Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:24 PM UTC

PDB ID	:	6P2K / pdb_00006p2k
Title	:	Crystal structure of AFV00434, an ancestral GH74 enzyme
Authors	:	Stogios, P.J.; Skarina, T.; Arnal, G.; Brumer, H.; Savchenko, A.
Deposited on	:	2019-05-21
Resolution	:	2.15 Å(reported)

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

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

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

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

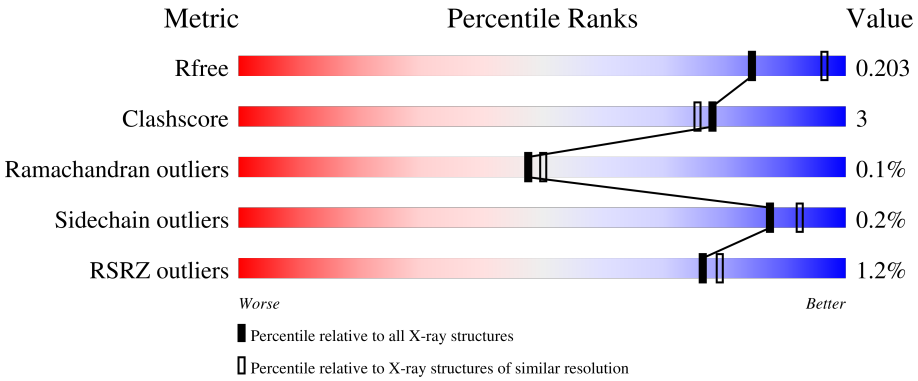
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	779	94% 5%
1	B	779	2% 91% 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14024 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.

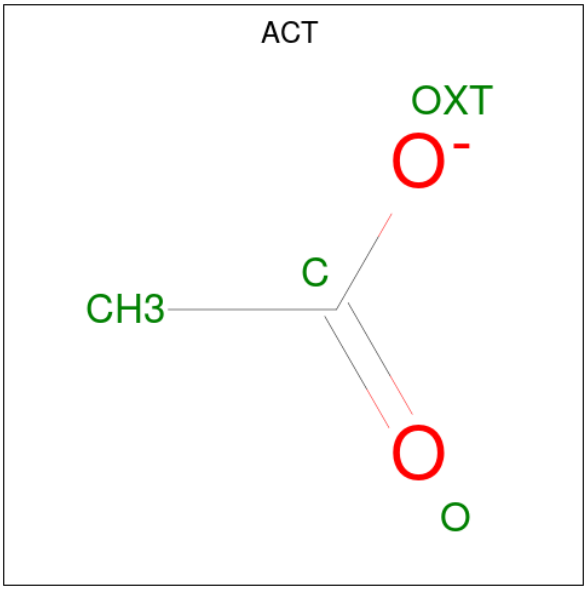
- Molecule 1 is a protein called Fibronectin type III domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	776	Total	C	N	O	S	0	5	0
			6043	3804	1049	1175	15			
1	B	778	Total	C	N	O	S	0	1	0
			6037	3798	1051	1173	15			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

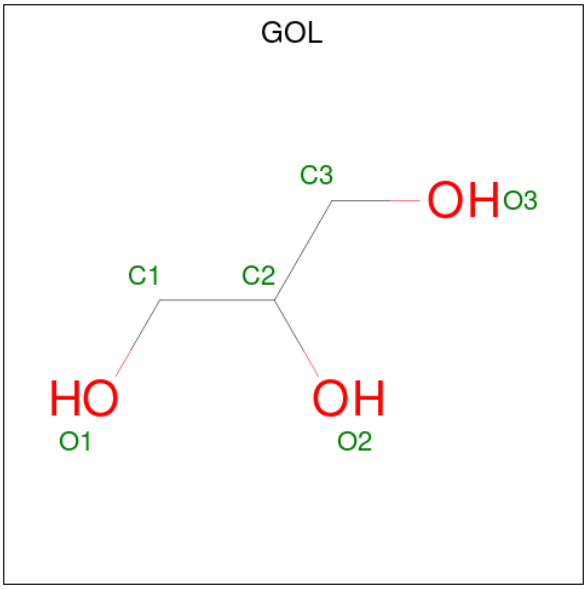
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



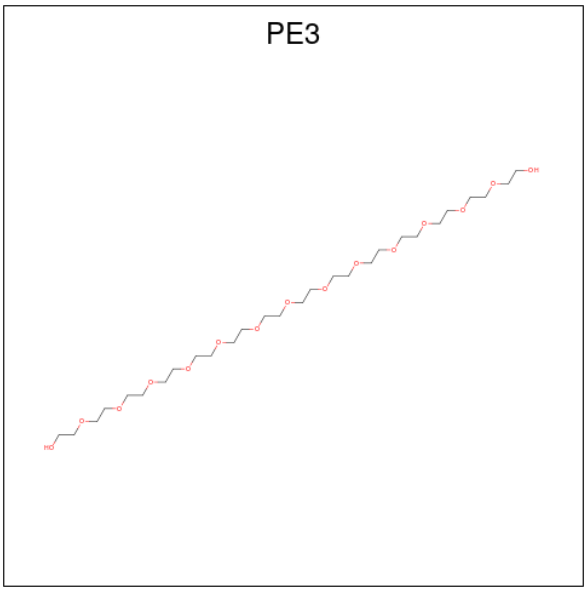
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAOXAHENTETRACONTANE-1 ,41-DIOL (CCD ID: PE3) (formula: $C_{28}H_{58}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 13 8 5	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 13 8 5	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	1	Total Cl 1 1	0	0

- Molecule 7 is water.

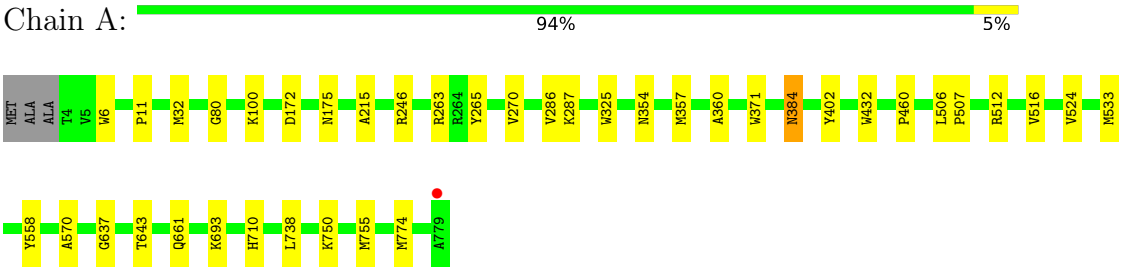
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	911	Total O 950 950	0	38
7	B	803	Total O 844 844	0	40

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.

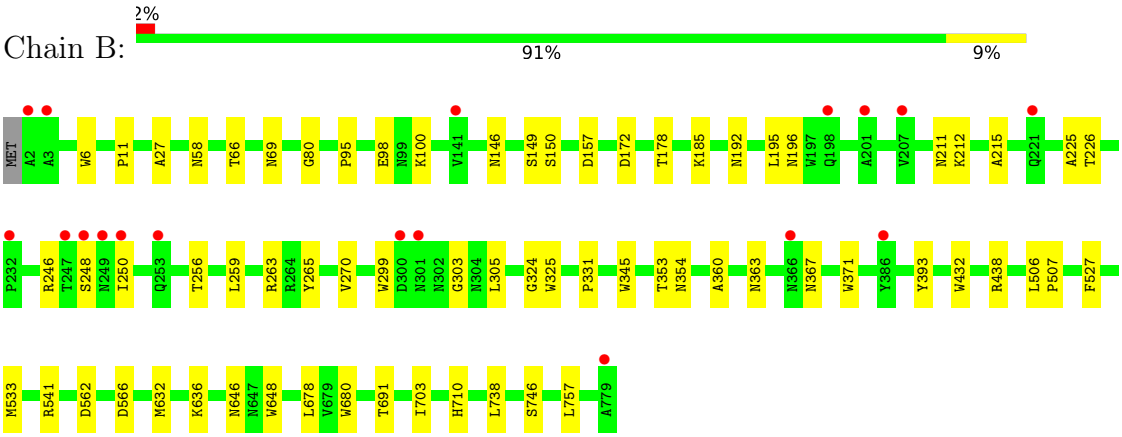
• Molecule 1: Fibronectin type III domain-containing protein

Chain A:



• Molecule 1: Fibronectin type III domain-containing protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	173.43Å 173.43Å 173.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.78 – 2.15 38.78 – 2.15	Depositor EDS
% Data completeness (in resolution range)	86.8 (38.78-2.15) 90.1 (38.78-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.15_3448: ???)	Depositor
R, R_{free}	0.154 , 0.204 0.155 , 0.203	Depositor DCC
R_{free} test set	2739 reflections (2.93%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 58.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14024	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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: CL, ZN, PE3, ACT, GOL

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	0.21	1/6235 (0.0%)	0.37	0/8510
1	B	0.18	1/6217 (0.0%)	0.39	0/8486
All	All	0.20	2/12452 (0.0%)	0.38	0/16996

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	ASN	C-O	-7.21	1.15	1.24
1	B	248	SER	C-O	-5.32	1.18	1.24

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	6043	0	5627	25	0
1	B	6037	0	5612	40	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	4	0	3	0	0
4	A	30	0	40	1	0
4	B	54	0	72	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	27	0	35	2	0
5	B	27	0	35	0	0
6	A	1	0	0	0	0
6	B	1	0	0	1	0
7	A	950	0	0	5	0
7	B	844	0	0	5	0
All	All	14024	0	11424	67	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 3.

All (67) 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)
4:B:815:GOL:H11	7:B:1548:HOH:O	1.89	0.73
1:A:533:MET:HB3	1:A:558:TYR:HB3	1.79	0.65
1:B:562:ASP:N	1:B:566:ASP:OD2	2.30	0.65
1:A:246:ARG:NH1	7:A:901:HOH:O	2.21	0.61
1:B:146:ASN:ND2	7:B:905:HOH:O	2.35	0.60
1:B:636:LYS:NZ	1:B:646:ASN:OD1	2.35	0.59
1:B:710:HIS:HB2	6:B:816:CL:CL	2.42	0.57
1:B:527:PHE:HD2	1:B:533:MET:HE3	1.70	0.56
1:A:11:PRO:HB3	1:A:432:TRP:HB2	1.85	0.56
1:B:215:ALA:HB1	1:B:270:VAL:HG23	1.89	0.54
1:B:95:PRO:HA	1:B:98:GLU:HG3	1.89	0.54
1:B:27:ALA:HA	1:B:345:TRP:CE2	2.42	0.54
1:A:215:ALA:HB1	1:A:270:VAL:HG23	1.91	0.53
1:B:192:ASN:ND2	1:B:196:ASN:HB2	2.23	0.53
1:B:11:PRO:HB3	1:B:432:TRP:HB2	1.92	0.52
1:B:438:ARG:NH2	7:B:912:HOH:O	2.40	0.51
1:B:58:ASN:ND2	7:B:919:HOH:O	2.43	0.51
1:A:755:MET:HG2	1:A:774:MET:SD	2.50	0.51
1:B:246:ARG:HD2	1:B:303:GLY:O	2.10	0.50
1:B:746:SER:HB3	1:B:757:LEU:HD11	1.93	0.50
1:B:146:ASN:OD1	1:B:149:SER:N	2.44	0.50
1:B:157:ASP:OD1	1:B:185:LYS:NZ	2.44	0.49
1:B:66:THR:OG1	1:B:69:ASN:O	2.29	0.49
1:A:506:LEU:HD12	1:A:507:PRO:HD2	1.95	0.49
1:B:256:THR:HA	1:B:259:LEU:HD12	1.94	0.49
1:A:402:TYR:CE2	4:A:805:GOL:H2	2.48	0.49
1:B:80:GLY:HA2	1:B:100:LYS:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:TRP:CE2	1:B:305:LEU:HD13	2.48	0.49
1:A:516:VAL:HG22	1:A:524:VAL:HG22	1.94	0.48
1:A:6:TRP:CD1	1:A:738:LEU:HB2	2.49	0.48
1:B:146:ASN:ND2	1:B:150:SER:OG	2.47	0.48
1:B:632:MET:HE2	1:B:703:ILE:HG23	1.96	0.48
1:B:648:TRP:CD1	1:B:691:THR:HG22	2.50	0.47
1:A:750:LYS:NZ	7:A:918:HOH:O	2.47	0.47
1:B:541:ARG:NH2	7:B:931[B]:HOH:O	2.34	0.47
1:A:80:GLY:HA2	1:A:100:LYS:O	2.15	0.47
1:B:211:ASN:ND2	1:B:225:ALA:HB1	2.30	0.47
1:B:192:ASN:HD21	1:B:196:ASN:HB2	1.79	0.47
1:A:637:GLY:HA2	1:A:643:THR:HG23	1.97	0.46
1:A:32:MET:HE1	7:A:1024:HOH:O	2.14	0.46
1:B:157:ASP:HB3	1:B:185:LYS:HZ2	1.81	0.46
1:A:460:PRO:HA	5:A:809:PE3:H412	1.98	0.45
1:A:661[A]:GLN:NE2	7:A:921:HOH:O	2.48	0.45
1:A:693:LYS:HD2	1:A:693:LYS:HA	1.68	0.45
1:B:192:ASN:OD1	1:B:192:ASN:N	2.50	0.45
1:B:263:ARG:HB2	1:B:265:TYR:CE2	2.52	0.45
1:A:32:MET:HE3	1:A:357:MET:SD	2.57	0.45
1:A:263:ARG:HB2	1:A:265:TYR:CE2	2.52	0.45
5:A:811:PE3:H322	5:A:811:PE3:H362	1.98	0.45
1:B:360:ALA:HB2	1:B:371:TRP:CD2	2.52	0.44
1:B:11:PRO:HB2	1:B:325:TRP:CD1	2.52	0.44
1:A:710:HIS:HB2	7:A:1650:HOH:O	2.17	0.44
1:A:286:VAL:HG22	1:A:287:LYS:HG3	1.98	0.44
1:B:363:ASN:O	1:B:367:ASN:N	2.51	0.44
1:A:172:ASP:HB3	1:A:175:ASN:O	2.17	0.44
1:A:11:PRO:HB2	1:A:325:TRP:CD1	2.53	0.43
1:A:360:ALA:HB2	1:A:371:TRP:CD2	2.53	0.43
1:B:192:ASN:HB2	1:B:195:LEU:H	1.83	0.43
1:B:6:TRP:CD1	1:B:738:LEU:HB2	2.54	0.42
1:B:331:PRO:HB3	1:B:353:THR:HG22	2.01	0.42
1:B:324:GLY:HA2	1:B:393:TYR:CE2	2.55	0.42
1:B:212:LYS:HB2	1:B:226:THR:OG1	2.20	0.42
1:A:360:ALA:HB2	1:A:371:TRP:CE3	2.55	0.41
1:A:512:ARG:HB2	1:A:570:ALA:O	2.21	0.41
1:B:172:ASP:HB3	1:B:178:THR:HB	2.02	0.41
1:B:678:LEU:HD13	1:B:680:TRP:CZ2	2.56	0.41
1:B:506:LEU:HD12	1:B:507:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	779/779 (100%)	752 (96%)	26 (3%)	1 (0%)	48 50
1	B	777/779 (100%)	749 (96%)	27 (4%)	1 (0%)	48 50
All	All	1556/1558 (100%)	1501 (96%)	53 (3%)	2 (0%)	48 50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	354	ASN
1	A	354	ASN

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	628/624 (101%)	627 (100%)	1 (0%)	87 92
1	B	624/624 (100%)	623 (100%)	1 (0%)	87 92
All	All	1252/1248 (100%)	1250 (100%)	2 (0%)	87 92

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

Mol	Chain	Res	Type
1	A	384	ASN
1	B	250	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	99	ASN
1	A	140	GLN
1	A	198	GLN
1	A	239	ASN
1	A	298	ASN
1	A	355	GLN
1	A	372	GLN
1	B	50	GLN
1	B	99	ASN
1	B	253	GLN
1	B	354	ASN
1	B	556	GLN
1	B	600	GLN
1	B	724	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 29 ligands modelled in this entry, 8 are monoatomic - leaving 21 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	$\#\|Z\|>2$
4	GOL	B	814	-	5,5,5	0.89	0	5,5,5	1.08	0
5	PE3	B	808	-	6,6,42	0.51	0	5,5,41	0.59	0
4	GOL	B	806	-	5,5,5	0.95	0	5,5,5	1.06	0
5	PE3	B	809	-	12,12,42	0.43	0	11,11,41	1.19	1 (9%)
5	PE3	A	810	-	6,6,42	0.57	0	5,5,41	0.33	0
5	PE3	A	811	-	12,12,42	0.62	0	11,11,41	1.39	1 (9%)
4	GOL	B	805	-	5,5,5	0.85	0	5,5,5	1.09	0
5	PE3	B	807	-	6,6,42	0.51	0	5,5,41	0.44	0
4	GOL	A	807	-	5,5,5	0.94	0	5,5,5	1.07	0
4	GOL	B	812	-	5,5,5	0.96	0	5,5,5	1.05	0
4	GOL	B	810	-	5,5,5	0.92	0	5,5,5	1.06	0
4	GOL	B	811	-	5,5,5	0.97	0	5,5,5	0.98	0
4	GOL	A	806	-	5,5,5	0.91	0	5,5,5	1.06	0
4	GOL	A	805	-	5,5,5	0.98	0	5,5,5	1.01	0
4	GOL	A	808	-	5,5,5	1.01	0	5,5,5	1.02	0
3	ACT	A	803	-	3,3,3	0.98	0	3,3,3	0.85	0
4	GOL	B	813	-	5,5,5	1.02	0	5,5,5	1.03	0
4	GOL	B	815	-	5,5,5	1.05	0	5,5,5	0.51	0
4	GOL	B	804	-	5,5,5	0.96	0	5,5,5	1.04	0
5	PE3	A	809	-	6,6,42	0.58	0	5,5,41	0.79	0
4	GOL	A	804	-	5,5,5	0.93	0	5,5,5	1.08	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
4	GOL	B	814	-	-	0/4/4/4	-
5	PE3	B	808	-	-	1/4/4/40	-
4	GOL	B	806	-	-	0/4/4/4	-
5	PE3	B	809	-	-	3/10/10/40	-
5	PE3	A	810	-	-	1/4/4/40	-
5	PE3	A	811	-	-	5/10/10/40	-
4	GOL	B	805	-	-	2/4/4/4	-
5	PE3	B	807	-	-	0/4/4/40	-
4	GOL	A	807	-	-	2/4/4/4	-
4	GOL	B	812	-	-	2/4/4/4	-
4	GOL	B	810	-	-	0/4/4/4	-
4	GOL	B	811	-	-	4/4/4/4	-
4	GOL	A	806	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	805	-	-	0/4/4/4	-
4	GOL	A	808	-	-	0/4/4/4	-
4	GOL	B	813	-	-	1/4/4/4	-
4	GOL	B	815	-	-	2/4/4/4	-
4	GOL	B	804	-	-	0/4/4/4	-
5	PE3	A	809	-	-	1/4/4/40	-
4	GOL	A	804	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	811	PE3	O34-C33-C32	3.09	123.73	110.11
5	B	809	PE3	O34-C35-C36	-2.06	100.97	110.35

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	807	GOL	C1-C2-C3-O3
4	B	805	GOL	C1-C2-C3-O3
4	B	811	GOL	C1-C2-C3-O3
4	B	812	GOL	O1-C1-C2-C3
4	B	815	GOL	C1-C2-C3-O3
4	B	811	GOL	O1-C1-C2-C3
4	B	811	GOL	O1-C1-C2-O2
4	B	811	GOL	O2-C2-C3-O3
4	B	815	GOL	O2-C2-C3-O3
4	A	807	GOL	O2-C2-C3-O3
4	B	805	GOL	O2-C2-C3-O3
5	A	811	PE3	C42-C41-O40-C39
4	B	812	GOL	O1-C1-C2-O2
5	B	809	PE3	C39-C38-O37-C36
5	A	810	PE3	C38-C39-O40-C41
5	A	809	PE3	C42-C41-O40-C39
5	B	808	PE3	C42-C41-O40-C39
5	A	811	PE3	C32-C33-O34-C35
5	B	809	PE3	O34-C35-C36-O37
5	A	811	PE3	C36-C35-O34-C33
5	B	809	PE3	O37-C38-C39-O40
5	A	811	PE3	O37-C38-C39-O40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	806	GOL	O2-C2-C3-O3
5	A	811	PE3	O34-C35-C36-O37
4	B	813	GOL	O2-C2-C3-O3

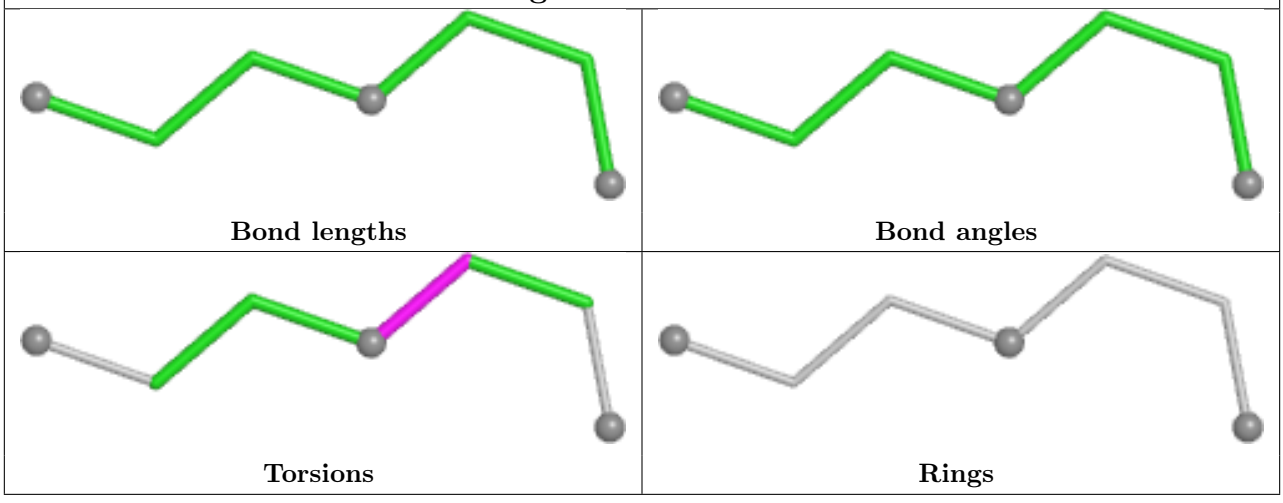
There are no ring outliers.

4 monomers are involved in 4 short contacts:

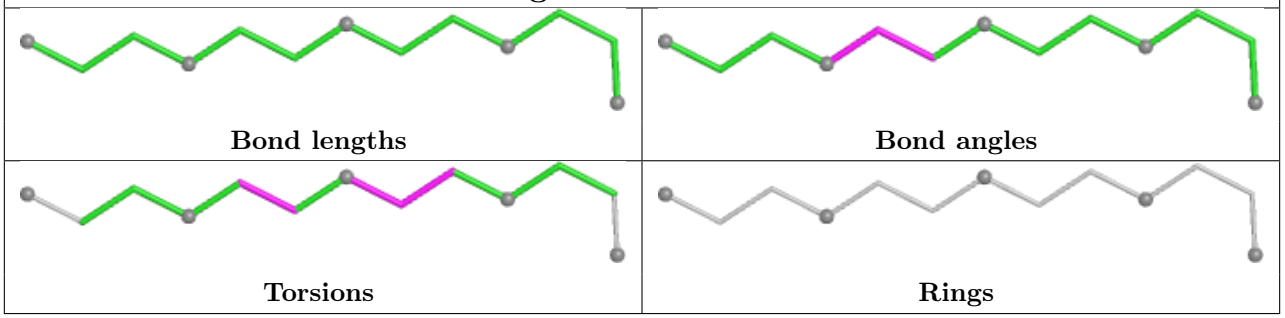
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	811	PE3	1	0
4	A	805	GOL	1	0
4	B	815	GOL	1	0
5	A	809	PE3	1	0

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.

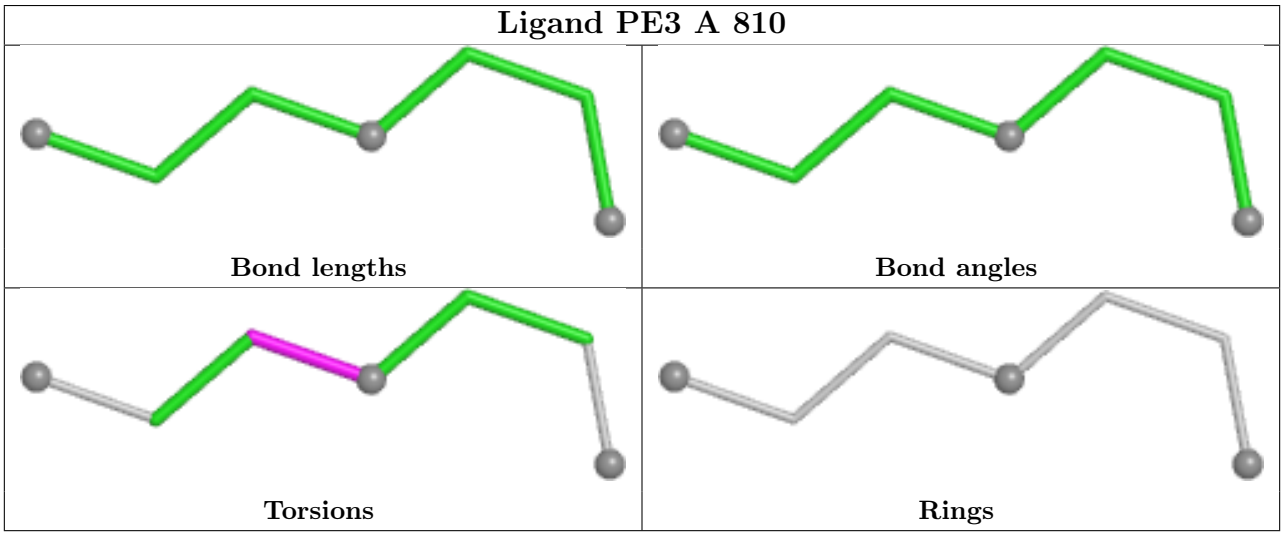
Ligand PE3 B 808



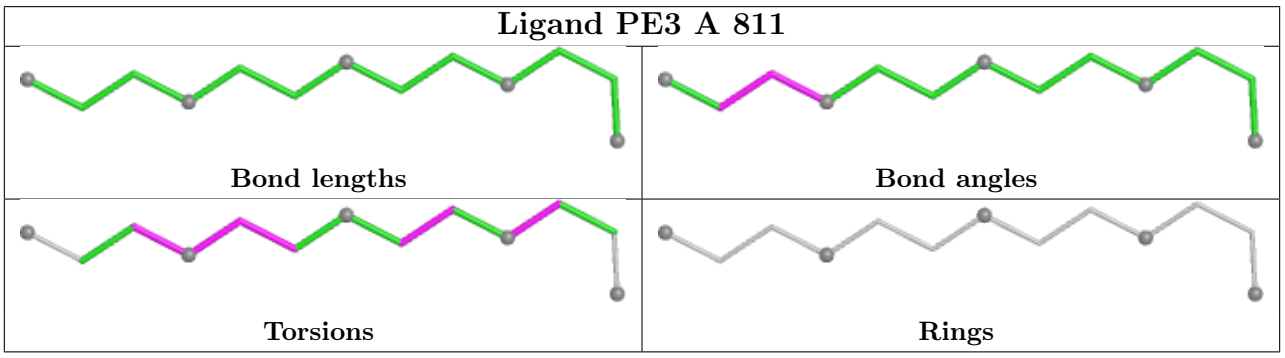
Ligand PE3 B 809



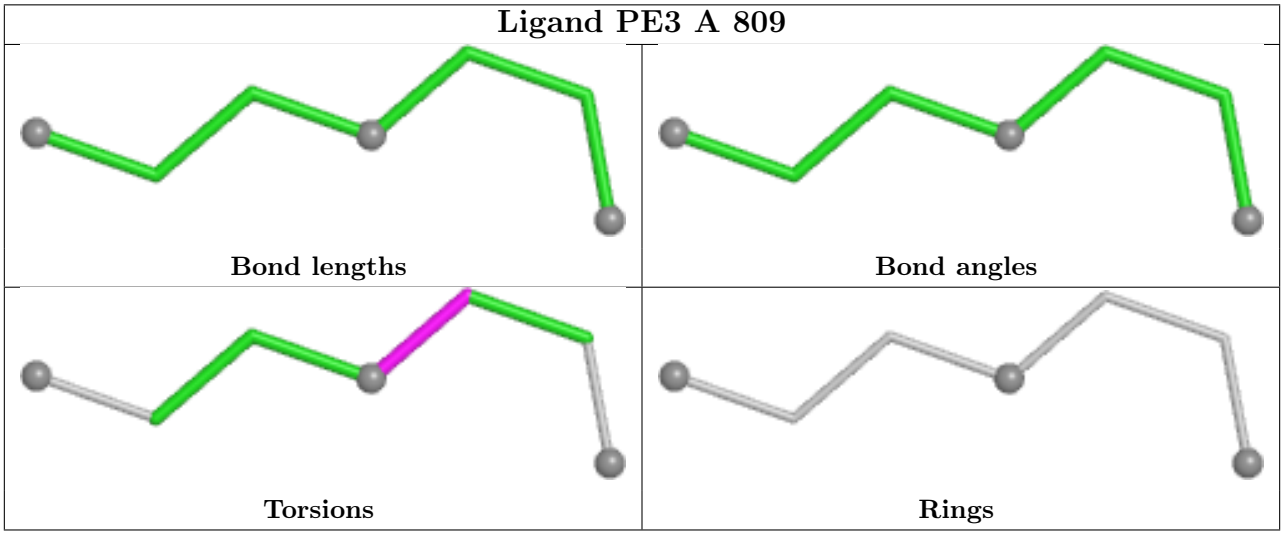
Ligand PE3 A 810



Ligand PE3 A 811



Ligand PE3 A 809



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, 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	776/779 (99%)	-0.53	1 (0%)	92	93	14, 28, 51, 111	5 (0%)
1	B	778/779 (99%)	-0.23	18 (2%)	61	64	15, 32, 72, 122	1 (0%)
All	All	1554/1558 (99%)	-0.38	19 (1%)	76	79	14, 30, 67, 122	6 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	779	ALA	3.3
1	B	2	ALA	3.3
1	B	198	GLN	3.0
1	B	249	ASN	2.9
1	A	779	ALA	2.9
1	B	3	ALA	2.8
1	B	232	PRO	2.8
1	B	248	SER	2.7
1	B	221	GLN	2.6
1	B	207	VAL	2.4
1	B	386	TYR	2.3
1	B	253	GLN	2.2
1	B	247	THR	2.2
1	B	250	ILE	2.1
1	B	141	VAL	2.1
1	B	201	ALA	2.1
1	B	300	ASP	2.0
1	B	301	ASN	2.0
1	B	366	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

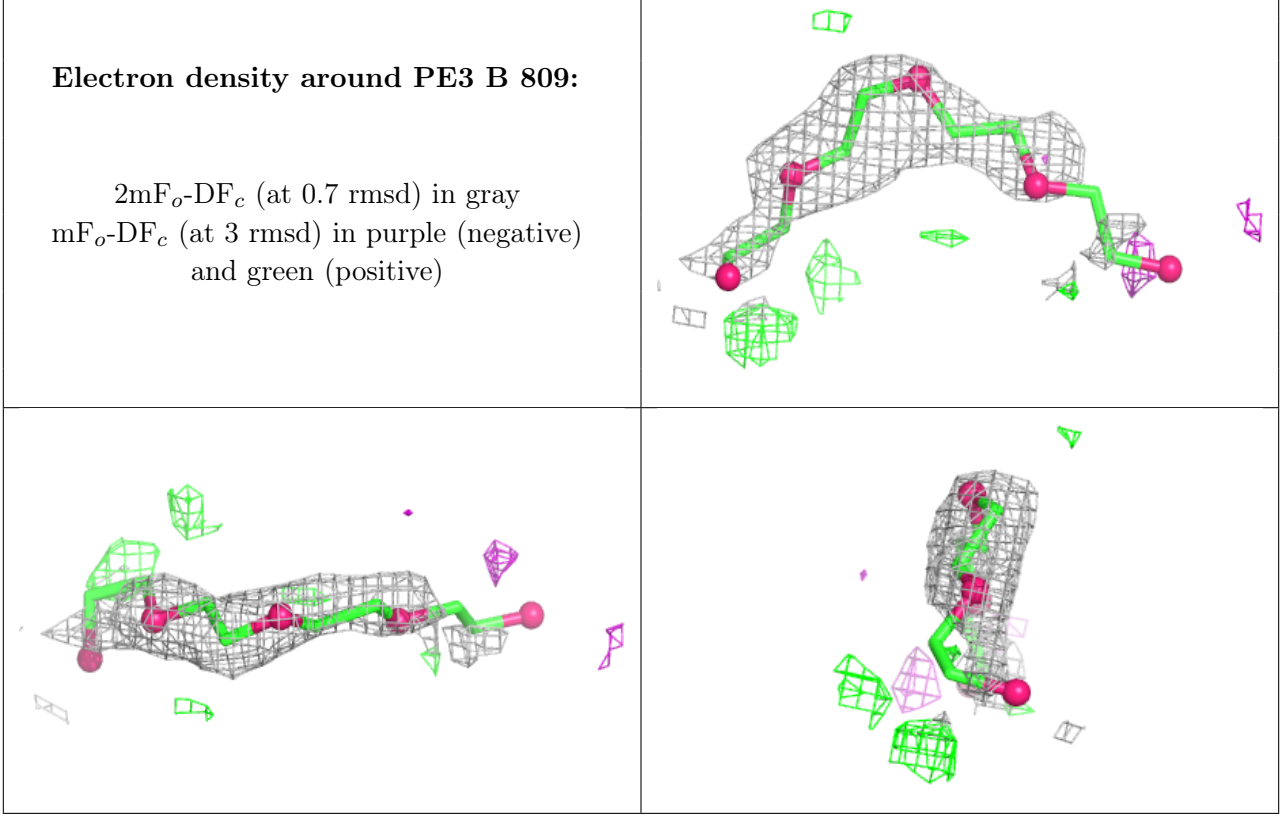
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	813	6/6	0.72	0.22	53,63,63,67	0
4	GOL	B	811	6/6	0.74	0.15	71,77,78,79	0
4	GOL	B	810	6/6	0.75	0.15	74,75,76,77	0
4	GOL	B	806	6/6	0.76	0.14	78,78,79,79	0
5	PE3	B	809	13/43	0.76	0.25	92,94,103,104	0
5	PE3	B	808	7/43	0.77	0.19	72,73,74,75	0
4	GOL	A	806	6/6	0.77	0.14	73,73,73,74	0
5	PE3	A	811	13/43	0.78	0.23	43,71,73,74	0
4	GOL	B	814	6/6	0.80	0.15	73,80,81,82	0
4	GOL	B	812	6/6	0.81	0.15	80,82,82,83	0
4	GOL	A	804	6/6	0.81	0.14	77,80,82,84	0
4	GOL	B	805	6/6	0.83	0.13	54,57,59,59	0
5	PE3	A	809	7/43	0.83	0.18	71,71,72,73	0
5	PE3	A	810	7/43	0.83	0.14	62,63,67,68	0
5	PE3	B	807	7/43	0.84	0.17	67,68,69,71	0
4	GOL	A	807	6/6	0.85	0.14	72,73,75,76	0
4	GOL	A	805	6/6	0.85	0.16	51,54,56,56	0
6	CL	A	812	1/1	0.87	0.16	52,52,52,52	0
4	GOL	B	815	6/6	0.88	0.14	54,57,58,61	0
4	GOL	A	808	6/6	0.88	0.13	54,57,57,59	0
2	ZN	B	802	1/1	0.89	0.28	69,69,69,69	1
4	GOL	B	804	6/6	0.90	0.12	57,59,61,61	0
2	ZN	A	813	1/1	0.91	0.08	36,36,36,36	1
6	CL	B	816	1/1	0.91	0.12	67,67,67,67	0
2	ZN	B	801	1/1	0.95	0.05	17,17,17,17	1
2	ZN	A	801	1/1	0.97	0.04	28,28,28,28	1
3	ACT	A	803	4/4	0.97	0.07	21,23,24,24	0
2	ZN	A	802	1/1	0.98	0.06	20,20,20,20	1
2	ZN	B	803	1/1	0.99	0.03	11,11,11,11	1

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.

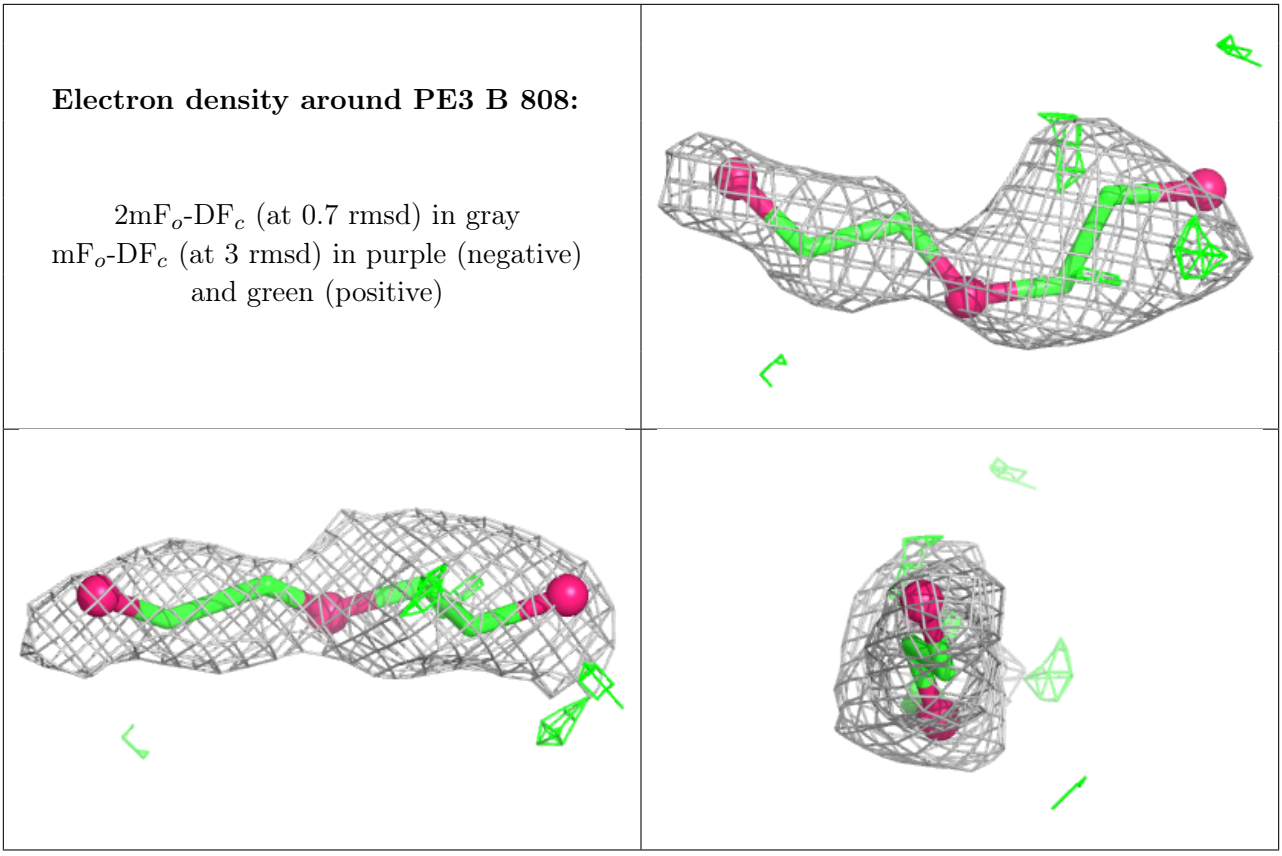
Electron density around PE3 B 809:

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



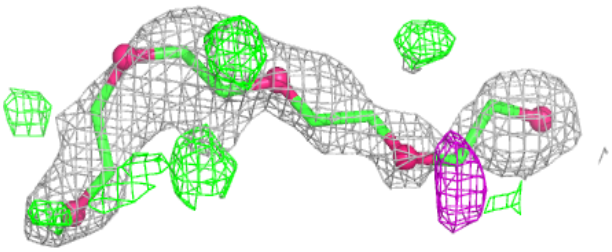
Electron density around PE3 B 808:

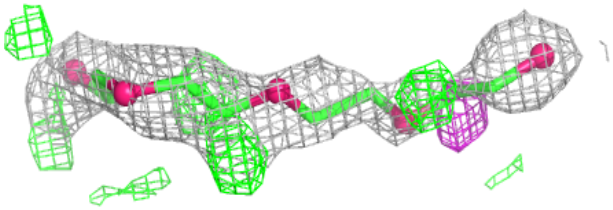
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

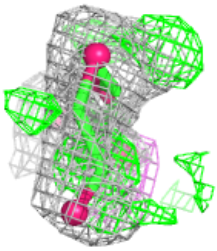


Electron density around PE3 A 811:

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

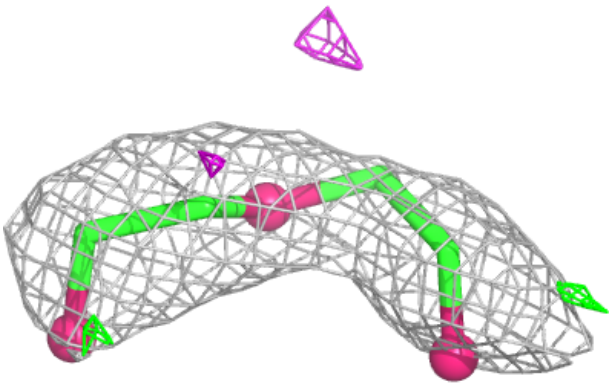


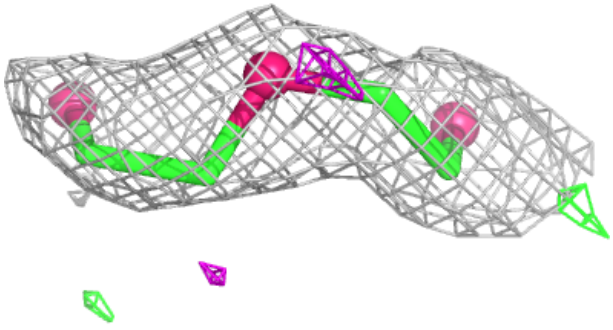


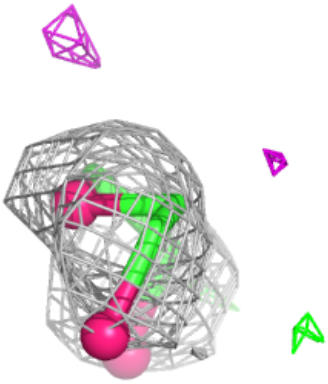


Electron density around PE3 A 809:

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

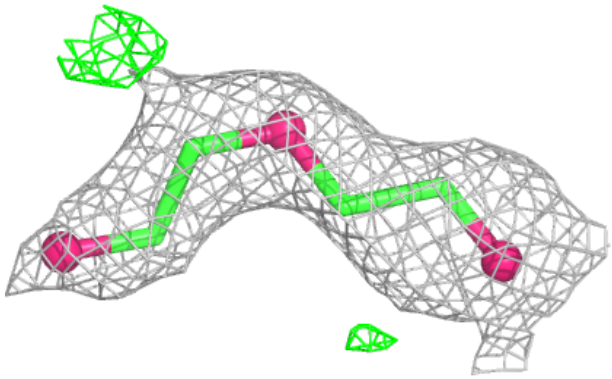


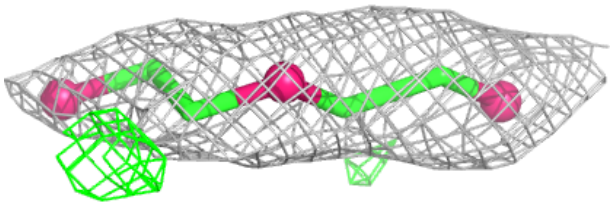


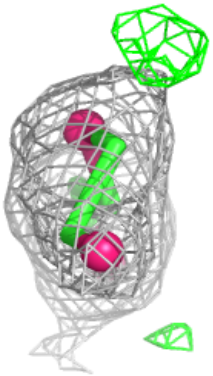


Electron density around PE3 A 810:

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







6.5 Other polymers

There are no such residues in this entry.