



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:49 PM UTC

PDB ID : 3DAO / pdb_00003dao
Title : CRYSTAL STRUCTURE OF A PUTATIVE PHOSPHATE (EUBREC_1417)
FROM EUBACTERIUM RECTALE AT 1.80 Å RESOLUTION
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2008-05-29
Resolution : 1.80 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
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

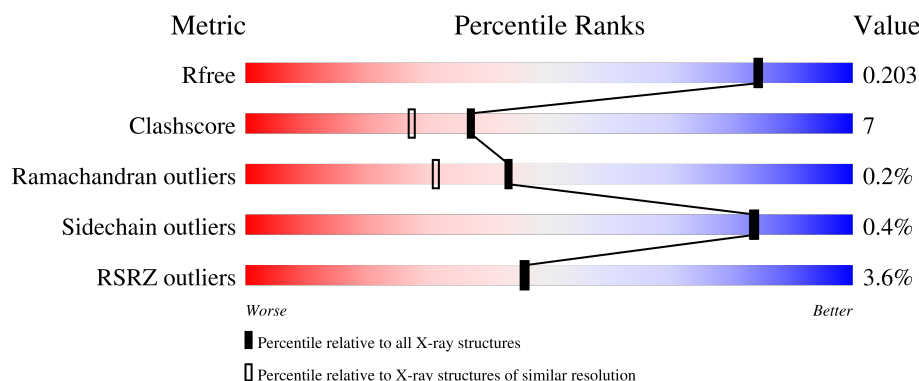
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	283	% 84% 10% 6%
1	B	283	6% 84% 12% ..

2 Entry composition [i](#)

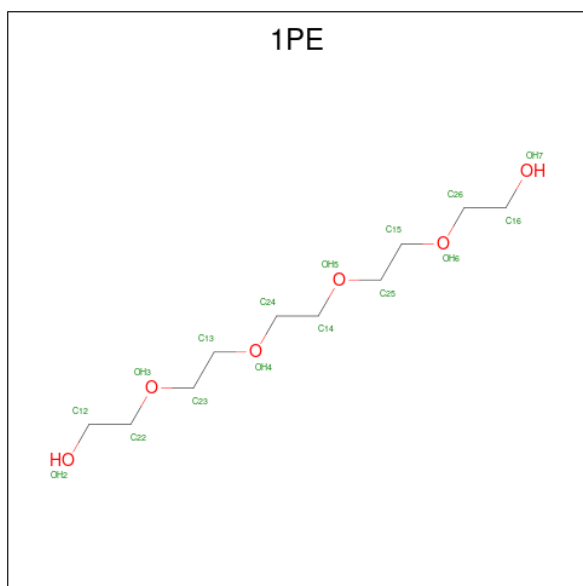
There are 4 unique types of molecules in this entry. The entry contains 5121 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative Phosphate.

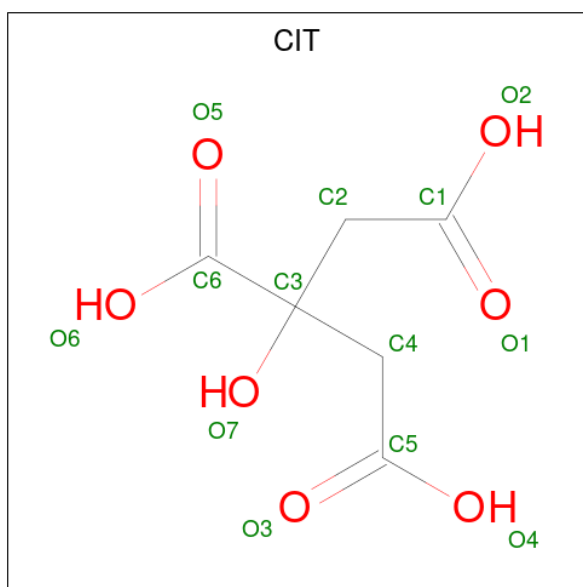
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	Se	0	12	0
			2148	1383	346	401	10	8			
1	B	274	Total	C	N	O	S	Se	0	17	0
			2260	1455	363	422	11	9			

- Molecule 2 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	335	Total	O	0	1
			336	336		
4	B	345	Total	O	0	3
			348	348		

i

- Molecule 1: Putative Phosphate



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.86Å 101.86Å 110.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 1.80 29.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.93-1.80) 100.0 (29.93-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.4.0067, PHENIX	Depositor
R, R_{free}	0.168 , 0.208 0.167 , 0.203	Depositor DCC
R_{free} test set	2772 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.9	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	5121	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.15% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, CIT

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	0.85	0/2226	1.02	6/3005 (0.2%)
1	B	0.91	0/2345	1.10	9/3162 (0.3%)
All	All	0.88	0/4571	1.06	15/6167 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	4

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209[A]	ASP	CA-C-N	9.60	139.07	122.56
1	B	209[A]	ASP	C-N-CA	9.60	139.07	122.56
1	B	209[B]	ASP	CA-C-N	9.60	139.07	122.56
1	B	209[B]	ASP	C-N-CA	9.60	139.07	122.56
1	B	209[A]	ASP	N-CA-C	7.05	120.98	112.38
1	B	209[B]	ASP	N-CA-C	7.05	120.98	112.38
1	A	167[A]	ILE	CA-C-N	-6.98	112.51	119.56
1	A	167[A]	ILE	C-N-CA	-6.98	112.51	119.56
1	A	167[B]	ILE	CA-C-N	-6.98	112.51	119.56
1	A	167[B]	ILE	C-N-CA	-6.98	112.51	119.56
1	A	43	SER	N-CA-C	6.24	118.25	108.96
1	B	132	GLU	N-CA-C	-6.15	98.50	108.41
1	B	167	ILE	N-CA-CB	6.12	115.22	110.45
1	B	43	SER	N-CA-C	6.00	118.29	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ASP	N-CA-CB	5.71	118.26	110.38

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	-1	GLN	Mainchain
1	B	207	LEU	Mainchain

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	2148	0	2132	17	0
1	B	2260	0	2227	39	0
2	A	16	0	22	6	0
3	B	13	0	5	3	0
4	A	336	0	0	3	0
4	B	348	0	0	3	0
All	All	5121	0	4386	63	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 7.

All (63) 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)
3:B:265:CIT:H41	4:B:482:HOH:O	1.42	1.19
2:A:265:1PE:H261	4:A:589:HOH:O	1.65	0.96
1:B:134[B]:ARG:HD3	1:B:135:GLU:N	1.83	0.92
1:B:217[A]:ASN:ND2	4:B:482:HOH:O	2.04	0.91
1:B:1[B]:MSE:HE2	1:B:209[B]:ASP:O	1.71	0.89
1:B:134[B]:ARG:CG	1:B:134[B]:ARG:HH11	1.94	0.78
1:B:134[B]:ARG:HH11	1:B:134[B]:ARG:HG2	1.47	0.77
1:B:207:LEU:C	1:B:209[B]:ASP:N	2.41	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134[B]:ARG:HB2	1:B:134[B]:ARG:NH1	2.05	0.71
1:A:149:LYS:HZ1	2:A:265:1PE:H141	1.57	0.69
1:B:115:GLU:OE2	1:B:137:ASP:O	2.10	0.69
1:B:208[A]:PRO:C	1:B:210:GLU:N	2.40	0.68
2:A:265:1PE:H251	4:A:589:HOH:O	1.94	0.67
1:B:134[B]:ARG:HH11	1:B:134[B]:ARG:HB2	1.59	0.65
1:A:133:MSE:O	1:A:134[B]:ARG:HD3	1.97	0.65
1:B:127[B]:ASP:OD1	1:B:128:SER:N	2.31	0.63
1:B:134[B]:ARG:HH11	1:B:134[B]:ARG:CB	2.10	0.63
1:A:167[B]:ILE:HD13	1:A:176:LEU:HD23	1.81	0.62
3:B:265:CIT:O3	3:B:265:CIT:C6	2.46	0.59
1:B:104:TYR:OH	1:B:139:ILE:HG21	2.03	0.59
1:B:207:LEU:C	1:B:209[B]:ASP:H	2.00	0.58
1:B:207:LEU:HB3	1:B:208[A]:PRO:CD	2.34	0.58
1:B:149:LYS:HE2	4:B:599:HOH:O	2.04	0.57
1:B:1[A]:MSE:HG3	1:B:2:ILE:N	2.20	0.53
1:A:10:ASP:HB3	1:A:16[A]:ASP:OD1	2.09	0.52
1:B:-2:PHE:CE1	1:B:262[B]:SER:OG	2.63	0.51
1:B:66:ASP:HB2	1:B:69[A]:THR:OG1	2.10	0.51
1:A:24:GLU:OE2	1:A:261:LYS:CE	2.59	0.50
1:B:123:HIS:ND1	1:B:127[B]:ASP:OD2	2.45	0.50
1:A:179:ALA:HB3	1:A:183:TRP:HB2	1.93	0.50
1:B:8[B]:ASP:OD1	3:B:265:CIT:C5	2.62	0.47
1:B:134[B]:ARG:HG2	1:B:134[B]:ARG:NH1	2.23	0.47
1:B:112[A]:CYS:SG	1:B:133:MSE:SE	3.22	0.47
1:B:134[B]:ARG:NH1	1:B:134[B]:ARG:CB	2.72	0.47
1:B:-5:ASN:CG	1:B:1[B]:MSE:SE	3.08	0.46
1:A:9:ILE:HD11	1:A:41:VAL:CG1	2.46	0.46
2:A:265:1PE:H141	2:A:265:1PE:H131	1.58	0.45
1:A:85:GLU:HG2	1:A:89:LYS:HD2	1.98	0.45
1:B:-5:ASN:ND2	1:B:1[B]:MSE:SE	3.00	0.45
1:B:-5:ASN:ND2	1:B:1[B]:MSE:HE1	2.32	0.44
1:A:212:CYS:HA	1:A:229:ILE:O	2.17	0.44
1:B:83[B]:MSE:HE3	1:B:187:ASN:C	2.43	0.44
1:A:59:HIS:NE2	1:A:60:LYS:HG3	2.33	0.43
2:A:265:1PE:H121	4:A:496:HOH:O	2.18	0.43
1:B:115:GLU:CD	1:B:137:ASP:O	2.61	0.43
1:B:157:LYS:HD3	1:B:157:LYS:HA	1.84	0.43
1:A:214:PHE:CD2	1:A:231:TYR:HB2	2.55	0.42
1:A:167[B]:ILE:CD1	1:A:176:LEU:HD23	2.48	0.42
1:B:220:ASP:O	1:B:224:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLU:OE2	1:A:261:LYS:HE2	2.19	0.42
1:B:1[A]:MSE:O	1:B:3:LYS:HG2	2.19	0.42
1:B:134[B]:ARG:CG	1:B:134[B]:ARG:NH1	2.64	0.41
1:B:207:LEU:HB3	1:B:208[A]:PRO:HD2	2.01	0.41
1:A:31:ARG:NH1	1:A:264:LEU:HD13	2.34	0.41
1:A:55:ALA:HB3	1:A:56:PRO:HD3	2.02	0.41
2:A:265:1PE:H261	2:A:265:1PE:H251	1.85	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	275/283 (97%)	268 (98%)	7 (2%)	0	100	100
1	B	289/283 (102%)	278 (96%)	9 (3%)	2 (1%)	18	8
All	All	564/566 (100%)	546 (97%)	16 (3%)	2 (0%)	43	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	208[A]	PRO
1	B	208[B]	PRO

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	237/238 (100%)	237 (100%)	0	100	100
1	B	251/238 (106%)	249 (99%)	2 (1%)	73	70
All	All	488/476 (102%)	486 (100%)	2 (0%)	84	83

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

Mol	Chain	Res	Type
1	B	75	LYS
1	B	138	ASP

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

Mol	Chain	Res	Type
1	A	46	GLN
1	B	-5	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	CIT	B	265	-	12,12,12	1.33	1 (8%)	17,17,17	1.68	4 (23%)
2	1PE	A	265	-	15,15,15	0.51	0	14,14,14	0.48	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	CIT	B	265	-	-	2/16/16/16	-
2	1PE	A	265	-	-	10/13/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	265	CIT	O3-C5	2.76	1.31	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	265	CIT	O6-C6-C3	3.90	120.61	113.14
3	B	265	CIT	O3-C5-C4	-2.85	114.89	122.95
3	B	265	CIT	C4-C3-C2	-2.12	103.88	109.31
3	B	265	CIT	O6-C6-O5	-2.07	117.25	123.86

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	265	1PE	C25-C15-OH6-C26
2	A	265	1PE	C14-C24-OH4-C13
2	A	265	1PE	OH4-C13-C23-OH3
2	A	265	1PE	OH2-C12-C22-OH3
2	A	265	1PE	C24-C14-OH5-C25
2	A	265	1PE	OH6-C15-C25-OH5
2	A	265	1PE	OH5-C14-C24-OH4
2	A	265	1PE	C12-C22-OH3-C23
3	B	265	CIT	O2-C1-C2-C3
2	A	265	1PE	C15-C25-OH5-C14
2	A	265	1PE	C13-C23-OH3-C22
3	B	265	CIT	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	265	CIT	3	0
2	A	265	1PE	6	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	258/283 (91%)	-0.12	3 (1%) 76 77	11, 20, 29, 47	11 (4%)
1	B	267/283 (94%)	0.07	16 (5%) 27 26	8, 18, 38, 51	15 (5%)
All	All	525/566 (92%)	-0.02	19 (3%) 46 46	8, 19, 32, 51	26 (4%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-7	HIS	4.4
1	B	131	PHE	4.3
1	B	-6	GLU	4.2
1	B	-8	HIS	4.0
1	B	-9	HIS	3.8
1	B	-2	PHE	3.8
1	B	127[A]	ASP	3.7
1	B	-3	TYR	3.5
1	B	130	GLY	3.3
1	B	-5	ASN	3.0
1	B	128	SER	2.8
1	B	126	ARG	2.8
1	B	-4	LEU	2.7
1	A	0	GLY	2.7
1	B	129	TYR	2.6
1	B	138	ASP	2.4
1	A	145[A]	ASN	2.2
1	A	2	ILE	2.0
1	B	134[A]	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	1PE	A	265	16/16	0.83	0.17	36,41,54,54	0
3	CIT	B	265	13/13	0.87	0.12	15,32,36,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.