Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2026 – 12:22 PM JST

PDB ID	:	46AQ / pdb_000046aq
Title	:	Crystal structure of the diaminopimelate dehydrogenase from Pyrococcus sp. in its apo form
Authors	:	Matyuta, I.O.; Bezsudnova, E.Y.; Popov, V.O.; Boyko, K.M.
Deposited on	:	2026-09-16
Resolution	:	2.50 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:

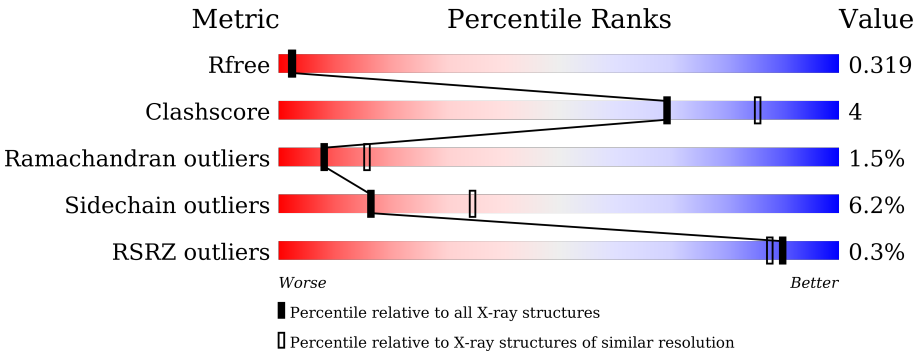
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	311	85% 9%
1	C	311	% 85% 10%
1	E	311	85% 9%

2 Entry composition

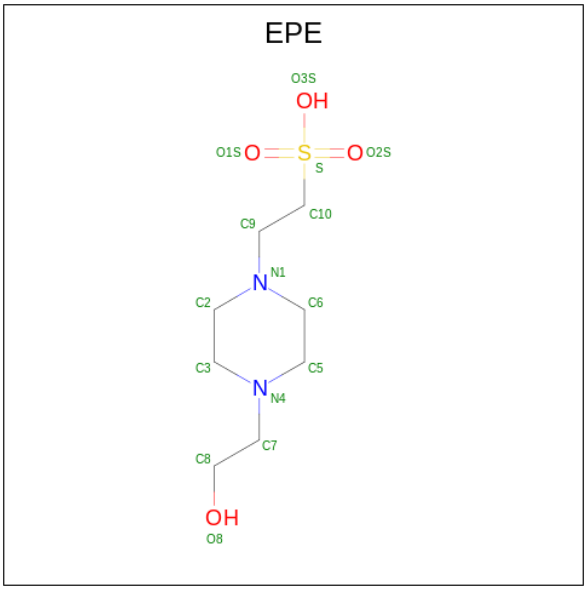
There are 3 unique types of molecules in this entry. The entry contains 6797 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Diaminopimelate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2244	1433	369	431	11			
1	C	303	Total	C	N	O	S	0	0	0
			2258	1448	373	426	11			
1	E	307	Total	C	N	O	S	0	0	0
			2249	1441	365	432	11			

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 3 is water.

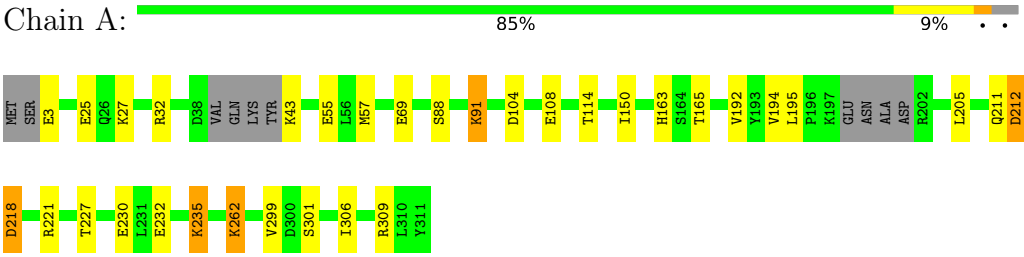
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O 1 1	0	0

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.

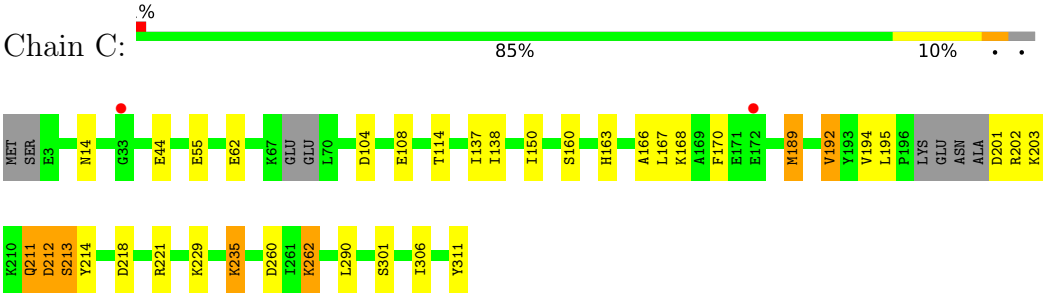
• Molecule 1: Diaminopimelate dehydrogenase

Chain A:



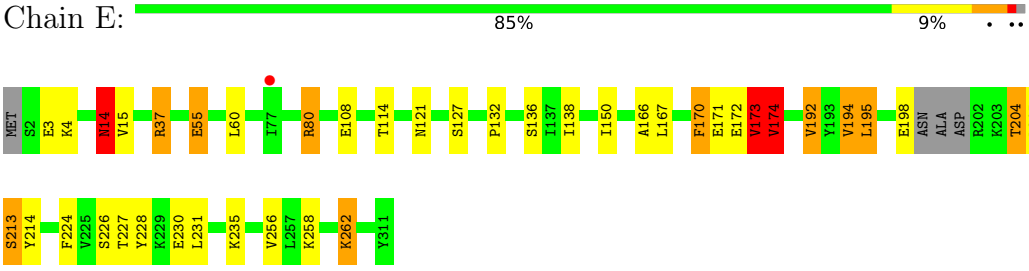
• Molecule 1: Diaminopimelate dehydrogenase

Chain C:



• Molecule 1: Diaminopimelate dehydrogenase

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	113.28Å 122.23Å 83.41Å 90.00° 96.21° 90.00°	Depositor
Resolution (Å)	23.08 – 2.50 23.08 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.9 (23.08-2.50) 93.9 (23.08-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0431	Depositor
R, R_{free}	0.286 , 0.314 0.287 , 0.319	Depositor DCC
R_{free} test set	1831 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 20.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.320 for -1/2*h+1/2*k-l,1/2*h-1/2*k-l,-1/2*h-1/2*k 0.317 for -1/2*h-1/2*k-l,-1/2*h-1/2*k+l,-1/2*h+1/2*k	Xtriage
Reported twinning fraction	0.490 for H, K, L 0.261 for -1/2H+1/2K-L, 1/2H-1/2K-L, -1/2H-1/2K 0.249 for -1/2H-1/2K-L, -1/2H-1/2K+L, -1/2H+1/2K	Depositor
Outliers	1 of 36842 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6797	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.10% 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: EPE

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	0.71	0/2286	1.40	12/3111 (0.4%)
1	C	0.72	0/2302	1.42	18/3133 (0.6%)
1	E	0.72	0/2292	1.48	21/3127 (0.7%)
All	All	0.72	0/6880	1.43	51/9371 (0.5%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	174	VAL	N-CA-CB	10.91	129.23	111.23
1	A	262	LYS	CG-CD-CE	10.04	134.40	111.30
1	C	206	GLU	N-CA-CB	9.54	126.61	110.49
1	E	206	GLU	N-CA-CB	8.97	125.65	110.49
1	C	262	LYS	CG-CD-CE	8.90	131.76	111.30
1	C	260	ASP	CA-CB-CG	8.71	121.31	112.60
1	E	173	VAL	N-CA-CB	8.56	125.36	111.23
1	E	172	GLU	CB-CG-CD	8.48	127.03	112.60
1	C	206	GLU	CB-CG-CD	8.26	126.64	112.60
1	E	170	PHE	CA-CB-CG	8.24	122.05	113.80
1	E	194	VAL	N-CA-CB	7.87	123.01	111.52
1	C	166	ALA	N-CA-C	-7.69	100.61	110.53
1	A	27	LYS	CB-CG-CD	7.47	128.49	111.30
1	C	235	LYS	CG-CD-CE	7.47	128.49	111.30
1	E	262	LYS	CG-CD-CE	7.39	128.31	111.30
1	A	235	LYS	CA-CB-CG	7.09	128.29	114.10
1	C	44	GLU	CB-CG-CD	-6.89	100.89	112.60
1	E	170	PHE	N-CA-CB	6.87	120.09	109.85
1	C	170	PHE	N-CA-CB	-6.67	99.21	110.49
1	C	170	PHE	CA-CB-CG	6.44	120.24	113.80
1	A	25	GLU	CB-CG-CD	-6.37	101.77	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	194	VAL	N-CA-CB	6.21	120.59	111.52
1	E	55	GLU	CB-CA-C	6.03	122.92	110.31
1	E	55	GLU	CB-CG-CD	6.01	122.81	112.60
1	E	198	GLU	N-CA-CB	5.99	120.68	110.50
1	C	55	GLU	CB-CG-CD	5.97	122.75	112.60
1	C	202	ARG	N-CA-CB	5.96	120.57	110.49
1	E	206	GLU	CB-CG-CD	5.95	122.72	112.60
1	E	108	GLU	N-CA-CB	-5.91	101.44	110.01
1	E	108	GLU	CB-CA-C	5.89	120.12	110.88
1	A	104	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	27	LYS	CG-CD-CE	5.74	124.49	111.30
1	E	80	ARG	N-CA-CB	5.70	119.00	110.22
1	E	3	GLU	CB-CA-C	-5.65	100.90	109.99
1	C	108	GLU	N-CA-CB	-5.64	101.83	110.01
1	C	168	LYS	N-CA-CB	5.63	118.25	109.97
1	C	62	GLU	CB-CG-CD	5.61	122.14	112.60
1	C	262	LYS	CB-CG-CD	5.60	124.18	111.30
1	E	14	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	55	GLU	CB-CG-CD	5.56	122.05	112.60
1	A	216	VAL	N-CA-CB	5.53	120.35	111.23
1	E	4	LYS	CB-CA-C	5.49	121.34	110.42
1	A	262	LYS	CB-CG-CD	5.44	123.80	111.30
1	C	108	GLU	CB-CA-C	5.42	119.38	110.88
1	E	262	LYS	CB-CG-CD	5.25	123.37	111.30
1	C	235	LYS	CA-CB-CG	5.22	124.54	114.10
1	A	218	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	211	GLN	N-CA-CB	-5.20	106.76	111.59
1	A	232	GLU	CB-CG-CD	5.13	121.32	112.60
1	E	172	GLU	CA-C-N	5.08	131.12	121.97
1	E	172	GLU	C-N-CA	5.08	131.12	121.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2244	0	2174	12	0
1	C	2258	0	2195	14	0
1	E	2249	0	2154	23	0
2	A	15	0	18	0	0
2	C	15	0	18	2	0
2	E	15	0	18	1	0
3	E	1	0	0	0	0
All	All	6797	0	6577	47	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 (47) 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:E:14:ASN:ND2	1:E:15:VAL:HG23	1.87	0.88
1:E:14:ASN:HD22	1:E:15:VAL:HG23	1.38	0.87
1:A:211:GLN:O	1:A:213:SER:N	2.21	0.69
1:A:299:VAL:HG21	1:A:306:ILE:HD12	1.77	0.67
1:A:227:THR:HG23	1:A:230:GLU:H	1.61	0.64
1:C:192:VAL:HG23	1:C:194:VAL:HG23	1.79	0.64
1:E:227:THR:HG23	1:E:230:GLU:H	1.63	0.64
1:E:170:PHE:O	1:E:171:GLU:HG2	1.98	0.64
1:E:14:ASN:HD22	1:E:15:VAL:N	1.99	0.61
1:E:14:ASN:HD22	1:E:15:VAL:H	1.48	0.59
1:E:166:ALA:O	1:E:170:PHE:HD2	1.86	0.58
1:E:192:VAL:HG23	1:E:194:VAL:HG13	1.85	0.58
1:E:206:GLU:HB2	1:E:224:PHE:HZ	1.68	0.58
1:A:299:VAL:HG21	1:A:306:ILE:CD1	2.34	0.57
1:C:167:LEU:HD22	1:C:209:ILE:HG12	1.89	0.55
1:E:195:LEU:HB2	1:E:231:LEU:HD22	1.89	0.53
1:A:32:ARG:HE	1:A:69:GLU:HB3	1.74	0.52
1:E:14:ASN:ND2	1:E:15:VAL:H	2.07	0.52
1:C:189:MET:SD	1:C:221:ARG:HG3	2.50	0.51
1:E:37:ARG:HE	1:E:60:LEU:HD11	1.75	0.51
1:C:211:GLN:O	1:C:213:SER:N	2.45	0.49
1:C:192:VAL:HG21	1:C:209:ILE:HG21	1.94	0.49
1:E:211:GLN:O	1:E:213:SER:N	2.45	0.49
1:C:160:SER:HA	2:C:401:EPE:O3S	2.13	0.48
1:A:301:SER:HB2	1:A:306:ILE:HD11	1.96	0.48
1:C:311:TYR:CE1	1:E:132:PRO:HB2	2.48	0.48
1:E:206:GLU:HB2	1:E:224:PHE:CZ	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:TYR:OH	1:E:127:SER:O	2.32	0.46
2:E:401:EPE:H102	2:E:401:EPE:H61	1.56	0.45
1:A:212:ASP:C	1:A:214:TYR:H	2.24	0.44
1:A:88:SER:O	1:A:91:LYS:HD2	2.18	0.44
1:A:227:THR:CG2	1:A:230:GLU:HG2	2.48	0.44
1:C:211:GLN:O	1:C:212:ASP:C	2.60	0.43
1:E:173:VAL:HB	1:E:174:VAL:H	1.28	0.43
1:E:212:ASP:O	1:E:214:TYR:N	2.48	0.43
1:A:306:ILE:HD13	1:A:309:ARG:NH1	2.34	0.43
1:A:43:LYS:NZ	1:A:57:MET:O	2.52	0.43
1:E:256:VAL:CG1	1:E:258:LYS:HE2	2.49	0.42
2:C:401:EPE:H102	2:C:401:EPE:H61	1.75	0.42
1:C:301:SER:HB2	1:C:306:ILE:HD11	2.01	0.42
1:C:138:ILE:HD12	1:E:138:ILE:HD12	2.02	0.41
1:E:171:GLU:C	1:E:173:VAL:H	2.28	0.41
1:C:137:ILE:HD11	1:C:290:LEU:HB3	2.01	0.41
1:C:201:ASP:C	1:C:203:LYS:H	2.29	0.41
1:E:227:THR:CG2	1:E:230:GLU:HG2	2.51	0.41
1:A:212:ASP:C	1:A:214:TYR:N	2.79	0.40
1:C:311:TYR:HA	1:E:136:SER:HB3	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	295/311 (95%)	285 (97%)	7 (2%)	3 (1%)	12 24
1	C	297/311 (96%)	282 (95%)	11 (4%)	4 (1%)	9 18
1	E	303/311 (97%)	287 (95%)	10 (3%)	6 (2%)	6 10
All	All	895/933 (96%)	854 (95%)	28 (3%)	13 (2%)	8 16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ASP
1	C	14	ASN
1	C	206	GLU
1	C	212	ASP
1	E	204	THR
1	E	206	GLU
1	E	212	ASP
1	A	213	SER
1	E	173	VAL
1	E	205	LEU
1	C	213	SER
1	E	213	SER
1	A	216	VAL

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	234/274 (85%)	220 (94%)	14 (6%)	17	36
1	C	234/274 (85%)	222 (95%)	12 (5%)	21	43
1	E	230/274 (84%)	213 (93%)	17 (7%)	13	27
All	All	698/822 (85%)	655 (94%)	43 (6%)	16	34

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	91	LYS
1	A	108	GLU
1	A	114	THR
1	A	150	ILE
1	A	163	HIS
1	A	165	THR
1	A	192	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	195	LEU
1	A	205	LEU
1	A	218	ASP
1	A	221	ARG
1	A	235	LYS
1	A	262	LYS
1	C	104	ASP
1	C	114	THR
1	C	150	ILE
1	C	163	HIS
1	C	189	MET
1	C	192	VAL
1	C	195	LEU
1	C	214	TYR
1	C	218	ASP
1	C	229	LYS
1	C	235	LYS
1	C	262	LYS
1	E	14	ASN
1	E	37	ARG
1	E	55	GLU
1	E	80	ARG
1	E	114	THR
1	E	121	ASN
1	E	150	ILE
1	E	167	LEU
1	E	173	VAL
1	E	174	VAL
1	E	192	VAL
1	E	195	LEU
1	E	204	THR
1	E	226	SER
1	E	228	TYR
1	E	235	LYS
1	E	262	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	185	ASN
1	A	271	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	120	HIS
1	C	271	GLN
1	E	14	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

3 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	EPE	E	401	-	15,15,15	1.00	1 (6%)	18,20,20	1.87	4 (22%)
2	EPE	A	401	-	15,15,15	0.96	1 (6%)	18,20,20	1.94	6 (33%)
2	EPE	C	401	-	15,15,15	0.71	0	18,20,20	1.45	4 (22%)

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	EPE	E	401	-	-	5/9/19/19	0/1/1/1
2	EPE	A	401	-	-	6/9/19/19	0/1/1/1
2	EPE	C	401	-	-	7/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	EPE	O3S-S	2.94	1.58	1.47
2	E	401	EPE	O3S-S	2.92	1.58	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	EPE	O3S-S-O1S	-5.63	97.51	111.27
2	A	401	EPE	C6-N1-C2	3.74	117.24	108.83
2	A	401	EPE	C5-C6-N1	3.48	117.78	110.64
2	A	401	EPE	O2S-S-O1S	3.43	125.82	113.95
2	C	401	EPE	O3S-S-C10	-3.11	100.73	105.77
2	C	401	EPE	O1S-S-C10	3.11	110.66	106.92
2	C	401	EPE	O3S-S-O1S	-2.96	104.04	111.27
2	A	401	EPE	C5-N4-C3	-2.84	102.43	108.83
2	E	401	EPE	O3S-S-O2S	2.74	117.96	111.27
2	C	401	EPE	O2S-S-O1S	2.67	123.20	113.95
2	E	401	EPE	O2S-S-O1S	2.58	122.89	113.95
2	E	401	EPE	O2S-S-C10	-2.57	103.82	106.92
2	A	401	EPE	C2-C3-N4	-2.18	106.16	110.64
2	A	401	EPE	O3S-S-O2S	-2.15	106.03	111.27

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	EPE	C10-C9-N1-C6
2	A	401	EPE	S-C10-C9-N1
2	A	401	EPE	C9-C10-S-O1S
2	A	401	EPE	C9-C10-S-O2S
2	A	401	EPE	C9-C10-S-O3S
2	C	401	EPE	C10-C9-N1-C6
2	C	401	EPE	S-C10-C9-N1
2	C	401	EPE	C9-C10-S-O2S
2	E	401	EPE	C10-C9-N1-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	401	EPE	S-C10-C9-N1
2	E	401	EPE	C9-C10-S-O1S
2	A	401	EPE	N4-C7-C8-O8
2	E	401	EPE	C10-C9-N1-C2
2	C	401	EPE	C9-C10-S-O3S
2	E	401	EPE	N4-C7-C8-O8
2	C	401	EPE	C8-C7-N4-C5
2	C	401	EPE	C9-C10-S-O1S
2	C	401	EPE	C8-C7-N4-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	EPE	1	0
2	C	401	EPE	2	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

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	301/311 (96%)	-0.27	0	100	100	22, 54, 97, 135	0
1	C	303/311 (97%)	-0.33	2 (0%)	84	81	23, 56, 86, 111	0
1	E	307/311 (98%)	-0.30	1 (0%)	90	87	27, 57, 84, 102	0
All	All	911/933 (97%)	-0.30	3 (0%)	90	87	22, 56, 88, 135	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	GLY	2.7
1	C	172	GLU	2.3
1	E	77	ILE	2.1

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

There are no oligosaccharides 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
2	EPE	A	401	15/15	0.98	0.05	24,28,58,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EPE	C	401	15/15	0.98	0.06	29,39,51,54	0
2	EPE	E	401	15/15	0.98	0.06	22,29,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.