Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 08:20 AM EST

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 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:

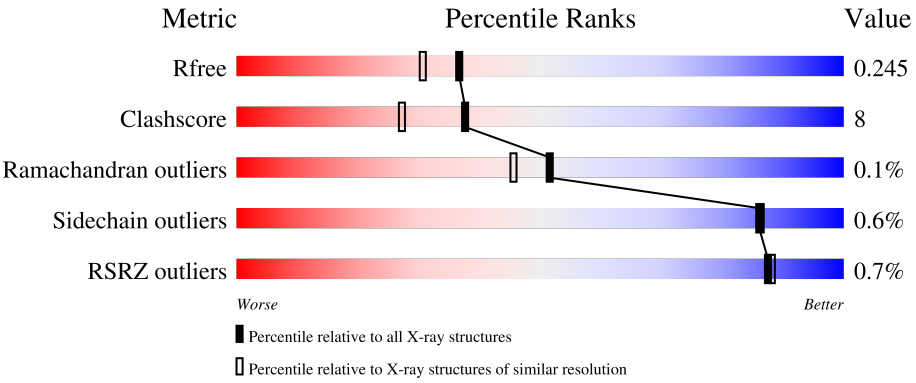
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.05 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}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (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 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	438	76% 18%
1	B	438	77% 18% 5%
1	C	438	79% 16%
1	D	438	79% 16% 5%

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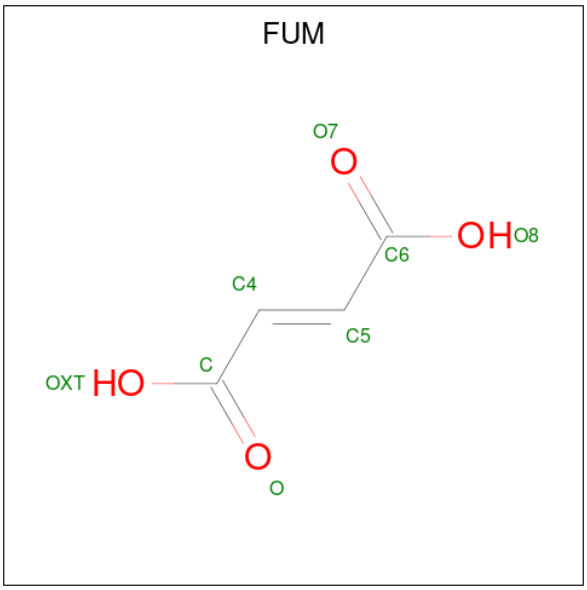
Chain	Residue	Modelled	Actual	Comment	Reference
D	436	ASN	-	expression tag	UNP Q5NIQ1
D	437	LEU	-	expression tag	UNP Q5NIQ1
D	438	TYR	-	expression tag	UNP Q5NIQ1

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

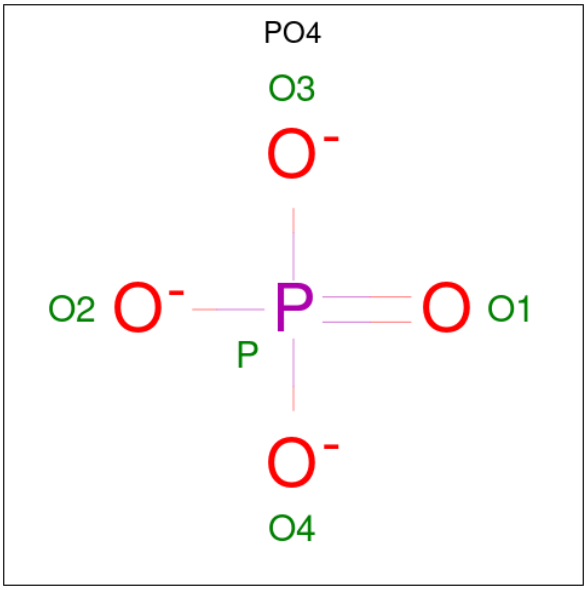
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0

- Molecule 3 is FUMARIC ACID (three-letter code: FUM) (formula: $C_4H_4O_4$).



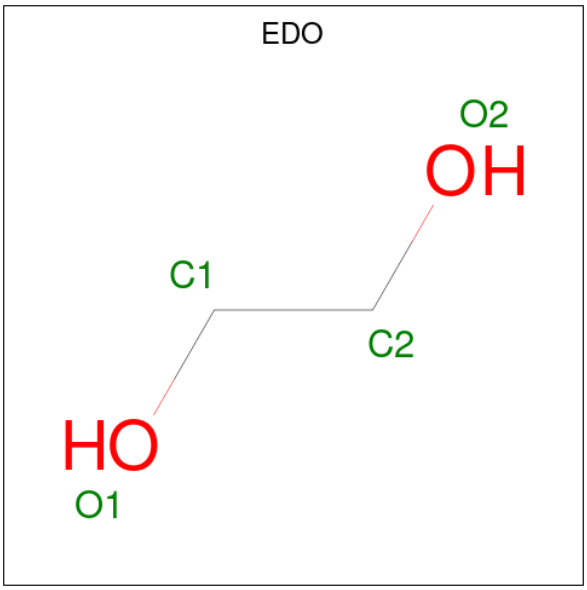
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 4 4	0	0
3	B	1	Total C O 8 4 4	0	0
3	C	1	Total C O 8 4 4	0	0

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



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

- 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.

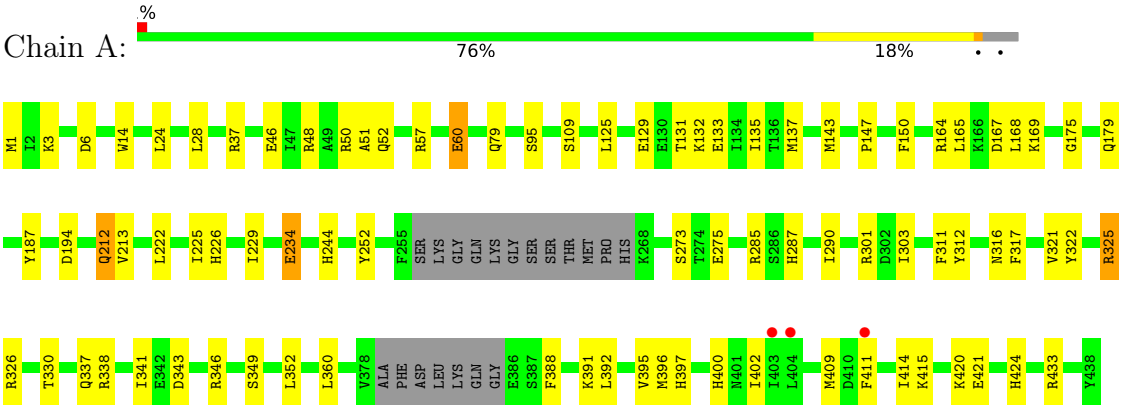
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	262	Total O 262 262	0	0
6	B	273	Total O 273 273	0	0
6	C	225	Total O 225 225	0	0
6	D	230	Total O 230 230	0	0

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.

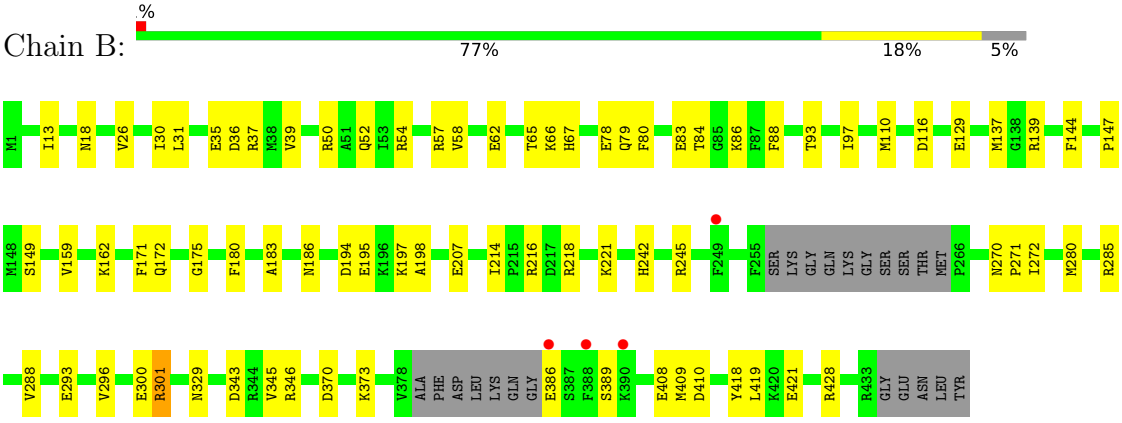
• Molecule 1: Adenylosuccinate lyase

Chain A:



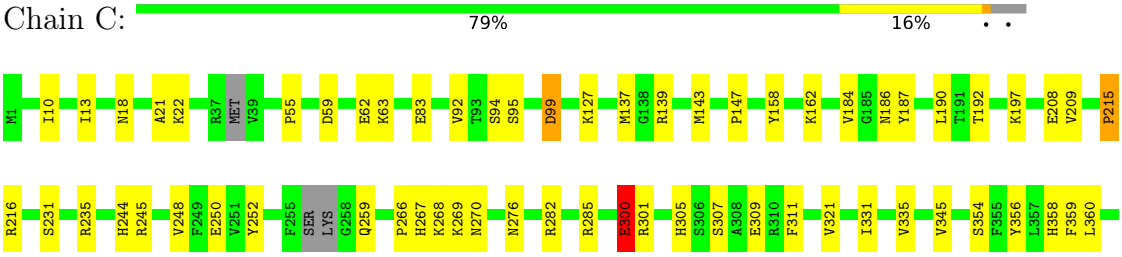
• Molecule 1: Adenylosuccinate lyase

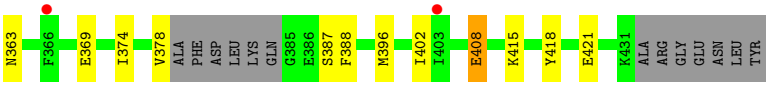
Chain B:



• Molecule 1: Adenylosuccinate lyase

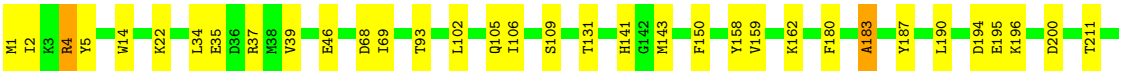
Chain C:

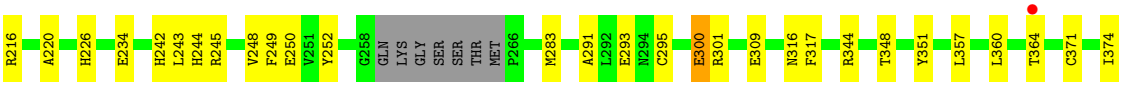


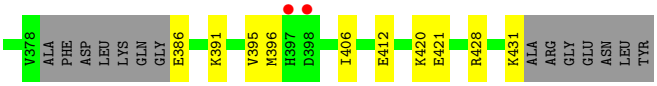


• Molecule 1: Adenylosuccinate lyase

Chain D:







4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.46 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.188 , 0.245 0.189 , 0.245	Depositor DCC
R_{free} test set	5773 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	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.*

[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 (i)

5.1 Standard geometry (i)

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

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

All (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
1	A	325	ARG	NE-CZ	-9.91	1.20	1.33
1	C	408	GLU	CD-OE2	-9.87	1.14	1.25
1	B	129	GLU	CD-OE1	-9.71	1.15	1.25
1	A	46	GLU	CD-OE1	-9.68	1.15	1.25
1	C	421	GLU	CD-OE1	-9.53	1.15	1.25
1	C	83	GLU	CD-OE2	-9.47	1.15	1.25
1	A	46	GLU	CD-OE2	-8.64	1.16	1.25
1	D	300	GLU	CD-OE1	-8.62	1.16	1.25
1	B	129	GLU	CD-OE2	-8.45	1.16	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	421	GLU	CD-OE2	-8.33	1.16	1.25
1	B	421	GLU	CD-OE2	-7.66	1.17	1.25
1	D	300	GLU	CD-OE2	-7.36	1.17	1.25
1	C	369	GLU	CD-OE1	-6.98	1.18	1.25
1	D	46	GLU	CD-OE1	-6.79	1.18	1.25
1	A	50	ARG	CZ-NH1	-6.70	1.24	1.33
1	A	50	ARG	NE-CZ	-6.65	1.24	1.33
1	C	62	GLU	CD-OE1	-6.46	1.18	1.25
1	A	60	GLU	CD-OE1	-6.46	1.18	1.25
1	A	60	GLU	CD-OE2	-6.38	1.18	1.25
1	A	325	ARG	CZ-NH2	-6.27	1.25	1.33
1	D	46	GLU	CD-OE2	-5.92	1.19	1.25
1	C	62	GLU	CD-OE2	-5.89	1.19	1.25
1	D	4	ARG	CZ-NH2	-5.88	1.25	1.33
1	C	300	GLU	CD-OE1	-5.82	1.19	1.25
1	D	4	ARG	NE-CZ	-5.79	1.25	1.33
1	C	215	PRO	N-CD	5.76	1.55	1.47
1	C	369	GLU	CD-OE2	-5.63	1.19	1.25
1	A	50	ARG	CZ-NH2	-5.58	1.25	1.33
1	D	234	GLU	CD-OE1	-5.54	1.19	1.25
1	D	4	ARG	CZ-NH1	-5.48	1.25	1.33
1	A	325	ARG	CD-NE	-5.27	1.37	1.46
1	A	234	GLU	CD-OE1	-5.26	1.19	1.25
1	D	234	GLU	CD-OE2	-5.22	1.20	1.25
1	A	234	GLU	CD-OE2	-5.05	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 (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	3340	0	3316	62	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	1	0	0
3	B	8	0	1	0	0
3	C	8	0	1	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	13245	206	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.

All (206) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ILE:HD13	1:D:283:MET:HE1	1.50	0.92
1:C:216:ARG:HH11	1:C:305:HIS:CE1	1.87	0.91
1:D:102:LEU:O	1:D:106:ILE:HD12	1.81	0.79
1:A:290:ILE:HD13	1:D:283:MET:CE	2.13	0.78
1:A:143:MET:HG3	1:C:270:ASN:HD22	1.48	0.77
1:A:415:LYS:NZ	6:A:601:HOH:O	2.21	0.73
1:C:13:ILE:HA	1:C:18:ASN:HD22	1.52	0.72
1:B:37:ARG:NH1	1:B:194:ASP:OD2	2.23	0.71
1:B:280:MET:SD	1:C:307:SER:HB2	2.31	0.71
1:C:387:SER:OG	1:C:408:GLU:OE2	2.10	0.69
1:B:52:GLN:H	1:B:79:GLN:NE2	1.90	0.69
1:B:214:ILE:O	1:B:216:ARG:NH2	2.25	0.69
1:A:212:GLN:HB3	1:A:301:ARG:HB3	1.75	0.69
1:A:338:ARG:NH2	6:A:601:HOH:O	2.25	0.69
1:D:220:ALA:HA	1:D:291:ALA:HB1	1.77	0.67
1:B:65:THR:HG23	1:B:67:HIS:H	1.61	0.66
1:A:343:ASP:HA	1:A:346:ARG:HD2	1.78	0.65
1:D:22:LYS:NZ	6:D:609:HOH:O	2.29	0.65
1:D:348:THR:HG23	1:D:351:TYR:HE2	1.62	0.65
1:C:231:SER:O	6:C:601:HOH:O	2.15	0.64
1:A:57:ARG:NH1	1:A:60:GLU:OE1	2.30	0.64
1:B:329:ASN:ND2	6:B:612:HOH:O	2.31	0.63
1:A:167:ASP:HB3	1:A:225:ILE:HD13	1.79	0.63
1:B:280:MET:HE1	1:C:311:PHE:HE2	1.63	0.63
1:D:420:LYS:HG3	1:D:421:GLU:HG2	1.80	0.62
1:A:273:SER:HG	1:A:330:THR:HG1	1.42	0.62
1:A:322:TYR:OH	1:A:326:ARG:NH1	2.33	0.61
1:C:92:VAL:HG12	1:C:190:LEU:HD11	1.83	0.61
1:D:386:GLU:N	6:D:613:HOH:O	2.33	0.60
1:A:95:SER:OG	1:A:301:ARG:NH1	2.35	0.60
1:A:321:VAL:O	1:A:325:ARG:HG3	2.03	0.59
1:C:94:SER:N	3:C:502:FUM:O	2.28	0.59
1:C:184:VAL:HB	1:C:300:GLU:HG2	1.84	0.58
1:A:420:LYS:HE3	1:A:421:GLU:HG2	1.84	0.58
1:B:35:GLU:HA	1:B:39:VAL:HB	1.86	0.57
1:A:290:ILE:CD1	1:D:283:MET:HE1	2.31	0.57
1:C:268:LYS:HE2	1:C:270:ASN:HD21	1.69	0.57
1:C:276:ASN:ND2	4:C:503:PO4:O1	2.30	0.57
1:D:4:ARG:HD3	1:D:5:TYR:CZ	2.40	0.57
1:C:21:ALA:O	6:C:602:HOH:O	2.17	0.56
1:A:125:LEU:O	1:A:129:GLU:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASN:HD22	1:D:141:HIS:HB2	1.70	0.56
1:C:374:ILE:O	1:C:378:VAL:HG23	2.04	0.56
1:A:234:GLU:HG2	1:B:296:VAL:HG11	1.87	0.56
1:C:305:HIS:ND1	1:C:309:GLU:OE2	2.30	0.56
1:D:35:GLU:HA	1:D:39:VAL:HB	1.88	0.55
1:C:208:GLU:O	1:D:428:ARG:NE	2.39	0.55
1:A:164:ARG:HB3	1:A:229:ILE:HG12	1.89	0.55
1:C:359:PHE:O	1:C:363:ASN:ND2	2.33	0.54
1:A:52:GLN:HB2	1:A:79:GLN:HE22	1.73	0.54
1:D:37:ARG:NH1	1:D:194:ASP:OD2	2.39	0.54
1:A:147:PRO:O	1:B:186:ASN:ND2	2.40	0.54
1:B:50:ARG:NH2	6:B:627:HOH:O	2.41	0.54
1:C:127:LYS:NZ	1:C:331:ILE:O	2.31	0.54
1:B:31:LEU:CD1	1:B:88:PHE:HA	2.39	0.53
1:D:374:ILE:HD13	1:D:396:MET:HE1	1.89	0.53
1:B:52:GLN:N	1:B:79:GLN:HE22	1.95	0.53
1:B:36:ASP:OD2	1:B:197:LYS:NZ	2.35	0.53
1:A:135:ILE:HB	1:A:415:LYS:HE3	1.90	0.53
1:D:158:TYR:CZ	1:D:162:LYS:HD2	2.44	0.52
1:D:180:PHE:HB2	1:D:195:GLU:HG3	1.92	0.52
1:C:215:PRO:O	6:C:603:HOH:O	2.19	0.52
1:A:226:HIS:ND1	1:A:316:ASN:OD1	2.29	0.52
1:D:244:HIS:CD2	1:D:252:TYR:HA	2.44	0.52
1:A:133:GLU:OE1	1:A:338:ARG:NH1	2.38	0.52
1:D:68:ASP:N	1:D:68:ASP:OD1	2.37	0.52
1:D:226:HIS:ND1	1:D:316:ASN:OD1	2.32	0.52
1:D:431:LYS:N	6:D:601:HOH:O	2.10	0.52
1:A:391:LYS:O	1:A:395:VAL:HG23	2.10	0.51
1:C:252:TYR:CD1	1:C:269:LYS:HD3	2.45	0.51
1:D:412:GLU:OE1	1:D:412:GLU:N	2.40	0.51
1:A:14:TRP:NE1	1:A:109:SER:OG	2.39	0.51
1:B:137:MET:HG2	1:B:345:VAL:HG22	1.93	0.51
1:A:179:GLN:HE22	1:A:213:VAL:HA	1.76	0.51
1:A:244:HIS:CD2	1:A:252:TYR:HA	2.45	0.51
1:D:93:THR:HB	1:D:183:ALA:HA	1.93	0.51
1:B:62:GLU:HA	1:B:65:THR:HG22	1.93	0.51
1:B:52:GLN:HG3	1:B:54:ARG:HH21	1.75	0.50
1:C:192:THR:N	6:C:631:HOH:O	2.44	0.50
1:B:207:GLU:OE2	1:B:218:ARG:NE	2.44	0.50
1:B:66:LYS:HB2	1:C:259:GLN:HG3	1.93	0.50
1:C:139:ARG:N	1:D:300:GLU:OE2	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:MET:HG3	1:C:270:ASN:ND2	2.24	0.49
1:B:139:ARG:NH1	6:B:631:HOH:O	2.43	0.49
1:C:215:PRO:HG3	6:C:747:HOH:O	2.12	0.49
1:A:57:ARG:HD2	1:A:60:GLU:OE1	2.12	0.49
1:B:186:ASN:OD1	1:B:186:ASN:N	2.41	0.49
1:A:132:LYS:NZ	1:A:433:ARG:HH22	2.11	0.48
1:B:83:GLU:O	1:B:86:LYS:NZ	2.26	0.48
1:B:116:ASP:O	6:B:601:HOH:O	2.19	0.48
1:C:18:ASN:OD1	1:C:22:LYS:NZ	2.38	0.48
1:A:212:GLN:HG2	1:A:301:ARG:HD2	1.94	0.48
1:D:34:LEU:HD21	1:D:190:LEU:HD22	1.95	0.48
1:D:187:TYR:OH	1:D:195:GLU:OE1	2.26	0.48
1:B:57:ARG:NE	1:B:78:GLU:OE2	2.46	0.47
1:D:243:LEU:HA	1:D:248:VAL:HG11	1.96	0.47
1:C:95:SER:OG	1:C:301:ARG:NH1	2.47	0.47
1:B:139:ARG:HE	1:B:144:PHE:HE1	1.61	0.47
1:B:171:PHE:O	1:B:175:GLY:N	2.47	0.47
1:C:162:LYS:HB3	1:C:162:LYS:HE3	1.63	0.47
1:C:374:ILE:HG21	1:C:396:MET:HE3	1.96	0.47
1:A:14:TRP:HE1	1:A:109:SER:HG	1.57	0.47
1:A:131:THR:HB	1:A:150:PHE:HD2	1.79	0.47
1:A:285:ARG:NH2	1:D:293:GLU:OE1	2.40	0.47
1:C:10:ILE:HG13	1:C:321:VAL:HG21	1.97	0.47
1:A:187:TYR:OH	1:B:428:ARG:NH2	2.41	0.47
1:C:209:VAL:HB	1:D:159:VAL:HG21	1.97	0.47
1:B:293:GLU:OE1	1:C:285:ARG:NH2	2.42	0.46
1:D:211:THR:HB	1:D:300:GLU:HB3	1.98	0.46
1:D:216:ARG:NE	1:D:309:GLU:OE2	2.48	0.46
1:B:180:PHE:HB2	1:B:195:GLU:HG3	1.98	0.46
1:D:14:TRP:HA	1:D:105:GLN:NE2	2.31	0.46
1:C:187:TYR:OH	1:D:428:ARG:NH2	2.31	0.46
1:C:266:PRO:HA	1:C:267:HIS:HA	1.48	0.46
6:B:629:HOH:O	1:C:268:LYS:NZ	2.48	0.46
1:A:396:MET:HA	1:A:400:HIS:HB2	1.98	0.45
1:A:397:HIS:HA	1:A:402:ILE:H	1.80	0.45
1:C:356:TYR:O	1:C:360:LEU:HG	2.15	0.45
1:A:411:PHE:C	1:A:411:PHE:CD1	2.89	0.45
1:A:1:MET:N	6:D:634:HOH:O	2.50	0.45
1:B:242:HIS:O	1:B:245:ARG:HG2	2.16	0.45
1:A:28:LEU:HB3	1:A:48:ARG:HH21	1.81	0.45
1:B:30:ILE:HA	1:B:198:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ARG:O	1:B:288:VAL:HG12	2.16	0.45
1:A:137:MET:HB3	6:A:608:HOH:O	2.16	0.45
1:B:50:ARG:HB2	1:B:80:PHE:CE2	2.52	0.45
1:B:80:PHE:HB3	1:B:84:THR:HB	1.98	0.45
1:D:109:SER:HB3	1:D:317:PHE:CD1	2.52	0.45
1:D:131:THR:HB	1:D:150:PHE:HD2	1.82	0.45
1:A:222:LEU:HD21	1:A:317:PHE:HZ	1.82	0.45
1:B:271:PRO:HD3	1:D:143:MET:HE3	1.99	0.45
1:C:248:VAL:HG12	1:C:250:GLU:HG3	1.99	0.45
1:A:301:ARG:HH21	1:A:303:ILE:HA	1.82	0.44
1:D:196:LYS:NZ	1:D:200:ASP:OD2	2.50	0.44
1:A:349:SER:OG	1:A:352:LEU:HD12	2.17	0.44
1:D:250:GLU:OE1	1:D:344:ARG:NH1	2.50	0.44
1:B:31:LEU:HD12	1:B:88:PHE:HA	1.98	0.44
1:D:2:ILE:HD11	1:D:5:TYR:CE2	2.52	0.44
1:A:167:ASP:OD1	1:B:221:LYS:NZ	2.46	0.44
1:C:59:ASP:O	1:C:63:LYS:HG3	2.18	0.44
1:D:360:LEU:O	1:D:364:THR:OG1	2.23	0.44
1:A:396:MET:O	1:A:402:ILE:N	2.48	0.44
1:C:99:ASP:OD2	1:C:99:ASP:N	2.51	0.44
1:B:147:PRO:HD2	1:B:418:TYR:CZ	2.52	0.43
1:B:408:GLU:HG3	1:B:410:ASP:H	1.83	0.43
1:B:110:MET:HG3	6:B:696:HOH:O	2.18	0.43
1:A:311:PHE:HE1	1:D:1:MET:HA	1.82	0.43
1:C:235:ARG:HD3	1:D:295:CYS:O	2.19	0.43
1:A:37:ARG:NH1	1:A:194:ASP:OD2	2.50	0.43
1:C:147:PRO:HG2	1:C:418:TYR:CG	2.53	0.43
1:D:300:GLU:N	1:D:300:GLU:CD	2.72	0.43
1:B:386:GLU:N	6:B:649:HOH:O	2.52	0.43
1:D:243:LEU:HD23	1:D:248:VAL:HG11	2.01	0.43
1:B:149:SER:HB2	1:B:419:LEU:HG	2.01	0.42
1:C:197:LYS:HA	1:C:197:LYS:HD2	1.84	0.42
1:A:225:ILE:HD12	6:A:802:HOH:O	2.20	0.42
1:A:165:LEU:HD11	1:A:169:LYS:HE3	2.01	0.42
1:B:54:ARG:O	1:B:58:VAL:HG23	2.20	0.42
1:C:137:MET:HG2	1:C:345:VAL:HG22	2.00	0.42
1:B:159:VAL:HA	1:B:162:LYS:HB2	2.02	0.42
1:B:172:GLN:HG3	6:B:817:HOH:O	2.20	0.42
1:D:357:LEU:HA	6:D:630:HOH:O	2.18	0.42
6:B:636:HOH:O	1:C:282:ARG:NH2	2.51	0.42
1:C:415:LYS:HD3	6:C:711:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:GLN:O	1:A:341:ILE:HG12	2.20	0.42
1:B:13:ILE:HA	1:B:18:ASN:HD22	1.83	0.42
1:B:245:ARG:HA	1:D:143:MET:HE2	2.01	0.42
1:B:270:ASN:HB2	1:B:272:ILE:HG23	2.01	0.42
1:C:192:THR:HG23	6:C:631:HOH:O	2.20	0.42
1:A:132:LYS:HZ2	1:A:433:ARG:HH22	1.67	0.42
1:B:343:ASP:OD1	1:B:346:ARG:NH1	2.52	0.42
1:A:409:MET:HE3	1:A:414:ILE:HA	2.02	0.41
1:D:371:CYS:HB3	6:D:630:HOH:O	2.20	0.41
1:A:3:LYS:HA	1:A:6:ASP:HB2	2.02	0.41
1:B:26:VAL:HG11	1:B:97:ILE:HA	2.03	0.41
1:C:158:TYR:OH	6:C:604:HOH:O	2.19	0.41
1:B:300:GLU:O	1:B:301:ARG:HB3	2.20	0.41
1:C:139:ARG:HA	1:C:143:MET:O	2.20	0.41
1:A:301:ARG:NH2	1:A:303:ILE:HG13	2.35	0.41
1:A:360:LEU:HD11	1:A:392:LEU:HD11	2.02	0.41
1:A:421:GLU:OE1	1:A:424:HIS:ND1	2.35	0.41
1:D:242:HIS:O	1:D:245:ARG:HG2	2.20	0.41
1:D:245:ARG:O	1:D:249:PHE:N	2.50	0.41
1:B:86:LYS:H	1:B:86:LYS:HG3	1.72	0.41
1:B:93:THR:HB	1:B:183:ALA:HA	2.03	0.41
1:A:275:GLU:OE2	6:A:602:HOH:O	2.22	0.41
1:C:186:ASN:OD1	1:C:186:ASN:N	2.47	0.41
1:C:244:HIS:O	1:C:244:HIS:ND1	2.45	0.41
1:D:391:LYS:O	1:D:395:VAL:HG23	2.21	0.41
1:D:69:ILE:HD12	1:D:69:ILE:HA	1.91	0.40
1:C:252:TYR:CZ	1:C:335:VAL:HG11	2.56	0.40
1:C:300:GLU:O	1:C:301:ARG:HB3	2.21	0.40
1:C:396:MET:O	1:C:402:ILE:N	2.53	0.40
1:A:234:GLU:HG2	1:B:296:VAL:CG1	2.51	0.40
1:A:287:HIS:CD2	1:A:312:TYR:HB2	2.56	0.40
1:A:24:LEU:HD21	1:A:51:ALA:HB1	2.03	0.40
1:C:139:ARG:NH1	6:C:624:HOH:O	2.52	0.40
1:C:245:ARG:NH1	6:C:620:HOH:O	2.38	0.40
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.87	0.40
1:B:389:SER:OG	1:B:409:MET:HG2	2.21	0.40
1:D:406:ILE:O	1:D:406:ILE:HD12	2.22	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	413/438 (94%)	395 (96%)	17 (4%)	1 (0%)	47 39
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%)	47 39
All	All	1651/1752 (94%)	1588 (96%)	61 (4%)	2 (0%)	51 45

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%)	86 86
1	B	357/386 (92%)	355 (99%)	2 (1%)	86 86
1	C	356/386 (92%)	353 (99%)	3 (1%)	81 81
1	D	359/386 (93%)	358 (100%)	1 (0%)	92 93
All	All	1432/1544 (93%)	1424 (99%)	8 (1%)	86 86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	388	PHE
1	B	301	ARG
1	B	370	ASP
1	C	99	ASP
1	C	300	GLU
1	C	388	PHE
1	D	301	ARG

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\|>2$
4	PO4	A	503	-	4,4,4	0.90	0	6,6,6	0.45	0
5	EDO	C	505	-	3,3,3	0.44	0	2,2,2	0.32	0
5	EDO	A	504	-	3,3,3	0.44	0	2,2,2	0.38	0
5	EDO	C	504	-	3,3,3	0.46	0	2,2,2	0.30	0
4	PO4	B	503	-	4,4,4	0.89	0	6,6,6	0.44	0
3	FUM	A	502	-	7,7,7	1.14	0	8,8,8	0.89	0
5	EDO	D	503	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	505	-	3,3,3	0.44	0	2,2,2	0.37	0
4	PO4	D	502	-	4,4,4	0.93	0	6,6,6	0.44	0
3	FUM	C	502	-	7,7,7	1.14	0	8,8,8	0.95	0
3	FUM	B	502	-	7,7,7	2.72	4 (57%)	8,8,8	1.44	1 (12%)
4	PO4	C	503	-	4,4,4	0.91	0	6,6,6	0.43	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
5	EDO	C	505	-	-	0/1/1/1	-
5	EDO	A	504	-	-	0/1/1/1	-
5	EDO	C	504	-	-	0/1/1/1	-
3	FUM	A	502	-	-	4/5/5/5	-
5	EDO	A	505	-	-	0/1/1/1	-
3	FUM	C	502	-	-	4/5/5/5	-
3	FUM	B	502	-	-	2/5/5/5	-
5	EDO	D	503	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	FUM	OXT-C	-3.84	1.20	1.30
3	B	502	FUM	O8-C6	-3.50	1.21	1.30
3	B	502	FUM	C4-C	-3.36	1.40	1.48
3	B	502	FUM	C5-C6	-3.14	1.41	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	FUM	C5-C4-C	-3.50	109.27	127.26

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	FUM	OXT-C-C4-C5
3	C	502	FUM	O-C-C4-C5
3	B	502	FUM	O-C-C4-C5
3	C	502	FUM	OXT-C-C4-C5
3	A	502	FUM	OXT-C-C4-C5
3	A	502	FUM	O-C-C4-C5
3	C	502	FUM	C4-C5-C6-O7
3	C	502	FUM	C4-C5-C6-O8
3	A	502	FUM	C4-C5-C6-O8
3	A	502	FUM	C4-C5-C6-O7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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

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	419/438 (95%)	-0.39	3 (0%)	87	88	12, 30, 68, 89	0
1	B	416/438 (94%)	-0.30	4 (0%)	82	83	10, 32, 76, 94	0
1	C	422/438 (96%)	-0.34	2 (0%)	91	91	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

All (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
1	C	403	ILE	2.7
1	A	404	LEU	2.7
1	B	386	GLU	2.7
1	D	398	ASP	2.5
1	D	364	THR	2.5
1	B	249	PHE	2.2
1	A	411	PHE	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 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
3	FUM	A	502	8/8	0.77	0.17	41,46,52,53	0
3	FUM	B	502	8/8	0.90	0.12	36,42,49,51	0
3	FUM	C	502	8/8	0.92	0.11	30,31,34,36	0
5	EDO	C	504	4/4	0.92	0.14	32,32,34,35	0
5	EDO	A	504	4/4	0.94	0.11	18,19,20,21	0
5	EDO	D	503	4/4	0.95	0.09	36,37,37,38	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
4	PO4	B	503	5/5	0.98	0.08	24,26,28,28	0
4	PO4	C	503	5/5	0.99	0.08	21,22,25,26	0
4	PO4	D	502	5/5	0.99	0.08	15,18,21,22	0
2	K	A	501	1/1	0.99	0.09	23,23,23,23	0
2	K	B	501	1/1	0.99	0.08	36,36,36,36	0
2	K	C	501	1/1	0.99	0.06	38,38,38,38	0
4	PO4	A	503	5/5	0.99	0.08	17,18,22,24	0
2	K	D	501	1/1	0.99	0.10	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.