



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 2, 2023 – 05:47 AM EDT

PDB ID : 1BOT  
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN ESCHERICHIA COLI GLYCEROL KINASE AND THE ALLOSTERIC REGULATOR FRUCTOSE 1,6-BISPHOSPHATE.  
Authors : Ormo, M.; Bystrom, C.E.; Remington, S.J.  
Deposited on : 1998-08-05  
Resolution : 3.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.34  
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) : 2.34

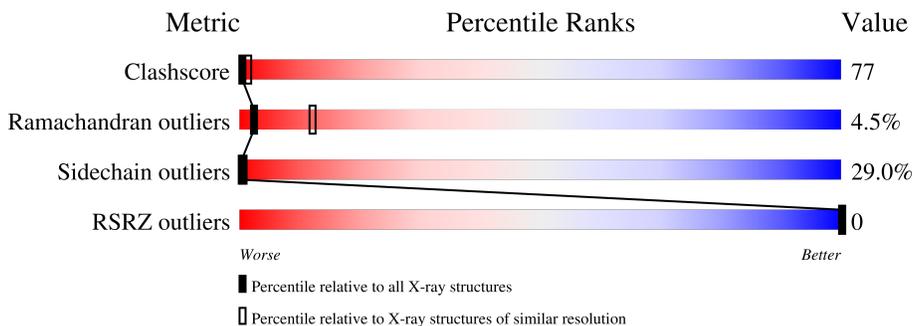
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	O	501	
1	Z	501	

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	O	601	-	-	X	-

## 2 Entry composition [i](#)

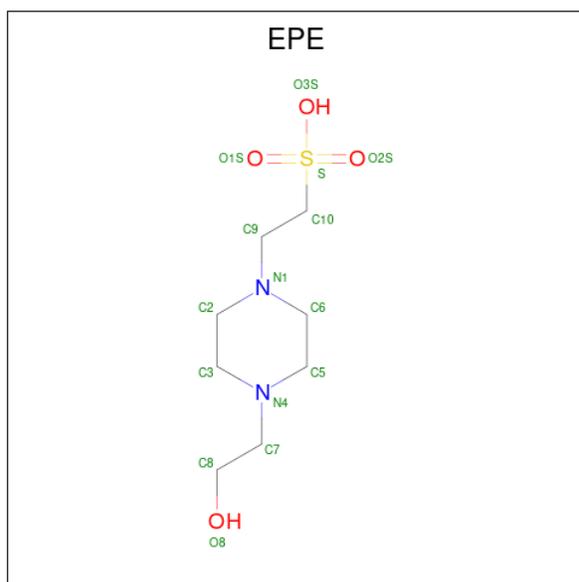
There are 3 unique types of molecules in this entry. The entry contains 7864 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (GLYCEROL KINASE).

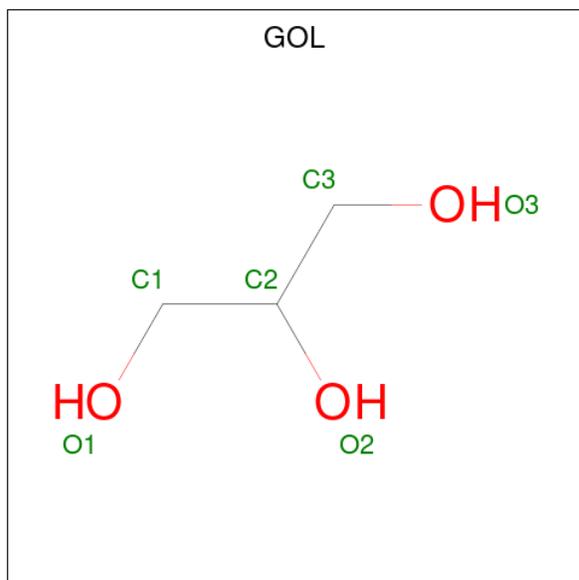
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	O	497	Total 3914	C 2469	N 686	O 740	S 19	0	0	0
1	Z	498	Total 3923	C 2474	N 687	O 743	S 19	0	0	0

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	O	1	Total 15	C 8	N 2	O 4	S 1	0	0

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



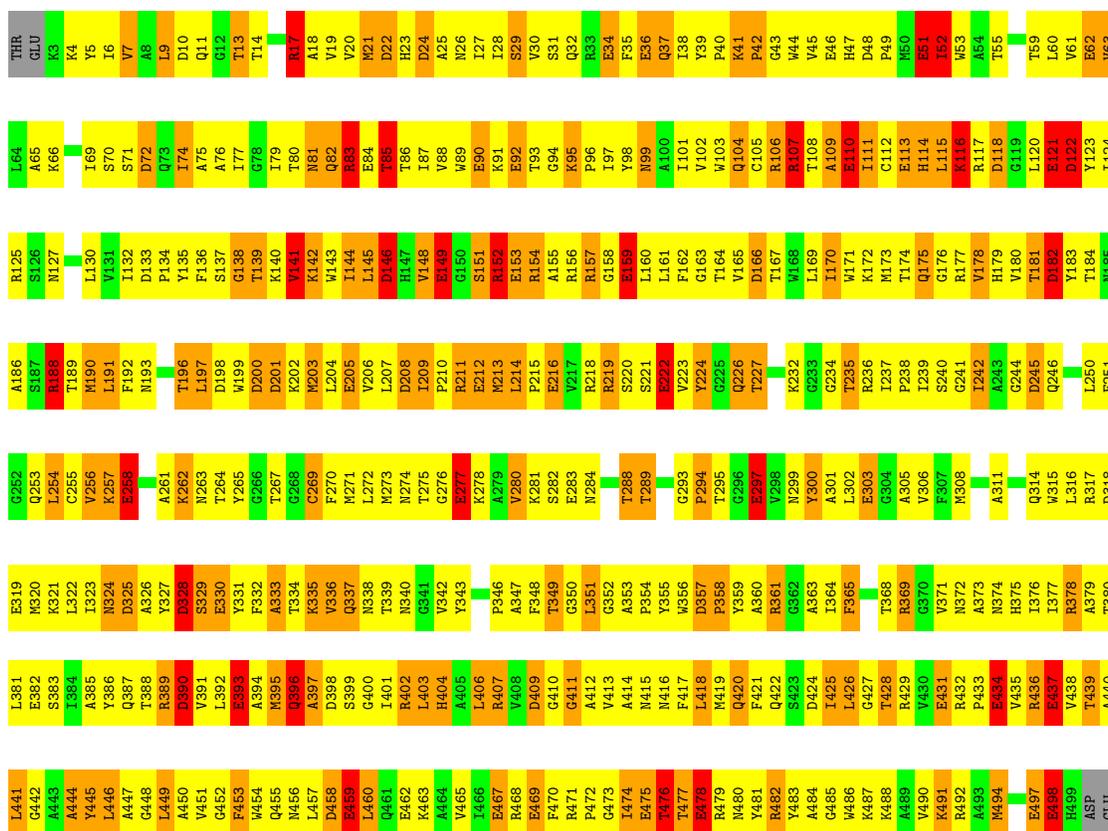
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	C	O	0	0
			6	3	3		
3	Z	1	Total	C	O	0	0
			6	3	3		

### 3 Residue-property plots

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.

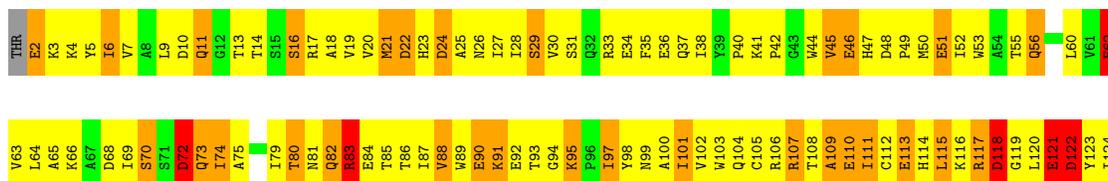
- Molecule 1: PROTEIN (GLYCEROL KINASE)

Chain O: 



- Molecule 1: PROTEIN (GLYCEROL KINASE)

Chain Z: 



GLU	R436	N374	S312	L250	W185	R125
E437	H375	I313	F210	F210	A186	S126
V438	I376	Q314	G277	G277	S187	M127
T439	R377	W315	E277	E277	R188	T128
A440	R378	L316	K278	K278	T189	G129
L441	L381	R317	G268	G268	G129	L130
G442	E382	D318	C289	C289	C255	W131
A443	S383	E319	F270	F270	L191	L132
A444	S383	N320	M271	M271	F192	D133
Y445	I384	K321	L272	L272	M193	P134
L446	A385	L322	M273	M273	H195	Y135
L449	Y386	I323	M274	M274	F196	F136
A450	Q387	N324	S209	S209	T197	S137
W451	T388	D325	I209	I209	G138	G138
G452	R389	A326	P210	P210	T139	T139
F453	D390	Y327	R211	R211	K140	K140
W454	V391	D328	E212	E212	V141	V141
Q455	L392	S329	M213	M213	K142	K142
M456	E393	E330	L214	L214	W143	W143
L457	A394	Y331	A279	A279	L144	L144
D458	N395	F332	V280	V280	L145	L145
E459	Q396	A333	K281	K281	D146	D146
L460	A397	T334	S282	S282	L147	L147
Q461	D398	K335	E283	E283	H147	H147
E462	S399	V336	L286	L286	V148	V148
K463	G400	Q337	T289	T289	E149	E149
V465	I401	N338	I290	I290	G150	G150
I466	R402	T339	A291	A291	S151	S151
E467	L403	N340	L351	L351	R152	R152
R468	L406	G341	G352	G352	E153	E153
E469	R407	V342	A353	A353	R154	R154
F470	W408	V343	P354	P354	A155	A155
R471	D409	V344	Y355	Y355	R156	R156
P472	G410	P346	W356	W356	R157	R157
G473	A411	A347	D357	D357	G158	G158
I474	V412	F348	P358	P358	E159	E159
E475	W413	T349	A360	A360	L160	L160
T476	A414	G350	R361	R361	L161	L161
T477	N415	L351	G362	G362	F162	F162
R478	N416	G352	A363	A363	G163	G163
R479	F417	A353	I364	I364	V165	V165
W480	L418	P354	F365	F365	D166	D166
Y481	M419	Y355	T368	T368	T167	T167
R482	Q420	W356	V371	V371	W168	W168
Y483	F421	D357	G310	G310	L169	L169
W486	Q422	P358	N308	N308	I170	I170
K488	S423	Y359	A309	A309	W171	W171
A489	D424	A360	G310	G310	K172	K172
V490	I425	R361	N372	N372	M173	M173
K491	L426	G362	A373	A373	T174	T174
R492	G427	A363	V368	V368	Q175	Q175
E497	T428	I364	G311	G311	G176	G176
E498	V430	F365	N308	N308	R177	R177
H499	E431	T368	A309	A309	V178	V178
ASP	R432	V371	G310	G310	H179	H179
	P433	A373	N372	N372	W180	W180
	E434		G310	G310	T181	T181
	V435		A373	A373	D182	D182
					Y183	Y183
					T184	T184

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.80Å 168.80Å 202.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.05 19.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	81.0 (20.00-3.05) 73.8 (19.98-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.88Å)	Xtrriage
Refinement program	TNT 5F	Depositor
R, $R_{free}$	0.219 , (Not available) 0.199 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtrriage
Anisotropy	0.128	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 107.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, GOL

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	O	1.20	34/3994 (0.9%)	1.57	57/5414 (1.1%)
1	Z	1.21	37/4003 (0.9%)	1.56	65/5426 (1.2%)
All	All	1.21	71/7997 (0.9%)	1.56	122/10840 (1.1%)

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	34	GLU	CD-OE2	11.22	1.38	1.25
1	O	216	GLU	CD-OE2	10.60	1.37	1.25
1	O	437	GLU	CD-OE1	8.56	1.35	1.25
1	Z	475	GLU	CD-OE2	8.45	1.34	1.25
1	O	462	GLU	CD-OE1	8.39	1.34	1.25

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	357	ASP	C-N-CD	-13.79	90.26	120.60
1	Z	152	ARG	NE-CZ-NH1	12.76	126.68	120.30
1	O	200	ASP	CB-CG-OD1	-9.71	109.56	118.30
1	O	409	ASP	CB-CG-OD2	-9.62	109.64	118.30
1	Z	10	ASP	CB-CG-OD1	-8.85	110.34	118.30

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	O	3914	0	3853	631	0
1	Z	3923	0	3859	572	0
2	O	15	0	18	2	0
3	O	6	0	8	4	0
3	Z	6	0	8	2	0
All	All	7864	0	7746	1204	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 77.

The worst 5 of 1204 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:Z:329:SER:HB2	1:Z:381:LEU:HD11	1.28	1.14
1:Z:84:GLU:HB2	1:Z:103:TRP:HB3	1.15	1.12
1:O:145:LEU:HD12	1:O:151:SER:HB2	1.23	1.11
1:Z:228:ASN:HB2	1:Z:236:ARG:HD2	1.28	1.09
1:O:17:ARG:HD2	1:O:32:GLN:HE21	1.17	1.07

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	O	495/501 (99%)	370 (75%)	94 (19%)	31 (6%)	1	7
1	Z	496/501 (99%)	397 (80%)	85 (17%)	14 (3%)	5	21
All	All	991/1002 (99%)	767 (77%)	179 (18%)	45 (4%)	2	12

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	99	ASN
1	O	109	ALA
1	O	149	GLU
1	O	151	SER
1	O	358	PRO

### 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	O	408/412 (99%)	293 (72%)	115 (28%)	0	1
1	Z	409/412 (99%)	287 (70%)	122 (30%)	0	0
All	All	817/824 (99%)	580 (71%)	237 (29%)	0	1

5 of 237 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	4	LYS
1	Z	460	LEU
1	Z	121	GLU
1	Z	456	ASN
1	Z	498	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	47	HIS
1	Z	455	GLN
1	Z	114	HIS
1	Z	404	HIS
1	Z	104	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands 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
2	EPE	O	602	-	15,15,15	2.10	3 (20%)	18,20,20	1.97	4 (22%)
3	GOL	Z	603	-	5,5,5	0.47	0	5,5,5	0.51	0
3	GOL	O	601	-	5,5,5	0.89	0	5,5,5	0.63	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	EPE	O	602	-	-	3/9/19/19	0/1/1/1
3	GOL	Z	603	-	-	0/4/4/4	-
3	GOL	O	601	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	602	EPE	O3S-S	5.74	1.67	1.47
2	O	602	EPE	C10-S	3.71	1.82	1.77
2	O	602	EPE	C5-N4	2.07	1.52	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	602	EPE	O3S-S-O1S	-4.38	100.58	111.27
2	O	602	EPE	O2S-S-C10	4.06	111.81	106.92
2	O	602	EPE	C2-C3-N4	2.93	116.65	110.64
2	O	602	EPE	O2S-S-O1S	2.44	122.41	113.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	602	EPE	C8-C7-N4-C5
3	O	601	GOL	C1-C2-C3-O3
3	O	601	GOL	O2-C2-C3-O3
2	O	602	EPE	C8-C7-N4-C3
2	O	602	EPE	N4-C7-C8-O8

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	602	EPE	2	0
3	Z	603	GOL	2	0
3	O	601	GOL	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 [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	O	497/501 (99%)	-0.94	0 100 100	12, 33, 66, 90	0
1	Z	498/501 (99%)	-0.97	0 100 100	11, 32, 66, 87	0
All	All	995/1002 (99%)	-0.96	0 100 100	11, 32, 66, 90	0

There are no RSRZ outliers to report.

### 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 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(Å <sup>2</sup> )	Q<0.9
2	EPE	O	602	15/15	0.92	0.28	84,84,84,84	0
3	GOL	O	601	6/6	0.97	0.11	10,11,69,71	0
3	GOL	Z	603	6/6	0.98	0.10	10,10,10,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.