Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 10:31 PM EST

PDB ID	:	5G0X
Title	:	Pseudomonas aeruginosa HDAH bound to acetate.
Authors	:	Kraemer, A.; Meyer-Almes, F.J.; Yildiz, O.
Deposited on	:	2016-03-23
Resolution	:	1.70 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
http://wwpdb.org/validation/2016/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:

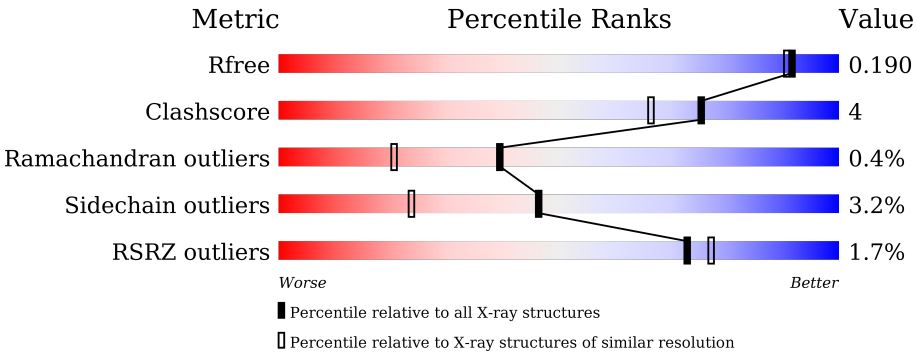
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 1.70 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	379	2% 87% 9%
1	C	379	2% 90% 9%

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
4	ACT	A	1375	-	-	-	X
4	ACT	C	1381	-	-	-	X
5	EPE	A	1376	-	-	-	X
5	EPE	A	1377	-	-	-	X
5	EPE	A	1378	-	-	-	X
5	EPE	C	1382	-	-	-	X
5	EPE	C	1383	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6307 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 HDAH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2819	1772	519	516	12			
1	C	376	Total	C	N	O	S	0	0	0
			2864	1801	527	524	12			

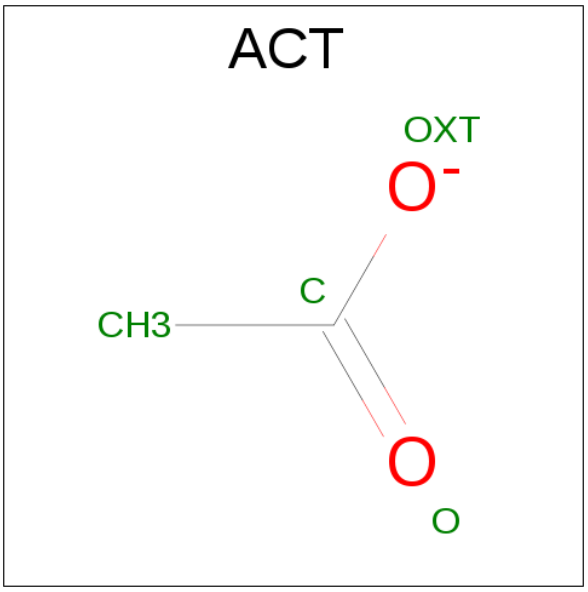
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

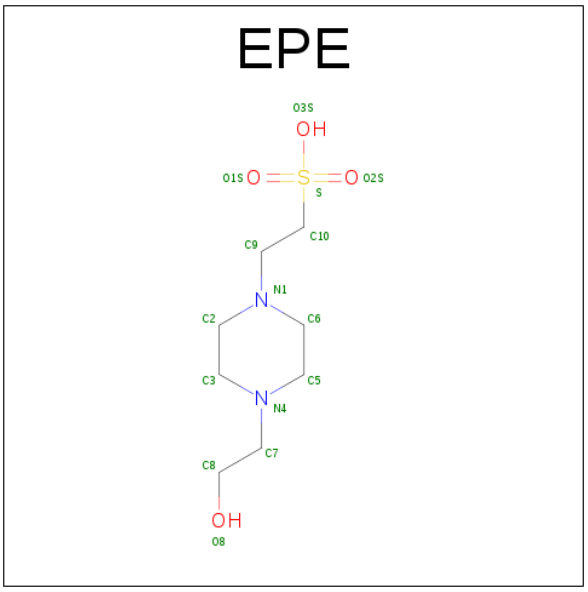
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	K	0	0
			2	2		
3	C	2	Total	K	0	0
			2	2		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

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

- Molecule 6 is water.

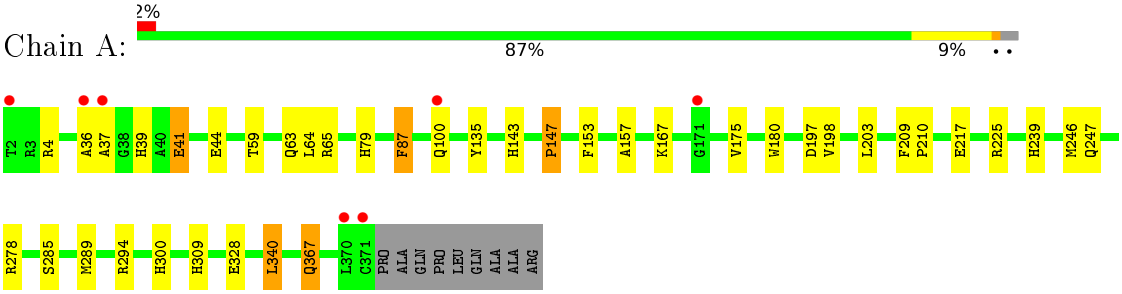
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	268	Total	O	0	0
			268	268		
6	C	267	Total	O	0	0
			267	267		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

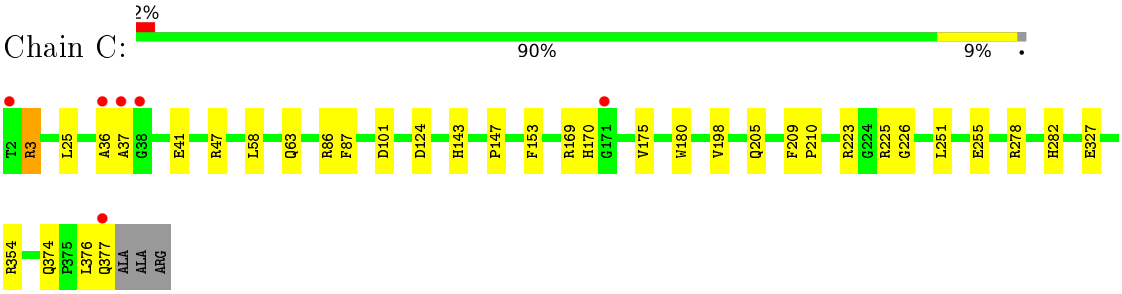
- Molecule 1: HDAH

Chain A:



- Molecule 1: HDAH

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	81.39Å 81.39Å 205.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.69 – 1.70 24.53 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (75.69-1.70) 100.0 (24.53-1.70)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.134 , 0.184 0.148 , 0.190	Depositor DCC
R_{free} test set	3852 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	14.0	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6307	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.06% 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: ZN, EPE, K, 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	0.59	0/2888	0.83	5/3922 (0.1%)
1	C	0.59	0/2935	0.82	6/3988 (0.2%)
All	All	0.59	0/5823	0.82	11/7910 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	225	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	C	225	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	225	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	C	354	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	86	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	225	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	47	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	87	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	C	86	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	278	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	87	PHE	CB-CG-CD1	5.02	124.31	120.80

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	2819	0	2739	28	0
1	C	2864	0	2785	18	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
4	A	4	0	3	0	0
4	C	4	0	3	0	0
5	A	45	0	54	0	0
5	C	30	0	36	2	0
6	A	268	0	0	8	0
6	C	267	0	0	6	0
All	All	6307	0	5620	44	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 (44) 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:294:ARG:NH1	1:A:328:GLU:OE2	2.08	0.85
1:C:205:GLN:HE22	1:C:278:ARG:H	1.28	0.78
1:A:300:HIS:HD2	6:A:2225:HOH:O	1.68	0.76
1:A:44:GLU:HG2	6:A:2038:HOH:O	1.92	0.68
1:A:100:GLN:O	6:A:2094:HOH:O	2.14	0.66
1:A:340:LEU:HD13	1:C:25:LEU:HD21	1.82	0.62
1:A:203:LEU:HD12	1:A:289:MET:HE1	1.83	0.61
1:A:367:GLN:NE2	6:A:2265:HOH:O	2.33	0.60
1:C:101:ASP:OD1	5:C:1383:EPE:H51	2.02	0.60
1:A:300:HIS:CD2	6:A:2225:HOH:O	2.47	0.58
1:A:39:HIS:CD2	1:A:41:GLU:H	2.22	0.57
1:C:226:GLY:HA2	6:C:2179:HOH:O	2.03	0.57
1:C:374:GLN:NE2	6:C:2265:HOH:O	2.37	0.57
1:C:124:ASP:OD1	1:C:170:HIS:HE1	1.88	0.56
1:C:205:GLN:NE2	1:C:278:ARG:H	2.02	0.55
1:A:59:THR:HG23	1:A:64:LEU:HD21	1.90	0.54
1:A:239:HIS:HD2	1:A:285:SER:OG	1.91	0.53
1:A:100:GLN:HG3	6:A:2096:HOH:O	2.10	0.51
1:A:246:MET:SD	1:A:289:MET:HE2	2.50	0.51
1:C:251:LEU:O	1:C:255:GLU:HG2	2.12	0.50
1:A:79:HIS:CE1	1:A:157:ALA:H	2.31	0.49
1:C:101:ASP:OD2	5:C:1383:EPE:H71	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:OH	1:A:309:HIS:HD2	1.97	0.48
1:A:135:TYR:OH	1:A:309:HIS:CD2	2.67	0.47
1:C:255:GLU:HG3	6:C:2264:HOH:O	2.14	0.47
1:A:167:LYS:HE3	1:A:197:ASP:OD2	2.14	0.47
1:C:223:ARG:NH2	6:C:2156:HOH:O	2.47	0.47
1:A:63:GLN:HE21	1:A:65:ARG:HD3	1.81	0.45
1:C:58:LEU:HD11	1:C:327:GLU:CG	2.47	0.45
1:A:79:HIS:HD2	1:A:147:PRO:O	2.00	0.45
1:A:209:PHE:HA	1:A:210:PRO:C	2.37	0.44
1:A:4:ARG:NE	1:A:63:GLN:OE1	2.51	0.44
1:C:282:HIS:HE1	6:C:2245:HOH:O	2.02	0.43
1:A:100:GLN:HA	1:A:100:GLN:OE1	2.19	0.43
1:A:217:GLU:H	1:A:217:GLU:CD	2.22	0.42
1:C:205:GLN:HE22	1:C:278:ARG:N	2.06	0.42
1:A:247:GLN:HG2	6:A:2191:HOH:O	2.19	0.41
1:A:175:VAL:O	1:A:198:VAL:HA	2.21	0.41
1:C:209:PHE:HA	1:C:210:PRO:C	2.41	0.41
1:A:79:HIS:HE1	1:A:157:ALA:H	1.66	0.41
1:C:3:ARG:HD3	6:C:2224:HOH:O	2.19	0.41
1:A:309:HIS:HE1	6:A:2040:HOH:O	2.03	0.40
1:C:175:VAL:O	1:C:198:VAL:HA	2.21	0.40
1:A:36:ALA:HB1	1:C:36:ALA:HB1	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	368/379 (97%)	356 (97%)	11 (3%)	1 (0%)	46	26
1	C	374/379 (99%)	361 (96%)	11 (3%)	2 (0%)	34	15
All	All	742/758 (98%)	717 (97%)	22 (3%)	3 (0%)	39	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ALA
1	C	37	ALA
1	C	3	ARG

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	282/288 (98%)	274 (97%)	8 (3%)	51	29
1	C	287/288 (100%)	277 (96%)	10 (4%)	43	20
All	All	569/576 (99%)	551 (97%)	18 (3%)	46	24

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	87	PHE
1	A	143	HIS
1	A	147	PRO
1	A	153	PHE
1	A	180	TRP
1	A	340	LEU
1	A	367	GLN
1	C	41	GLU
1	C	63	GLN
1	C	87	PHE
1	C	143	HIS
1	C	147	PRO
1	C	153	PHE
1	C	169	ARG
1	C	180	TRP
1	C	376	LEU
1	C	377	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	79	HIS
1	A	149	GLN
1	A	228	ASN
1	A	230	ASN
1	A	239	HIS
1	A	309	HIS
1	C	82	HIS
1	C	158	ASN
1	C	170	HIS
1	C	205	GLN
1	C	228	ASN
1	C	282	HIS
1	C	300	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	ACT	A	1375	2	0,3,3	0.00	-	0,3,3	0.00	-
5	EPE	A	1376	-	15,15,15	1.62	1 (6%)	19,20,20	2.38	1 (5%)
5	EPE	A	1377	-	15,15,15	1.90	1 (6%)	19,20,20	1.55	2 (10%)
5	EPE	A	1378	-	15,15,15	1.80	1 (6%)	19,20,20	1.43	3 (15%)
4	ACT	C	1381	2	0,3,3	0.00	-	0,3,3	0.00	-
5	EPE	C	1382	-	15,15,15	1.66	1 (6%)	19,20,20	1.93	2 (10%)
5	EPE	C	1383	-	15,15,15	1.64	1 (6%)	19,20,20	1.59	4 (21%)

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	ACT	A	1375	2	-	0/0/0/0	0/0/0/0
5	EPE	A	1376	-	-	0/9/19/19	0/1/1/1
5	EPE	A	1377	-	-	0/9/19/19	0/1/1/1
5	EPE	A	1378	-	-	0/9/19/19	0/1/1/1
4	ACT	C	1381	2	-	0/0/0/0	0/0/0/0
5	EPE	C	1382	-	-	0/9/19/19	0/1/1/1
5	EPE	C	1383	-	-	0/9/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1377	EPE	C10-S	-6.99	1.67	1.77
5	A	1378	EPE	C10-S	-6.46	1.67	1.77
5	C	1382	EPE	C10-S	-5.82	1.68	1.77
5	C	1383	EPE	C10-S	-5.65	1.69	1.77
5	A	1376	EPE	C10-S	-5.52	1.69	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1378	EPE	O2S-S-O1S	-2.23	107.66	113.96
5	C	1383	EPE	C5-N4-C3	2.02	113.39	108.87
5	A	1378	EPE	O3S-S-C10	2.06	109.28	104.99
5	C	1383	EPE	C2-C3-N4	2.37	115.28	110.65
5	C	1382	EPE	O3S-S-C10	2.69	110.59	104.99
5	C	1383	EPE	O3S-S-C10	3.12	111.47	104.99
5	A	1377	EPE	O2S-S-C10	3.22	109.14	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1383	EPE	O2S-S-C10	3.32	109.22	106.87
5	A	1378	EPE	O1S-S-C10	4.08	109.75	106.87
5	A	1377	EPE	O1S-S-C10	4.51	110.05	106.87
5	C	1382	EPE	O2S-S-C10	6.66	111.57	106.87
5	A	1376	EPE	O2S-S-C10	9.62	113.67	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1383	EPE	2	0

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	370/379 (97%)	-0.17	7 (1%) 70 74	9, 14, 29, 57	0
1	C	376/379 (99%)	-0.22	6 (1%) 74 79	8, 14, 30, 59	0
All	All	746/758 (98%)	-0.20	13 (1%) 73 77	8, 14, 30, 59	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	ALA	8.9
1	C	2	THR	7.1
1	A	371	CYS	6.7
1	C	37	ALA	6.5
1	A	2	THR	3.9
1	A	171	GLY	3.7
1	C	36	ALA	3.7
1	C	38	GLY	3.4
1	C	171	GLY	3.2
1	C	377	GLN	3.0
1	A	36	ALA	3.0
1	A	370	LEU	2.4
1	A	100	GLN	2.3

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
5	EPE	C	1382	15/15	0.94	0.23	10.80	20,36,47,48	0
4	ACT	A	1375	4/4	0.90	0.15	7.84	17,19,23,23	0
4	ACT	C	1381	4/4	0.92	0.16	6.57	17,19,21,23	0
5	EPE	A	1377	15/15	0.84	0.25	6.16	34,42,70,74	0
5	EPE	C	1383	15/15	0.61	0.28	4.24	36,41,82,85	0
5	EPE	A	1378	15/15	0.77	0.21	2.29	33,39,56,59	0
5	EPE	A	1376	15/15	0.94	0.21	2.26	20,34,47,50	0
2	ZN	C	1378	1/1	1.00	0.05	-1.32	10,10,10,10	1
3	K	A	1374	1/1	1.00	0.05	-2.10	11,11,11,11	0
3	K	C	1379	1/1	1.00	0.05	-2.54	11,11,11,11	0
3	K	A	1373	1/1	1.00	0.04	-3.04	10,10,10,10	0
3	K	C	1380	1/1	1.00	0.03	-3.34	10,10,10,10	0
2	ZN	A	1372	1/1	1.00	0.03	-3.55	10,10,10,10	1

6.5 Other polymers

There are no such residues in this entry.