Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 04:55 AM EDT

PDB ID	:	3B87
Title	:	Complex of T57A Substituted Droposphila LUSH protein with Butanol
Authors	:	Jones, D.N.M.; Thode, A.B.
Deposited on	:	2007-10-31
Resolution	:	2.00 Å(reported)

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

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

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

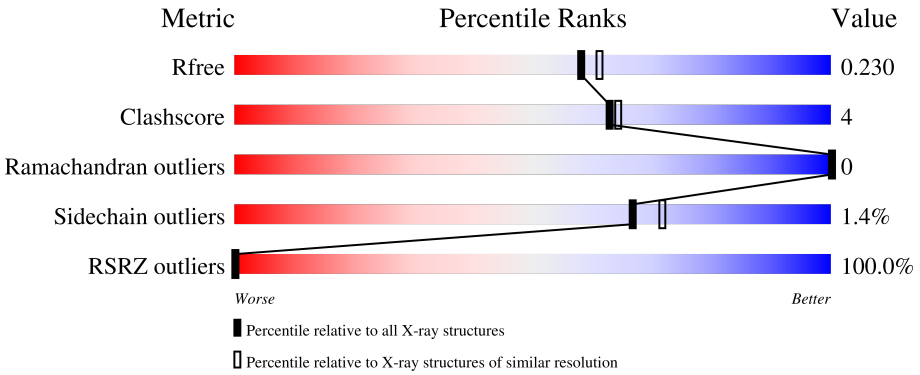
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	124	100% 87% 11% •
1	B	124	100% 92% 8%

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
2	ACT	A	704	-	-	-	X
2	ACT	B	703	-	-	-	X
3	PE8	A	224	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2212 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.

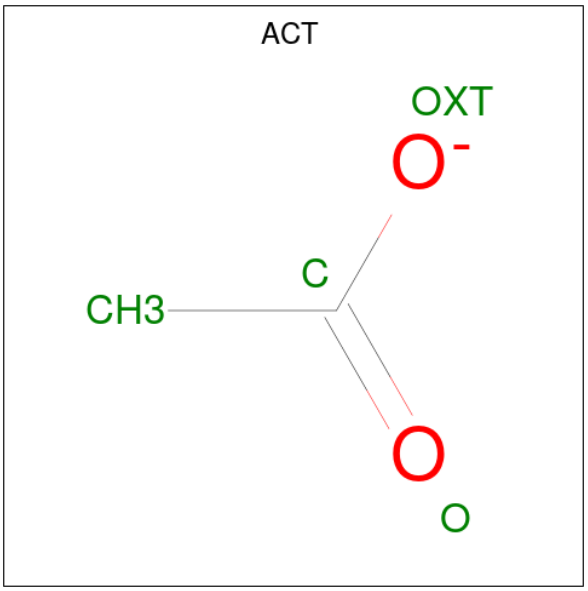
- Molecule 1 is a protein called General odorant-binding protein lush.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			980	615	167	183	15			
1	B	124	Total	C	N	O	S	0	4	0
			1007	629	172	191	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ALA	THR	engineered mutation	UNP O02372
B	57	ALA	THR	engineered mutation	UNP O02372

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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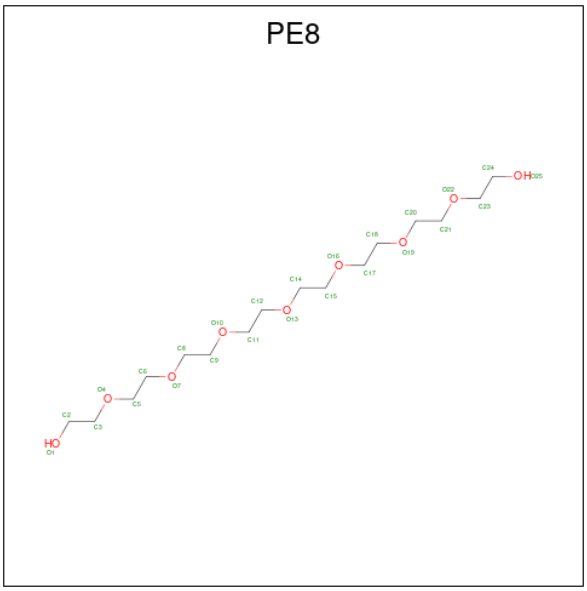
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: $C_{16}H_{34}O_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 25 16 9	0	0

- Molecule 4 is water.

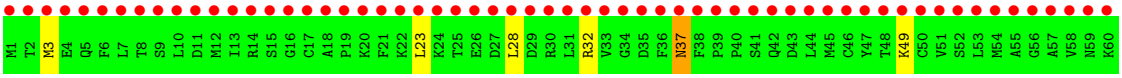
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	98	Total O 98 98	0	0
4	B	90	Total O 90 90	0	0

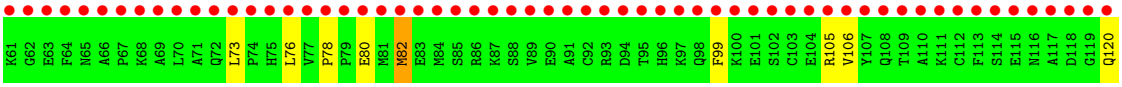
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: General odorant-binding protein lush

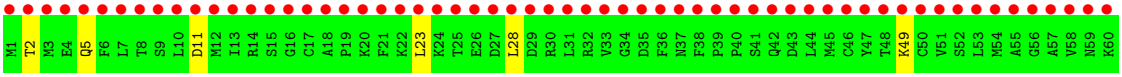
Chain A:

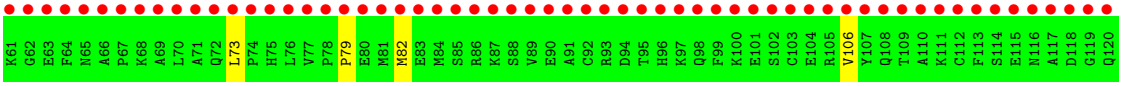




• Molecule 1: General odorant-binding protein lush

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	42.66Å 45.70Å 114.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 45.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.00) 99.9 (45.70-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.43 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.229 0.187 , 0.230	Depositor DCC
R_{free} test set	1587 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2212	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.61% 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: PE8, ACT

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	0.47	0/1001	0.57	0/1343
1	B	0.46	0/1028	0.58	0/1380
All	All	0.47	0/2029	0.57	0/2723

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	980	0	958	13	0
1	B	1007	0	971	5	0
2	A	8	0	6	1	0
2	B	4	0	3	0	0
3	A	25	0	34	1	0
4	A	98	0	0	1	0
4	B	90	0	0	0	0
All	All	2212	0	1972	17	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HB3	1:A:82:MET:HE1	1.51	0.90
1:A:76:LEU:HD22	3:A:224:PE8:H182	1.64	0.79
1:A:82:MET:HA	1:A:82:MET:HE3	1.67	0.75
1:A:80:GLU:OE2	2:A:702:ACT:H3	1.91	0.70
1:A:82:MET:HA	1:A:82:MET:CE	2.27	0.65
1:A:23:LEU:HD13	1:A:28:LEU:HD21	1.91	0.53
1:B:2:THR:OG1	1:B:5[A]:GLN:HG3	2.09	0.52
1:B:49:LYS:HA	1:B:106:VAL:HG11	1.92	0.50
1:A:99:PHE:O	1:A:105:ARG:NH1	2.45	0.49
1:B:23:LEU:HD13	1:B:28:LEU:HD21	1.95	0.48
1:A:120:GLN:NE2	1:B:11[B]:ASP:OD2	2.43	0.47
1:A:32:ARG:HA	1:A:123:TRP:O	2.18	0.43
1:A:105:ARG:NH1	4:A:801:HOH:O	2.52	0.43
1:B:79:PRO:HA	1:B:82:MET:HG3	2.01	0.42
1:A:37:ASN:HD22	1:A:37:ASN:C	2.23	0.41
1:A:49:LYS:HA	1:A:106:VAL:HG11	2.03	0.41
1:A:3:MET:SD	1:A:78:PRO:HG2	2.62	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	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	B	126/124 (102%)	126 (100%)	0	0	100	100
All	All	248/248 (100%)	247 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	109/110 (99%)	107 (98%)	2 (2%)	59 63
1	B	112/110 (102%)	111 (99%)	1 (1%)	78 83
All	All	221/220 (100%)	218 (99%)	3 (1%)	67 72

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

Mol	Chain	Res	Type
1	A	37	ASN
1	A	82	MET
1	B	73	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	116	ASN
1	B	98	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
2	ACT	A	704	-	1,3,3	1.31	0	0,3,3	-	-
3	PE8	A	224	-	24,24,24	0.54	0	23,23,23	0.27	0
2	ACT	A	702	-	1,3,3	0.58	0	0,3,3	-	-
2	ACT	B	703	-	1,3,3	1.40	0	0,3,3	-	-

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	PE8	A	224	-	-	10/22/22/22	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

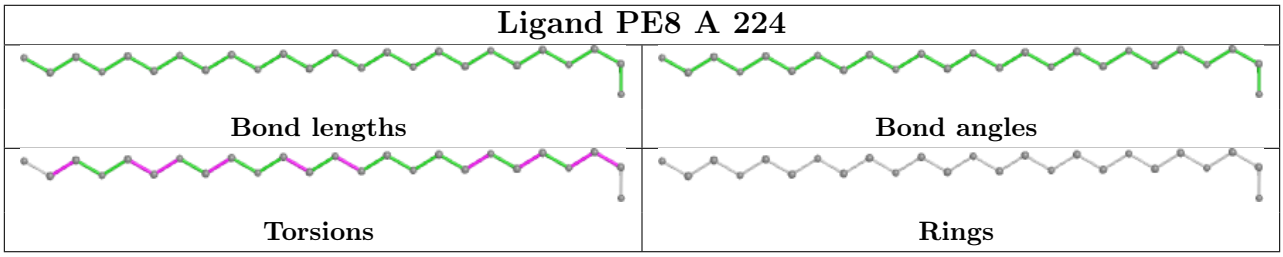
Mol	Chain	Res	Type	Atoms
3	A	224	PE8	O13-C14-C15-O16
3	A	224	PE8	O19-C20-C21-O22
3	A	224	PE8	O1-C2-C3-O4
3	A	224	PE8	O4-C5-C6-O7
3	A	224	PE8	C9-C8-O7-C6
3	A	224	PE8	C21-C20-O19-C18
3	A	224	PE8	C2-C3-O4-C5
3	A	224	PE8	C11-C12-O13-C14
3	A	224	PE8	O22-C23-C24-O25
3	A	224	PE8	O16-C17-C18-O19

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	224	PE8	1	0
2	A	702	ACT	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 (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	124/124 (100%)	21.35	124 (100%)	0	0	11, 19, 28, 35	0
1	B	124/124 (100%)	22.60	124 (100%)	0	0	11, 18, 31, 38	0
All	All	248/248 (100%)	21.98	248 (100%)	0	0	11, 19, 30, 38	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	TRP	78.2
1	B	6	PHE	72.1
1	A	77	VAL	68.0
1	B	70	LEU	66.3
1	B	2	THR	62.1
1	B	123	TRP	60.6
1	B	23	LEU	59.7
1	A	70	LEU	58.0
1	A	67	PRO	57.8
1	B	78	PRO	57.4
1	B	43	ASP	57.2
1	A	107	TYR	56.6
1	A	66	ALA	56.3
1	A	64	PHE	55.4
1	A	31	LEU	55.0
1	B	38	PHE	54.8
1	B	99	PHE	54.7
1	B	77	VAL	53.2
1	A	19	PRO	52.6
1	B	73	LEU	52.5
1	B	109	THR	52.4
1	B	107	TYR	51.9
1	A	27	ASP	51.5
1	B	3	MET	51.4

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Mol	Chain	Res	Type	RSRZ
1	A	118	ASP	50.6
1	A	69	ALA	50.4
1	A	73	LEU	50.2
1	B	96	HIS	49.9
1	A	16	GLY	47.5
1	A	17	CYS	46.8
1	A	29	ASP	46.2
1	B	97	LYS	44.3
1	A	106	VAL	44.1
1	B	74	PRO	43.7
1	B	66	ALA	42.8
1	A	26	GLU	42.7
1	B	104	GLU	42.7
1	A	6	PHE	42.6
1	B	118	ASP	42.0
1	A	102	SER	41.7
1	B	7	LEU	41.5
1	B	64	PHE	41.3
1	B	35	ASP	41.2
1	A	20	LYS	41.0
1	B	42	GLN	40.4
1	B	110	ALA	38.2
1	A	28	LEU	37.9
1	B	22	LYS	37.5
1	B	119	GLY	37.3
1	A	15	SER	37.1
1	B	33	VAL	36.9
1	A	74	PRO	36.2
1	A	5	GLN	35.5
1	B	47	TYR	34.8
1	B	106	VAL	34.6
1	A	8	THR	34.6
1	B	1	MET	34.5
1	B	30	ARG	33.1
1	A	109	THR	32.5
1	A	98	GLN	32.3
1	B	54	MET	32.2
1	B	60	LYS	32.2
1	A	32	ARG	31.6
1	B	4	GLU	31.5
1	A	116	ASN	31.3
1	A	103	CYS	30.7

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Mol	Chain	Res	Type	RSRZ
1	B	95	THR	30.7
1	B	67	PRO	30.3
1	B	108	GLN	30.3
1	A	44	LEU	30.3
1	B	53	LEU	30.1
1	A	122	MET	29.8
1	B	69	ALA	29.6
1	B	10	LEU	28.9
1	A	62	GLY	28.4
1	B	93	ARG	28.2
1	B	11[A]	ASP	27.9
1	B	39	PRO	27.6
1	A	119	GLY	26.8
1	B	124	PRO	26.6
1	B	117	ALA	26.5
1	B	36	PHE	26.2
1	B	122	MET	26.1
1	A	21	PHE	25.8
1	A	78	PRO	25.7
1	A	117	ALA	25.7
1	B	37[A]	ASN	25.0
1	A	18	ALA	24.9
1	A	63	GLU	24.8
1	B	94	ASP	24.1
1	A	65	ASN	24.0
1	B	46	CYS	23.6
1	B	45	MET	23.5
1	A	110	ALA	23.3
1	A	42	GLN	22.9
1	B	71	ALA	22.4
1	A	10	LEU	22.4
1	A	25	THR	22.2
1	B	17	CYS	22.2
1	B	14	ARG	22.2
1	B	18	ALA	22.1
1	B	48	THR	22.1
1	B	50	CYS	22.0
1	A	101	GLU	21.9
1	A	124	PRO	21.5
1	A	45	MET	20.9
1	B	12	MET	20.7
1	A	79	PRO	20.5

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	20.2
1	A	71	ALA	20.1
1	B	31	LEU	19.6
1	A	40	PRO	19.3
1	A	39	PRO	19.0
1	A	80	GLU	18.9
1	B	44	LEU	18.8
1	B	21	PHE	18.5
1	A	95	THR	18.5
1	A	61	LYS	18.3
1	A	48	THR	18.3
1	B	76	LEU	18.1
1	A	41	SER	17.7
1	B	79	PRO	17.4
1	A	108	GLN	17.3
1	B	98	GLN	17.3
1	B	116	ASN	17.0
1	A	7	LEU	16.7
1	B	105	ARG	16.6
1	A	115	GLU	16.4
1	B	8	THR	16.3
1	A	82	MET	15.8
1	A	94	ASP	15.7
1	A	50	CYS	15.7
1	A	12	MET	15.2
1	B	113	PHE	14.9
1	A	46	CYS	14.8
1	B	15[A]	SER	14.7
1	B	34	GLY	14.7
1	A	99	PHE	14.4
1	A	59	ASN	14.2
1	A	96	HIS	14.1
1	A	54	MET	14.0
1	A	89	VAL	13.9
1	A	2	THR	13.8
1	A	24	LYS	13.6
1	B	89	VAL	13.4
1	A	9	SER	13.1
1	B	41	SER	13.0
1	A	113	PHE	13.0
1	B	103	CYS	12.9
1	A	53	LEU	12.7

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Mol	Chain	Res	Type	RSRZ
1	A	38	PHE	12.6
1	A	81	MET	12.6
1	A	76	LEU	12.4
1	A	60	LYS	12.3
1	B	32	ARG	12.1
1	A	105	ARG	11.7
1	B	16	GLY	11.7
1	B	13	ILE	11.5
1	B	115	GLU	11.1
1	B	28	LEU	10.8
1	B	61	LYS	10.7
1	A	43	ASP	10.6
1	B	87	LYS	10.4
1	B	82	MET	10.1
1	B	59	ASN	9.8
1	A	30	ARG	9.7
1	A	3	MET	9.7
1	B	9	SER	9.5
1	A	36	PHE	9.2
1	A	4	GLU	9.1
1	B	121	PHE	9.1
1	A	87	LYS	9.0
1	B	92	CYS	8.8
1	B	51	VAL	8.8
1	A	83	GLU	8.7
1	A	93	ARG	8.7
1	B	5[A]	GLN	8.7
1	A	92	CYS	8.5
1	B	40	PRO	8.4
1	A	91	ALA	8.4
1	A	97	LYS	8.0
1	A	85	SER	7.9
1	A	68	LYS	7.8
1	A	58	VAL	7.6
1	A	112	CYS	7.5
1	A	11	ASP	7.4
1	A	13	ILE	7.2
1	A	33	VAL	7.2
1	A	22	LYS	7.0
1	A	104	GLU	6.9
1	A	52	SER	6.8
1	B	55	ALA	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	100	LYS	6.4
1	B	25	THR	6.4
1	B	120	GLN	6.4
1	B	112	CYS	6.3
1	A	14	ARG	6.2
1	B	52	SER	6.2
1	A	47	TYR	6.2
1	B	114	SER	6.1
1	B	111	LYS	5.9
1	A	121	PHE	5.9
1	B	65	ASN	5.9
1	B	85	SER	5.7
1	B	24	LYS	5.7
1	A	72	GLN	5.6
1	A	120	GLN	5.5
1	A	57	ALA	5.5
1	A	75	HIS	5.5
1	B	29	ASP	5.5
1	B	58	VAL	5.5
1	A	37	ASN	5.4
1	B	68	LYS	5.3
1	A	88	SER	5.2
1	A	114	SER	5.2
1	B	20	LYS	5.2
1	B	62	GLY	5.1
1	B	72	GLN	5.1
1	B	81	MET	5.0
1	A	23	LEU	5.0
1	B	19	PRO	4.8
1	B	49	LYS	4.8
1	A	49	LYS	4.7
1	A	51	VAL	4.7
1	A	84	MET	4.7
1	B	56	GLY	4.6
1	B	101	GLU	4.6
1	A	55	ALA	4.6
1	A	111	LYS	4.6
1	B	75	HIS	4.6
1	B	102	SER	4.5
1	A	34	GLY	4.3
1	B	88	SER	4.3
1	B	57	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	86	ARG	4.1
1	B	84	MET	4.0
1	B	91	ALA	3.6
1	A	100	LYS	3.4
1	A	90	GLU	3.4
1	B	83	GLU	3.2
1	A	86	ARG	3.2
1	B	63	GLU	3.1
1	B	80	GLU	3.1
1	A	35	ASP	3.1
1	B	27	ASP	2.9
1	A	56	GLY	2.8
1	B	90	GLU	2.6
1	B	26	GLU	2.6

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)

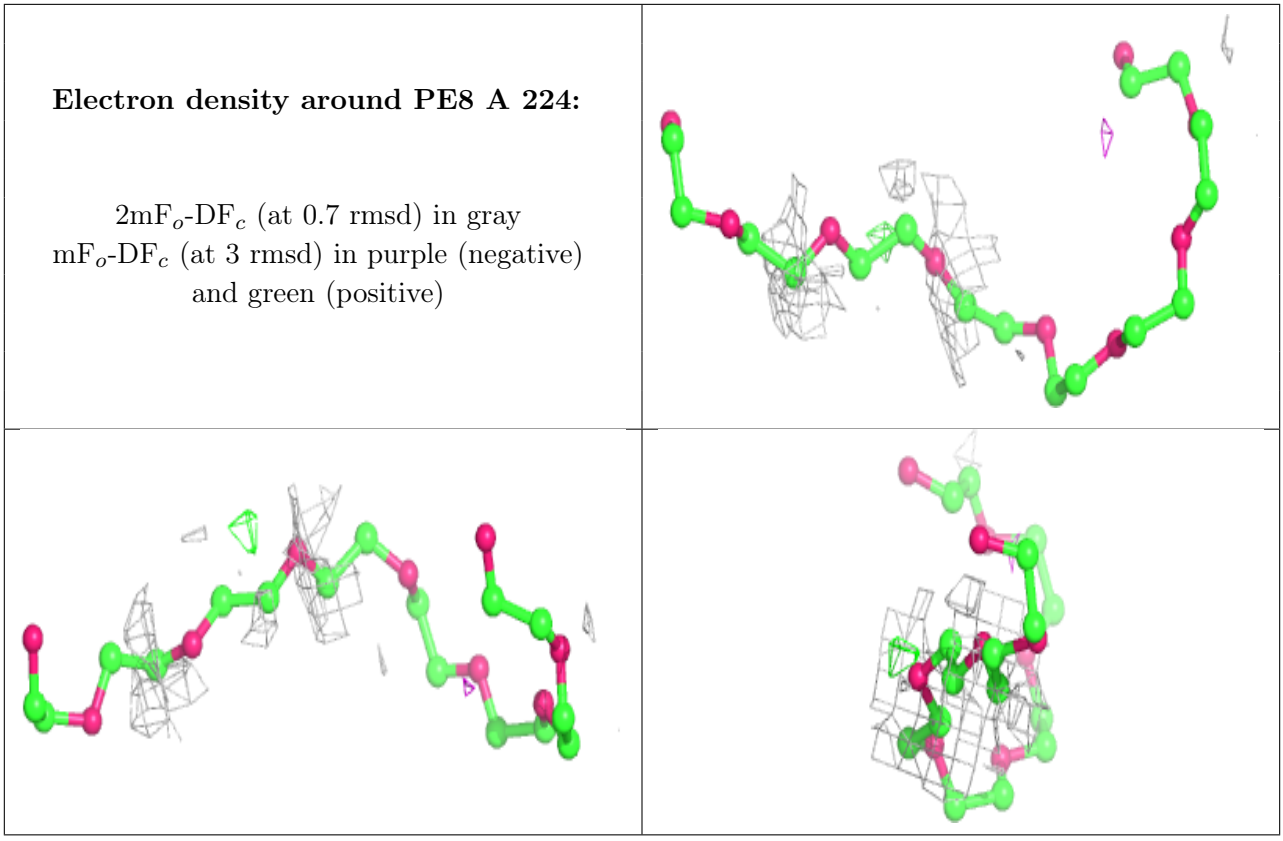
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	ACT	A	704	4/4	-0.35	2.47	26,27,27,28	0
2	ACT	A	702	4/4	-0.34	0.36	23,23,24,27	0
2	ACT	B	703	4/4	-0.05	0.63	58,58,58,58	0
3	PE8	A	224	25/25	0.02	1.50	32,37,45,46	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 PE8 A 224:

$2mF_o$-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.