



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 03:59 AM UTC

PDB ID : 1BOT / pdb_00001bot
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

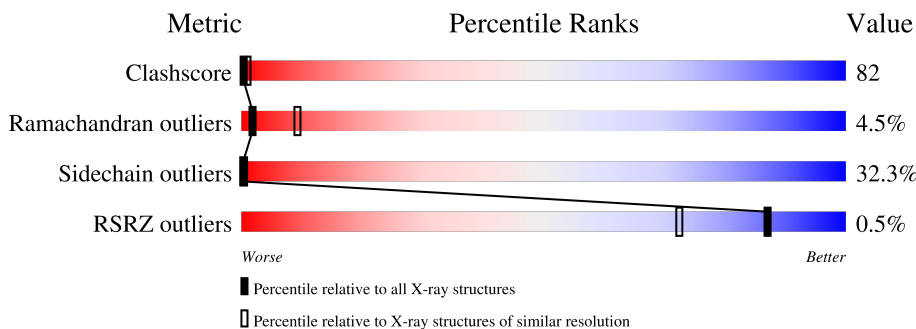
1 Overall quality at a glance

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	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (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 ≥ 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	 14% 50% 28% 7% .
1	Z	501	 16% 50% 30% 4% .

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](#)

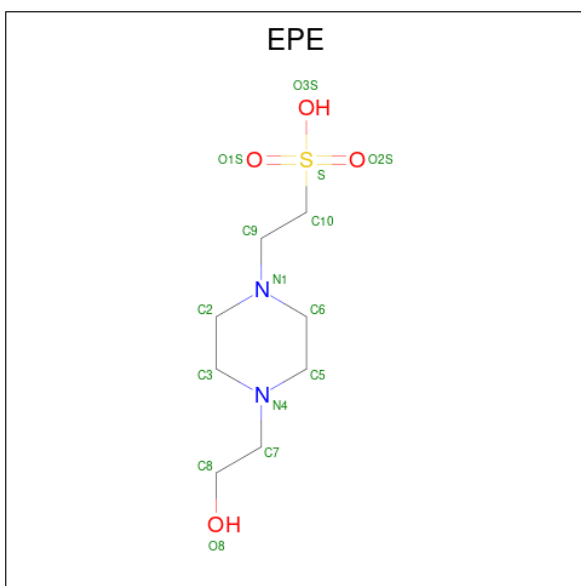
There are 3 unique types of molecules in this entry. The entry contains 7864 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).

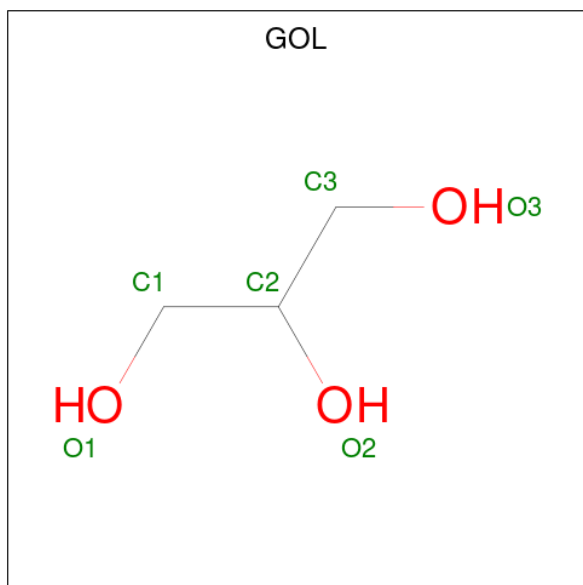
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	O	497	Total 3914	C 2469	N 686	O 740	S 19	0	0	0
1	Z	498	Total 3923	C 2474	N 687	O 743	S 19	0	0	0

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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 (CCD ID: GOL) (formula: $C_3H_8O_3$).

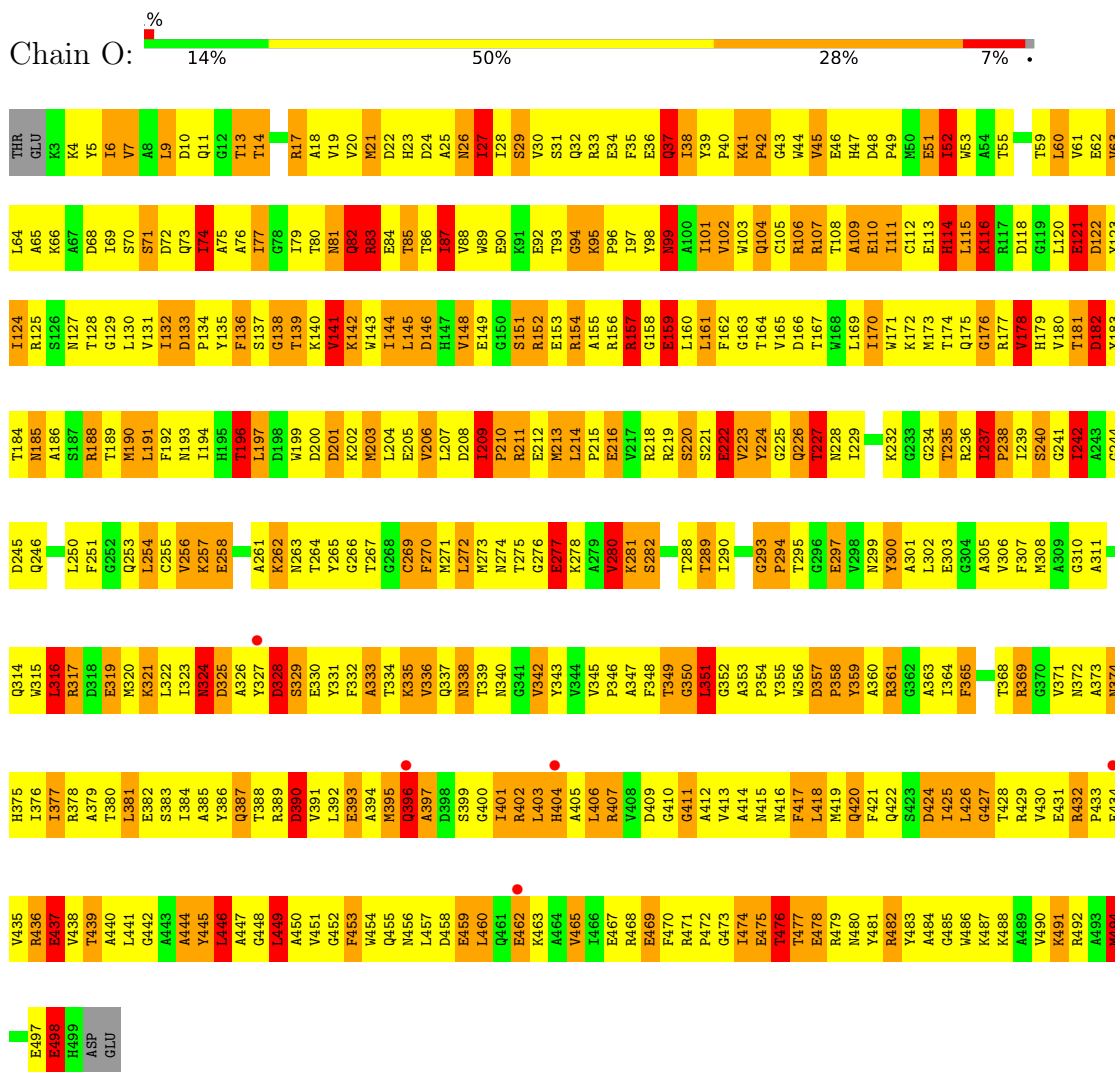


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	C	O	0	0
			6	3	3		
3	Z	1	Total	C	O	0	0
			6	3	3		

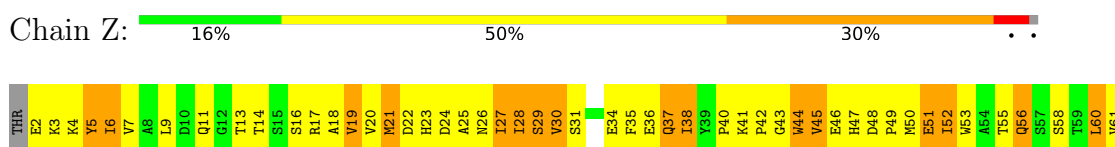
3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PROTEIN (GLYCEROL KINASE)



• Molecule 1: PROTEIN (GLYCEROL KINASE)



L441	L442	A443	A444	Y445	L446	L449	A450	V451	G452	F453	W454	Q455	M456	L457	D458	F459	L460	Q461	E462	K463	A464	V465	I466	E467	R468	E469	F470	R471	P472	G473	I474	E475	T476	T477	E478	R479	N480	Y481	R482	Y483	A484	G485	W486	R487	K488	A489	V490	K491	R492	E497	E498	H499	ASP	GLU						
L381	E382	S383	I384	A385	Y386	Q387	T388	R389	D390	V391	L392	E393	A394	M395	Q396	A397	R398	S399	G400	I401	R402	L403	L406	R407	V408	D409	G410	G411	A412	V413	A414	N415	N416	F417	L418	M419	Q420	F421	Q422	S423	D424	I425	L426	G427	T428	R429	V430	E431	R432	P433	E434	V435	R436	E437	E438	H439	ASP	GLU		
R317	D318	E319	M320	K321	L322	I323	M324	D325	A326	Y327	D328	S329	E330	Y331	F332	A333	T334	K335	V336	Q337	N338	T339	M340	G341	V342	Y343	V344	V345	P346	A347	F348	T349	G350	L351	G352	A353	P354	Y355	W356	D357	P358	Y359	A360	R361	G362	A363	I364	F365	T368	R369	G370	V371	G310	A311	N372	A373	N374	H375	I376	I377
F251	G252	Q253	L254	C255	V256	K257	M260	A261	K262	M263	T264	Y265	G266	T267	G268	C269	F270	M271	L272	M273	M274	T275	K278	A279	V280	K281	L286	T289	I290	A291	S221	E222	V223	Y224	G225	Q226	T227	M228	I229	T235	R236	I237	P238	T239	S240	G241	M308	A309	G310	A311	S312	I313	G314	W315	L316					
A186	S187	R188	T189	M190	L191	F192	M193	I194	H195	T196	L197	D198	M199	D200	D201	K202	M203	L204	E205	V206	L207	D208	I209	P210	R211	E212	M213	L214	P215	E216	V217	R218	R219	S220	S221	E222	V223	Y224	G225	Q226	T227	M228	I229	T235	R236	I237	P238	T239	S240	G241	M308	A309	G310	A311	S312	I313	G314	W315	L316	
E62	V63	L64	A65	I69	S70	S71	D72	Q73	I74	A75	I79	T80	N81	Q82	R83	E84	T85	T86	I87	V88	W89	E90	E91	K91	E92	T93	G94	K95	P96	I97	Y98	N99	A100	I101	F102	M103	Q104	C105	R106	R107	T108	A109	E110	I111	C112	E113	H114	L115	K116	R117	D118	G119	L120	E121	D122	Y123	I124	N125		
S126	M127	T128	G129	L130	V131	I132	D133	P134	Y135	F136	S137	G138	T139	K140	V141	K142	W143	L144	L145	D146	H147	V148	E149	G150	S151	R152	E153	R154	A155	P156	R157	G158	E159	A160	L161	F162	G163	T164	V165	D166	T167	W168	L169	I170	M171	K172	M173	T174	Q175	G176	R177	V178	H179	V180	T181	D182	Y183	I184	N185	

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	168.80Å 168.80Å 202.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.05 20.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	81.0 (20.00-3.05) 80.9 (20.00-3.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.88Å)	Xtrriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.219 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtrriage
Anisotropy	0.128	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 123.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7864	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.46	15/3994 (0.4%)	1.89	109/5414 (2.0%)
1	Z	1.48	10/4003 (0.2%)	1.87	107/5426 (2.0%)
All	All	1.47	25/7997 (0.3%)	1.88	216/10840 (2.0%)

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	44	TRP	CA-C	-7.10	1.44	1.52
1	Z	34	GLU	CD-OE2	6.65	1.38	1.25
1	O	270	PHE	CA-C	-6.34	1.46	1.53
1	O	216	GLU	CD-OE2	6.29	1.37	1.25
1	O	345	VAL	CA-CB	-6.21	1.48	1.54

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	404	HIS	CA-CB-CG	-9.99	103.81	113.80
1	Z	237	ILE	CA-C-N	9.68	129.44	119.76
1	Z	237	ILE	C-N-CA	9.68	129.44	119.76
1	Z	136	PHE	CA-C-N	9.04	132.75	120.54
1	Z	136	PHE	C-N-CA	9.04	132.75	120.54

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	673	0
1	Z	3923	0	3859	606	0
2	O	15	0	18	2	0
3	O	6	0	8	4	0
3	Z	6	0	8	3	0
All	All	7864	0	7746	1278	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 82.

The worst 5 of 1278 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:O:271:MET:HE1	1:O:392:LEU:HA	1.14	1.10
1:Z:228:ASN:HB2	1:Z:236:ARG:HD2	1.28	1.09

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 5
1	Z	496/501 (99%)	397 (80%)	85 (17%)	14 (3%)	4 16
All	All	991/1002 (99%)	767 (77%)	179 (18%)	45 (4%)	2 9

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%)	276 (68%)	132 (32%)	0	0
1	Z	409/412 (99%)	277 (68%)	132 (32%)	0	0
All	All	817/824 (99%)	553 (68%)	264 (32%)	0	0

5 of 264 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	398	ASP
1	Z	423	SER
1	Z	479	ARG
1	O	351	LEU
1	O	335	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	47	HIS
1	Z	420	GLN
1	Z	104	GLN
1	Z	455	GLN
1	Z	337	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 oligosaccharides 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	2.07	3 (20%)	19,20,20	1.87	5 (26%)
3	GOL	O	601	-	5,5,5	0.92	0	5,5,5	0.65	0
3	GOL	Z	603	-	5,5,5	0.49	0	5,5,5	0.54	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	O	601	-	-	2/4/4/4	-
3	GOL	Z	603	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	602	EPE	O3S-S	5.49	1.67	1.47
2	O	602	EPE	C10-S	3.70	1.82	1.77
2	O	602	EPE	C5-N4	2.13	1.52	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	602	EPE	O3S-S-O1S	-4.32	100.58	111.40
2	O	602	EPE	O2S-S-C10	3.36	111.81	106.73
2	O	602	EPE	C2-C3-N4	2.97	116.65	110.65
2	O	602	EPE	O2S-S-O1S	2.64	122.41	113.82
2	O	602	EPE	C6-N1-C2	2.07	113.29	108.84

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	601	GOL	C1-C2-C3-O3
2	O	602	EPE	C8-C7-N4-C5
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 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	602	EPE	2	0
3	O	601	GOL	4	0
3	Z	603	GOL	3	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, 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	O	497/501 (99%)	-0.37	5 (1%) 79 59	12, 33, 66, 90	0
1	Z	498/501 (99%)	-0.44	0 100 100	11, 32, 66, 87	0
All	All	995/1002 (99%)	-0.41	5 (0%) 87 72	11, 32, 66, 90	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	404	HIS	3.0
1	O	327	TYR	2.7
1	O	396	GLN	2.6
1	O	462	GLU	2.1
1	O	434	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 oligosaccharides 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, 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	B-factors(\AA^2)	Q<0.9
2	EPE	O	602	15/15	0.88	0.18	84,84,84,84	0
3	GOL	O	601	6/6	0.98	0.06	10,11,69,71	0
3	GOL	Z	603	6/6	0.98	0.06	10,10,10,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.