Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:27 am BST

PDB ID	:	5TXT
Title	:	Structure of asymmetric apo/holo ALAS dimer from S. cerevisiae
Authors	:	Brown, B.L.; Grant, R.A.; Kardon, J.R.; Sauer, R.T.; Baker, T.A.
Deposited on	:	2016-11-17
Resolution	:	2.70 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:

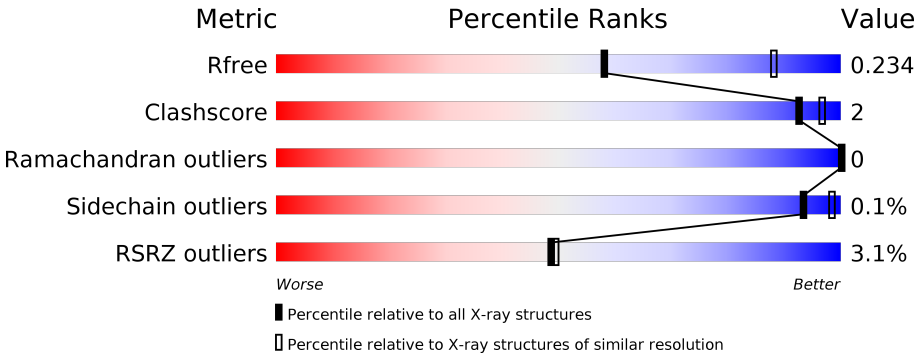
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	491	89% · 9%
1	D	491	86% · 10%
1	E	491	4% 89% · 9%
2	B	491	3% 87% 7% 6%
2	C	491	2% 89% · 7%
2	F	491	7% 89% 5% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 42498 atoms, of which 21004 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.

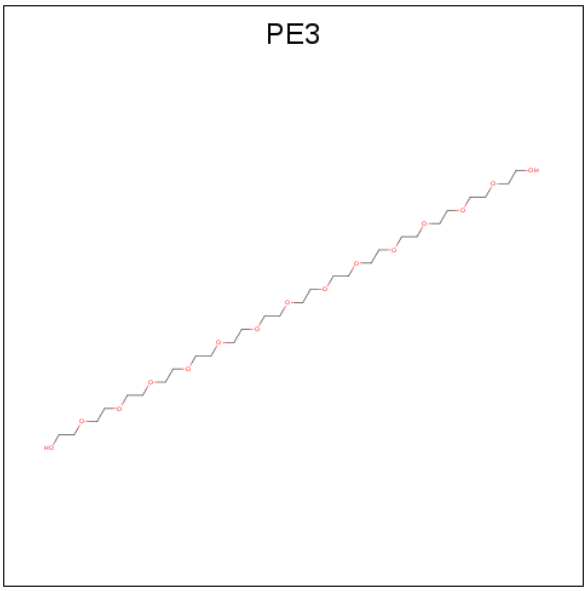
- Molecule 1 is a protein called 5-aminolevulinate synthase, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	448	Total	C	H	N	O	S	0	0	0
			6870	2180	3427	594	655	14			
1	D	441	Total	C	H	N	O	S	0	0	0
			6769	2146	3381	586	642	14			
1	E	448	Total	C	H	N	O	S	0	0	0
			6870	2180	3427	594	655	14			

- Molecule 2 is a protein called 5-aminolevulinate synthase, mitochondrial.

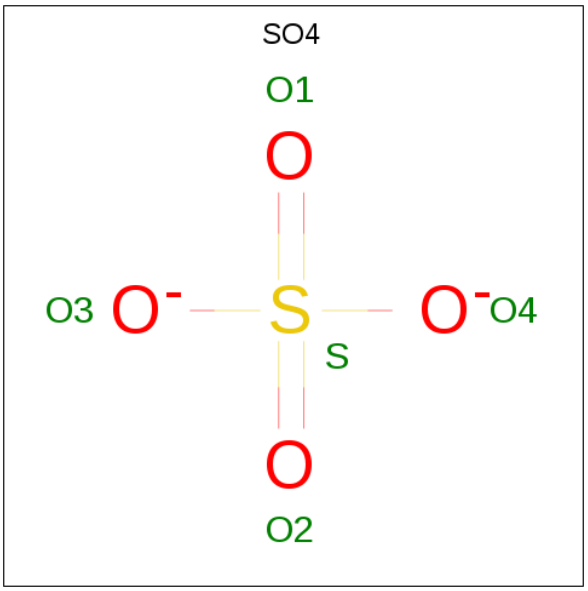
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	B	460	Total	C	H	N	O	P	S	0	0	0
			7160	2278	3564	622	681	1	14			
2	C	457	Total	C	H	N	O	P	S	0	0	0
			7112	2262	3538	619	678	1	14			
2	F	460	Total	C	H	N	O	P	S	0	0	0
			7160	2278	3564	622	681	1	14			

- Molecule 3 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1 ,41-DIOL (three-letter code: PE3) (formula: $C_{28}H_{58}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C H O 38 12 20 6	0	0
3	B	1	Total C H O 65 18 37 10	0	0
3	B	1	Total C O 8 5 3	0	0
3	C	1	Total C H O 38 12 20 6	0	0
3	C	1	Total C H O 30 11 14 5	0	0
3	C	1	Total C H O 20 8 8 4	0	0
3	F	1	Total C H O 23 12 4 7	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

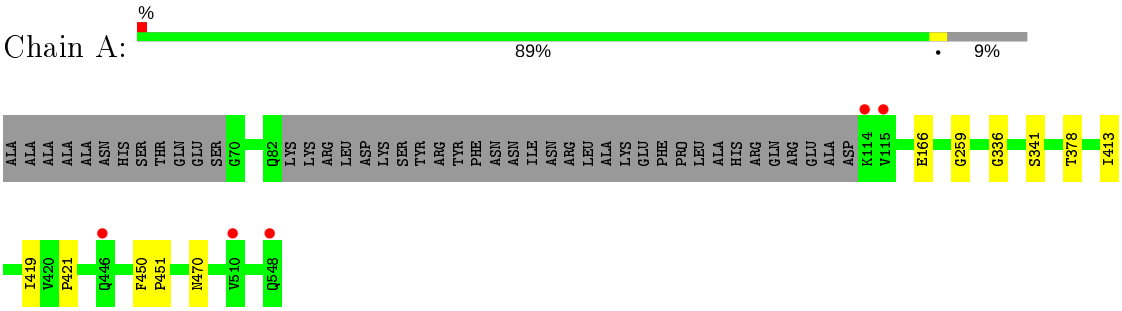
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	59	Total O 59 59	0	0
5	B	47	Total O 47 47	0	0
5	D	90	Total O 90 90	0	0
5	C	64	Total O 64 64	0	0
5	E	39	Total O 39 39	0	0
5	F	31	Total O 31 31	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

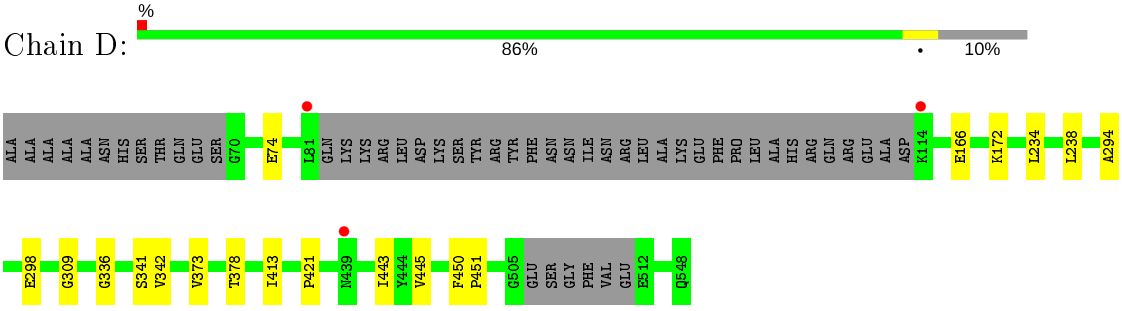
- Molecule 1: 5-aminolevulinate synthase, mitochondrial

Chain A:



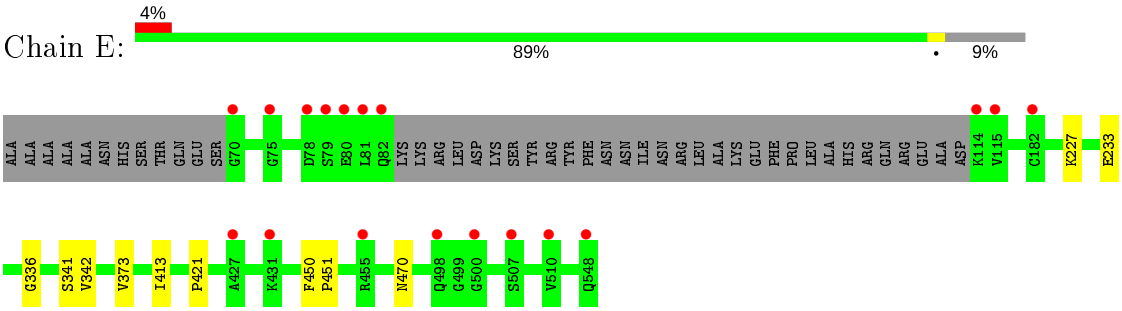
- Molecule 1: 5-aminolevulinate synthase, mitochondrial

Chain D:



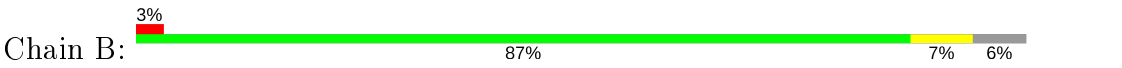
- Molecule 1: 5-aminolevulinate synthase, mitochondrial

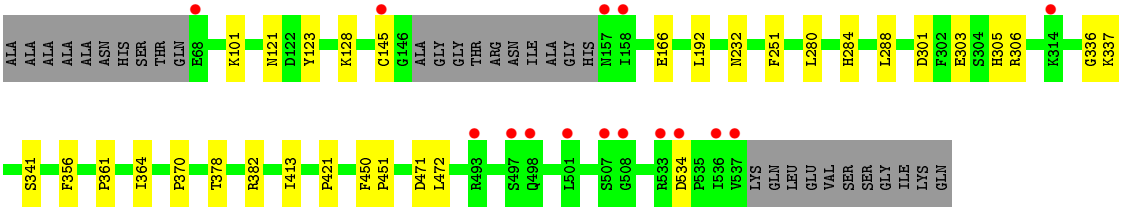
Chain E:



- Molecule 2: 5-aminolevulinate synthase, mitochondrial

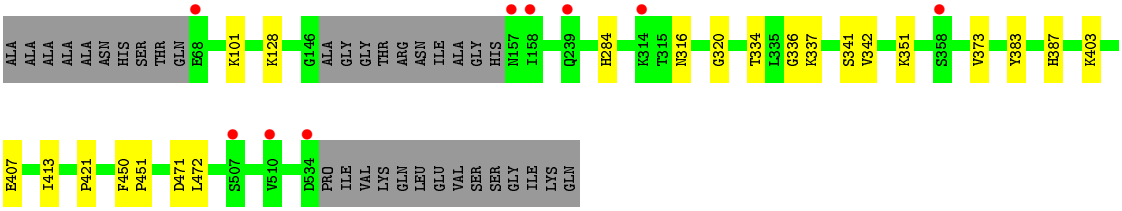
Chain B:





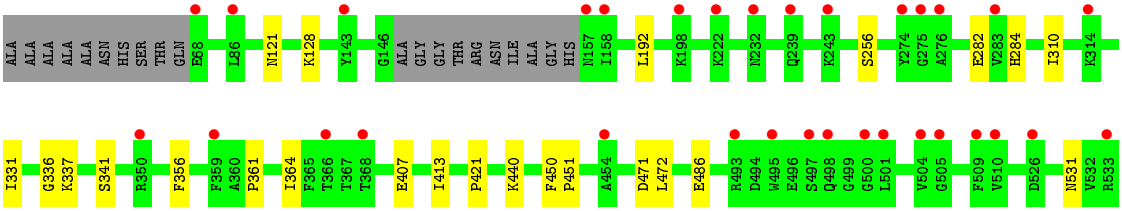
- Molecule 2: 5-aminolevulinate synthase, mitochondrial

Chain C:



- Molecule 2: 5-aminolevulinate synthase, mitochondrial

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	63.49Å 113.81Å 119.34Å 116.52° 98.18° 92.56°	Depositor
Resolution (Å)	35.00 – 2.70 35.00 – 2.69	Depositor EDS
% Data completeness (in resolution range)	94.3 (35.00-2.70) 94.3 (35.00-2.69)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.186 , 0.232 0.188 , 0.234	Depositor DCC
R_{free} test set	2007 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,k,-k-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	42498	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: LLP, SO4, PE3

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	0.27	0/3514	0.45	0/4764
1	D	0.28	0/3457	0.45	0/4686
1	E	0.27	0/3514	0.45	0/4764
2	B	0.28	0/3647	0.45	0/4942
2	C	0.29	0/3624	0.46	0/4909
2	F	0.27	0/3647	0.45	0/4942
All	All	0.28	0/21403	0.45	0/29007

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3443	3427	3427	6	0
1	D	3388	3381	3380	10	0
1	E	3443	3427	3427	6	0
2	B	3596	3564	3564	16	1
2	C	3574	3538	3537	14	0
2	F	3596	3564	3564	14	1
3	B	54	57	67	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	46	42	54	1	0
3	F	19	4	24	0	0
4	D	5	0	0	0	0
5	A	59	0	0	0	0
5	B	47	0	0	0	0
5	C	64	0	0	0	0
5	D	90	0	0	0	0
5	E	39	0	0	0	0
5	F	31	0	0	0	0
All	All	21494	21004	21044	65	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 2.

All (65) 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)
2:F:284:HIS:HE2	2:F:337:LLP:HO3	1.14	0.89
2:C:284:HIS:HE2	2:C:337:LLP:HO3	1.19	0.87
2:F:284:HIS:NE2	2:F:337:LLP:O3	2.08	0.80
2:B:284:HIS:NE2	2:B:337:LLP:O3	2.22	0.72
3:C:602:PE3:H322	3:C:603:PE3:H301	1.81	0.62
2:C:334:THR:HG21	2:C:337:LLP:HG2	1.81	0.61
1:D:74:GLU:OE2	2:C:351:LYS:NZ	2.35	0.60
2:F:471:ASP:OD1	2:F:472:LEU:N	2.35	0.59
2:B:471:ASP:OD1	2:B:472:LEU:N	2.36	0.59
1:E:413:ILE:HB	1:E:421:PRO:HG2	1.89	0.54
1:A:470:ASN:HB2	2:C:101:LYS:O	2.08	0.54
1:D:413:ILE:HB	1:D:421:PRO:HG2	1.91	0.53
1:A:336:GLY:HA2	1:A:341:SER:O	2.08	0.53
2:F:413:ILE:HB	2:F:421:PRO:HG2	1.92	0.52
2:C:342:VAL:HG12	2:C:373:VAL:HG11	1.92	0.51
2:B:121:ASN:HB3	2:B:337:LLP:HG2	1.93	0.51
1:E:336:GLY:HA2	1:E:341:SER:O	2.10	0.51
2:C:336:GLY:HA2	2:C:341:SER:O	2.10	0.50
1:D:336:GLY:HA2	1:D:341:SER:O	2.11	0.50
2:F:361:PRO:O	2:F:364:ILE:HG13	2.11	0.50
2:C:413:ILE:HB	2:C:421:PRO:HG2	1.94	0.48
2:C:284:HIS:NE2	2:C:337:LLP:O3	2.25	0.48
2:F:336:GLY:HA2	2:F:341:SER:O	2.13	0.47
2:B:413:ILE:HB	2:B:421:PRO:HG2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:VAL:HG12	1:D:373:VAL:HG11	1.96	0.47
2:B:166:GLU:HG3	2:B:378:THR:HG23	1.96	0.47
1:A:413:ILE:HB	1:A:421:PRO:HG2	1.96	0.47
1:A:166:GLU:HG3	1:A:378:THR:HG23	1.97	0.47
2:F:121:ASN:HB3	2:F:337:LLP:HG2	1.97	0.46
2:B:192:LEU:HD23	2:B:356:PHE:HD1	1.81	0.45
1:D:450:PHE:CG	1:D:451:PRO:HA	2.52	0.45
2:C:284:HIS:CD2	2:C:337:LLP:HO3	2.28	0.45
1:A:450:PHE:CG	1:A:451:PRO:HA	2.52	0.45
2:B:361:PRO:O	2:B:364:ILE:HG12	2.17	0.44
2:F:284:HIS:CE1	2:F:337:LLP:HO3	2.25	0.44
1:D:294:ALA:HB3	1:D:298:GLU:HB2	2.00	0.44
2:F:192:LEU:HD23	2:F:356:PHE:HD1	1.82	0.43
2:B:101:LYS:O	1:E:470:ASN:HB2	2.19	0.43
2:F:256:SER:HB3	2:F:284:HIS:CE1	2.54	0.43
2:B:303:GLU:OE2	2:B:306:ARG:NH2	2.52	0.43
1:D:172:LYS:NZ	1:D:309:GLY:O	2.43	0.43
2:F:282:GLU:HG3	2:F:331:ILE:HG23	2.01	0.42
2:B:123:TYR:CD2	2:B:288:LEU:HD11	2.54	0.42
2:C:471:ASP:OD1	2:C:472:LEU:N	2.52	0.42
1:D:166:GLU:HG3	1:D:378:THR:HG23	2.01	0.42
2:B:336:GLY:HA2	2:B:341:SER:O	2.19	0.42
1:D:443:ILE:HG22	1:D:445:VAL:HG23	2.01	0.42
1:E:342:VAL:HG12	1:E:373:VAL:HG11	2.01	0.42
1:E:450:PHE:CG	1:E:451:PRO:HA	2.55	0.42
2:B:450:PHE:CG	2:B:451:PRO:HA	2.55	0.42
2:B:382:ARG:NH2	2:B:534:ASP:OD1	2.53	0.42
2:C:403:LYS:O	2:C:407:GLU:HG3	2.20	0.42
3:B:601:PE3:H352	3:B:603:PE3:H211	2.02	0.41
2:C:383:TYR:CE2	2:C:387:HIS:CE1	3.08	0.41
2:F:450:PHE:CG	2:F:451:PRO:HA	2.55	0.41
2:B:301:ASP:O	2:B:305:HIS:CD2	2.74	0.41
1:E:227:LYS:HG2	1:E:233:GLU:OE1	2.20	0.41
2:F:310:ILE:HG22	2:F:531:ASN:CG	2.40	0.41
1:A:259:GLY:HA2	1:A:419:ILE:HD12	2.01	0.41
2:C:450:PHE:CG	2:C:451:PRO:HA	2.56	0.41
2:F:440:LYS:NZ	2:F:486:GLU:OE2	2.51	0.41
2:B:251:PHE:CE2	2:B:280:LEU:HD13	2.56	0.40
2:C:316:ASN:OD1	2:C:320:GLY:N	2.48	0.40
1:D:234:LEU:O	1:D:238:LEU:HG	2.21	0.40
2:B:145:CYS:O	2:B:370:PRO:HB3	2.21	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)
2:B:232:ASN:HD22	2:F:407:GLU:OE2[1_666]	1.46	0.14

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	444/491 (90%)	438 (99%)	6 (1%)	0	100	100
1	D	435/491 (89%)	429 (99%)	6 (1%)	0	100	100
1	E	444/491 (90%)	438 (99%)	6 (1%)	0	100	100
2	B	455/491 (93%)	448 (98%)	7 (2%)	0	100	100
2	C	452/491 (92%)	445 (98%)	7 (2%)	0	100	100
2	F	455/491 (93%)	448 (98%)	7 (2%)	0	100	100
All	All	2685/2946 (91%)	2646 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	376/411 (92%)	376 (100%)	0	100	100
1	D	370/411 (90%)	370 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	376/411 (92%)	376 (100%)	0	100	100
2	B	390/410 (95%)	389 (100%)	1 (0%)	92	98
2	C	387/410 (94%)	386 (100%)	1 (0%)	92	98
2	F	390/410 (95%)	389 (100%)	1 (0%)	92	98
All	All	2289/2463 (93%)	2286 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	128	LYS
2	C	128	LYS
2	F	128	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	121	ASN
1	E	121	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	LLP	B	337	2	23,24,25	1.72	3 (13%)	25,32,34	1.03	2 (8%)
2	LLP	C	337	2	23,24,25	1.71	3 (13%)	25,32,34	1.05	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LLP	F	337	2	23,24,25	1.74	3 (13%)	25,32,34	0.96	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LLP	B	337	2	-	8/16/17/19	0/1/1/1
2	LLP	C	337	2	-	7/16/17/19	0/1/1/1
2	LLP	F	337	2	-	7/16/17/19	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	337	LLP	C4-C4'	5.08	1.56	1.46
2	C	337	LLP	C4-C4'	4.86	1.55	1.46
2	F	337	LLP	C4-C4'	4.75	1.55	1.46
2	F	337	LLP	C4-C5	-4.01	1.36	1.42
2	F	337	LLP	C4-C3	-3.57	1.35	1.40
2	C	337	LLP	C4-C3	-3.40	1.35	1.40
2	C	337	LLP	C4-C5	-3.35	1.37	1.42
2	B	337	LLP	C4-C5	-3.33	1.37	1.42
2	B	337	LLP	C4-C3	-3.32	1.35	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	337	LLP	CE-NZ-C4'	3.14	128.54	118.90
2	B	337	LLP	CE-NZ-C4'	2.99	128.07	118.90
2	F	337	LLP	CE-NZ-C4'	2.32	126.03	118.90
2	F	337	LLP	C5-C6-N1	-2.29	120.00	123.82
2	B	337	LLP	C5-C6-N1	-2.18	120.19	123.82
2	C	337	LLP	C5-C6-N1	-2.07	120.38	123.82

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	337	LLP	C4-C4'-NZ-CE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	337	LLP	C-CA-CB-CG
2	B	337	LLP	O-C-CA-CB
2	B	337	LLP	CG-CD-CE-NZ
2	C	337	LLP	C4-C4'-NZ-CE
2	F	337	LLP	C4-C4'-NZ-CE
2	F	337	LLP	C-CA-CB-CG
2	F	337	LLP	O-C-CA-CB
2	C	337	LLP	CG-CD-CE-NZ
2	F	337	LLP	CG-CD-CE-NZ
2	B	337	LLP	C3-C4-C4'-NZ
2	C	337	LLP	C3-C4-C4'-NZ
2	F	337	LLP	C3-C4-C4'-NZ
2	F	337	LLP	CE-CD-CG-CB
2	B	337	LLP	CE-CD-CG-CB
2	C	337	LLP	CA-CB-CG-CD
2	C	337	LLP	CE-CD-CG-CB
2	B	337	LLP	CD-CE-NZ-C4'
2	C	337	LLP	CD-CE-NZ-C4'
2	F	337	LLP	CD-CE-NZ-C4'
2	C	337	LLP	C5-C4-C4'-NZ
2	B	337	LLP	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	337	LLP	2	0
2	C	337	LLP	4	0
2	F	337	LLP	4	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
3	PE3	F	601	-	18,18,42	0.53	0	17,17,41	0.34	0
3	PE3	C	603	-	11,11,42	0.53	0	10,10,41	0.42	0
3	PE3	B	601	-	17,17,42	0.54	0	16,16,41	0.30	0
3	PE3	C	602	-	15,15,42	0.53	0	14,14,41	0.26	0
3	PE3	B	602	-	27,27,42	0.54	0	26,26,41	0.44	0
3	PE3	B	603	-	7,7,42	0.49	0	6,6,41	0.23	0
4	SO4	D	601	-	4,4,4	0.14	0	6,6,6	0.05	0
3	PE3	C	601	-	17,17,42	0.54	0	16,16,41	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PE3	F	601	-	-	10/16/16/40	-
3	PE3	C	603	-	-	3/9/9/40	-
3	PE3	B	601	-	-	5/15/15/40	-
3	PE3	C	602	-	-	4/13/13/40	-
3	PE3	B	602	-	-	10/25/25/40	-
3	PE3	B	603	-	-	1/5/5/40	-
3	PE3	C	601	-	-	8/15/15/40	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	PE3	C20-C21-O22-C23
3	B	602	PE3	O31-C32-C33-O34
3	C	602	PE3	O28-C29-C30-O31
3	B	603	PE3	O19-C20-C21-O22
3	C	601	PE3	O31-C32-C33-O34
3	B	602	PE3	O16-C17-C18-O19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	F	601	PE3	O13-C14-C15-O16
3	B	601	PE3	O25-C26-C27-O28
3	F	601	PE3	O16-C17-C18-O19
3	C	601	PE3	O25-C26-C27-O28
3	F	601	PE3	O22-C23-C24-O25
3	B	602	PE3	O37-C38-C39-O40
3	F	601	PE3	O10-C11-C12-O13
3	C	601	PE3	O28-C29-C30-O31
3	C	603	PE3	O31-C32-C33-O34
3	C	603	PE3	O28-C29-C30-O31
3	B	602	PE3	O22-C23-C24-O25
3	F	601	PE3	O25-C26-C27-O28
3	B	602	PE3	O40-C41-C42-O43
3	B	601	PE3	C23-C24-O25-C26
3	C	601	PE3	C23-C24-O25-C26
3	F	601	PE3	O19-C20-C21-O22
3	F	601	PE3	C27-C26-O25-C24
3	B	602	PE3	C23-C24-O25-C26
3	B	601	PE3	C26-C27-O28-C29
3	C	601	PE3	C36-C35-O34-C33
3	F	601	PE3	C14-C15-O16-C17
3	B	602	PE3	C32-C33-O34-C35
3	C	601	PE3	C33-C32-O31-C30
3	F	601	PE3	C15-C14-O13-C12
3	C	603	PE3	C36-C35-O34-C33
3	C	602	PE3	C23-C24-O25-C26
3	C	601	PE3	C30-C29-O28-C27
3	F	601	PE3	C18-C17-O16-C15
3	B	601	PE3	O31-C32-C33-O34
3	B	602	PE3	C38-C39-O40-C41
3	C	601	PE3	C26-C27-O28-C29
3	B	602	PE3	O25-C26-C27-O28
3	C	602	PE3	C32-C33-O34-C35
3	C	602	PE3	O34-C35-C36-O37
3	B	601	PE3	C36-C35-O34-C33

There are no ring outliers.

4 monomers are involved in 2 short contacts:

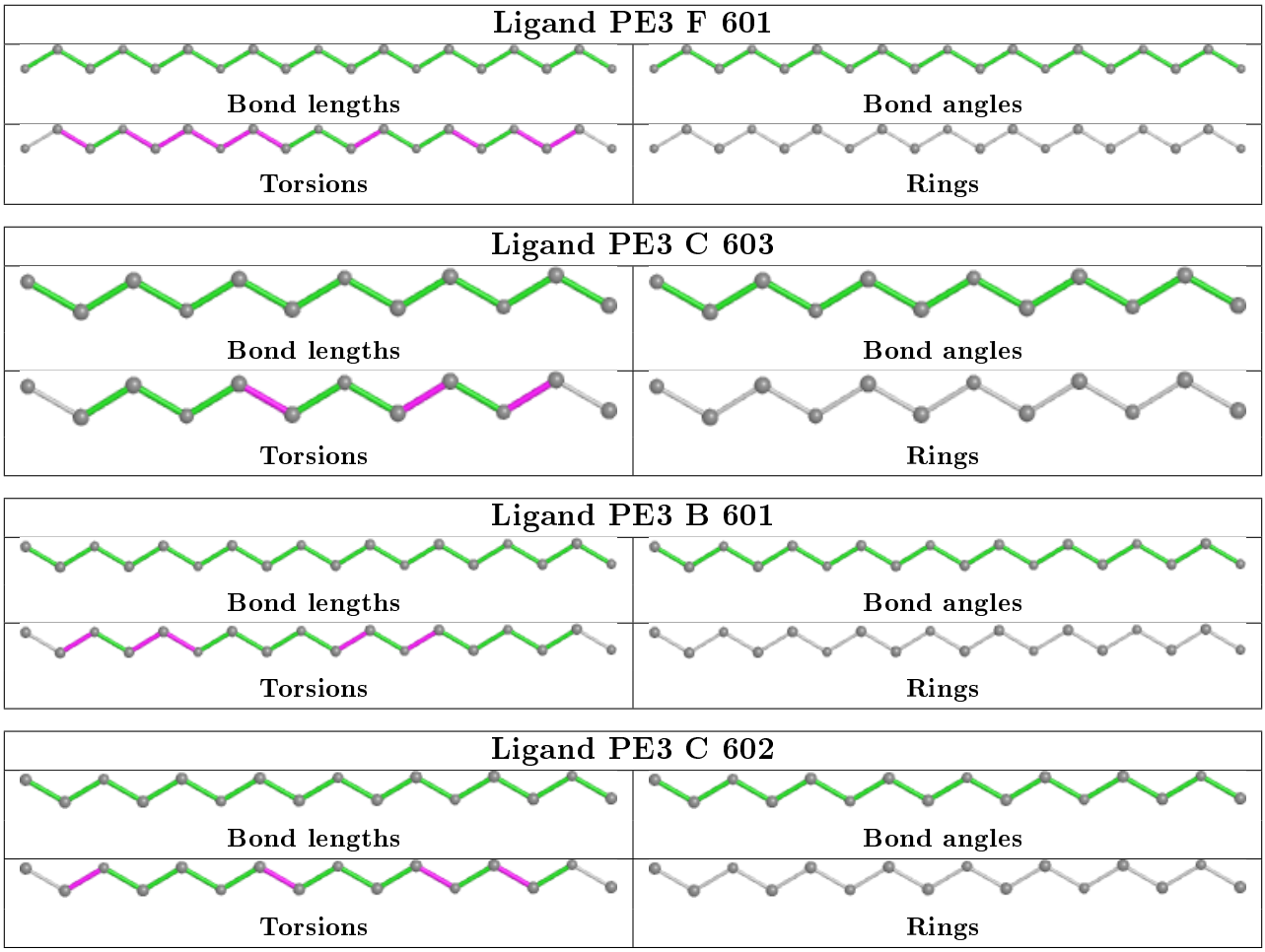
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	PE3	1	0
3	B	601	PE3	1	0

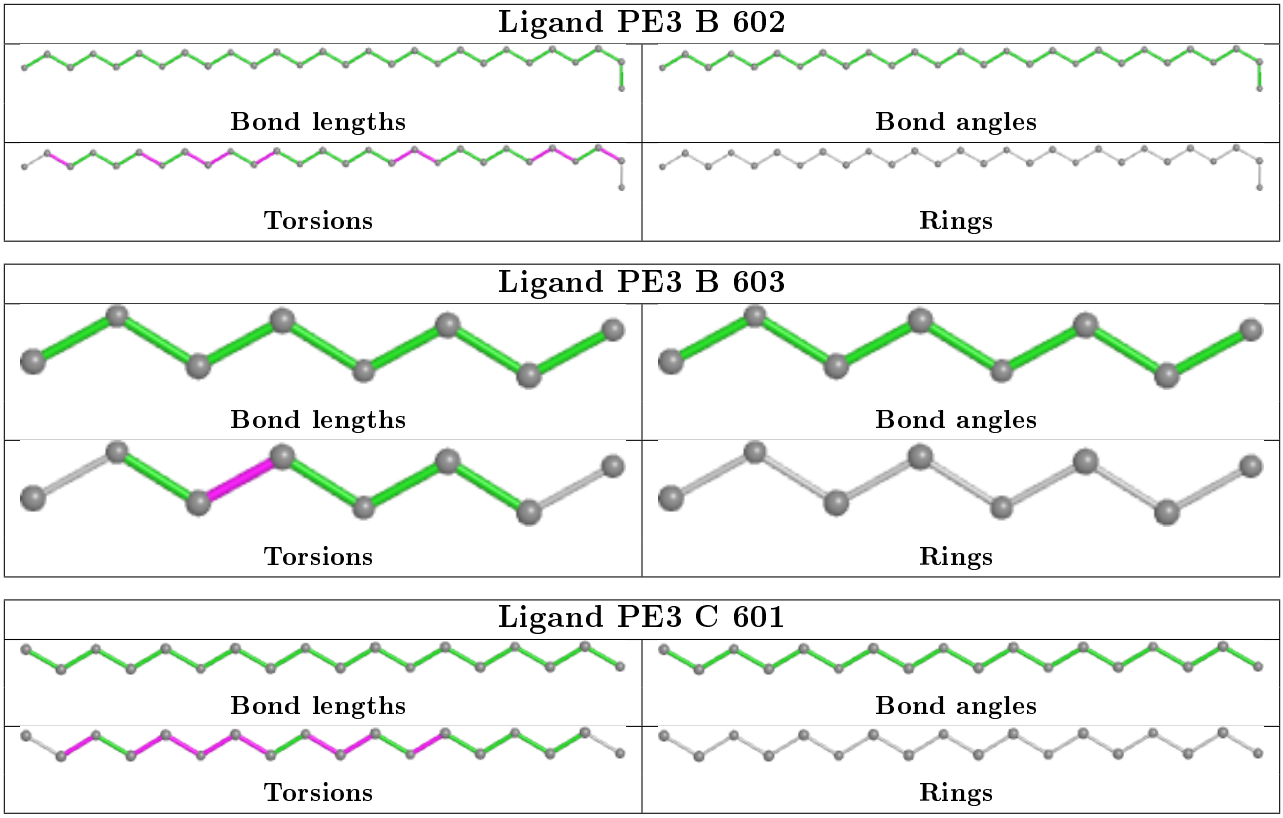
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	PE3	1	0
3	B	603	PE3	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.





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	448/491 (91%)	-0.28	5 (1%)	80	82	11, 31, 63, 82	1 (0%)
1	D	441/491 (89%)	-0.27	3 (0%)	87	89	11, 30, 57, 80	0
1	E	448/491 (91%)	-0.08	18 (4%)	38	37	16, 36, 66, 102	0
2	B	459/491 (93%)	-0.10	15 (3%)	46	46	12, 38, 71, 125	0
2	C	456/491 (92%)	-0.15	9 (1%)	65	67	15, 35, 70, 101	0
2	F	459/491 (93%)	0.38	35 (7%)	13	12	22, 52, 95, 135	0
All	All	2711/2946 (92%)	-0.08	85 (3%)	49	49	11, 36, 74, 135	1 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	536	ILE	5.8
2	F	239	GLN	5.3
2	B	68	GLU	5.1
1	E	548	GLN	4.7
1	E	115	VAL	4.5
1	E	81	LEU	4.0
1	D	81	LEU	3.5
2	B	507	SER	3.5
2	F	533	ARG	3.5
2	F	68	GLU	3.5
2	B	536	ILE	3.4
1	E	79	SER	3.3
1	D	114	LYS	3.2
2	B	158	ILE	3.2
2	F	314	LYS	3.2
2	F	509	PHE	3.1
2	F	537	VAL	3.1
2	B	501	LEU	3.1
2	C	507	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	70	GLY	3.0
2	F	497	SER	3.0
1	A	115	VAL	3.0
2	F	510	VAL	2.9
1	E	114	LYS	2.8
2	F	198	LYS	2.8
2	F	498	GLN	2.8
1	E	78	ASP	2.8
2	F	495	TRP	2.8
2	B	493	ARG	2.7
2	B	537	VAL	2.7
2	C	158	ILE	2.7
1	A	114	LYS	2.7
1	E	455	ARG	2.6
2	F	368	THR	2.6
2	F	232	ASN	2.6
2	B	145	CYS	2.6
2	C	157	ASN	2.5
2	F	501	LEU	2.5
2	F	143	TYR	2.5
2	B	533	ARG	2.5
2	F	222	LYS	2.5
2	F	505	GLY	2.5
2	C	358	SER	2.5
2	C	534	ASP	2.5
2	F	534	ASP	2.5
1	E	75	GLY	2.5
2	F	158	ILE	2.5
2	F	359	PHE	2.5
1	E	82	GLN	2.4
2	F	274	TYR	2.4
2	F	157	ASN	2.4
2	B	498	GLN	2.3
2	C	510	VAL	2.3
2	B	534	ASP	2.3
2	B	497	SER	2.3
1	A	446	GLN	2.3
1	E	500	GLY	2.3
1	A	548	GLN	2.3
2	F	350	ARG	2.2
1	E	498	GLN	2.2
1	E	427	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	526	ASP	2.2
2	B	508	GLY	2.2
2	F	500	GLY	2.2
1	E	510	VAL	2.2
2	F	493	ARG	2.2
2	F	243	LYS	2.2
1	E	80	GLU	2.1
2	F	504	VAL	2.1
2	F	86	LEU	2.1
2	F	454	ALA	2.1
2	F	275	GLY	2.1
2	B	314	LYS	2.1
1	D	439	ASN	2.1
2	B	157	ASN	2.1
2	F	283	VAL	2.1
2	C	239	GLN	2.1
2	F	276	ALA	2.1
1	E	507	SER	2.1
1	E	182	CYS	2.0
1	A	510	VAL	2.0
2	C	68	GLU	2.0
2	F	366	THR	2.0
1	E	431	LYS	2.0
2	C	314	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
2	LLP	F	337	24/25	0.95	0.28	23,41,55,63	0
2	LLP	B	337	24/25	0.96	0.22	16,29,43,44	0
2	LLP	C	337	24/25	0.97	0.22	18,26,49,50	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

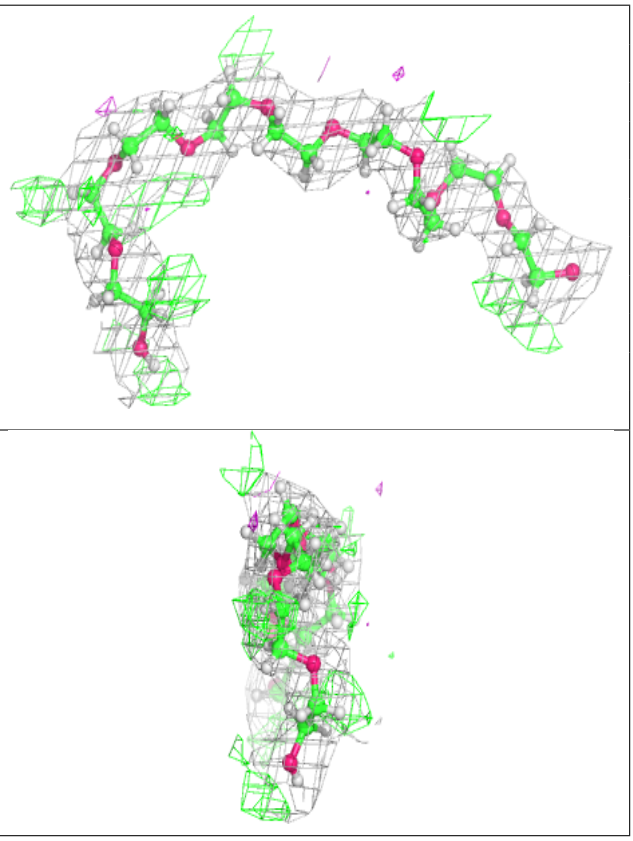
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	PE3	B	602	28/43	0.83	0.19	27,46,56,56	0
3	PE3	C	601	18/43	0.84	0.17	38,52,64,66	0
3	PE3	F	601	19/43	0.86	0.17	43,51,61,64	0
3	PE3	B	603	8/43	0.87	0.14	36,41,46,48	0
4	SO4	D	601	5/5	0.88	0.21	93,93,93,93	0
3	PE3	C	602	16/43	0.89	0.17	24,49,59,60	0
3	PE3	C	603	12/43	0.90	0.24	36,44,55,55	0
3	PE3	B	601	18/43	0.93	0.15	23,36,47,48	0

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

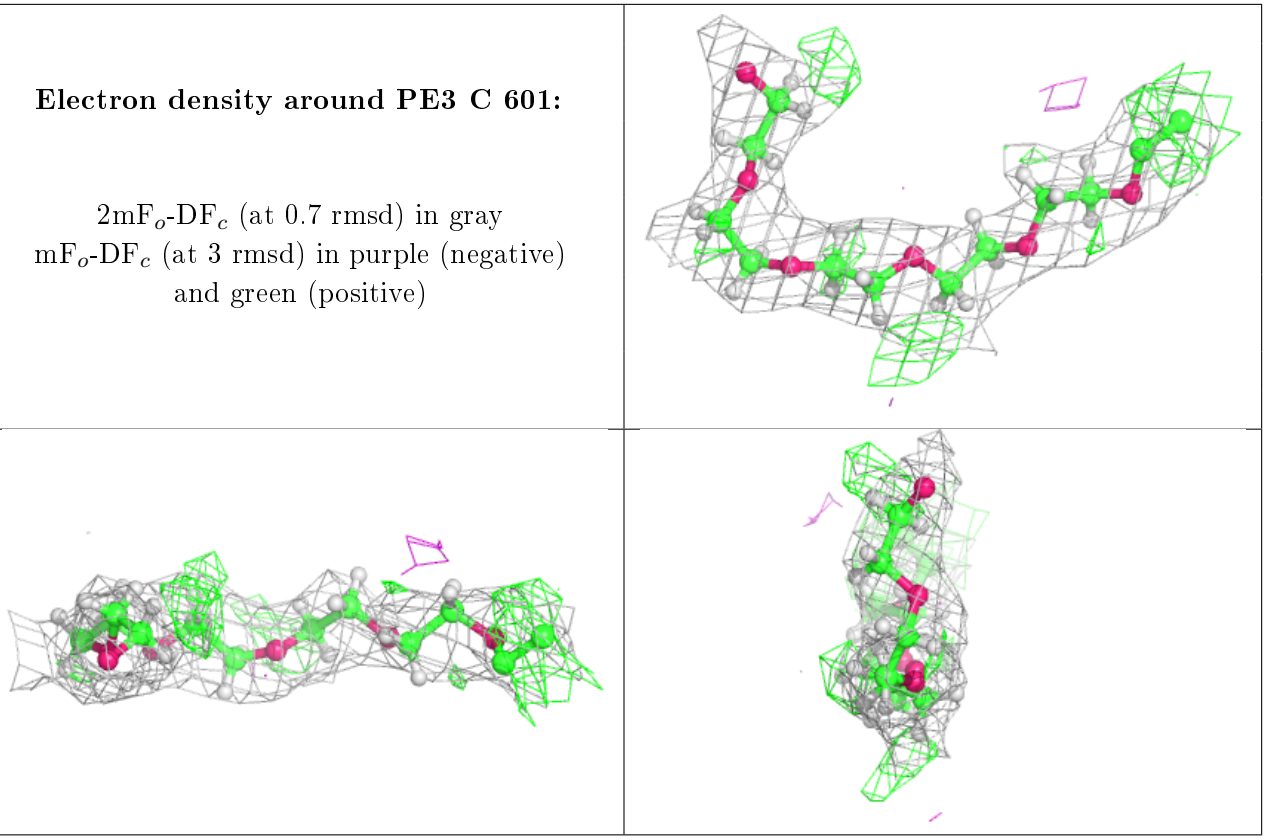
Electron density around PE3 B 602:

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



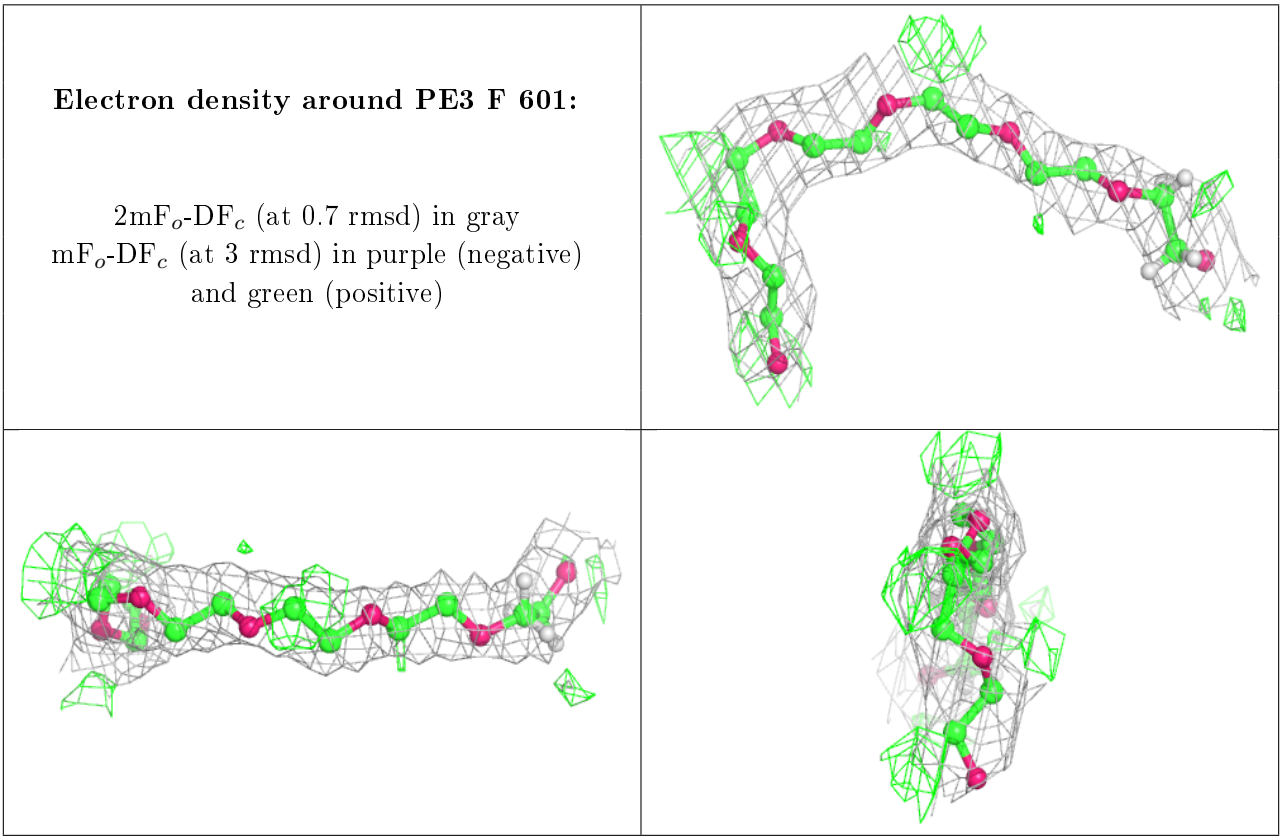
Electron density around PE3 C 601:

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



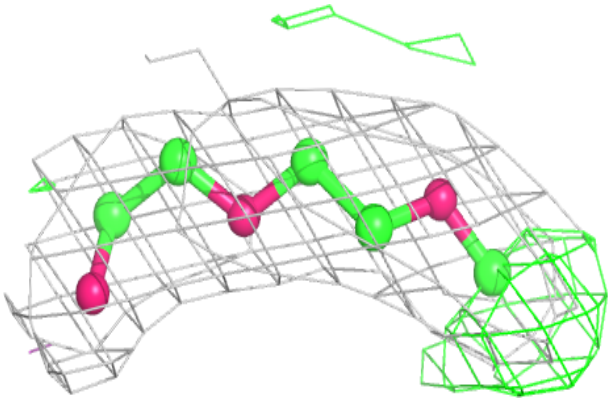
Electron density around PE3 F 601:

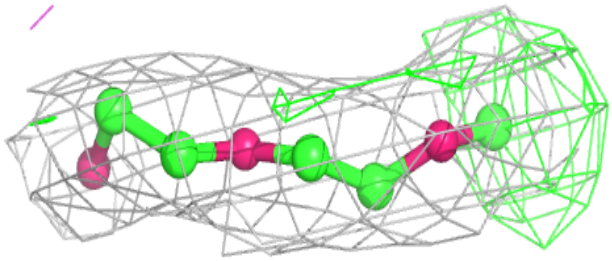
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

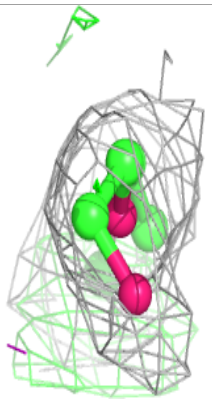


Electron density around PE3 B 603:

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

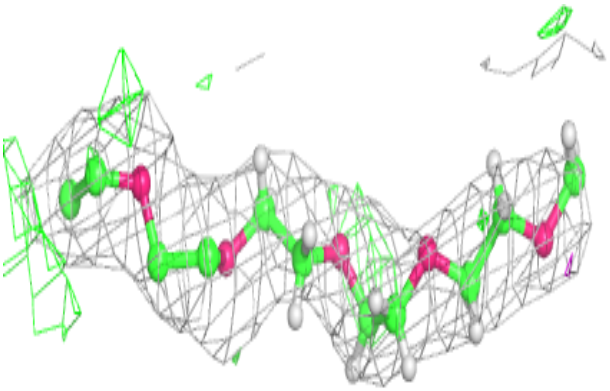


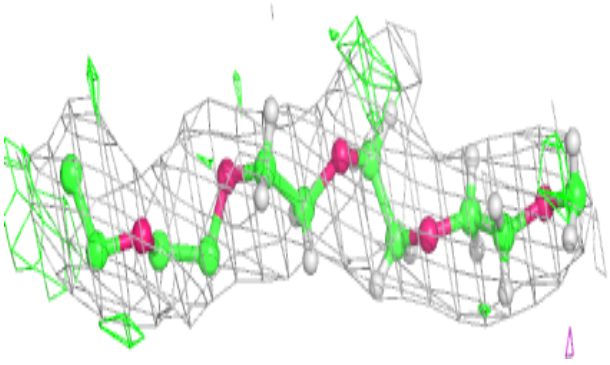


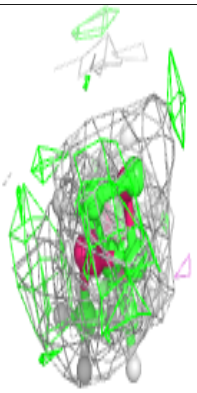


Electron density around PE3 C 602:

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

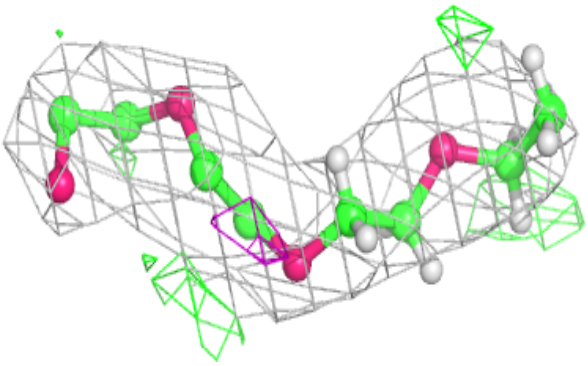


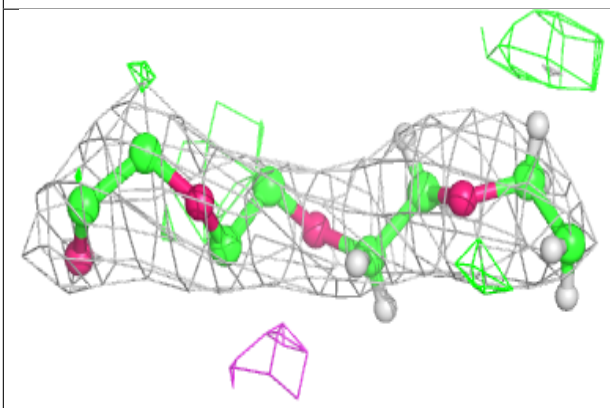


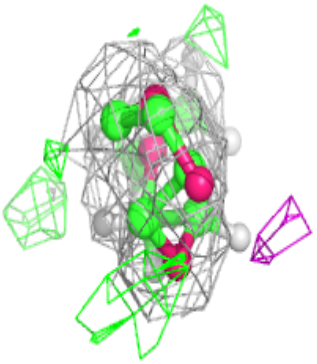


Electron density around PE3 C 603:

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

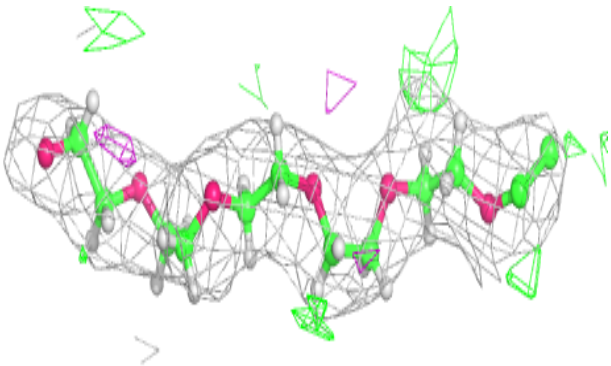


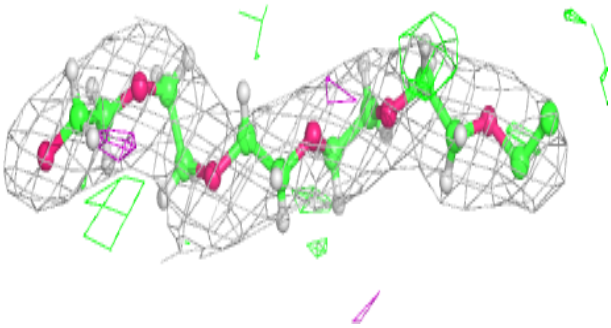


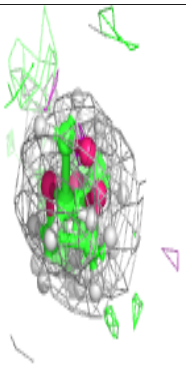


Electron density around PE3 B 601:

$2mF_o$-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.