



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:41 AM GMT

PDB ID : 3MQH
Title : crystal structure of the 3-N-acetyl transferase WlbB from Bordetella petrii in complex with CoA and UDP-3-amino-2-acetamido-2,3-dideoxy glucuronic acid
Authors : thoden, J.B.; holden, H.M.
Deposited on : 2010-04-28
Resolution : 1.43 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

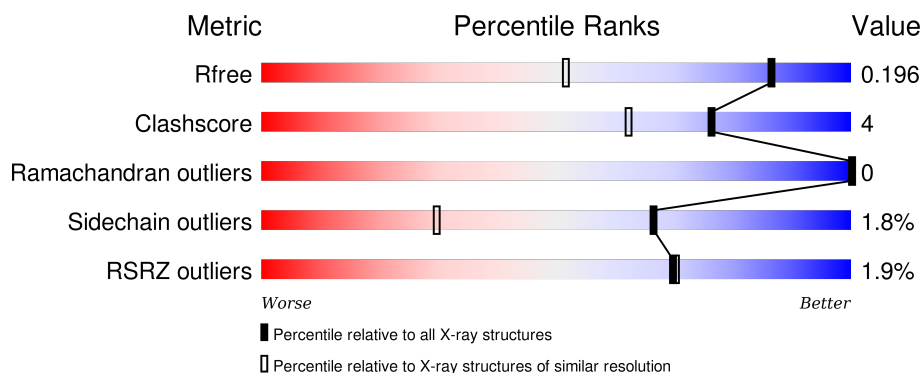
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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.



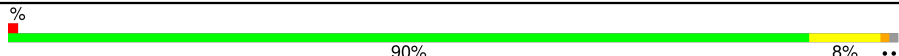
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1164 (1.46-1.42)
Clashscore	102246	1219 (1.46-1.42)
Ramachandran outliers	100387	1200 (1.46-1.42)
Sidechain outliers	100360	1200 (1.46-1.42)
RSRZ outliers	91569	1166 (1.46-1.42)

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	192	<div> <div>2%</div> <div>94%</div> <div>5% ..</div> </div>
1	B	192	<div> <div>%</div> <div>93%</div> <div>5% ..</div> </div>
1	C	192	<div> <div>3%</div> <div>93%</div> <div>6% .</div> </div>
1	D	192	<div> <div>3%</div> <div>95%</div> <div>. .</div> </div>
1	E	192	<div> <div>2%</div> <div>93%</div> <div>6% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	192	

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	193	-	-	-	X
4	EDO	A	195	-	-	-	X
4	EDO	B	194	-	-	X	X
4	EDO	C	196	-	-	-	X
4	EDO	D	195	-	-	-	X
6	PO4	C	193	-	-	-	X
6	PO4	F	193	-	-	-	X
7	PE4	C	197	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11106 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 Lipopolysaccharides biosynthesis acetyltransferase.

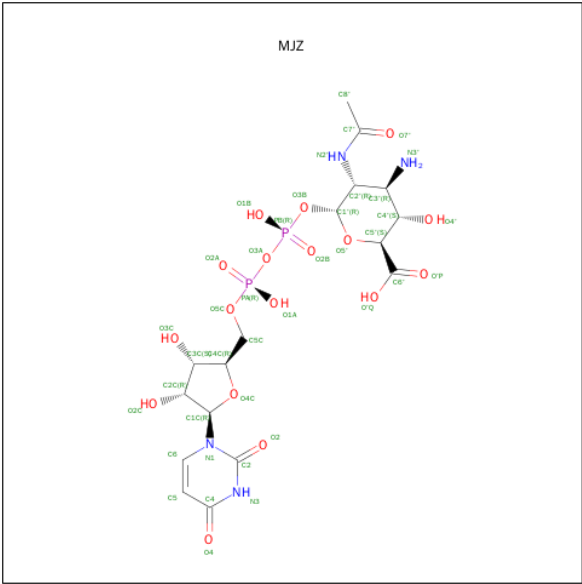
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	2	0
			1464	913	276	265	10			
1	B	189	Total	C	N	O	S	0	5	0
			1467	916	271	271	9			
1	C	192	Total	C	N	O	S	0	4	0
			1477	924	276	268	9			
1	D	192	Total	C	N	O	S	0	2	0
			1467	918	273	266	10			
1	E	192	Total	C	N	O	S	0	3	0
			1475	920	273	272	10			
1	F	190	Total	C	N	O	S	0	1	0
			1446	902	269	266	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP A9IH93
A	0	HIS	-	EXPRESSION TAG	UNP A9IH93
B	-1	GLY	-	EXPRESSION TAG	UNP A9IH93
B	0	HIS	-	EXPRESSION TAG	UNP A9IH93
C	-1	GLY	-	EXPRESSION TAG	UNP A9IH93
C	0	HIS	-	EXPRESSION TAG	UNP A9IH93
D	-1	GLY	-	EXPRESSION TAG	UNP A9IH93
D	0	HIS	-	EXPRESSION TAG	UNP A9IH93
E	-1	GLY	-	EXPRESSION TAG	UNP A9IH93
E	0	HIS	-	EXPRESSION TAG	UNP A9IH93
F	-1	GLY	-	EXPRESSION TAG	UNP A9IH93
F	0	HIS	-	EXPRESSION TAG	UNP A9IH93

- Molecule 2 is (2S,3S,4R,5R,6R)-5-(ACETYLAMINO)-4-AMINO-6-{{[(R)-{[(R)-{[(2R,3S,4R,5R)-5-(2,4-DIOXO-3,4-DIHYDROPYRIMIDIN-1(2H)-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHOXY}(HYDROXY)PHOSPHORYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-3-HYDROXYTETRAHYDRO-2H-PYRAN-2-CARBOXYLIC ACID

(three-letter code: MJZ) (formula: C₁₇H₂₆N₄O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			40	17	4	17	2		
2	B	1	Total	C	N	O	P	0	0
			40	17	4	17	2		
2	C	1	Total	C	N	O	P	0	0
			40	17	4	17	2		
2	D	1	Total	C	N	O	P	0	0
			40	17	4	17	2		
2	E	1	Total	C	N	O	P	0	0
			40	17	4	17	2		
2	F	1	Total	C	N	O	P	0	0
			40	17	4	17	2		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

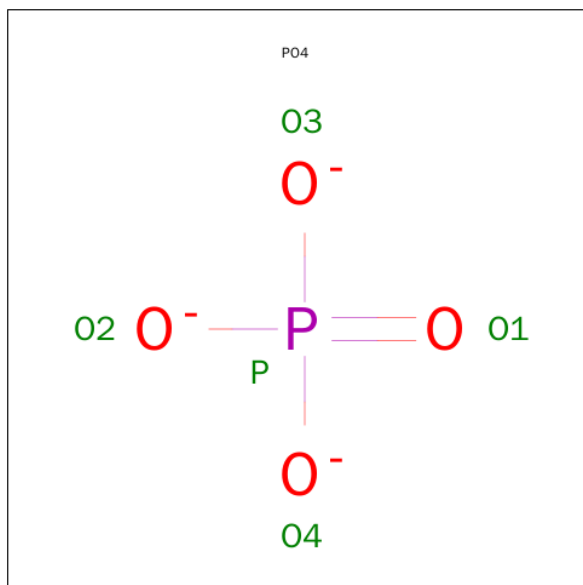


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total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

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

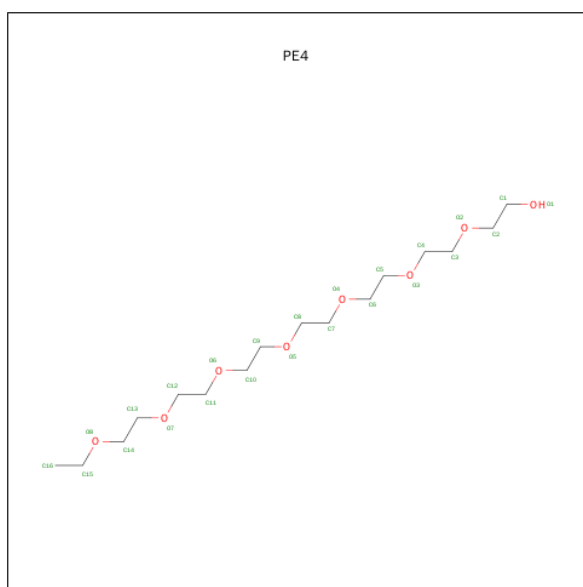
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			5	4	1		
6	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			24	16	8		

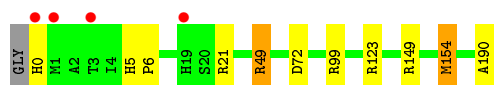
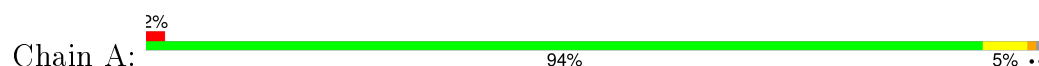
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	277	Total O 277 277	0	0
8	B	281	Total O 281 281	0	0
8	C	280	Total O 280 280	0	0
8	D	280	Total O 280 280	0	0
8	E	285	Total O 285 285	0	0
8	F	295	Total O 295 295	0	0

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.

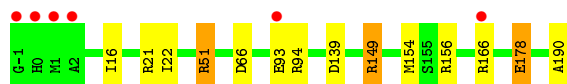
- Molecule 1: Lipopolysaccharides biosynthesis acetyltransferase



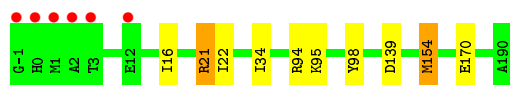
- Molecule 1: Lipopolysaccharides biosynthesis acetyltransferase



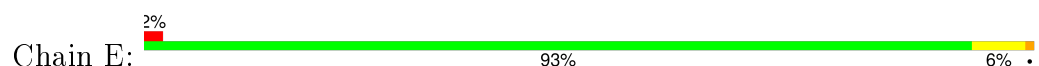
- Molecule 1: Lipopolysaccharides biosynthesis acetyltransferase



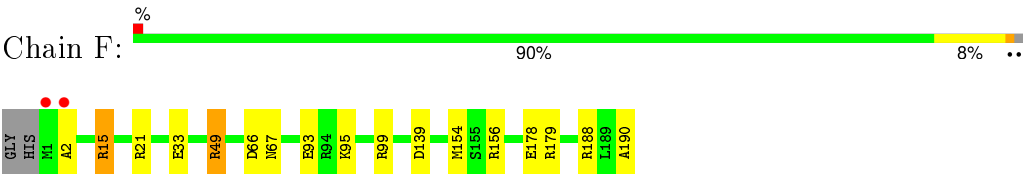
- Molecule 1: Lipopolysaccharides biosynthesis acetyltransferase



- Molecule 1: Lipopolysaccharides biosynthesis acetyltransferase



- Molecule 1: Lipopolysaccharides biosynthesis acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.47Å 107.89Å 91.27Å 90.00° 102.55° 90.00°	Depositor
Resolution (Å)	30.00 – 1.43 25.07 – 1.43	Depositor EDS
% Data completeness (in resolution range)	89.9 (30.00-1.43) 89.9 (25.07-1.43)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.38 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.174 , 0.206 0.166 , 0.196	Depositor DCC
R_{free} test set	10686 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	8.8	Xtriage
Anisotropy	0.892	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 62.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	7 of 213775 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11106	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.99 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6290e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PE4, NA, PO4, EDO, COA, MJZ

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	0.56	0/1499	1.03	4/2034 (0.2%)
1	B	0.55	0/1511	1.00	4/2051 (0.2%)
1	C	0.56	0/1519	1.07	7/2062 (0.3%)
1	D	0.54	0/1503	0.98	3/2041 (0.1%)
1	E	0.55	0/1514	1.02	4/2055 (0.2%)
1	F	0.59	0/1478	1.09	6/2008 (0.3%)
All	All	0.56	0/9024	1.03	28/12251 (0.2%)

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	E	0	1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	179	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	A	72	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	C	66	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	C	94	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	E	139	ASP	CB-CG-OD1	6.79	124.41	118.30
1	E	72	ASP	CB-CG-OD1	6.68	124.31	118.30
1	F	139	ASP	CB-CG-OD1	6.61	124.25	118.30
1	D	139	ASP	CB-CG-OD1	6.25	123.93	118.30
1	F	179	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	C	139	ASP	CB-CG-OD1	6.09	123.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	99	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	D	94	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	F	15	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	F	66	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	B	72	ASP	CB-CG-OD1	5.93	123.63	118.30
1	F	188	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	C	178	GLU	CG-CD-OE1	-5.54	107.23	118.30
1	A	154	MET	CA-CB-CG	5.49	122.63	113.30
1	A	99	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	C	66	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	123	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	51	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	B	73	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	B	11	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	E	179	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	D	154	MET	CG-SD-CE	5.03	108.24	100.20
1	C	94	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	B	99	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	-1	GLY	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	1464	0	1447	6	0
1	B	1467	0	1444	14	0
1	C	1477	0	1462	11	0
1	D	1467	0	1451	9	0
1	E	1475	0	1447	15	1
1	F	1446	0	1418	15	1
2	A	40	0	23	0	0
2	B	40	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	40	0	23	0	0
2	D	40	0	23	0	0
2	E	40	0	23	0	0
2	F	40	0	23	0	0
3	A	48	0	32	0	0
3	B	48	0	32	0	0
3	C	48	0	32	0	0
3	D	48	0	32	0	0
3	E	48	0	32	0	0
3	F	48	0	32	0	0
4	A	8	0	12	0	0
4	B	8	0	12	9	0
4	C	12	0	18	0	0
4	D	12	0	18	0	0
4	E	4	0	6	0	0
4	F	4	0	6	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	C	5	0	0	0	0
6	F	5	0	0	0	0
7	C	24	0	34	1	0
8	A	277	0	0	3	2
8	B	281	0	0	3	3
8	C	280	0	0	3	3
8	D	280	0	0	3	1
8	E	285	0	0	7	0
8	F	295	0	0	6	1
All	All	11106	0	9105	70	6

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 (70) 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:148:ALA:HB3	4:B:194:EDO:C2	1.77	1.14
1:E:149:ARG:HH11	1:E:149:ARG:HG3	1.14	1.12
1:F:95:LYS:NZ	8:F:965:HOH:O	1.83	1.11
1:E:149:ARG:HD3	8:E:1441:HOH:O	1.52	1.08
1:D:95:LYS:NZ	8:D:1747:HOH:O	1.87	1.07
1:B:148:ALA:HB3	4:B:194:EDO:H22	1.08	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:ARG:HH11	1:E:149:ARG:CG	1.69	1.04
1:D:170:GLU:OE1	8:D:792:HOH:O	1.90	0.89
1:C:149[A]:ARG:HG3	1:C:149[A]:ARG:HH11	1.39	0.88
1:C:149[A]:ARG:HH11	1:C:149[A]:ARG:CG	1.88	0.87
1:E:135:LYS:NZ	8:E:1435:HOH:O	2.07	0.86
1:B:149:ARG:NH2	8:B:2400:HOH:O	1.99	0.85
1:D:16[B]:ILE:HD13	1:D:22[B]:ILE:HD11	1.63	0.81
1:F:15:ARG:NH1	1:F:33:GLU:HG3	2.01	0.75
1:E:149:ARG:HG3	1:E:149:ARG:NH1	1.91	0.74
1:C:190:ALA:O	8:C:2417:HOH:O	2.06	0.74
1:F:15:ARG:HH12	1:F:33:GLU:HG3	1.52	0.74
1:D:21:ARG:HH21	1:D:21:ARG:HG3	1.53	0.73
1:E:156:ARG:NH2	1:E:178:GLU:OE2	2.20	0.71
1:E:149:ARG:NH1	8:E:710:HOH:O	2.23	0.71
1:C:16:ILE:HD13	1:C:22[B]:ILE:HD11	1.74	0.70
1:C:149[A]:ARG:NH1	8:C:2125:HOH:O	1.74	0.67
1:C:21:ARG:HG3	1:C:21:ARG:HH11	1.61	0.66
1:E:149:ARG:CD	8:E:1441:HOH:O	2.22	0.66
1:E:149:ARG:NH1	1:E:149:ARG:CG	2.41	0.66
1:A:190:ALA:O	8:A:2145:HOH:O	2.14	0.65
1:D:16[B]:ILE:HD13	1:D:22[B]:ILE:CD1	2.26	0.65
1:F:15:ARG:HH12	1:F:33:GLU:CG	2.08	0.65
1:C:156:ARG:NH2	1:C:178:GLU:OE1	2.27	0.65
1:F:156:ARG:NH2	1:F:178:GLU:OE1	2.28	0.65
1:B:133:VAL:HG13	4:B:194:EDO:C1	2.26	0.64
1:B:21:ARG:NH2	8:B:427:HOH:O	2.30	0.64
1:B:133:VAL:HG13	4:B:194:EDO:H11	1.79	0.63
1:E:149:ARG:NE	8:E:1441:HOH:O	2.33	0.61
1:C:16:ILE:HD13	1:C:22[B]:ILE:CD1	2.32	0.58
1:F:21:ARG:NH2	8:F:1059:HOH:O	2.16	0.58
1:C:51:ARG:HH21	7:C:197:PE4:H42	1.69	0.57
1:B:148:ALA:CB	4:B:194:EDO:C2	2.70	0.57
1:F:15:ARG:HH12	1:F:33:GLU:CB	2.18	0.57
1:C:149[A]:ARG:NH1	1:C:149[A]:ARG:CG	2.58	0.56
1:F:15:ARG:HH12	1:F:33:GLU:HB2	1.72	0.55
1:E:149:ARG:HG2	1:E:149:ARG:HH11	1.67	0.54
1:B:148:ALA:HB3	4:B:194:EDO:H21	1.80	0.53
1:E:156:ARG:NH1	8:E:1407:HOH:O	2.43	0.51
1:A:0:HIS:CB	8:A:1232:HOH:O	2.58	0.51
1:B:148:ALA:O	4:B:194:EDO:H21	2.11	0.51
1:F:15:ARG:HH11	1:F:15:ARG:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:ARG:CG	1:D:21:ARG:HH21	2.22	0.50
1:C:149[A]:ARG:NH2	8:C:2125:HOH:O	2.47	0.48
1:F:95:LYS:NZ	8:F:1299:HOH:O	2.37	0.48
1:B:21:ARG:HD2	8:B:2122:HOH:O	2.12	0.48
1:E:188:ARG:NE	8:E:1337:HOH:O	2.27	0.47
1:B:133:VAL:HG13	4:B:194:EDO:H12	1.96	0.47
1:A:5:HIS:CG	1:A:6:PRO:HD2	2.49	0.47
1:A:149:ARG:NH2	8:A:2138:HOH:O	2.01	0.47
1:B:133:VAL:HA	4:B:194:EDO:H22	1.97	0.46
1:F:95:LYS:CE	8:F:1299:HOH:O	2.64	0.46
1:B:135:LYS:HE3	1:B:135:LYS:HB3	1.30	0.44
1:F:156:ARG:NH1	8:F:1372:HOH:O	2.51	0.44
1:B:95:LYS:HA	1:B:98:TYR:CE1	2.53	0.43
1:D:16[A]:ILE:CD1	1:D:34:ILE:HD12	2.49	0.42
1:F:49:ARG:HD2	1:F:67:ASN:OD1	2.20	0.42
1:A:21:ARG:HH11	1:A:21:ARG:HG3	1.86	0.41
1:E:49:ARG:HE	1:E:49:ARG:HB2	1.65	0.41
1:D:95:LYS:HA	1:D:98:TYR:CE1	2.56	0.41
1:D:170:GLU:CD	8:D:792:HOH:O	2.50	0.41
1:F:2:ALA:O	8:F:1519:HOH:O	2.21	0.41
1:E:168:ASN:HA	1:E:182:LEU:O	2.21	0.40
1:F:15:ARG:NH1	1:F:15:ARG:HB2	2.36	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:ARG:NH2	8:F:1760:HOH:O[2_655]	1.72	0.48
8:A:1907:HOH:O	8:C:2063:HOH:O[2_554]	1.89	0.31
8:B:1150:HOH:O	8:C:1710:HOH:O[2_554]	1.89	0.31
8:B:662:HOH:O	8:C:1698:HOH:O[2_554]	1.92	0.28
8:A:1678:HOH:O	8:B:1216:HOH:O[1_455]	2.12	0.08
1:F:190:ALA:O	8:D:901:HOH:O[2_545]	2.19	0.01

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	191/192 (100%)	188 (98%)	3 (2%)	0	100	100
1	B	192/192 (100%)	189 (98%)	3 (2%)	0	100	100
1	C	194/192 (101%)	190 (98%)	4 (2%)	0	100	100
1	D	192/192 (100%)	188 (98%)	4 (2%)	0	100	100
1	E	193/192 (100%)	190 (98%)	3 (2%)	0	100	100
1	F	189/192 (98%)	184 (97%)	5 (3%)	0	100	100
All	All	1151/1152 (100%)	1129 (98%)	22 (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	152/151 (101%)	149 (98%)	3 (2%)	63	25
1	B	154/151 (102%)	153 (99%)	1 (1%)	90	73
1	C	154/151 (102%)	149 (97%)	5 (3%)	46	11
1	D	153/151 (101%)	151 (99%)	2 (1%)	76	44
1	E	154/151 (102%)	150 (97%)	4 (3%)	54	16
1	F	150/151 (99%)	147 (98%)	3 (2%)	63	25
All	All	917/906 (101%)	899 (98%)	18 (2%)	66	25

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

Mol	Chain	Res	Type
1	A	49[A]	ARG
1	A	49[B]	ARG
1	A	154	MET

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Mol	Chain	Res	Type
1	B	135	LYS
1	C	93	GLU
1	C	149[A]	ARG
1	C	149[B]	ARG
1	C	154	MET
1	C	166	ARG
1	D	21	ARG
1	D	154	MET
1	E	0	HIS
1	E	134	ASN
1	E	135	LYS
1	E	149	ARG
1	F	49	ARG
1	F	93	GLU
1	F	154	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	134	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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
2	MJZ	A	191	-	30,42,42	0.94	1 (3%)	42,64,64	1.57	4 (9%)
3	COA	A	192	-	40,50,50	0.81	2 (5%)	50,75,75	1.55	8 (16%)
4	EDO	A	193	-	3,3,3	0.48	0	2,2,2	0.53	0
4	EDO	A	195	-	3,3,3	0.51	0	2,2,2	0.29	0
2	MJZ	B	191	-	30,42,42	0.98	1 (3%)	42,64,64	1.33	4 (9%)
3	COA	B	192	-	40,50,50	0.87	1 (2%)	50,75,75	1.43	6 (12%)
4	EDO	B	193	-	3,3,3	0.46	0	2,2,2	0.17	0
4	EDO	B	194	-	3,3,3	0.40	0	2,2,2	0.47	0
3	COA	C	191	-	40,50,50	0.82	1 (2%)	50,75,75	1.86	10 (20%)
2	MJZ	C	192	-	30,42,42	0.98	1 (3%)	42,64,64	1.78	4 (9%)
6	PO4	C	193	-	4,4,4	1.10	1 (25%)	6,6,6	0.35	0
4	EDO	C	194	-	3,3,3	0.45	0	2,2,2	0.46	0
4	EDO	C	195	-	3,3,3	0.39	0	2,2,2	0.52	0
4	EDO	C	196	-	3,3,3	0.53	0	2,2,2	0.69	0
7	PE4	C	197	-	23,23,23	0.49	0	22,22,22	0.88	1 (4%)
2	MJZ	D	191	-	30,42,42	1.11	2 (6%)	42,64,64	1.63	5 (11%)
3	COA	D	192	-	40,50,50	0.86	1 (2%)	50,75,75	1.50	5 (10%)
4	EDO	D	193	-	3,3,3	0.55	0	2,2,2	0.45	0
4	EDO	D	194	-	3,3,3	0.46	0	2,2,2	0.41	0
4	EDO	D	195	-	3,3,3	0.47	0	2,2,2	0.52	0
2	MJZ	E	191	-	30,42,42	0.88	1 (3%)	42,64,64	1.31	5 (11%)
3	COA	E	192	-	40,50,50	0.86	1 (2%)	50,75,75	2.31	11 (22%)
4	EDO	E	193	-	3,3,3	0.53	0	2,2,2	0.46	0
3	COA	F	191	-	40,50,50	0.80	1 (2%)	50,75,75	1.53	9 (18%)
2	MJZ	F	192	-	30,42,42	1.01	1 (3%)	42,64,64	1.79	7 (16%)
6	PO4	F	193	-	4,4,4	1.04	0	6,6,6	0.33	0
4	EDO	F	194	-	3,3,3	0.44	0	2,2,2	0.51	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
2	MJZ	A	191	-	-	0/20/65/65	0/3/3/3
3	COA	A	192	-	-	0/44/64/64	0/3/3/3
4	EDO	A	193	-	-	0/1/1/1	0/0/0/0
4	EDO	A	195	-	-	0/1/1/1	0/0/0/0
2	MJZ	B	191	-	-	0/20/65/65	0/3/3/3
3	COA	B	192	-	-	0/44/64/64	0/3/3/3
4	EDO	B	193	-	-	0/1/1/1	0/0/0/0
4	EDO	B	194	-	-	0/1/1/1	0/0/0/0
3	COA	C	191	-	-	0/44/64/64	0/3/3/3
2	MJZ	C	192	-	-	0/20/65/65	0/3/3/3
6	PO4	C	193	-	-	0/0/0/0	0/0/0/0
4	EDO	C	194	-	-	0/1/1/1	0/0/0/0
4	EDO	C	195	-	-	0/1/1/1	0/0/0/0
4	EDO	C	196	-	-	0/1/1/1	0/0/0/0
7	PE4	C	197	-	-	0/21/21/21	0/0/0/0
2	MJZ	D	191	-	-	0/20/65/65	0/3/3/3
3	COA	D	192	-	-	0/44/64/64	0/3/3/3
4	EDO	D	193	-	-	0/1/1/1	0/0/0/0
4	EDO	D	194	-	-	0/1/1/1	0/0/0/0
4	EDO	D	195	-	-	0/1/1/1	0/0/0/0
2	MJZ	E	191	-	-	0/20/65/65	0/3/3/3
3	COA	E	192	-	-	0/44/64/64	0/3/3/3
4	EDO	E	193	-	-	0/1/1/1	0/0/0/0
3	COA	F	191	-	-	0/44/64/64	0/3/3/3
2	MJZ	F	192	-	-	0/20/65/65	0/3/3/3
6	PO4	F	193	-	-	0/0/0/0	0/0/0/0
4	EDO	F	194	-	-	0/1/1/1	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	192	COA	O4B-C1B	2.07	1.43	1.41
3	A	192	COA	OAP-CAP	2.08	1.46	1.42
6	C	193	PO4	P-O4	2.10	1.60	1.53
3	A	192	COA	C5A-C4A	2.24	1.45	1.40
3	B	192	COA	C5A-C4A	2.36	1.45	1.40
2	D	191	MJZ	O4C-C1C	2.49	1.44	1.41
3	D	192	COA	C5A-C4A	2.53	1.46	1.40
3	F	191	COA	C5A-C4A	2.60	1.46	1.40
3	C	191	COA	C5A-C4A	2.62	1.46	1.40
2	E	191	MJZ	C3'-N3'	3.18	1.52	1.47
2	A	191	MJZ	C3'-N3'	3.26	1.52	1.47
2	F	192	MJZ	C3'-N3'	3.77	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	192	MJZ	C3'-N3'	4.03	1.53	1.47
2	B	191	MJZ	C3'-N3'	4.09	1.53	1.47
2	D	191	MJZ	C3'-N3'	4.22	1.53	1.47

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	192	COA	N3A-C2A-N1A	-9.30	121.77	128.89
3	C	191	COA	N3A-C2A-N1A	-7.58	123.09	128.89
3	B	192	COA	N3A-C2A-N1A	-5.22	124.89	128.89
2	A	191	MJZ	O5'-C1'-O3B	-5.20	104.50	111.36
3	A	192	COA	N3A-C2A-N1A	-4.79	125.23	128.89
3	D	192	COA	C1B-N9A-C4A	-4.71	119.83	126.94
3	E	192	COA	C2P-C3P-N4P	-4.52	103.44	112.37
3	D	192	COA	N3A-C2A-N1A	-4.23	125.65	128.89
2	F	192	MJZ	C8'-C7'-N2'	-4.09	108.28	116.11
3	F	191	COA	C1B-N9A-C4A	-3.96	120.96	126.94
3	E	192	COA	C3P-N4P-C5P	-3.63	115.65	122.79
2	C	192	MJZ	O5'-C1'-O3B	-3.59	106.62	111.36
3	E	192	COA	O9A-P3B-O8A	-3.59	93.72	107.38
3	A	192	COA	C2B-C1B-N9A	-3.56	108.86	114.29
2	F	192	MJZ	O5'-C1'-O3B	-3.43	106.83	111.36
3	F	191	COA	C7P-C6P-C5P	-3.37	106.76	112.31
2	D	191	MJZ	O4'-C4'-C3'	-3.27	104.78	110.31
3	C	191	COA	C1B-N9A-C4A	-3.25	122.04	126.94
3	C	191	COA	CDP-CBP-CAP	-3.15	103.60	109.34
2	B	191	MJZ	O4'-C4'-C3'	-3.14	105.00	110.31
3	E	192	COA	O9A-P3B-O7A	-3.05	100.75	110.58
3	A	192	COA	C4B-O4B-C1B	-3.02	106.39	109.72
3	C	191	COA	C2B-C1B-N9A	-3.00	109.71	114.29
3	D	192	COA	C7P-C6P-C5P	-2.95	107.45	112.31
3	C	191	COA	C7P-C6P-C5P	-2.88	107.57	112.31
3	B	192	COA	C7P-C6P-C5P	-2.87	107.58	112.31
3	C	191	COA	C3P-N4P-C5P	-2.75	117.38	122.79
2	C	192	MJZ	C8'-C7'-N2'	-2.71	110.92	116.11
3	D	192	COA	O4B-C1B-N9A	-2.63	102.60	108.10
3	B	192	COA	C1B-N9A-C4A	-2.62	122.98	126.94
3	A	192	COA	C7P-C6P-C5P	-2.53	108.14	112.31
3	C	191	COA	O3B-P3B-O7A	-2.50	100.88	107.11
2	D	191	MJZ	C8'-C7'-N2'	-2.48	111.35	116.11
3	A	192	COA	CDP-CBP-CAP	-2.44	104.90	109.34
2	E	191	MJZ	O5'-C1'-O3B	-2.43	108.16	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	191	MJZ	O4'-C4'-C3'	-2.37	106.31	110.31
2	F	192	MJZ	O2C-C2C-C3C	-2.36	104.14	111.83
3	F	191	COA	N3A-C2A-N1A	-2.35	127.10	128.89
2	E	191	MJZ	O4C-C4C-C3C	-2.34	100.44	105.15
3	A	192	COA	O4B-C1B-N9A	-2.30	103.28	108.10
3	F	191	COA	CDP-CBP-CAP	-2.28	105.18	109.34
3	F	191	COA	C4A-C5A-N7A	-2.27	107.39	109.48
3	E	192	COA	O5P-C5P-C6P	-2.24	118.11	121.98
3	C	191	COA	C2P-C3P-N4P	-2.19	108.04	112.37
3	A	192	COA	C1B-N9A-C4A	-2.17	123.66	126.94
7	C	197	PE4	O6-C10-C9	-2.17	100.71	110.36
3	B	192	COA	O3B-C3B-C2B	-2.15	103.15	111.51
3	F	191	COA	O4B-C1B-N9A	-2.11	103.68	108.10
2	B	191	MJZ	O5'-C5'-C4'	-2.10	105.16	108.76
3	D	192	COA	CDP-CBP-CAP	-2.09	105.52	109.34
2	E	191	MJZ	O3A-PA-O5C	-2.03	97.55	102.94
2	B	191	MJZ	O7'-C7'-N2'	2.01	125.96	121.86
2	D	191	MJZ	PB-O3A-PA	2.06	138.50	132.73
3	B	192	COA	O2B-C2B-C3B	2.11	117.25	111.16
2	C	192	MJZ	PB-O3A-PA	2.14	138.73	132.73
3	F	191	COA	CEP-CBP-CAP	2.14	113.25	109.34
3	E	192	COA	O2B-C2B-C3B	2.21	117.55	111.16
2	A	191	MJZ	C1'-O5'-C5'	2.25	115.67	112.17
2	E	191	MJZ	C4C-O4C-C1C	2.33	112.28	109.72
2	F	192	MJZ	PB-O3A-PA	2.40	139.46	132.73
3	B	192	COA	O8A-P3B-O7A	2.42	118.36	110.58
3	E	192	COA	C2A-N1A-C6A	2.43	123.11	118.77
2	F	192	MJZ	O1B-PB-O2B	2.43	125.72	112.53
3	F	191	COA	O8A-P3B-O7A	2.65	119.11	110.58
3	A	192	COA	CEP-CBP-CAP	2.75	114.36	109.34
2	D	191	MJZ	C1'-O5'-C5'	2.77	116.48	112.17
2	F	192	MJZ	O7'-C7'-N2'	2.83	127.63	121.86
3	E	192	COA	CEP-CBP-CAP	2.93	114.69	109.34
3	C	191	COA	C2A-N1A-C6A	3.01	124.15	118.77
3	C	191	COA	CDP-CBP-CCP	3.36	112.86	108.50
3	F	191	COA	CDP-CBP-CCP	3.39	112.89	108.50
3	E	192	COA	C7P-N8P-C9P	3.70	129.85	122.53
2	B	191	MJZ	C4-N3-C2	4.78	118.87	114.14
2	E	191	MJZ	C4-N3-C2	4.81	118.90	114.14
2	A	191	MJZ	C4-N3-C2	6.20	120.28	114.14
2	D	191	MJZ	C4-N3-C2	6.65	120.72	114.14
3	E	192	COA	O8A-P3B-O7A	7.13	133.53	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	192	MJZ	C4-N3-C2	7.36	121.43	114.14
2	C	192	MJZ	C4-N3-C2	8.53	122.59	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	194	EDO	9	0
7	C	197	PE4	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, 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	191/192 (99%)	0.13	4 (2%) 67 68	5, 10, 18, 30	0
1	B	189/192 (98%)	0.11	1 (0%) 91 93	5, 9, 22, 29	0
1	C	192/192 (100%)	0.03	6 (3%) 52 53	5, 9, 20, 33	0
1	D	192/192 (100%)	0.02	6 (3%) 52 53	5, 9, 19, 33	0
1	E	192/192 (100%)	0.10	3 (1%) 74 75	5, 9, 22, 37	0
1	F	190/192 (98%)	0.06	2 (1%) 82 83	5, 9, 21, 29	0
All	All	1146/1152 (99%)	0.08	22 (1%) 70 70	5, 9, 21, 37	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-1	GLY	6.3
1	E	0	HIS	6.3
1	D	1	MET	6.3
1	E	-1	GLY	5.9
1	F	1	MET	5.2
1	C	1	MET	5.0
1	D	-1	GLY	4.2
1	D	2	ALA	4.0
1	C	0	HIS	3.9
1	D	0	HIS	3.5
1	E	1	MET	3.4
1	C	2	ALA	3.2
1	A	1	MET	3.1
1	A	0	HIS	3.1
1	F	2	ALA	2.7
1	C	166	ARG	2.4
1	D	12	GLU	2.3
1	B	3	THR	2.2
1	A	3	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	3	THR	2.1
1	A	19	HIS	2.1
1	C	93	GLU	2.0

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
4	EDO	A	193	4/4	0.92	0.12	7.05	13,14,17,17	0
6	PO4	C	193	5/5	0.89	0.17	7.02	20,21,25,31	0
6	PO4	F	193	5/5	0.93	0.14	4.33	20,22,25,35	0
4	EDO	A	195	4/4	0.89	0.23	3.42	22,28,30,35	0
4	EDO	C	196	4/4	0.90	0.11	2.60	19,21,23,23	0
7	PE4	C	197	24/24	0.89	0.12	2.48	18,25,32,38	0
4	EDO	B	194	4/4	0.96	0.16	2.26	15,21,25,26	0
4	EDO	D	195	4/4	0.94	0.10	2.11	19,19,20,20	0
4	EDO	E	193	4/4	0.94	0.09	1.88	14,14,19,21	0
4	EDO	D	193	4/4	0.93	0.09	1.10	11,14,19,20	0
4	EDO	B	193	4/4	0.97	0.07	0.51	13,14,15,19	0
3	COA	C	191	48/48	0.96	0.08	0.30	5,8,24,30	0
3	COA	D	192	48/48	0.96	0.08	0.22	5,7,21,27	0
3	COA	A	192	48/48	0.95	0.09	0.20	5,9,25,29	0
3	COA	F	191	48/48	0.96	0.09	0.11	5,9,30,35	0
4	EDO	F	194	4/4	0.96	0.08	-0.04	17,17,18,21	0
3	COA	B	192	48/48	0.96	0.09	-0.11	4,7,27,31	0
5	NA	D	196	1/1	0.99	0.07	-0.13	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	COA	E	192	48/48	0.96	0.08	-0.15	3,7,23,27	0
2	MJZ	D	191	40/40	0.97	0.07	-0.33	6,9,13,16	0
4	EDO	C	194	4/4	0.98	0.07	-0.34	11,15,15,17	0
2	MJZ	B	191	40/40	0.97	0.08	-0.35	6,8,12,16	0
2	MJZ	A	191	40/40	0.97	0.07	-0.50	7,9,13,15	0
2	MJZ	C	192	40/40	0.98	0.07	-0.80	5,8,11,13	0
4	EDO	D	194	4/4	0.98	0.06	-0.86	13,14,14,17	0
2	MJZ	E	191	40/40	0.98	0.06	-1.03	6,8,13,15	0
2	MJZ	F	192	40/40	0.98	0.06	-1.20	4,8,12,15	0
5	NA	A	194	1/1	1.00	0.06	-1.43	9,9,9,9	0
4	EDO	C	195	4/4	0.98	0.05	-1.64	16,16,17,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.