



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:12 am GMT

PDB ID : 5HW2
Title : Crystal Structure of Adenylosuccinate Lyase from *Francisella tularensis* Complexed with fumaric acid
Authors : Chang, C.; Maltseva, N.; Kim, Y.; Shatsman, S.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2016-01-28
Resolution : 2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

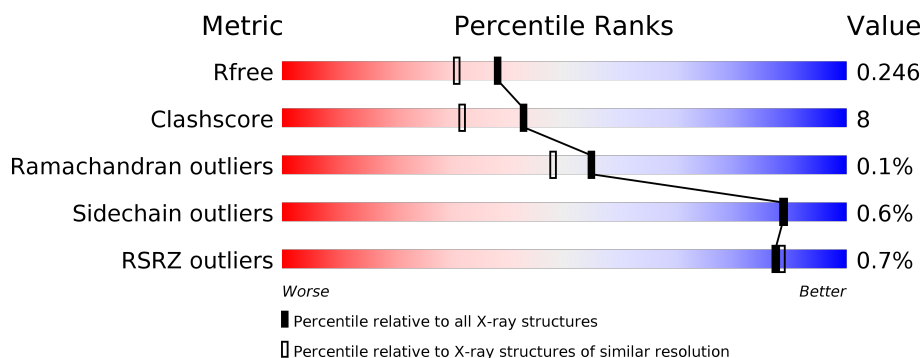
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	100719	2028 (2.08-2.04)
Clashscore	112137	2143 (2.08-2.04)
Ramachandran outliers	110173	2126 (2.08-2.04)
Sidechain outliers	110143	2126 (2.08-2.04)
RSRZ outliers	101464	2035 (2.08-2.04)

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 $\leq 5\%$. 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	438	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 76%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> % 76% 19% • • </div> </div>
1	B	438	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 77%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> % 77% 18% 5% </div> </div>
1	C	438	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 16%, green 79%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> % 79% 16% • • </div> </div>
1	D	438	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 79%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> % 79% 16% • 5% </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FUM	A	502	-	-	-	X
5	EDO	C	504	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14356 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 Adenylosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3340	2120	573	630	17			
1	B	416	Total	C	N	O	S	0	1	0
			3311	2099	569	624	19			
1	C	422	Total	C	N	O	S	0	0	0
			3326	2110	572	627	17			
1	D	417	Total	C	N	O	S	0	2	0
			3321	2104	571	627	19			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	433	ARG	-	expression tag	UNP Q5NIQ1
A	434	GLY	-	expression tag	UNP Q5NIQ1
A	435	GLU	-	expression tag	UNP Q5NIQ1
A	436	ASN	-	expression tag	UNP Q5NIQ1
A	437	LEU	-	expression tag	UNP Q5NIQ1
A	438	TYR	-	expression tag	UNP Q5NIQ1
B	433	ARG	-	expression tag	UNP Q5NIQ1
B	434	GLY	-	expression tag	UNP Q5NIQ1
B	435	GLU	-	expression tag	UNP Q5NIQ1
B	436	ASN	-	expression tag	UNP Q5NIQ1
B	437	LEU	-	expression tag	UNP Q5NIQ1
B	438	TYR	-	expression tag	UNP Q5NIQ1
C	433	ARG	-	expression tag	UNP Q5NIQ1
C	434	GLY	-	expression tag	UNP Q5NIQ1
C	435	GLU	-	expression tag	UNP Q5NIQ1
C	436	ASN	-	expression tag	UNP Q5NIQ1
C	437	LEU	-	expression tag	UNP Q5NIQ1
C	438	TYR	-	expression tag	UNP Q5NIQ1
D	433	ARG	-	expression tag	UNP Q5NIQ1
D	434	GLY	-	expression tag	UNP Q5NIQ1
D	435	GLU	-	expression tag	UNP Q5NIQ1

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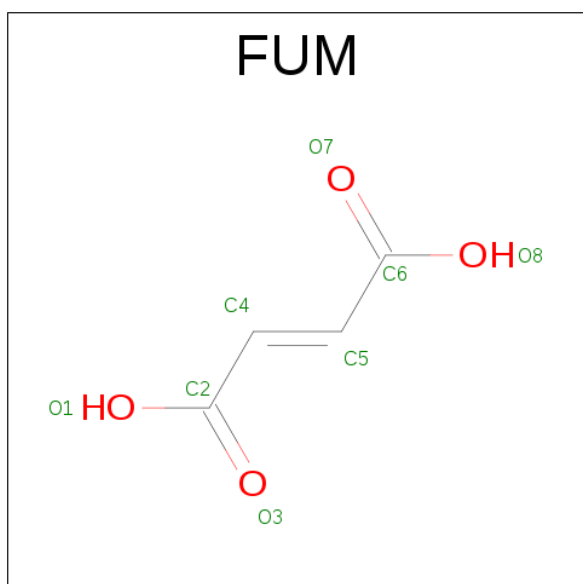
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Chain	Residue	Modelled	Actual	Comment	Reference
D	436	ASN	-	expression tag	UNP Q5NIQ1
D	437	LEU	-	expression tag	UNP Q5NIQ1
D	438	TYR	-	expression tag	UNP Q5NIQ1

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

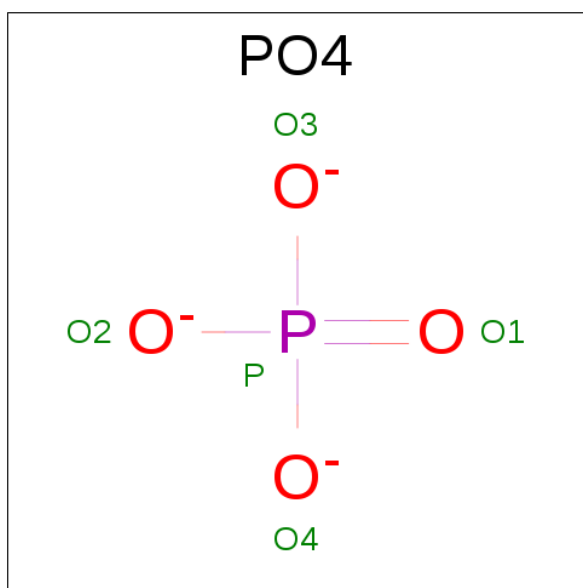
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0

- Molecule 3 is FUMARIC ACID (three-letter code: FUM) (formula: C₄H₄O₄).



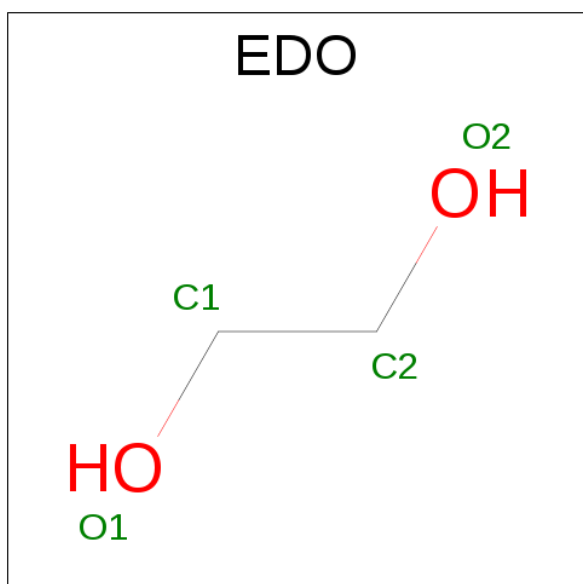
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 4 4	0	0
3	B	1	Total C O 8 4 4	0	0
3	C	1	Total C O 8 4 4	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

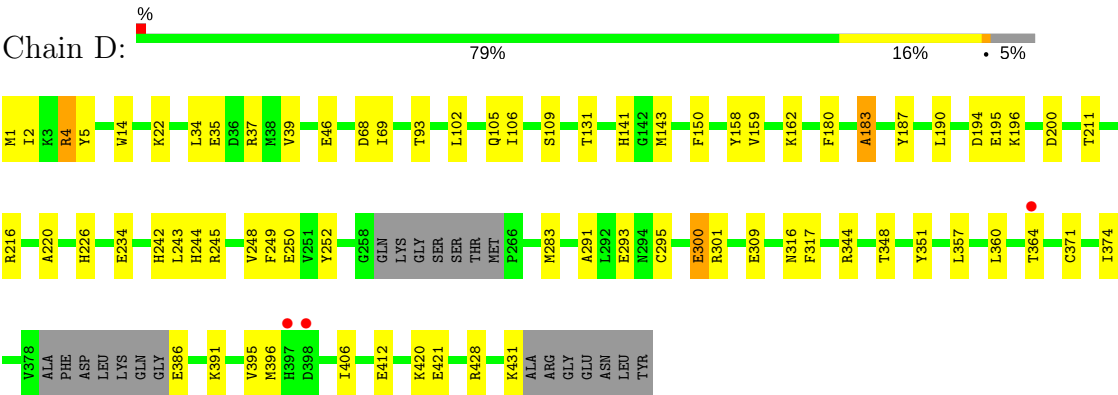


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	262	Total O 262 262	0	0
6	B	273	Total O 273 273	0	0
6	C	225	Total O 225 225	0	0
6	D	230	Total O 230 230	0	0

● Molecule 1: Adenylosuccinate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	88.68Å 88.68Å 255.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.43 – 2.05 36.43 – 2.05	Depositor EDS
% Data completeness (in resolution range)	93.2 (36.43-2.05) 93.0 (36.43-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.10_ 2155: ???)	Depositor
R, R_{free}	0.188 , 0.245 0.188 , 0.246	Depositor DCC
R_{free} test set	5772 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
Reported twinning fraction	0.490 for -h,k,-l	Depositor
Outliers	0 of 113636 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14356	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 4.94% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, FUM, PO4, EDO

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	0.55	13/3397 (0.4%)	0.41	1/4575 (0.0%)
1	B	0.49	4/3365 (0.1%)	0.40	0/4530
1	C	0.70	13/3381 (0.4%)	0.44	1/4554 (0.0%)
1	D	0.49	9/3375 (0.3%)	0.40	0/4545
All	All	0.56	39/13518 (0.3%)	0.41	2/18204 (0.0%)

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	1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	55	PRO	N-CD	-15.73	1.25	1.47
1	C	408	GLU	CD-OE1	-11.75	1.12	1.25
1	C	83	GLU	CD-OE1	-10.88	1.13	1.25
1	A	325	ARG	CZ-NH1	-10.35	1.19	1.33
1	B	421	GLU	CD-OE1	-10.17	1.14	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	PRO	N-CD-CG	6.47	112.91	103.20
1	A	325	ARG	NE-CZ-NH1	-5.88	117.36	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	373	LYS	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	3340	0	3316	63	0
1	B	3311	0	3297	57	0
1	C	3326	0	3293	57	0
1	D	3321	0	3306	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	2	1	0
3	B	8	0	2	0	0
3	C	8	0	2	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
5	A	8	0	12	0	0
5	C	8	0	12	0	0
5	D	4	0	6	0	0
6	A	262	0	0	5	0
6	B	273	0	0	9	0
6	C	225	0	0	10	0
6	D	230	0	0	7	0
All	All	14356	0	13248	207	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 8.

The worst 5 of 207 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:C:354:SER:O	1:C:358:HIS:HD2	1.12	1.33
1:C:354:SER:O	1:C:358:HIS:CD2	1.97	1.16
1:D:162:LYS:NZ	6:D:601:HOH:O	1.95	0.98
1:D:248:VAL:HG12	1:D:250:GLU:HG3	1.48	0.94
1:B:52:GLN:H	1:B:79:GLN:HE22	1.14	0.93

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	413/438 (94%)	395 (96%)	17 (4%)	1 (0%)	51	42
1	B	411/438 (94%)	391 (95%)	20 (5%)	0	100	100
1	C	414/438 (94%)	403 (97%)	11 (3%)	0	100	100
1	D	413/438 (94%)	399 (97%)	13 (3%)	1 (0%)	51	42
All	All	1651/1752 (94%)	1588 (96%)	61 (4%)	2 (0%)	55	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	GLY
1	D	183	ALA

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	360/386 (93%)	358 (99%)	2 (1%)	89	89
1	B	357/386 (92%)	355 (99%)	2 (1%)	89	89
1	C	356/386 (92%)	353 (99%)	3 (1%)	85	84
1	D	359/386 (93%)	358 (100%)	1 (0%)	94	94
All	All	1432/1544 (93%)	1424 (99%)	8 (1%)	89	89

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	370	ASP
1	D	301	ARG
1	C	300	GLU
1	B	301	ARG
1	C	99	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	79	GLN
1	B	393	GLN
1	C	358	HIS
1	C	400	HIS
1	D	18	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
3	FUM	A	502	-	1,7,7	0.30	0	0,8,8	0.00	-
4	PO4	A	503	-	4,4,4	0.75	0	6,6,6	0.41	0
5	EDO	A	504	-	3,3,3	0.44	0	2,2,2	0.41	0
5	EDO	A	505	-	3,3,3	0.44	0	2,2,2	0.40	0
3	FUM	B	502	-	1,7,7	0.55	0	0,8,8	0.00	-
4	PO4	B	503	-	4,4,4	0.74	0	6,6,6	0.40	0
3	FUM	C	502	-	1,7,7	0.30	0	0,8,8	0.00	-
4	PO4	C	503	-	4,4,4	0.76	0	6,6,6	0.39	0
5	EDO	C	504	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	C	505	-	3,3,3	0.44	0	2,2,2	0.35	0
4	PO4	D	502	-	4,4,4	0.77	0	6,6,6	0.40	0
5	EDO	D	503	-	3,3,3	0.45	0	2,2,2	0.37	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	FUM	A	502	-	-	0/0/5/5	0/0/0/0
4	PO4	A	503	-	-	0/0/0/0	0/0/0/0
5	EDO	A	504	-	-	0/1/1/1	0/0/0/0
5	EDO	A	505	-	-	0/1/1/1	0/0/0/0
3	FUM	B	502	-	-	0/0/5/5	0/0/0/0
4	PO4	B	503	-	-	0/0/0/0	0/0/0/0
3	FUM	C	502	-	-	0/0/5/5	0/0/0/0
4	PO4	C	503	-	-	0/0/0/0	0/0/0/0
5	EDO	C	504	-	-	0/1/1/1	0/0/0/0
5	EDO	C	505	-	-	0/1/1/1	0/0/0/0
4	PO4	D	502	-	-	0/0/0/0	0/0/0/0
5	EDO	D	503	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	FUM	1	0
3	C	502	FUM	1	0
4	C	503	PO4	1	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	419/438 (95%)	-0.39	3 (0%) 87 88	12, 30, 68, 89	0
1	B	416/438 (94%)	-0.30	4 (0%) 82 84	10, 32, 76, 94	0
1	C	422/438 (96%)	-0.34	2 (0%) 90 92	13, 33, 69, 90	0
1	D	417/438 (95%)	-0.33	3 (0%) 87 88	17, 34, 67, 97	0
All	All	1674/1752 (95%)	-0.34	12 (0%) 87 88	10, 33, 70, 97	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	ILE	4.8
1	B	388	PHE	3.7
1	D	397	HIS	3.0
1	C	366	PHE	2.9
1	B	390	LYS	2.9

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 carbohydrates 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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	FUM	A	502	8/8	0.77	0.17	7.96	41,46,52,53	0
5	EDO	C	504	4/4	0.92	0.14	3.35	32,32,34,35	0
5	EDO	A	504	4/4	0.94	0.11	1.10	18,19,20,21	0
3	FUM	B	502	8/8	0.90	0.12	0.66	36,42,49,51	0
3	FUM	C	502	8/8	0.92	0.11	0.10	30,31,34,36	0
2	K	D	501	1/1	0.99	0.10	0.07	29,29,29,29	0
2	K	A	501	1/1	0.99	0.09	-0.20	23,23,23,23	0
4	PO4	D	502	5/5	0.99	0.08	-0.63	15,18,21,22	0
4	PO4	C	503	5/5	0.99	0.08	-0.70	21,22,25,26	0
2	K	B	501	1/1	0.99	0.08	-0.81	36,36,36,36	0
4	PO4	A	503	5/5	0.99	0.08	-0.84	17,18,22,24	0
4	PO4	B	503	5/5	0.98	0.08	-0.94	24,26,28,28	0
5	EDO	D	503	4/4	0.95	0.09	-0.98	36,37,37,38	0
2	K	C	501	1/1	0.99	0.06	-2.88	38,38,38,38	0
5	EDO	C	505	4/4	0.96	0.16	-	34,34,34,34	0
5	EDO	A	505	4/4	0.97	0.09	-	11,12,12,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.