



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 12:28 AM EDT

PDB ID : 4IED  
Title : Crystal Structure of FUS-1 (OXA-85), a Class D beta-lactamase from *Fusobacterium nucleatum* subsp. *polymorphum*  
Authors : Mangani, S.; Benvenuti, M.; Docquier, J.D.  
Deposited on : 2012-12-13  
Resolution : 1.50 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

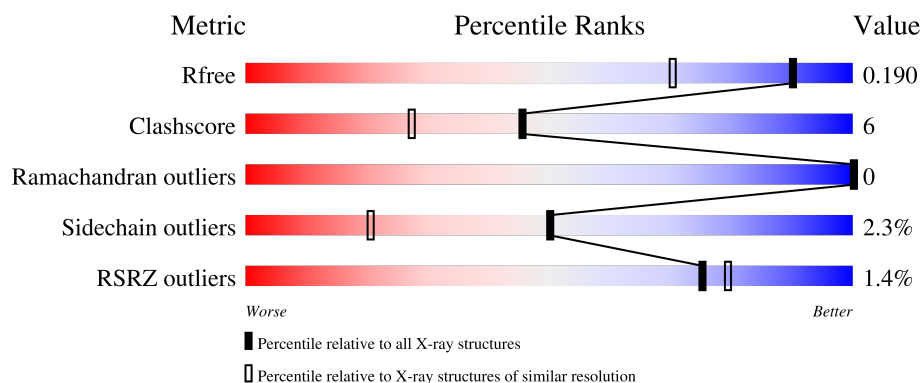
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	254	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 80%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>80%</span> <span>14%</span> <span>•• 5%</span> </div> </div>
1	B	254	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 13%, green 81%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>81%</span> <span>13%</span> <span>• •</span> </div> </div>
1	C	254	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 14%, green 83%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>83%</span> <span>14%</span> <span>• •</span> </div> </div>
1	D	254	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 9%, green 85%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>9%</span> <span>• 5%</span> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	305	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10027 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 Class D beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	10	0
			2066	1346	335	380	5			
1	B	245	Total	C	N	O	S	0	13	0
			2109	1376	341	387	5			
1	C	247	Total	C	N	O	S	0	5	0
			2068	1345	334	384	5			
1	D	242	Total	C	N	O	S	0	11	0
			2069	1349	333	382	5			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	3	Total	Mg	0	0
			3	3		
2	C	4	Total	Mg	0	0
			4	4		
2	D	3	Total	Mg	0	0
			3	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

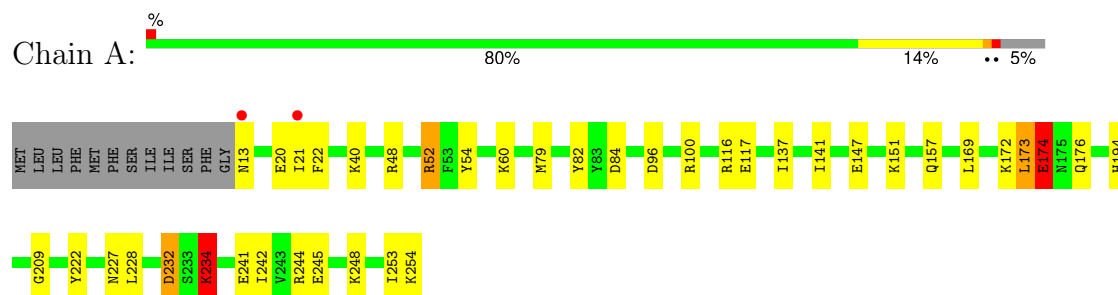
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	472	Total	O	0	0
			472	472		
6	B	416	Total	O	0	0
			416	416		
6	C	397	Total	O	0	0
			397	397		
6	D	404	Total	O	0	0
			404	404		

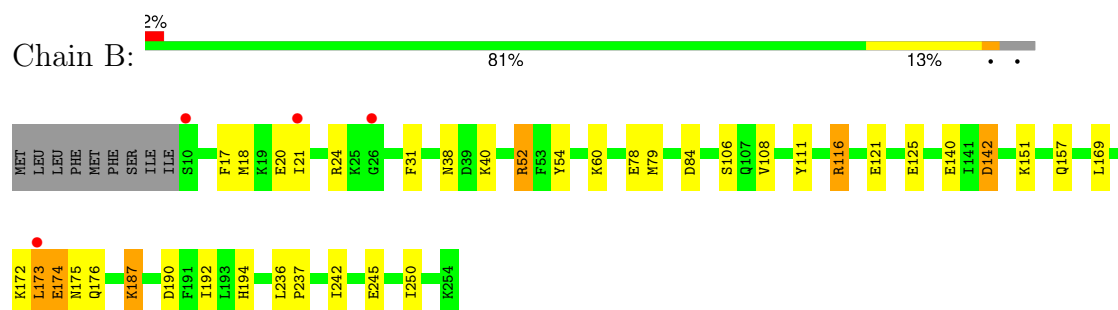
### 3 Residue-property plots [i](#)

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.

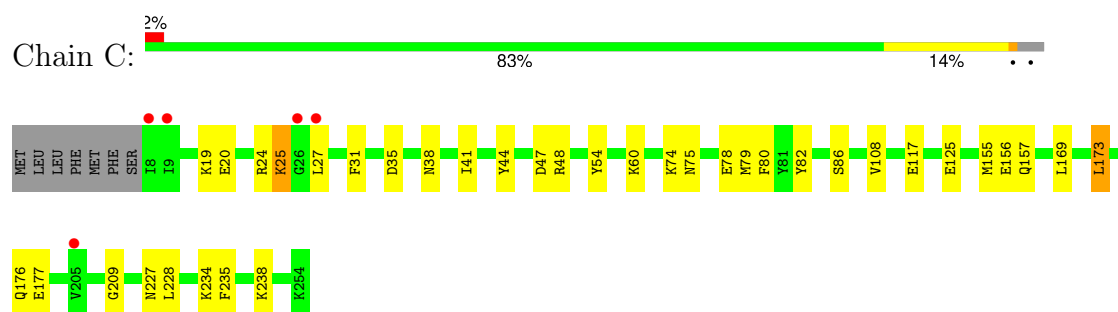
- Molecule 1: Class D beta-lactamase



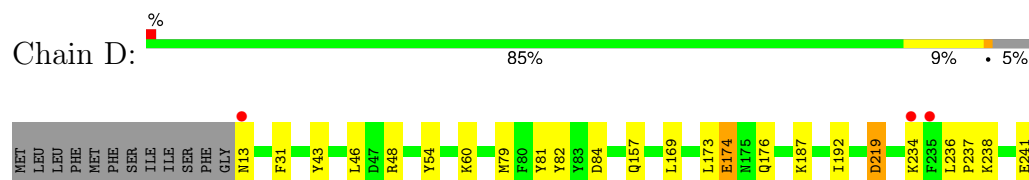
- Molecule 1: Class D beta-lactamase



- Molecule 1: Class D beta-lactamase



- Molecule 1: Class D beta-lactamase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.95Å 65.67Å 91.70Å 84.59° 82.91° 70.12°	Depositor
Resolution (Å)	37.59 – 1.50 37.59 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.5 (37.59-1.50) 95.5 (37.59-1.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.95 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.146 , 0.184 0.155 , 0.190	Depositor DCC
$R_{free}$ test set	13309 reflections (9.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.4	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10027	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL, KCX, MG, 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	1.18	4/2126 (0.2%)	1.25	16/2853 (0.6%)
1	B	1.18	5/2182 (0.2%)	1.22	18/2927 (0.6%)
1	C	1.19	7/2114 (0.3%)	1.16	9/2842 (0.3%)
1	D	1.04	0/2132	1.03	6/2861 (0.2%)
All	All	1.15	16/8554 (0.2%)	1.17	49/11483 (0.4%)

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	A	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	GLU	CD-OE1	-8.02	1.16	1.25
1	A	241	GLU	CD-OE1	6.99	1.33	1.25
1	A	82	TYR	CG-CD2	-6.51	1.30	1.39
1	B	38	ASN	CG-ND2	-6.51	1.16	1.32
1	C	54	TYR	CE1-CZ	-6.22	1.30	1.38
1	C	117	GLU	CD-OE1	6.10	1.32	1.25
1	C	125	GLU	CD-OE1	6.03	1.32	1.25
1	C	156	GLU	CD-OE2	5.61	1.31	1.25
1	C	44	TYR	CE1-CZ	-5.52	1.31	1.38
1	C	86	SER	CB-OG	-5.45	1.35	1.42
1	B	125[A]	GLU	CD-OE2	5.35	1.31	1.25
1	B	125[B]	GLU	CD-OE2	5.35	1.31	1.25
1	B	54	TYR	CG-CD2	-5.32	1.32	1.39
1	A	20	GLU	CD-OE2	5.30	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	GLU	CD-OE2	-5.17	1.20	1.25
1	A	147	GLU	CD-OE2	5.00	1.31	1.25

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	ASP	CB-CG-OD1	11.72	128.85	118.30
1	C	47	ASP	CB-CG-OD2	-11.39	108.05	118.30
1	A	100	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	B	40[A]	LYS	CD-CE-NZ	10.90	136.77	111.70
1	B	40[B]	LYS	CD-CE-NZ	10.90	136.77	111.70
1	A	234	LYS	CD-CE-NZ	9.48	133.51	111.70
1	C	173	LEU	CB-CG-CD1	8.71	125.80	111.00
1	A	48	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	B	142	ASP	CB-CG-OD2	8.17	125.65	118.30
1	B	84	ASP	CB-CG-OD1	7.99	125.49	118.30
1	A	232	ASP	CB-CG-OD2	7.80	125.32	118.30
1	B	84	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	A	173	LEU	CB-CG-CD1	7.22	123.28	111.00
1	B	140	GLU	OE1-CD-OE2	-6.97	114.94	123.30
1	C	35	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	A	48	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	147	GLU	OE1-CD-OE2	6.53	131.13	123.30
1	D	219[A]	ASP	CB-CG-OD1	6.46	124.12	118.30
1	D	219[B]	ASP	CB-CG-OD1	6.46	124.12	118.30
1	A	116[A]	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	116[B]	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	173[A]	LEU	CB-CG-CD2	-6.21	100.45	111.00
1	B	173[B]	LEU	CB-CG-CD2	-6.21	100.45	111.00
1	C	234	LYS	CD-CE-NZ	6.20	125.95	111.70
1	A	52	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	174	GLU	OE1-CD-OE2	6.11	130.63	123.30
1	A	84	ASP	CB-CG-OD1	6.06	123.76	118.30
1	C	228	LEU	CB-CG-CD2	-6.04	100.72	111.00
1	B	78	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	D	54	TYR	CB-CG-CD1	5.62	124.37	121.00
1	B	111	TYR	CB-CG-CD1	5.60	124.36	121.00
1	C	31	PHE	CB-CG-CD1	5.59	124.72	120.80
1	C	117	GLU	OE1-CD-OE2	5.56	129.98	123.30
1	C	48	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	142	ASP	OD1-CG-OD2	-5.52	112.81	123.30
1	A	54	TYR	CB-CG-CD2	-5.51	117.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	190	ASP	CB-CG-OD2	5.47	123.23	118.30
1	D	31	PHE	CB-CG-CD1	5.38	124.56	120.80
1	A	222	TYR	CG-CD2-CE2	-5.37	117.00	121.30
1	D	48	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	244	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	116[A]	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	116[B]	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	116[C]	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	31	PHE	CB-CG-CD1	5.18	124.43	120.80
1	B	54	TYR	CG-CD2-CE2	5.17	125.44	121.30
1	A	228	LEU	CB-CG-CD2	-5.13	102.28	111.00
1	D	84	ASP	CB-CG-OD1	-5.07	113.74	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	253	ILE	Peptide

## 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	2066	0	2109	31	0
1	B	2109	0	2161	28	0
1	C	2068	0	2084	29	0
1	D	2069	0	2113	18	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
3	A	1	0	0	0	0
4	A	8	0	12	9	0
4	B	4	0	6	2	0
5	B	1	0	0	0	0
6	A	472	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	416	0	0	17	0
6	C	397	0	0	8	0
6	D	404	0	0	7	0
All	All	10027	0	8485	107	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 6.

All (107) 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:B:21:ILE:HD12	1:B:242:ILE:HG23	1.41	1.00
1:A:79[B]:MET:HG2	4:A:305:EDO:O2	1.72	0.90
1:D:174:GLU:HG3	6:D:616:HOH:O	1.72	0.88
1:C:25:LYS:CG	1:C:27:LEU:HG	2.04	0.86
1:B:17:PHE:O	1:B:20[A]:GLU:HG3	1.79	0.83
1:C:25:LYS:HG3	1:C:27:LEU:HG	1.59	0.83
1:B:116[A]:ARG:NH2	1:B:142:ASP:OD2	2.12	0.81
1:A:79[B]:MET:CG	4:A:305:EDO:HO2	1.94	0.79
1:C:19[A]:LYS:HD3	6:C:572:HOH:O	1.80	0.79
1:A:117[A]:GLU:HG3	6:A:520:HOH:O	1.84	0.77
1:A:141:ILE:H	1:C:38:ASN:HD21	1.30	0.76
1:A:245[A]:GLU:HG3	6:A:609:HOH:O	1.86	0.76
1:B:21:ILE:CD1	1:B:242:ILE:HG23	2.17	0.74
1:C:79[B]:MET:CE	1:C:82:TYR:CE1	2.72	0.73
1:B:245[A]:GLU:HG3	6:B:571:HOH:O	1.90	0.72
1:A:248:LYS:NZ	6:A:852:HOH:O	2.21	0.72
1:A:137:ILE:HG22	6:A:716:HOH:O	1.90	0.72
1:D:79[B]:MET:HE2	1:D:82:TYR:CE1	2.25	0.72
1:A:79[B]:MET:HG2	4:A:305:EDO:HO2	1.48	0.72
1:D:174:GLU:CG	6:D:616:HOH:O	2.35	0.72
4:A:304:EDO:H22	1:B:236:LEU:HD13	1.73	0.71
1:C:108:VAL:CG2	6:C:795:HOH:O	2.38	0.71
1:D:79[B]:MET:HE2	1:D:82:TYR:CD1	2.26	0.70
1:A:232:ASP:OD1	1:A:234:LYS:HD3	1.92	0.70
1:C:79[B]:MET:HE2	1:C:82:TYR:CE1	2.27	0.69
1:C:177[A]:GLU:OE2	6:C:715:HOH:O	2.10	0.69
1:A:174:GLU:HG3	6:A:542:HOH:O	1.93	0.68
1:D:169:LEU:H	1:D:176:GLN:HE22	1.42	0.66
1:A:21[A]:ILE:HD12	1:A:22:PHE:N	2.10	0.66
1:B:192[A]:ILE:HG13	6:B:508:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:305:EDO:C1	6:B:786:HOH:O	2.45	0.65
1:B:108:VAL:HG21	6:B:540:HOH:O	1.99	0.63
1:B:108:VAL:CG2	6:B:540:HOH:O	2.47	0.63
1:D:192[A]:ILE:HG13	6:D:789:HOH:O	1.97	0.63
1:A:172[A]:LYS:HG2	6:A:542:HOH:O	2.00	0.62
1:B:245[A]:GLU:HG2	6:B:791:HOH:O	1.99	0.61
1:D:192[A]:ILE:CG1	6:D:789:HOH:O	2.48	0.61
1:D:79[B]:MET:CE	1:D:82:TYR:CD1	2.82	0.61
1:C:169:LEU:H	1:C:176:GLN:HE22	1.47	0.60
1:C:235:PHE:CE1	1:C:238:LYS:HG3	2.37	0.60
1:A:96:ASP:OD2	4:A:305:EDO:H22	2.02	0.60
1:C:79[B]:MET:HE1	1:C:82:TYR:CE1	2.37	0.59
1:A:96:ASP:OD2	4:A:305:EDO:C2	2.50	0.58
1:C:108:VAL:HG21	6:C:795:HOH:O	1.99	0.58
1:A:169:LEU:H	1:A:176:GLN:HE22	1.51	0.57
1:B:169:LEU:H	1:B:176:GLN:HE22	1.53	0.57
1:B:192[A]:ILE:CG1	6:B:508:HOH:O	2.51	0.57
1:A:79[B]:MET:CG	4:A:305:EDO:O2	2.46	0.57
1:D:79[B]:MET:CE	1:D:82:TYR:CE1	2.88	0.57
1:C:108:VAL:HG22	6:C:795:HOH:O	2.01	0.56
1:A:174:GLU:CG	6:A:542:HOH:O	2.53	0.56
1:A:174:GLU:CD	6:A:705:HOH:O	2.44	0.56
4:B:305:EDO:H12	6:B:786:HOH:O	2.06	0.56
1:B:17:PHE:CE1	1:B:20[A]:GLU:OE1	2.59	0.55
1:A:141:ILE:H	1:C:38:ASN:ND2	2.01	0.55
1:B:194:HIS:HE1	6:B:561:HOH:O	1.90	0.54
1:C:25:LYS:HG2	1:C:27:LEU:HG	1.87	0.54
1:C:238:LYS:HG2	6:C:651:HOH:O	2.06	0.54
1:D:187[A]:LYS:HG2	1:D:192[A]:ILE:HG12	1.90	0.53
1:C:25:LYS:H	1:C:25:LYS:HD2	1.74	0.53
1:A:174:GLU:CD	6:A:542:HOH:O	2.46	0.53
1:C:79[B]:MET:CE	1:C:82:TYR:CZ	2.92	0.53
1:C:79[B]:MET:HE3	1:C:80:PHE:N	2.24	0.52
1:B:172[A]:LYS:NZ	6:B:623:HOH:O	2.29	0.52
1:D:13:ASN:HB3	1:D:43:TYR:OH	2.09	0.51
1:B:20[A]:GLU:OE2	1:B:24:ARG:NH2	2.44	0.51
1:B:79[A]:MET:HG2	6:B:576:HOH:O	2.10	0.51
1:D:238[A]:LYS:HD2	6:D:607:HOH:O	2.12	0.50
1:C:19[A]:LYS:CD	6:C:572:HOH:O	2.51	0.49
1:C:19[A]:LYS:CG	6:C:572:HOH:O	2.61	0.49
4:A:304:EDO:C1	6:A:458:HOH:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:HIS:HE1	6:A:533:HOH:O	1.96	0.48
1:D:79[B]:MET:HE1	1:D:81:TYR:O	2.13	0.47
1:A:137:ILE:CG2	6:A:716:HOH:O	2.56	0.47
1:D:192[A]:ILE:HD11	6:D:789:HOH:O	2.14	0.47
1:A:209:GLY:O	1:A:227:ASN:HA	2.16	0.46
1:C:25:LYS:HG3	1:C:27:LEU:CG	2.39	0.46
1:B:18:MET:O	1:B:21:ILE:HG12	2.17	0.44
1:A:172[A]:LYS:HD2	1:A:174:GLU:OE1	2.17	0.44
1:A:52:ARG:HB3	1:A:151:LYS:HB3	1.98	0.44
1:C:20:GLU:O	1:C:24:ARG:HG3	2.18	0.44
1:C:79[B]:MET:HE1	1:C:82:TYR:CD1	2.52	0.44
1:D:238[A]:LYS:HD3	1:D:241:GLU:OE1	2.18	0.44
1:A:79[B]:MET:SD	4:A:305:EDO:O2	2.67	0.44
1:B:108:VAL:HG22	6:B:540:HOH:O	2.17	0.44
1:C:41:ILE:HD13	1:C:155:MET:SD	2.58	0.44
1:C:74:LYS:HE3	1:C:75:ASN:ND2	2.33	0.44
1:C:79[B]:MET:HE2	1:C:79[B]:MET:HB3	1.87	0.43
1:B:172[A]:LYS:HE2	6:B:590:HOH:O	2.17	0.43
1:A:21[A]:ILE:CD1	1:A:242:ILE:HG23	2.48	0.43
1:B:187[A]:LYS:HD3	6:B:560:HOH:O	2.19	0.42
1:B:174:GLU:OE2	1:B:175:ASN:OD1	2.36	0.42
1:C:235:PHE:CZ	1:C:238:LYS:HG3	2.54	0.42
1:C:209:GLY:O	1:C:227:ASN:HA	2.20	0.41
1:D:254:LYS:NZ	6:D:633:HOH:O	2.51	0.41
1:D:43:TYR:CE1	1:D:46:LEU:HB2	2.55	0.41
1:B:121:GLU:OE2	6:B:539:HOH:O	2.22	0.41
1:A:172[A]:LYS:HD2	1:A:174:GLU:CD	2.41	0.41
1:B:250:ILE:HG23	6:B:642:HOH:O	2.19	0.41
1:B:174:GLU:HG2	6:B:482:HOH:O	2.20	0.41
1:A:172[A]:LYS:CD	1:A:174:GLU:OE1	2.69	0.41
1:B:21:ILE:HD13	1:B:21:ILE:HG21	1.88	0.41
1:B:52:ARG:HB3	1:B:151:LYS:HB3	2.02	0.41
1:B:236:LEU:N	1:B:237:PRO:CD	2.84	0.41
1:A:21[A]:ILE:HD13	1:A:242:ILE:HG23	2.02	0.40
1:D:236:LEU:N	1:D:237:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	249/254 (98%)	244 (98%)	5 (2%)	0	100	100
1	B	256/254 (101%)	252 (98%)	4 (2%)	0	100	100
1	C	249/254 (98%)	246 (99%)	3 (1%)	0	100	100
1	D	250/254 (98%)	245 (98%)	5 (2%)	0	100	100
All	All	1004/1016 (99%)	987 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	228/229 (100%)	221 (97%)	7 (3%)	40	11
1	B	234/229 (102%)	227 (97%)	7 (3%)	41	12
1	C	227/229 (99%)	224 (99%)	3 (1%)	69	44
1	D	229/229 (100%)	223 (97%)	6 (3%)	46	16
All	All	918/916 (100%)	895 (98%)	23 (2%)	50	18

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	40	LYS

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Mol	Chain	Res	Type
1	A	157	GLN
1	A	173	LEU
1	A	174	GLU
1	A	234	LYS
1	A	254	LYS
1	B	106	SER
1	B	157	GLN
1	B	173[A]	LEU
1	B	173[B]	LEU
1	B	174	GLU
1	B	187[A]	LYS
1	B	187[B]	LYS
1	C	25	LYS
1	C	157	GLN
1	C	173	LEU
1	D	157	GLN
1	D	173	LEU
1	D	174	GLU
1	D	219[A]	ASP
1	D	219[B]	ASP
1	D	234	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	124	GLN
1	A	157	GLN
1	A	176	GLN
1	A	194	HIS
1	B	13	ASN
1	B	28	ASN
1	B	124	GLN
1	B	157	GLN
1	B	176	GLN
1	B	194	HIS
1	B	203	ASN
1	C	13	ASN
1	C	38	ASN
1	C	70	ASN
1	C	124	GLN
1	C	157	GLN

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Mol	Chain	Res	Type
1	C	176	GLN
1	D	28	ASN
1	D	38	ASN
1	D	70	ASN
1	D	124	GLN
1	D	157	GLN
1	D	176	GLN
1	D	194	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
1	KCX	B	60	1	10,11,12	1.03	0	6,12,14	2.16	1 (16%)
1	KCX	D	60	1	10,11,12	1.86	2 (20%)	6,12,14	1.63	2 (33%)
1	KCX	A	60	1	10,11,12	1.01	1 (10%)	6,12,14	2.04	2 (33%)
1	KCX	C	60	1	10,11,12	0.64	0	6,12,14	1.23	1 (16%)

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
1	KCX	B	60	1	-	0/9/10/12	-
1	KCX	D	60	1	-	0/9/10/12	-
1	KCX	A	60	1	-	2/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	C	60	1	-	1/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	60	KCX	CX-NZ	4.51	1.43	1.35
1	D	60	KCX	CB-CA	2.23	1.57	1.53
1	A	60	KCX	OQ1-CX	2.15	1.25	1.21

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	KCX	OQ1-CX-NZ	-4.88	117.51	124.92
1	A	60	KCX	OQ1-CX-NZ	-3.92	118.97	124.92
1	D	60	KCX	OQ1-CX-NZ	-3.23	120.02	124.92
1	A	60	KCX	CE-NZ-CX	3.00	127.07	121.98
1	C	60	KCX	OQ1-CX-NZ	-2.92	120.48	124.92
1	D	60	KCX	CE-NZ-CX	2.03	125.42	121.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	60	KCX	O-C-CA-CB
1	C	60	KCX	O-C-CA-CB
1	A	60	KCX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 14 are monoatomic - leaving 3 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	EDO	A	304	-	3,3,3	0.98	0	2,2,2	1.76	1 (50%)
4	EDO	B	305	-	3,3,3	0.30	0	2,2,2	0.40	0
4	EDO	A	305	-	3,3,3	0.70	0	2,2,2	0.73	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
4	EDO	A	304	-	-	1/1/1/1	-
4	EDO	B	305	-	-	0/1/1/1	-
4	EDO	A	305	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	304	EDO	O1-C1-C2	-2.40	94.11	112.39

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	304	EDO	O1-C1-C2-O2
4	A	305	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	EDO	2	0
4	B	305	EDO	2	0
4	A	305	EDO	7	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	241/254 (94%)	-0.13	2 (0%) 86 89	5, 7, 17, 34	0
1	B	244/254 (96%)	-0.10	4 (1%) 72 77	4, 8, 21, 36	0
1	C	246/254 (96%)	-0.11	5 (2%) 65 70	5, 10, 21, 35	0
1	D	241/254 (94%)	-0.18	3 (1%) 79 82	7, 11, 21, 32	0
All	All	972/1016 (95%)	-0.13	14 (1%) 75 79	4, 9, 21, 36	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	8	ILE	3.4
1	C	205	VAL	3.3
1	B	21	ILE	3.2
1	A	13	ASN	3.2
1	C	27	LEU	3.1
1	C	26	GLY	2.9
1	B	10	SER	2.9
1	D	234	LYS	2.6
1	B	26	GLY	2.6
1	B	173[A]	LEU	2.4
1	D	235	PHE	2.3
1	C	9	ILE	2.2
1	A	21[A]	ILE	2.2
1	D	13	ASN	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KCX	C	60	12/13	0.97	0.07	6,7,9,10	0
1	KCX	D	60	12/13	0.97	0.07	6,7,10,13	0
1	KCX	A	60	12/13	0.98	0.08	4,4,5,6	0
1	KCX	B	60	12/13	0.98	0.07	4,4,6,7	0

### 6.3 Carbohydrates [i](#)

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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	305	4/4	0.78	0.22	14,18,23,26	0
2	MG	D	303	1/1	0.87	0.32	38,38,38,38	0
4	EDO	B	305	4/4	0.92	0.26	23,23,25,26	0
4	EDO	A	304	4/4	0.93	0.16	15,17,17,17	0
2	MG	B	304	1/1	0.97	0.20	40,40,40,40	0
2	MG	C	303	1/1	0.97	0.14	32,32,32,32	0
2	MG	B	303	1/1	0.97	0.13	28,28,28,28	0
2	MG	C	304	1/1	0.98	0.25	23,23,23,23	0
2	MG	D	302	1/1	0.98	0.22	17,17,17,17	0
2	MG	A	301	1/1	0.98	0.28	19,19,19,19	0
2	MG	A	302	1/1	0.99	0.19	17,17,17,17	0
2	MG	C	301	1/1	0.99	0.08	13,13,13,13	0
2	MG	D	301	1/1	0.99	0.04	18,18,18,18	0
2	MG	C	302	1/1	0.99	0.14	14,14,14,14	0
5	NA	B	301	1/1	0.99	0.04	16,16,16,16	0
2	MG	B	302	1/1	1.00	0.07	7,7,7,7	0
3	CL	A	303	1/1	1.00	0.05	12,12,12,12	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.