



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 07:26 pm BST

PDB ID : 3OYT  
Title : 1.84 Angstrom resolution crystal structure of 3-oxoacyl-(acyl carrier protein) synthase I (fabB) from Yersinia pestis CO92  
Authors : Halavaty, A.S.; Wawrzak, Z.; Onopriyenko, O.; Peterson, S.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CS-GID)  
Deposited on : 2010-09-23  
Resolution : 1.84 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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

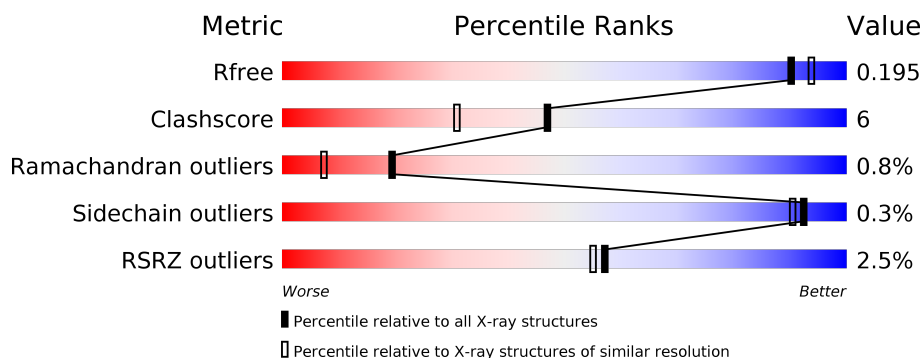
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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  $\geq 3$ , 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	410	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div></div> </div> </div>
1	B	410	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </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
5	PEG	A	415	-	-	X	-
5	PEG	A	416	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6809 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 3-oxoacyl-[acyl-carrier-protein] synthase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	Se	0	6	0
			3037	1880	527	602	7	21			
1	B	398	Total	C	N	O	S	Se	0	5	0
			2976	1845	518	588	6	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q7CJB1
A	-1	ASN	-	EXPRESSION TAG	UNP Q7CJB1
A	0	ALA	-	EXPRESSION TAG	UNP Q7CJB1
B	-2	SER	-	EXPRESSION TAG	UNP Q7CJB1
B	-1	ASN	-	EXPRESSION TAG	UNP Q7CJB1
B	0	ALA	-	EXPRESSION TAG	UNP Q7CJB1

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

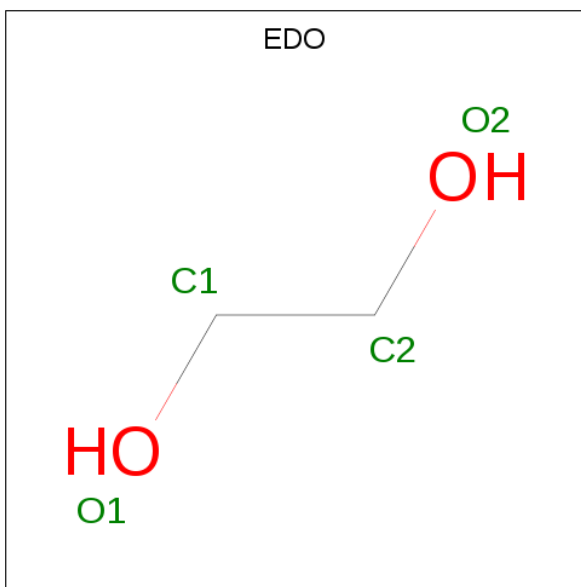
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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



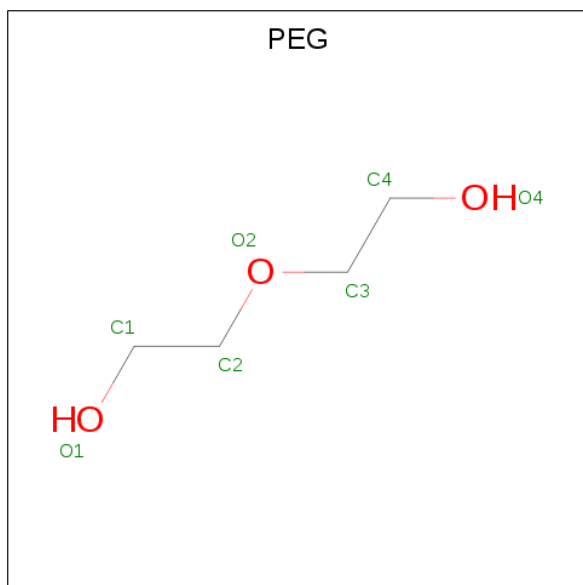
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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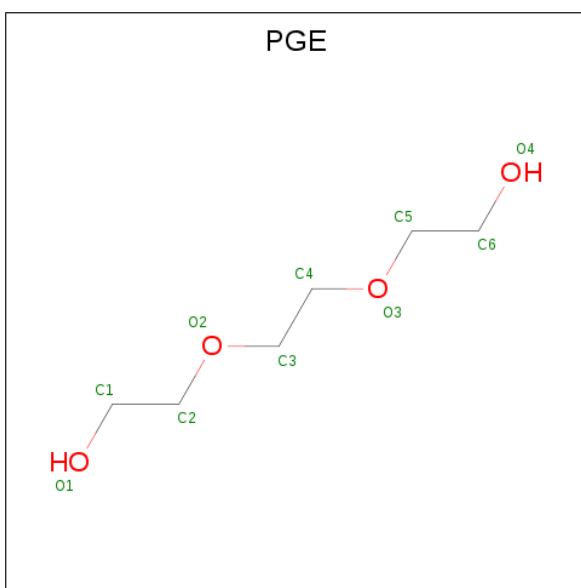
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



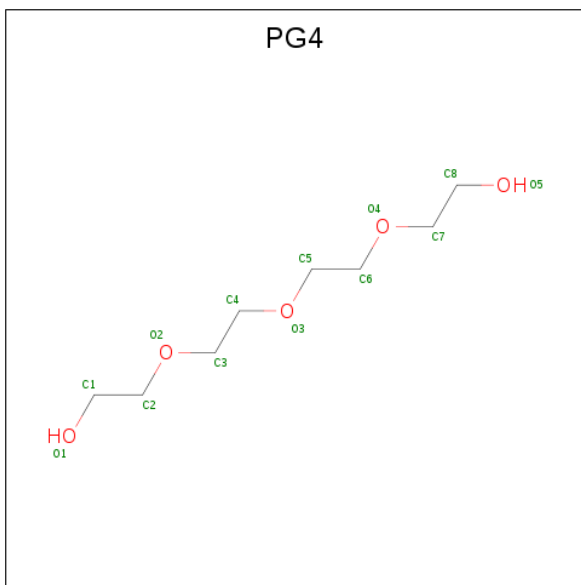
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is water.

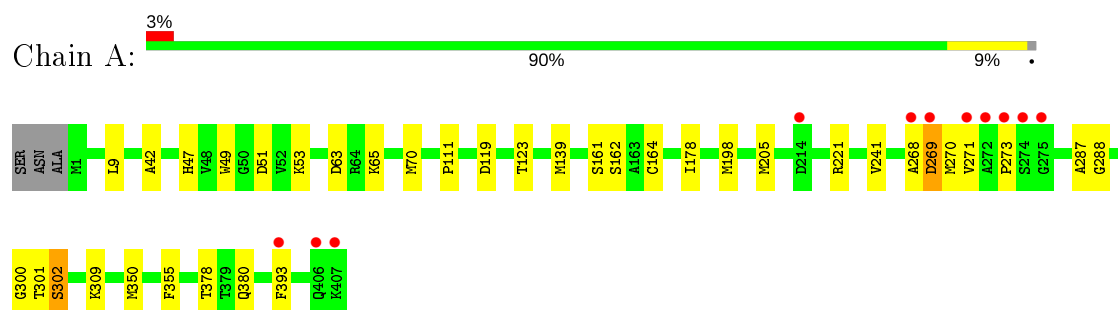
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	337	Total 349	O 349	0	12
8	B	314	Total 322	O 322	0	8



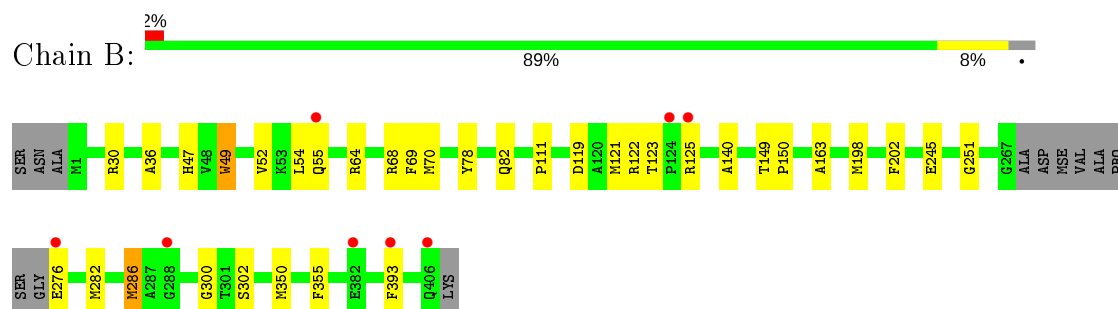
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 3-oxoacyl-[acyl-carrier-protein] synthase I



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase I



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.65Å 114.61Å 59.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.58 – 1.84 28.65 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.58-1.84) 98.9 (28.65-1.84)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.155 , 0.193 0.159 , 0.195	Depositor DCC
$R_{free}$ test set	3270 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.794	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	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 59.73 % 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 1.6914e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PO4, EDO, PG4, PEG, K

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	0/3064	0.77	2/4101 (0.0%)
1	B	0.57	0/3003	0.78	1/4020 (0.0%)
All	All	0.56	0/6067	0.78	3/8121 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	MSE	CG-SE-CE	-5.81	86.13	98.90
1	A	221	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	70	MSE	N-CA-C	5.19	125.02	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	3037	0	2977	43	0
1	B	2976	0	2913	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	1	0
3	B	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	6	0	0
4	B	12	0	18	0	0
5	A	42	0	60	12	0
5	B	14	0	20	0	0
6	B	10	0	14	1	0
7	B	26	0	36	2	0
8	A	349	0	0	9	0
8	B	322	0	0	7	0
All	All	6809	0	6044	76	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 (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164[B]:CYS:SG	8:A:482:HOH:O	2.29	0.89
1:A:51:ASP:HB2	8:A:601:HOH:O	1.78	0.82
1:A:205:MSE:HE1	1:A:271:VAL:HG11	1.62	0.81
1:A:139[A]:MSE:HE3	1:B:202:PHE:CE1	2.18	0.79
1:A:205:MSE:HE1	1:A:271:VAL:CG1	2.14	0.77
1:A:380:GLN:HG3	5:A:414:PEG:H32	1.66	0.77
1:A:51:ASP:HB2	8:A:505:HOH:O	1.87	0.75
1:A:139[B]:MSE:HE1	1:B:163:ALA:HB2	1.70	0.74
1:A:139[A]:MSE:HE3	1:B:202:PHE:CZ	2.23	0.73
1:B:52:VAL:HG12	1:B:54:LEU:HD13	1.71	0.72
1:A:63:ASP:OD2	1:A:65:LYS:NZ	2.21	0.72
1:A:139[A]:MSE:CE	1:B:202:PHE:CE1	2.73	0.72
1:B:55[B]:GLN:HE21	1:B:55[B]:GLN:HA	1.56	0.69
1:B:125:ARG:NH1	8:B:466:HOH:O	2.26	0.67
1:B:123:THR:OG1	1:B:125:ARG:HG2	1.96	0.65
1:B:55[B]:GLN:HA	1:B:55[B]:GLN:NE2	2.11	0.65
5:A:416:PEG:C4	8:A:566:HOH:O	2.45	0.65
5:A:416:PEG:H31	8:A:566:HOH:O	1.97	0.65
1:A:270:MSE:HG2	1:B:69:PHE:CD1	2.33	0.63
1:A:287:ALA:HA	5:A:415:PEG:H32	1.82	0.62
1:B:52:VAL:HG12	1:B:54:LEU:CD1	2.30	0.62
1:A:119:ASP:OD2	1:B:122:ARG:NH1	2.31	0.61
5:A:416:PEG:C3	8:A:566:HOH:O	2.50	0.60
1:A:288:GLY:H	5:A:415:PEG:C3	2.15	0.59
1:B:47:HIS:ND1	3:B:410:PO4:O1	2.25	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139[A]:MSE:HE1	1:B:198:MSE:CG	2.34	0.58
5:A:416:PEG:H42	8:A:566:HOH:O	2.03	0.57
1:A:205:MSE:CE	1:A:271:VAL:HG11	2.34	0.57
1:A:380:GLN:CG	5:A:414:PEG:H32	2.33	0.56
1:A:139[B]:MSE:HE2	8:B:582:HOH:O	2.06	0.55
1:B:163:ALA:HB2	1:B:393[A]:PHE:CE2	2.41	0.55
1:A:288:GLY:H	5:A:415:PEG:H31	1.72	0.54
1:A:47:HIS:ND1	3:A:409:PO4:O1	2.28	0.54
1:A:139[A]:MSE:HE1	1:B:202:PHE:HE1	1.73	0.54
1:A:139[A]:MSE:CE	1:B:202:PHE:HE1	2.21	0.54
1:A:350:MSE:HB3	1:A:355:PHE:O	2.09	0.53
1:B:111:PRO:HG2	1:B:198:MSE:HB2	1.89	0.53
1:A:205:MSE:HE1	1:A:271:VAL:HG13	1.92	0.52
1:B:282:MSE:O	1:B:286:MSE:HG3	2.10	0.52
1:A:51:ASP:OD1	1:A:53:LYS:NZ	2.33	0.51
1:B:30:ARG:NH1	8:B:669:HOH:O	2.27	0.51
1:B:52:VAL:CG1	1:B:54:LEU:CD1	2.88	0.51
1:B:70:MSE:HE1	1:B:78:TYR:CD1	2.46	0.50
1:A:273:PRO:HG2	8:A:474:HOH:O	2.12	0.50
1:A:111:PRO:HG2	1:A:198:MSE:HB2	1.93	0.50
1:A:139[B]:MSE:HE1	1:B:163:ALA:CB	2.42	0.49
1:A:9:LEU:HD12	1:A:9:LEU:C	2.32	0.49
1:A:139[A]:MSE:HE1	1:B:202:PHE:CE1	2.47	0.49
1:A:268:ALA:O	1:A:269:ASP:O	2.30	0.49
1:A:178:ILE:HD12	1:A:241:VAL:HG12	1.95	0.48
1:A:139[B]:MSE:CE	1:B:163:ALA:HB2	2.40	0.47
1:B:52:VAL:CG1	1:B:54:LEU:HD13	2.42	0.47
1:A:271:VAL:HG13	1:A:393:PHE:CE1	2.49	0.46
1:A:139[A]:MSE:HE1	1:B:198:MSE:HG3	1.97	0.46
1:A:288:GLY:H	5:A:415:PEG:H32	1.80	0.46
1:B:350:MSE:HB3	1:B:355:PHE:O	2.16	0.45
1:A:301:THR:O	1:A:302:SER:CB	2.65	0.45
1:A:42:ALA:O	1:B:121:MSE:HE3	2.17	0.44
1:B:82[A]:GLN:NE2	8:B:551:HOH:O	2.27	0.44
5:A:415:PEG:H12	8:A:594:HOH:O	2.18	0.43
1:B:245[A]:GLU:OE1	7:B:417:PG4:H41	2.17	0.43
1:A:378:THR:HG22	5:A:414:PEG:H31	2.00	0.43
1:B:245[A]:GLU:OE1	7:B:417:PG4:C4	2.67	0.43
1:A:273:PRO:O	1:A:309:LYS:HG3	2.19	0.42
1:B:251:GLY:HA2	8:B:515:HOH:O	2.19	0.42
1:B:119:ASP:O	1:B:123:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:THR:OG1	1:B:125:ARG:CG	2.67	0.42
1:A:161:SER:OG	1:B:140:ALA:HB3	2.19	0.42
1:B:64:ARG:O	1:B:68:ARG:HG3	2.19	0.42
1:B:149:THR:HB	1:B:150:PRO:HD3	2.02	0.42
1:B:276:GLU:N	8:B:555:HOH:O	2.52	0.42
1:A:119:ASP:O	1:A:123:THR:HG23	2.20	0.41
1:B:36:ALA:HB2	1:B:49:TRP:CG	2.55	0.41
1:B:393[A]:PHE:C	1:B:393[A]:PHE:CD1	2.94	0.41
1:B:55[B]:GLN:CA	1:B:55[B]:GLN:NE2	2.78	0.41
6:B:416:PGE:H52	8:B:589:HOH:O	2.20	0.41

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	411/410 (100%)	400 (97%)	7 (2%)	4 (1%)	15	5
1	B	399/410 (97%)	389 (98%)	8 (2%)	2 (0%)	29	15
All	All	810/820 (99%)	789 (97%)	15 (2%)	6 (1%)	19	9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	ASP
1	B	300	GLY
1	A	300	GLY
1	A	162	SER
1	A	302	SER
1	B	302	SER

### 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	319/295 (108%)	318 (100%)	1 (0%)	92	90
1	B	312/295 (106%)	311 (100%)	1 (0%)	92	90
All	All	631/590 (107%)	629 (100%)	2 (0%)	92	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	TRP
1	B	49	TRP

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

Mol	Chain	Res	Type
1	A	94	GLN
1	A	225	GLN
1	A	368	GLN
1	A	370	GLN
1	B	368	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	B	413	-	3,3,3	0.51	0	2,2,2	0.08	0
6	PGE	B	416	-	9,9,9	0.45	0	8,8,8	0.25	0
3	PO4	B	410	-	4,4,4	0.92	0	6,6,6	0.46	0
5	PEG	A	412	-	6,6,6	0.45	0	5,5,5	0.31	0
3	PO4	A	409	-	4,4,4	0.95	0	6,6,6	0.41	0
4	EDO	A	410	-	3,3,3	0.44	0	2,2,2	0.34	0
5	PEG	A	414	-	6,6,6	0.51	0	5,5,5	0.30	0
4	EDO	B	412	-	3,3,3	0.49	0	2,2,2	0.27	0
5	PEG	A	411	-	6,6,6	0.44	0	5,5,5	0.26	0
5	PEG	B	414	-	6,6,6	0.49	0	5,5,5	0.29	0
5	PEG	B	415	-	6,6,6	0.45	0	5,5,5	0.17	0
5	PEG	A	415	-	6,6,6	0.38	0	5,5,5	0.60	0
7	PG4	B	418	-	12,12,12	0.45	0	11,11,11	0.26	0
7	PG4	B	417	-	12,12,12	0.53	0	11,11,11	0.34	0
3	PO4	B	409	-	4,4,4	0.83	0	6,6,6	0.53	0
4	EDO	B	411	-	3,3,3	0.49	0	2,2,2	0.26	0
5	PEG	A	416	-	6,6,6	0.56	0	5,5,5	0.33	0
5	PEG	A	413	-	6,6,6	0.39	0	5,5,5	0.33	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	B	413	-	-	1/1/1/1	-
6	PGE	B	416	-	-	4/7/7/7	-
5	PEG	A	413	-	-	1/4/4/4	-
4	EDO	A	410	-	-	1/1/1/1	-
5	PEG	A	414	-	-	3/4/4/4	-
4	EDO	B	412	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	411	-	-	1/4/4/4	-
5	PEG	B	414	-	-	0/4/4/4	-
5	PEG	B	415	-	-	3/4/4/4	-
5	PEG	A	415	-	-	2/4/4/4	-
7	PG4	B	418	-	-	3/10/10/10	-
7	PG4	B	417	-	-	3/10/10/10	-
5	PEG	A	412	-	-	1/4/4/4	-
4	EDO	B	411	-	-	0/1/1/1	-
5	PEG	A	416	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	415	PEG	O2-C3-C4-O4
5	A	416	PEG	O2-C3-C4-O4
5	A	412	PEG	O1-C1-C2-O2
5	B	415	PEG	O1-C1-C2-O2
7	B	418	PG4	O1-C1-C2-O2
5	A	411	PEG	O2-C3-C4-O4
6	B	416	PGE	O1-C1-C2-O2
5	A	414	PEG	O2-C3-C4-O4
4	A	410	EDO	O1-C1-C2-O2
6	B	416	PGE	O3-C5-C6-O4
5	A	414	PEG	O1-C1-C2-O2
5	A	415	PEG	O2-C3-C4-O4
5	A	416	PEG	O1-C1-C2-O2
4	B	413	EDO	O1-C1-C2-O2
6	B	416	PGE	C3-C4-O3-C5
5	A	414	PEG	C1-C2-O2-C3
5	B	415	PEG	C1-C2-O2-C3
5	A	416	PEG	C1-C2-O2-C3
6	B	416	PGE	O2-C3-C4-O3
7	B	417	PG4	C1-C2-O2-C3
7	B	417	PG4	C8-C7-O4-C6
7	B	417	PG4	O3-C5-C6-O4
5	A	415	PEG	O1-C1-C2-O2
7	B	418	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
7	B	418	PG4	C1-C2-O2-C3
5	A	413	PEG	C4-C3-O2-C2

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	416	PGE	1	0
3	B	410	PO4	1	0
3	A	409	PO4	1	0
5	A	414	PEG	3	0
5	A	415	PEG	5	0
7	B	417	PG4	2	0
5	A	416	PEG	4	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<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	387/410 (94%)	-0.04	11 (2%) 53 51	10, 16, 26, 41	3 (0%)
1	B	379/410 (92%)	-0.07	8 (2%) 63 62	10, 16, 28, 41	0
All	All	766/820 (93%)	-0.05	19 (2%) 57 55	10, 16, 27, 41	3 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	VAL	6.4
1	B	55[A]	GLN	4.7
1	B	406	GLN	4.7
1	A	268	ALA	4.6
1	A	274	SER	4.4
1	A	272	ALA	4.3
1	B	125	ARG	4.2
1	A	269	ASP	3.6
1	A	275	GLY	3.3
1	A	273	PRO	3.0
1	A	406	GLN	2.9
1	B	382	GLU	2.9
1	B	124	PRO	2.7
1	B	393[A]	PHE	2.7
1	B	288	GLY	2.3
1	A	407	LYS	2.3
1	B	276	GLU	2.1
1	A	214	ASP	2.0
1	A	393	PHE	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> )	Q<0.9
5	PEG	A	411	7/7	0.67	0.32	58,58,59,59	0
7	PG4	B	417	13/13	0.68	0.22	39,46,51,52	0
5	PEG	A	416	7/7	0.73	0.20	34,37,39,40	0
5	PEG	A	412	7/7	0.75	0.14	48,48,50,50	0
5	PEG	B	414	7/7	0.76	0.18	40,41,42,43	0
4	EDO	B	411	4/4	0.76	0.19	44,44,45,46	0
4	EDO	B	412	4/4	0.76	0.13	40,40,40,41	0
5	PEG	A	414	7/7	0.76	0.23	44,45,46,47	0
5	PEG	B	415	7/7	0.79	0.27	48,48,50,50	0
6	PGE	B	416	10/10	0.80	0.15	38,41,43,43	0
5	PEG	A	413	7/7	0.82	0.18	50,51,51,52	0
4	EDO	A	410	4/4	0.84	0.15	44,44,44,45	0
7	PG4	B	418	13/13	0.85	0.19	41,42,46,47	0
5	PEG	A	415	7/7	0.86	0.16	42,42,43,44	0
4	EDO	B	413	4/4	0.87	0.19	43,44,44,45	0
3	PO4	B	410	5/5	0.88	0.29	50,50,50,51	5
3	PO4	A	409	5/5	0.90	0.25	40,41,41,42	5
3	PO4	B	409	5/5	0.93	0.15	60,60,60,60	0
2	K	B	408	1/1	0.99	0.04	15,15,15,15	0
2	K	A	408	1/1	1.00	0.06	15,15,15,15	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.