	GLN	2.5
1	E	249	GLU	2.5
1	F	25	LEU	2.4
1	C	178	LEU	2.4
1	F	21	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	177	LYS	2.4
1	E	158	LEU	2.4
1	E	11	ILE	2.3
1	F	169	HIS	2.3
1	A	175	ASP	2.2
1	A	179	VAL	2.2
1	F	133	VAL	2.2
1	F	159	MET	2.2
1	D	172	ILE	2.2
1	E	222	ARG	2.2
1	D	164	TYR	2.2
1	E	7	LYS	2.2
1	C	172	ILE	2.2
1	F	109	PRO	2.1
1	F	141	LEU	2.1
1	E	256	SER	2.1
1	E	78	VAL	2.1
1	F	247	CYS	2.1
1	F	47	ALA	2.1
1	E	199	TRP	2.1
1	F	222	ARG	2.1
1	D	175	ASP	2.1
1	D	252	ALA	2.1
1	E	187	ASP	2.0
1	D	257	ILE	2.0
1	C	245	ALA	2.0
1	F	171	THR	2.0
1	F	236	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	E	302	1/1	0.39	0.11	175,175,175,175	1
6	EDO	D	314	4/4	0.56	0.31	138,141,147,153	0
6	EDO	A	315	4/4	0.67	0.40	102,112,115,116	0
6	EDO	C	306	4/4	0.69	0.29	97,97,99,99	0
6	EDO	F	305	4/4	0.72	0.24	105,106,107,108	0
6	EDO	E	306	4/4	0.74	0.32	82,91,92,96	0
7	PE3	B	314	16/43	0.75	0.36	98,106,115,116	0
2	LLL	E	301	31/31	0.76	0.25	137,163,171,172	0
7	PE3	C	315	10/43	0.77	0.40	112,120,128,129	0
6	EDO	E	308	4/4	0.78	0.37	128,130,131,136	0
6	EDO	C	310	4/4	0.78	0.35	85,91,97,97	0
2	LLL	F	301	31/31	0.79	0.29	138,155,163,165	0
6	EDO	B	309	4/4	0.79	0.22	82,85,89,93	0
7	PE3	D	315	16/43	0.79	0.33	72,118,133,137	0
6	EDO	C	314	4/4	0.80	0.38	121,121,122,124	0
6	EDO	C	309	4/4	0.81	0.25	82,83,84,91	0
2	LLL	A	301	31/31	0.81	0.24	113,143,155,158	0
5	GOL	D	306	6/6	0.83	0.20	96,106,111,112	0
5	GOL	D	305	6/6	0.83	0.28	94,103,105,105	0
6	EDO	E	305	4/4	0.83	0.27	89,89,90,93	0
6	EDO	C	313	4/4	0.83	0.42	95,97,99,100	0
6	EDO	E	307	4/4	0.83	0.29	93,94,94,95	0
2	LLL	C	301	31/31	0.84	0.19	115,135,144,146	0
6	EDO	A	312	4/4	0.84	0.44	99,101,102,104	0
6	EDO	B	307	4/4	0.85	0.16	92,92,97,103	0
6	EDO	A	313	4/4	0.85	0.18	87,88,92,92	0
6	EDO	D	313	4/4	0.85	0.29	110,113,115,116	0
6	EDO	B	313	4/4	0.85	0.24	86,89,90,97	0
2	LLL	B	301	31/31	0.86	0.19	82,126,139,144	0
6	EDO	A	307	4/4	0.86	0.24	93,95,99,100	0
6	EDO	A	310	4/4	0.86	0.16	72,76,76,84	0
2	LLL	D	301	31/31	0.86	0.18	126,137,147,149	0
6	EDO	A	314	4/4	0.87	0.17	86,87,93,98	0
5	GOL	A	305	6/6	0.87	0.34	100,106,109,112	0
6	EDO	A	309	4/4	0.88	0.23	80,96,97,100	0
5	GOL	C	305	6/6	0.88	0.20	79,88,99,105	0
6	EDO	A	316	4/4	0.88	0.34	94,97,99,101	0
6	EDO	B	306	4/4	0.88	0.23	80,82,83,83	0
6	EDO	D	308	4/4	0.88	0.17	69,73,79,82	0
6	EDO	D	312	4/4	0.88	0.26	80,81,82,83	0
6	EDO	C	307	4/4	0.88	0.18	75,79,79,83	0

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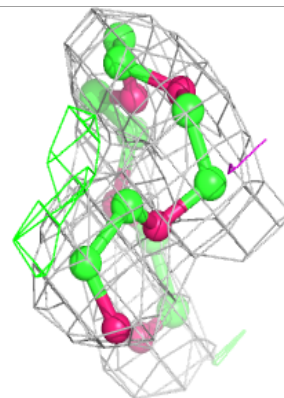
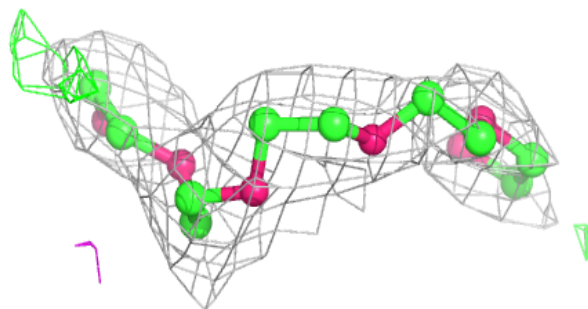
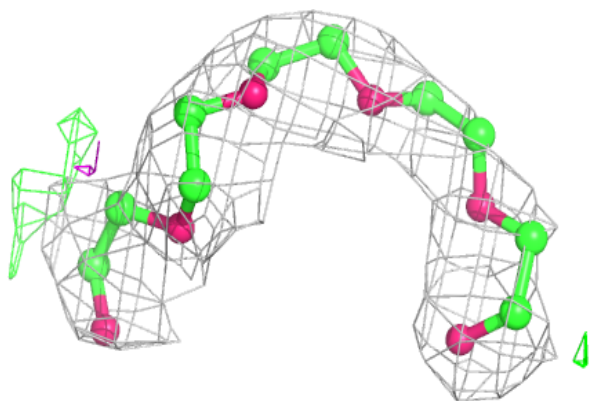
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	C	308	4/4	0.88	0.32	106,108,111,114	0
6	EDO	C	312	4/4	0.89	0.19	81,83,86,98	0
6	EDO	B	310	4/4	0.90	0.13	87,87,89,89	0
6	EDO	A	311	4/4	0.90	0.30	93,95,100,104	0
6	EDO	D	307	4/4	0.90	0.41	92,100,103,105	0
5	GOL	B	305	6/6	0.91	0.18	75,80,81,84	0
6	EDO	B	312	4/4	0.91	0.23	95,96,99,108	0
6	EDO	D	311	4/4	0.92	0.32	97,102,102,105	0
6	EDO	C	311	4/4	0.92	0.16	92,92,99,100	0
6	EDO	B	308	4/4	0.92	0.15	60,76,81,82	0
3	ZN	F	302	1/1	0.92	0.05	147,147,147,147	1
4	EPE	F	304	15/15	0.93	0.24	87,123,133,134	0
6	EDO	B	311	4/4	0.93	0.25	80,84,86,88	0
6	EDO	A	308	4/4	0.93	0.18	53,58,65,72	0
6	EDO	D	310	4/4	0.93	0.28	72,72,76,78	0
4	EPE	D	304	15/15	0.94	0.23	83,109,134,135	0
4	EPE	E	304	15/15	0.94	0.23	92,114,137,140	0
4	EPE	E	303	15/15	0.95	0.19	67,98,127,127	0
6	EDO	D	309	4/4	0.95	0.15	64,71,71,75	0
4	EPE	A	304	15/15	0.95	0.21	79,94,109,113	0
4	EPE	C	303	15/15	0.95	0.20	70,85,103,104	0
4	EPE	A	303	15/15	0.95	0.22	52,84,118,125	0
6	EDO	A	306	4/4	0.96	0.14	63,78,82,83	0
4	EPE	C	304	15/15	0.96	0.16	55,85,120,121	0
4	EPE	B	304	15/15	0.96	0.16	80,95,113,115	0
4	EPE	F	303	15/15	0.96	0.20	71,105,136,138	0
3	ZN	D	302	1/1	0.97	0.09	86,86,86,86	1
4	EPE	D	303	15/15	0.97	0.17	51,80,117,119	0
3	ZN	A	302	1/1	0.98	0.20	94,94,94,94	0
4	EPE	B	303	15/15	0.98	0.16	58,83,118,122	0
3	ZN	C	302	1/1	0.98	0.08	57,57,57,57	1
3	ZN	B	302	1/1	0.99	0.13	79,79,79,79	0

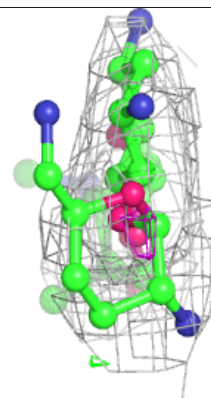
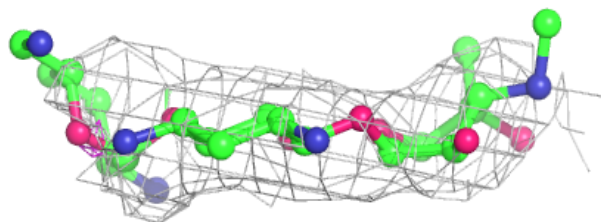
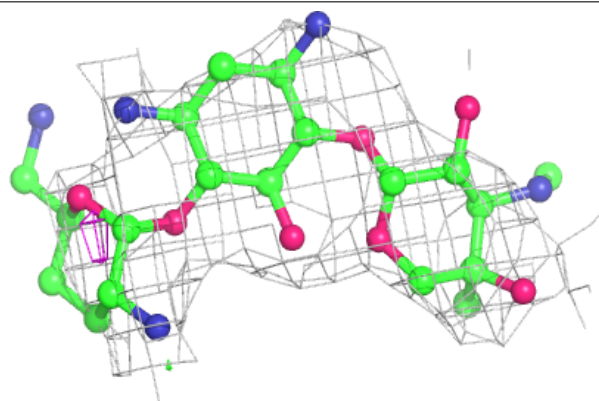
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PE3 B 314:

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

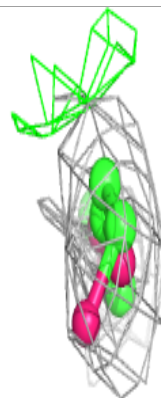
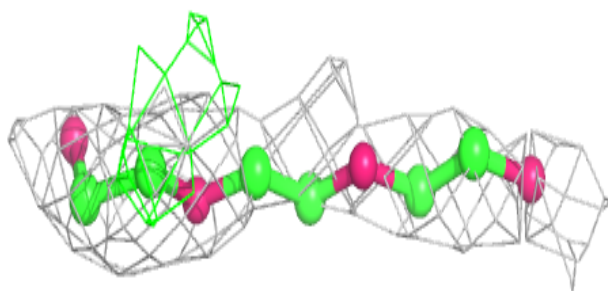
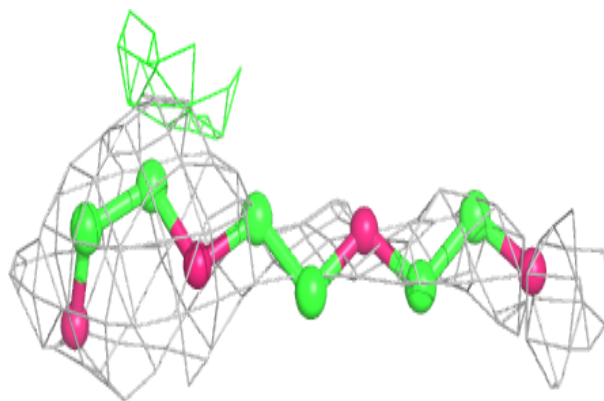
**Electron density around LLL E 301:**

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

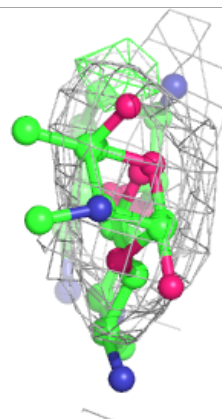
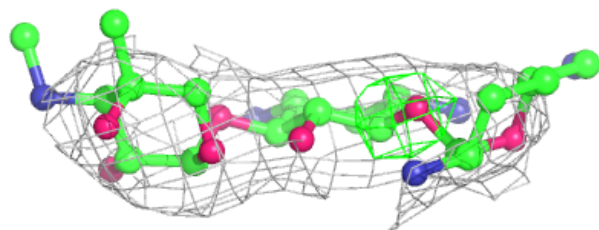
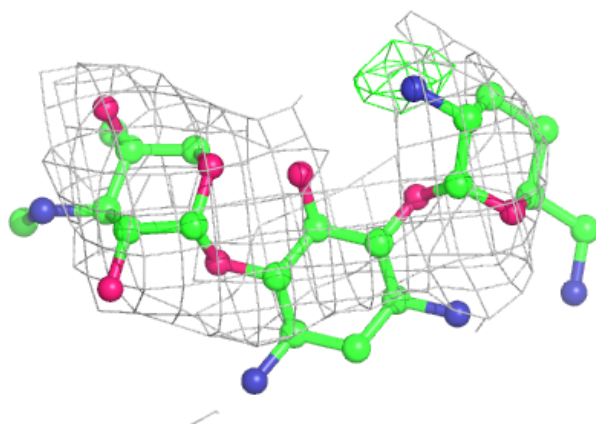


Electron density around PE3 C 315:

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

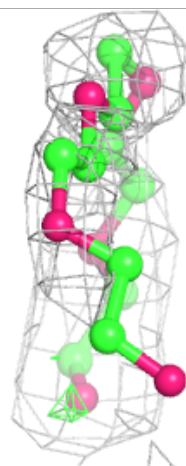
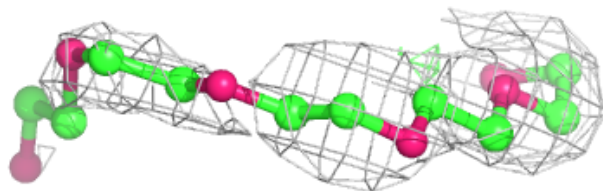
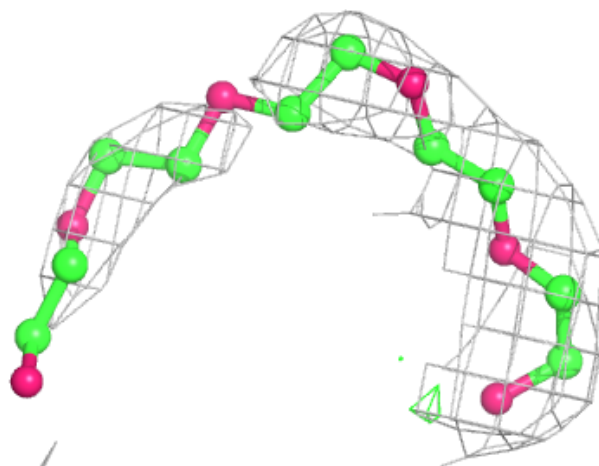
**Electron density around LLL F 301:**

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



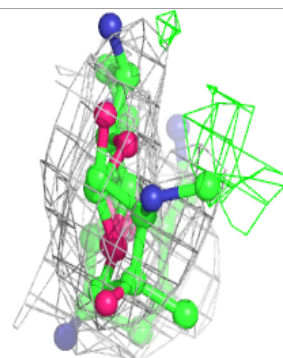
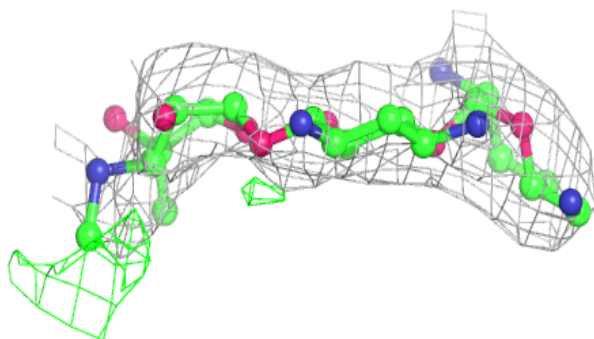
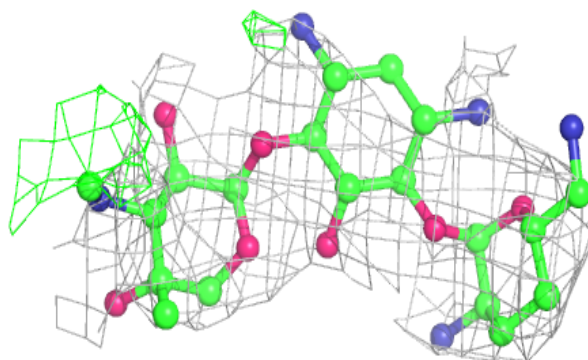
Electron density around PE3 D 315:

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

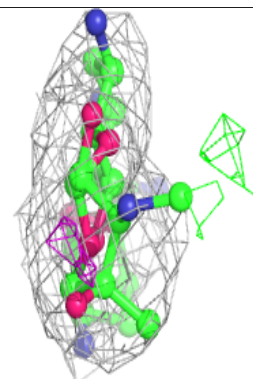
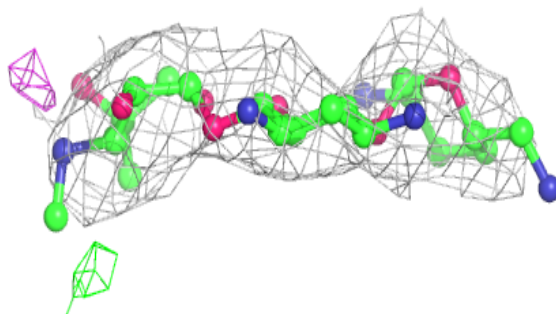
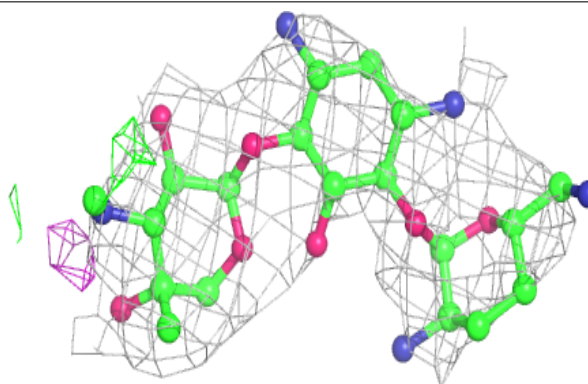


Electron density around LLL A 301:

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

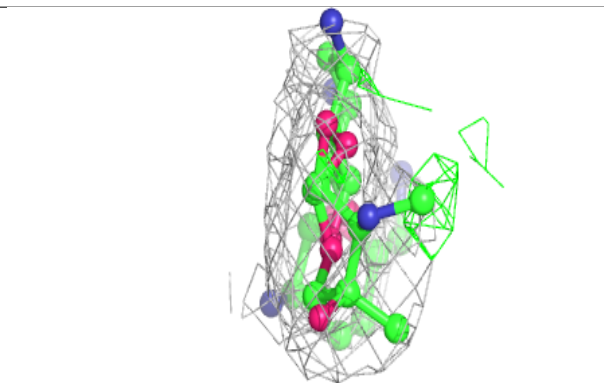
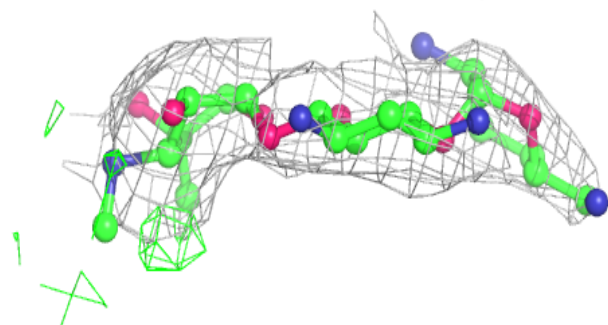
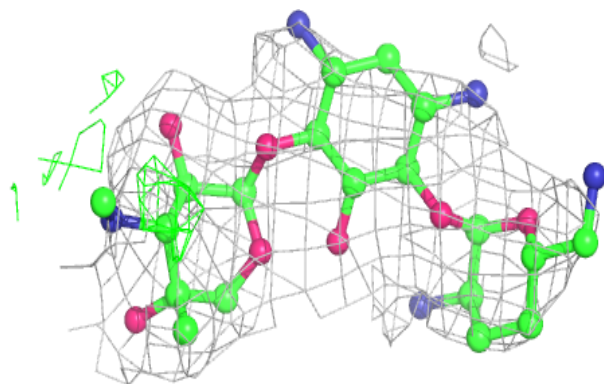
**Electron density around LLL C 301:**

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

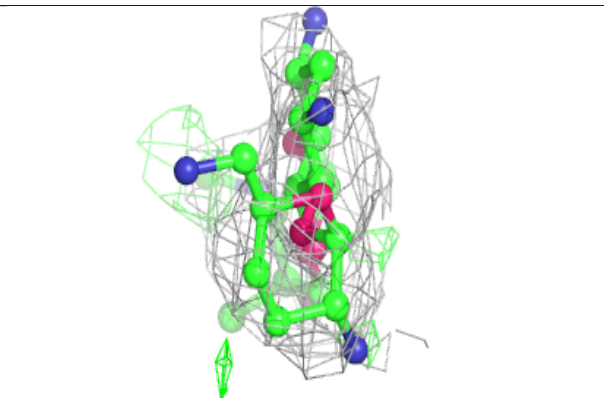
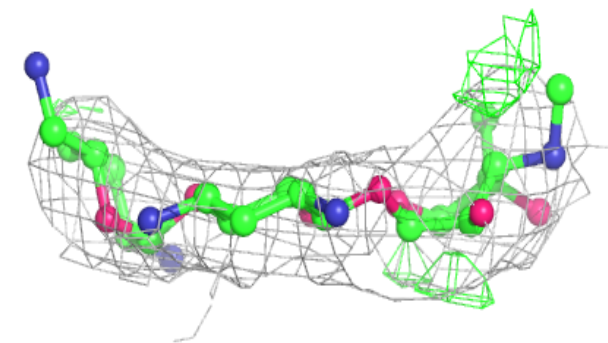
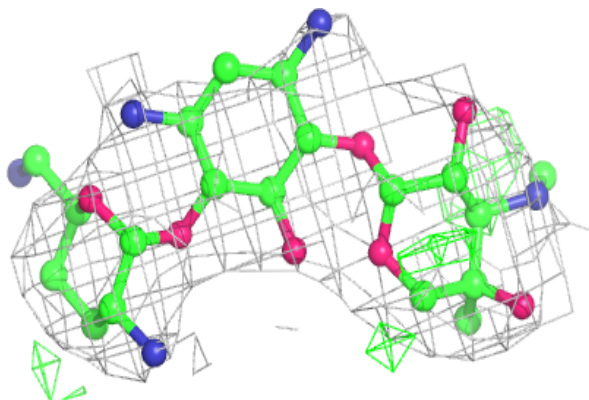


Electron density around LLL B 301:

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

**Electron density around LLL 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.