



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:59 pm BST

PDB ID : 5A5G  
Title : Crystal structure of FTHFS2 from T.acetoxydans Re1  
Authors : Bergdahl, R.; Jacobson, F.; Muller, B.; Mikkelsen, N.; Schurer, A.; Sandgren, M.  
Deposited on : 2015-06-17  
Resolution : 2.30 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 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

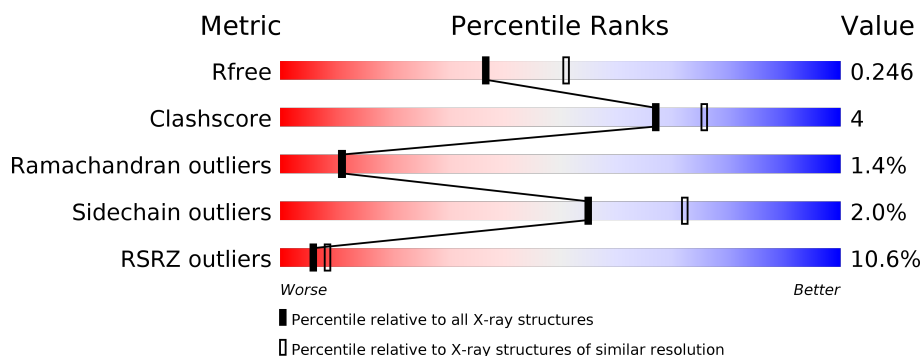
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	558	<div> <div>9%</div> <div>91%</div> <div>7%</div> <div>..</div> </div>
1	B	558	<div> <div>11%</div> <div>91%</div> <div>7%</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
3	GOL	A	1563	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8974 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 FORMATE--TETRAHYDROFOLATE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	3	0
			4178	2651	719	790	18			
1	B	555	Total	C	N	O	S	0	2	0
			4192	2662	720	793	17			

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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 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
4	A	1	Total	C	O	0	0
			7	4	3		

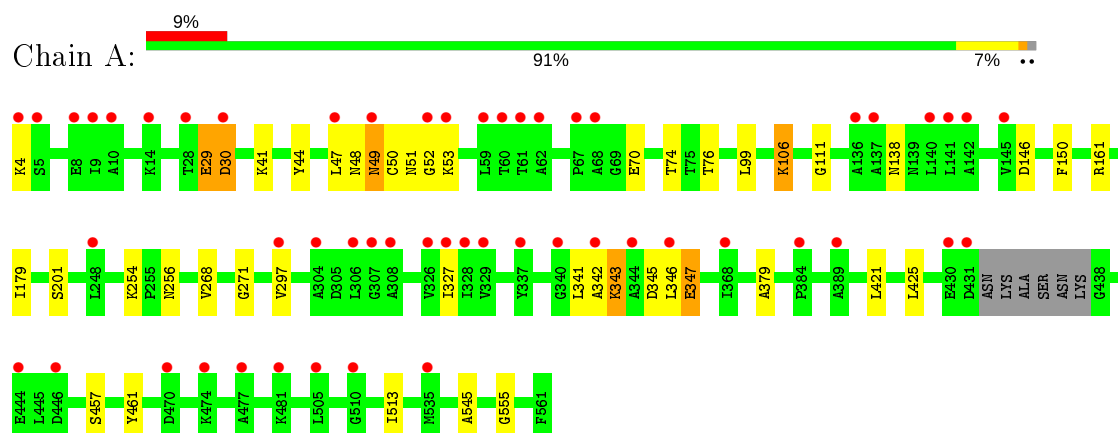
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	314	Total	O	0	0
			314	314		
5	B	273	Total	O	0	0
			273	273		

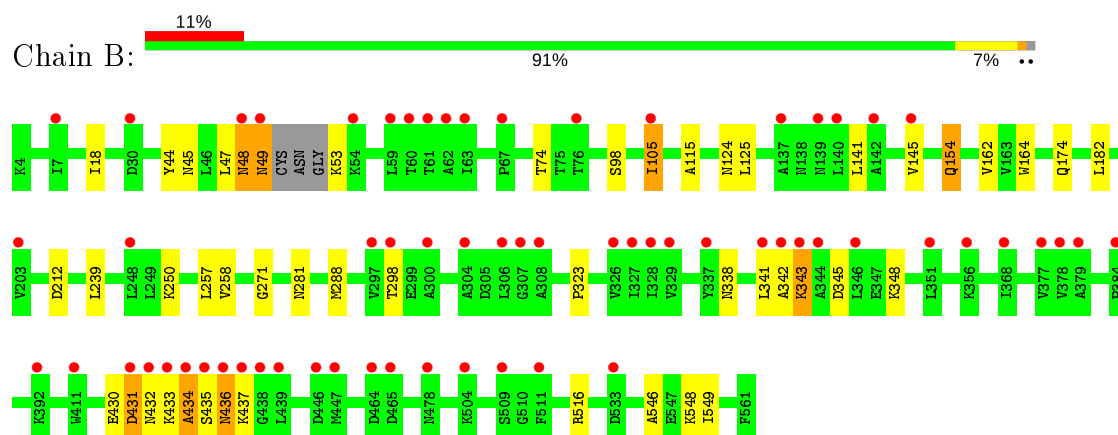
### 3 Residue-property plots [i](#)

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: FORMATE--TETRAHYDROFOLATE LIGASE



#### • Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.04Å 98.12Å 108.76Å 90.00° 101.51° 90.00°	Depositor
Resolution (Å)	29.66 – 2.30 29.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.66-2.30) 98.3 (29.64-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.184 , 0.246 0.189 , 0.246	Depositor DCC
$R_{free}$ test set	2596 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8974	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: GOL, K, PEG

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	0.34	0/4236	0.57	2/5726 (0.0%)
1	B	0.34	0/4250	0.55	0/5744
All	All	0.34	0/8486	0.56	2/11470 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	GLU	N-CA-C	5.37	125.51	111.00
1	A	29	GLU	C-N-CA	5.22	134.76	121.70

There are no chirality outliers.

There are no planarity outliers.

### 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	4178	0	4304	34	0
1	B	4192	0	4328	34	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	8	7	0
4	A	7	0	10	0	0
5	A	314	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	273	0	0	2	0
All	All	8974	0	8650	66	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 4.

All (66) 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:154[A]:GLN:NE2	1:B:154[A]:GLN:H	1.41	1.18
1:A:52:GLY:HA2	1:A:53:LYS:HB2	1.27	1.14
1:B:154[A]:GLN:HE21	1:B:154[A]:GLN:N	1.68	0.92
1:A:52:GLY:CA	1:A:53:LYS:HB2	2.01	0.89
1:A:161[B]:ARG:HH11	1:A:161[B]:ARG:HG2	1.37	0.88
1:B:154[A]:GLN:NE2	1:B:154[A]:GLN:N	2.22	0.87
1:B:154[A]:GLN:HE21	1:B:154[A]:GLN:H	0.88	0.84
1:A:345:ASP:O	1:A:347:GLU:N	2.15	0.77
1:A:146:ASP:O	3:A:1563:GOL:O3	2.09	0.70
1:B:430:GLU:O	1:B:432:ASN:N	2.23	0.70
1:A:161[B]:ARG:NH1	1:A:161[B]:ARG:HG2	2.06	0.68
1:B:49:ASN:HD22	1:B:49:ASN:C	1.97	0.68
1:B:154[B]:GLN:HE21	1:B:154[B]:GLN:C	1.98	0.67
1:B:141:LEU:HD23	1:B:164:TRP:CE2	2.29	0.67
1:B:124:ASN:O	5:B:2069:HOH:O	2.14	0.64
1:A:146:ASP:C	3:A:1563:GOL:H12	2.20	0.62
1:B:431:ASP:O	1:B:432:ASN:OD1	2.19	0.61
1:A:342:ALA:O	1:A:343:LYS:O	2.20	0.59
1:A:50:CYS:SG	1:A:51:ASN:N	2.78	0.57
3:A:1563:GOL:O2	1:B:174:GLN:OE1	2.12	0.56
1:B:45:ASN:O	1:B:48:ASN:ND2	2.39	0.56
1:A:343:LYS:O	1:A:345:ASP:N	2.39	0.55
1:B:516:ARG:NH1	5:B:2245:HOH:O	2.39	0.55
1:B:345:ASP:OD1	1:B:348:LYS:NZ	2.39	0.54
1:A:51:ASN:OD1	1:A:52:GLY:O	2.25	0.54
1:B:436:ASN:C	1:B:436:ASN:HD22	2.11	0.54
1:B:343:LYS:C	1:B:345:ASP:H	2.11	0.54
1:B:105:ILE:O	1:B:105:ILE:HG23	2.09	0.53
1:B:281:ASN:ND2	1:B:298:THR:OG1	2.42	0.53
1:B:141:LEU:HD23	1:B:164:TRP:CZ2	2.45	0.52
1:A:29:GLU:CG	1:A:30:ASP:HB2	2.39	0.52
1:A:457:SER:HA	1:A:461:TYR:CD2	2.45	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASN:O	1:A:49:ASN:C	2.48	0.52
1:A:70[B]:GLU:OE1	1:A:70[B]:GLU:N	2.42	0.51
1:A:29:GLU:N	1:A:30:ASP:CB	2.73	0.51
1:A:138:ASN:ND2	1:A:201:SER:OG	2.44	0.50
1:B:47:LEU:HD21	1:B:288:MET:HA	1.93	0.50
1:A:29:GLU:N	1:A:30:ASP:HB2	2.26	0.50
1:B:430:GLU:O	1:B:431:ASP:C	2.48	0.50
1:A:555:GLY:O	1:B:250:LYS:HD2	2.12	0.49
1:B:18:ILE:HD11	1:B:257:LEU:HG	1.93	0.49
1:B:436:ASN:ND2	1:B:436:ASN:C	2.66	0.48
1:B:546:ALA:HA	1:B:549:ILE:HD12	1.96	0.48
1:A:256:ASN:HB2	1:A:268:VAL:O	2.14	0.47
1:B:433:LYS:O	1:B:434:ALA:C	2.52	0.47
1:B:432:ASN:O	1:B:433:LYS:C	2.52	0.47
1:B:435:SER:C	1:B:437:LYS:N	2.68	0.47
1:A:161[B]:ARG:CG	1:A:161[B]:ARG:NH1	2.76	0.46
1:B:74:THR:HG23	1:B:115:ALA:HB3	1.96	0.46
1:A:146:ASP:HB3	3:A:1563:GOL:H12	1.98	0.46
1:A:74:THR:HG22	1:A:111:GLY:C	2.37	0.45
1:A:146:ASP:HB3	3:A:1563:GOL:C1	2.46	0.44
1:A:76:THR:HG23	1:A:297:VAL:HG12	1.99	0.44
1:A:461:TYR:HD2	1:A:513:ILE:CD1	2.32	0.43
1:A:461:TYR:CD2	1:A:513:ILE:CD1	3.02	0.43
1:A:379:ALA:HB2	1:A:421:LEU:HD13	2.02	0.42
1:A:106:LYS:HG3	1:A:545:ALA:HB1	2.01	0.42
1:A:41:LYS:HD3	1:A:254:LYS:HB2	2.02	0.42
1:A:179:ILE:HG12	1:B:182:LEU:HD11	2.02	0.42
1:B:548[B]:LYS:HG3	1:B:548[B]:LYS:O	2.21	0.41
1:B:49:ASN:ND2	1:B:49:ASN:C	2.69	0.41
1:A:327:ILE:HD11	1:A:425:LEU:HD11	2.03	0.41
3:A:1563:GOL:H32	1:B:174:GLN:OE1	2.21	0.40
1:B:145:VAL:HG22	1:B:239:LEU:CD1	2.51	0.40
1:A:150:PHE:HB2	3:A:1563:GOL:C3	2.52	0.40
1:A:70[A]:GLU:CA	1:A:70[A]:GLU:OE1	2.70	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	551/558 (99%)	517 (94%)	26 (5%)	8 (2%)	10	10
1	B	553/558 (99%)	522 (94%)	24 (4%)	7 (1%)	12	12
All	All	1104/1116 (99%)	1039 (94%)	50 (4%)	15 (1%)	11	11

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	49	ASN
1	A	343	LYS
1	A	346	LEU
1	B	431	ASP
1	B	343	LYS
1	B	434	ALA
1	A	47	LEU
1	A	347	GLU
1	B	125	LEU
1	B	342	ALA
1	A	106	LYS
1	A	271	GLY
1	B	271	GLY
1	B	258	VAL

### 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	436/438 (100%)	432 (99%)	4 (1%)	78	89
1	B	438/438 (100%)	424 (97%)	14 (3%)	39	54
All	All	874/876 (100%)	856 (98%)	18 (2%)	55	70

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

Mol	Chain	Res	Type
1	A	4	LYS
1	A	44	TYR
1	A	99	LEU
1	A	341	LEU
1	B	44	TYR
1	B	48	ASN
1	B	49	ASN
1	B	53	LYS
1	B	98	SER
1	B	105	ILE
1	B	154[A]	GLN
1	B	154[B]	GLN
1	B	162	VAL
1	B	212	ASP
1	B	323	PRO
1	B	338	ASN
1	B	341	LEU
1	B	436	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	281	ASN
1	B	48	ASN
1	B	49	ASN
1	B	281	ASN
1	B	436	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	A	1563	-	5,5,5	0.36	0	5,5,5	1.06	0
4	PEG	A	1565	-	6,6,6	0.49	0	5,5,5	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1563	-	-	4/4/4/4	-
4	PEG	A	1565	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1563	GOL	O1-C1-C2-O2
3	A	1563	GOL	O1-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	1563	GOL	C1-C2-C3-O3
3	A	1563	GOL	O2-C2-C3-O3
4	A	1565	PEG	C1-C2-O2-C3
4	A	1565	PEG	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1563	GOL	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

### 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	552/558 (98%)	0.61	53 (9%) <b>8</b> <b>10</b>	28, 50, 79, 87	18 (3%)
1	B	555/558 (99%)	0.63	64 (11%) <b>4</b> <b>7</b>	26, 51, 79, 97	16 (2%)
All	All	1107/1116 (99%)	0.62	117 (10%) <b>6</b> <b>8</b>	26, 51, 79, 97	34 (3%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	437	LYS	8.3
1	A	431	ASP	7.3
1	B	434	ALA	7.1
1	B	436	ASN	7.0
1	B	435	SER	6.8
1	B	433	LYS	6.1
1	B	432	ASN	5.9
1	A	52	GLY	5.8
1	B	327	ILE	5.1
1	A	328	ILE	4.9
1	B	344	ALA	4.8
1	B	328	ILE	4.6
1	B	61	THR	4.4
1	A	4	LYS	4.2
1	A	327	ILE	4.2
1	A	67	PRO	4.1
1	B	67	PRO	4.0
1	B	59	LEU	3.9
1	A	342	ALA	3.8
1	A	59	LEU	3.8
1	A	60	THR	3.8
1	B	431	ASP	3.8
1	B	342	ALA	3.7
1	A	326	VAL	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	62	ALA	3.6
1	B	438	GLY	3.6
1	A	535	MET	3.5
1	B	60	THR	3.5
1	A	430	GLU	3.5
1	B	464	ASP	3.4
1	B	304	ALA	3.4
1	B	447	MET	3.4
1	A	47	LEU	3.3
1	B	346	LEU	3.3
1	B	379	ALA	3.2
1	A	329	VAL	3.2
1	B	511	PHE	3.1
1	A	142	ALA	3.1
1	A	49	ASN	3.0
1	B	439	LEU	3.0
1	A	61	THR	3.0
1	A	340	GLY	3.0
1	A	8	GLU	3.0
1	B	326	VAL	3.0
1	B	48	ASN	3.0
1	A	304	ALA	2.9
1	A	297	VAL	2.9
1	B	49	ASN	2.9
1	B	137	ALA	2.9
1	B	465	ASP	2.9
1	A	308	ALA	2.9
1	A	368	ILE	2.8
1	A	5	SER	2.8
1	A	510	GLY	2.8
1	A	446	ASP	2.8
1	B	329	VAL	2.8
1	A	307	GLY	2.8
1	B	337	TYR	2.8
1	A	30	ASP	2.8
1	A	384	PRO	2.8
1	B	478	ASN	2.8
1	B	509	SER	2.8
1	B	341	LEU	2.8
1	A	470	ASP	2.8
1	B	307	GLY	2.8
1	A	389	ALA	2.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	7	ILE	2.7
1	A	10	ALA	2.7
1	B	343	LYS	2.7
1	A	141	LEU	2.7
1	B	351	LEU	2.7
1	B	308	ALA	2.7
1	A	28	THR	2.6
1	A	136	ALA	2.6
1	B	300	ALA	2.6
1	B	63	ILE	2.6
1	A	145	VAL	2.5
1	B	297	VAL	2.5
1	B	446	ASP	2.5
1	A	9	ILE	2.4
1	A	344	ALA	2.4
1	B	105	ILE	2.4
1	A	346	LEU	2.4
1	B	248	LEU	2.4
1	A	53	LYS	2.4
1	A	140	LEU	2.4
1	A	444	GLU	2.3
1	A	477	ALA	2.3
1	B	145	VAL	2.3
1	B	533	ASP	2.3
1	B	504	LYS	2.3
1	B	392	LYS	2.3
1	A	68	ALA	2.3
1	B	377	VAL	2.3
1	A	62	ALA	2.3
1	B	298	THR	2.2
1	B	411	TRP	2.2
1	B	356	LYS	2.2
1	A	137	ALA	2.2
1	B	76	THR	2.2
1	B	140	LEU	2.2
1	B	378	VAL	2.2
1	B	54	LYS	2.1
1	B	203	VAL	2.1
1	B	142	ALA	2.1
1	A	248	LEU	2.1
1	A	474	LYS	2.1
1	A	481	LYS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	139	ASN	2.1
1	A	337	TYR	2.1
1	A	306	LEU	2.1
1	A	14	LYS	2.0
1	B	384	PRO	2.0
1	A	505	LEU	2.0
1	B	306	LEU	2.0
1	B	368	ILE	2.0
1	B	30	ASP	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. 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	PEG	A	1565	7/7	0.66	0.31	68,75,79,81	1
3	GOL	A	1563	6/6	0.93	0.64	53,59,61,65	0
2	K	B	1563	1/1	0.93	0.27	74,74,74,74	0
2	K	A	1564	1/1	0.96	0.11	76,76,76,76	0
2	K	B	1562	1/1	0.99	0.12	37,37,37,37	0
2	K	A	1562	1/1	0.99	0.15	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.