



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:57 PM UTC

PDB ID : 7ZHT / pdb_00007zht
Title : Leishmania donovani Glucose 6-Phosphate Dehydrogenase apo form
Authors : Fritz-Wolf, K.; Berneburg, I.
Deposited on : 2022-04-07
Resolution : 2.80 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

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

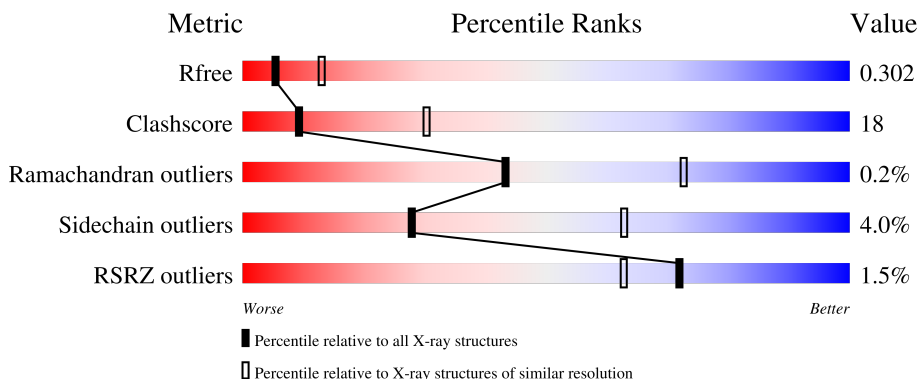
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	A	562	
1	B	562	
1	C	562	
1	D	562	

2 Entry composition [i](#)

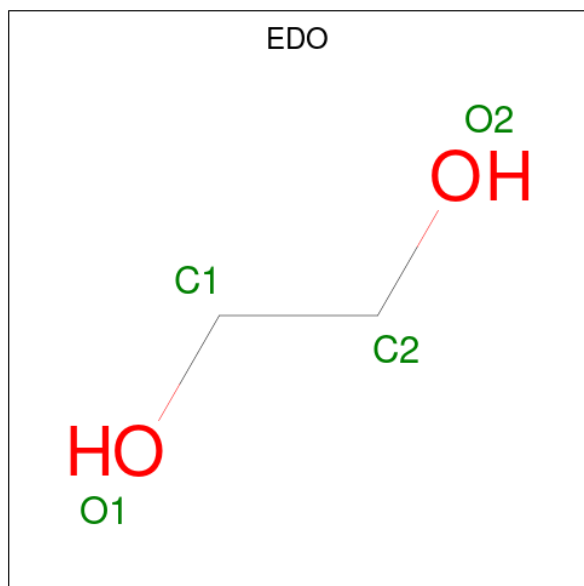
There are 4 unique types of molecules in this entry. The entry contains 16104 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glucose-6-phosphate 1-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4208	2676	724	792	16			
1	B	525	Total	C	N	O	S	0	0	0
			4158	2647	713	782	16			
1	C	483	Total	C	N	O	S	0	0	0
			3823	2432	656	718	17			
1	D	485	Total	C	N	O	S	0	0	0
			3838	2442	658	721	17			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



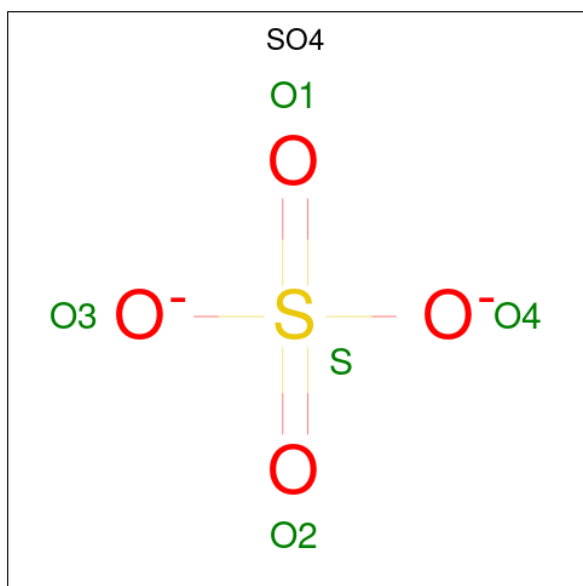
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

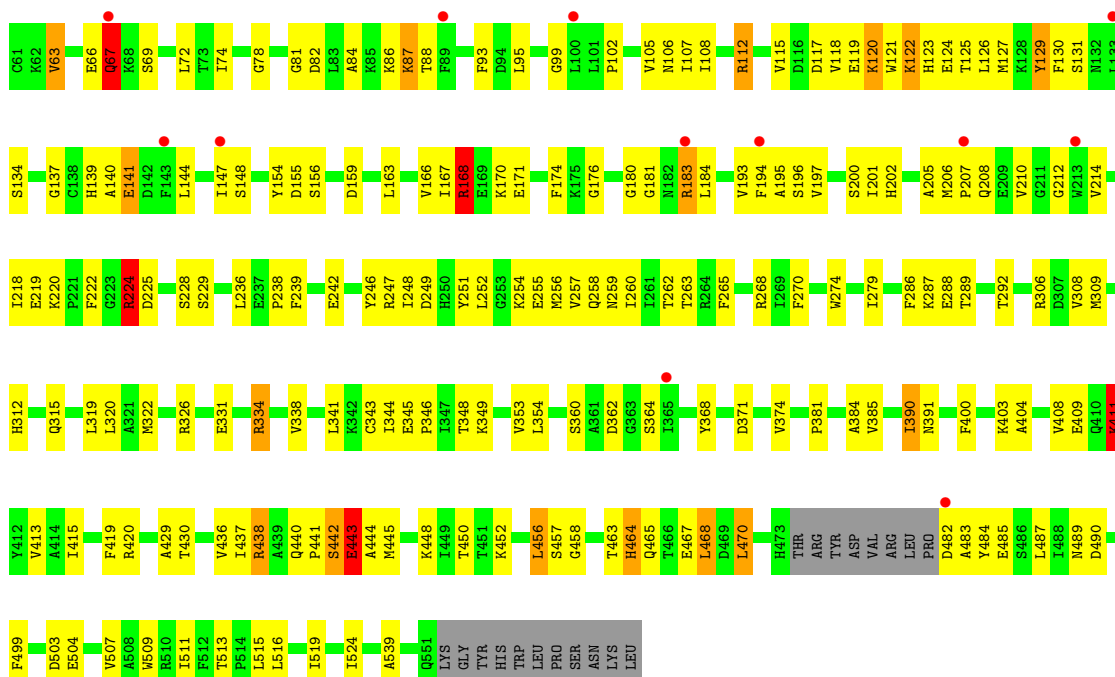
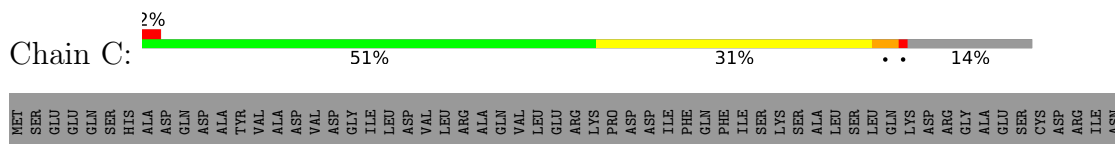


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

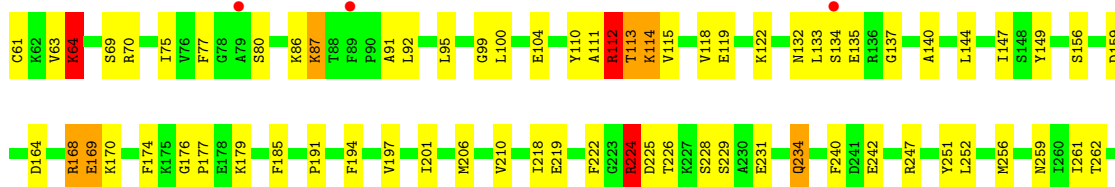
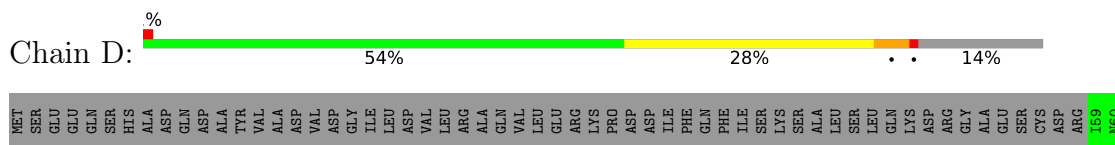
- Molecule 4 is water.

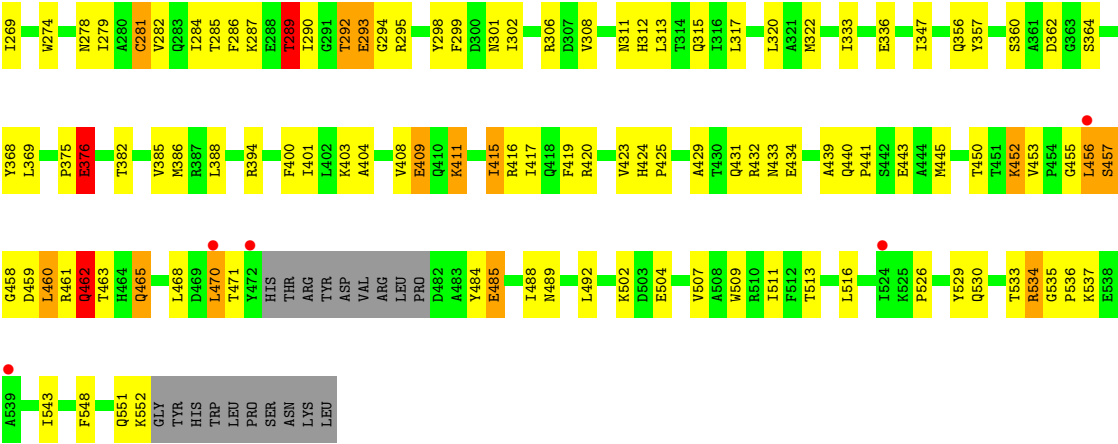
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	O 3	0	0
4	B	14	Total 14	O 14	0	0
4	C	4	Total 4	O 4	0	0
4	D	5	Total 5	O 5	0	0

- Molecule 1: Glucose-6-phosphate 1-dehydrogenase



- Molecule 1: Glucose-6-phosphate 1-dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.69Å 65.82Å 189.22Å 90.00° 92.35° 90.00°	Depositor
Resolution (Å)	39.20 – 2.80 39.20 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.20-2.80) 98.4 (39.20-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.244 , 0.304 0.244 , 0.302	Depositor DCC
R_{free} test set	7073 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16104	wwPDB-VP
Average B, all atoms (Å ²)	91.0	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 29.63 % 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 1.4996e-03. 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, 0.333 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: SO4, EDO

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	0.38	3/4296 (0.1%)	0.89	25/5810 (0.4%)
1	B	0.28	0/4244	0.66	9/5740 (0.2%)
1	C	0.48	5/3905 (0.1%)	1.08	42/5281 (0.8%)
1	D	0.44	3/3919 (0.1%)	1.04	42/5299 (0.8%)
All	All	0.40	11/16364 (0.1%)	0.93	118/22130 (0.5%)

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	A	0	17
1	C	0	6
1	D	1	7
All	All	1	30

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	326	ARG	CD-NE	-7.01	1.36	1.46
1	D	462	GLN	CB-CG	-6.71	1.32	1.52
1	C	326	ARG	CZ-NH2	6.58	1.42	1.33
1	A	326	ARG	CZ-NH2	6.23	1.41	1.33
1	A	112	ARG	CG-CD	-5.94	1.34	1.52

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	534	ARG	CB-CG-CD	-18.64	68.43	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	ALA	CA-C-N	-16.20	95.75	122.65
1	C	140	ALA	C-N-CA	-16.20	95.75	122.65
1	A	376	GLU	CG-CD-OE1	15.10	153.12	118.40
1	A	376	GLU	CG-CD-OE2	-14.37	85.36	118.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	289	THR	CB

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	GLU	Peptide
1	A	134	SER	Peptide
1	A	20	ILE	Peptide
1	A	67	GLN	Sidechain,Peptide
1	A	69	SER	Mainchain

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	4208	0	4181	149	2
1	B	4158	0	4135	125	0
1	C	3823	0	3791	176	1
1	D	3838	0	3814	158	0
2	A	8	0	11	2	0
2	B	12	0	18	0	0
2	C	12	0	18	0	0
2	D	4	0	6	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	3	0	0	3	0
4	B	14	0	0	2	0
4	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	5	0	0	0	0
All	All	16104	0	15974	579	2

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 18.

The worst 5 of 579 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:C:120:LYS:HD3	1:C:124:GLU:OE1	1.32	1.23
1:D:112:ARG:NH1	1:D:113:THR:HG23	1.57	1.18
1:D:112:ARG:HH12	1:D:113:THR:CG2	1.57	1.17
1:D:112:ARG:NH1	1:D:113:THR:CG2	2.09	1.14
1:D:112:ARG:HH12	1:D:113:THR:HG22	1.13	1.04

All (2) 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:A:112:ARG:NH1	1:C:159:ASP:OD1[2_646]	1.93	0.27
1:A:175:LYS:NZ	1:A:526:PRO:O[1_545]	2.16	0.04

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	526/562 (94%)	488 (93%)	34 (6%)	4 (1%)	16	44
1	B	519/562 (92%)	493 (95%)	26 (5%)	0	100	100
1	C	479/562 (85%)	451 (94%)	27 (6%)	1 (0%)	43	72
1	D	481/562 (86%)	457 (95%)	24 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2005/2248 (89%)	1889 (94%)	111 (6%)	5 (0%)	43 72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	LEU
1	A	376	GLU
1	C	443	GLU
1	A	33	PRO
1	A	34	ASP

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	454/482 (94%)	430 (95%)	24 (5%)	20 52
1	B	449/482 (93%)	438 (98%)	11 (2%)	43 77
1	C	412/482 (86%)	395 (96%)	17 (4%)	27 62
1	D	414/482 (86%)	396 (96%)	18 (4%)	26 60
All	All	1729/1928 (90%)	1659 (96%)	70 (4%)	28 63

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	289	THR
1	D	360	SER
1	D	462	GLN
1	B	14	VAL
1	A	468	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	315	GLN
1	C	67	GLN
1	D	440	GLN
1	B	440	GLN
1	C	495	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	EDO	D	601	-	3,3,3	0.43	0	2,2,2	0.41	0
3	SO4	B	1004	-	4,4,4	0.24	0	6,6,6	0.07	0
2	EDO	A	601	-	3,3,3	0.46	0	2,2,2	0.27	0
2	EDO	A	602	-	3,3,3	0.44	0	2,2,2	0.37	0
2	EDO	B	1002	-	3,3,3	0.45	0	2,2,2	0.43	0
3	SO4	C	604	-	4,4,4	0.26	0	6,6,6	0.18	0
2	EDO	C	601	-	3,3,3	0.47	0	2,2,2	0.26	0
2	EDO	C	603	-	3,3,3	0.44	0	2,2,2	0.37	0
3	SO4	A	603	-	4,4,4	0.25	0	6,6,6	0.04	0
2	EDO	B	1001	-	3,3,3	0.43	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	1003	-	3,3,3	0.44	0	2,2,2	0.36	0
2	EDO	C	602	-	3,3,3	0.44	0	2,2,2	0.37	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	EDO	D	601	-	-	0/1/1/1	-
2	EDO	A	601	-	-	1/1/1/1	-
2	EDO	A	602	-	-	0/1/1/1	-
2	EDO	B	1002	-	-	1/1/1/1	-
2	EDO	C	601	-	-	0/1/1/1	-
2	EDO	C	603	-	-	1/1/1/1	-
2	EDO	B	1001	-	-	0/1/1/1	-
2	EDO	B	1003	-	-	1/1/1/1	-
2	EDO	C	602	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	602	EDO	O1-C1-C2-O2
2	A	601	EDO	O1-C1-C2-O2
2	B	1003	EDO	O1-C1-C2-O2
2	C	603	EDO	O1-C1-C2-O2
2	B	1002	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	EDO	1	0
2	A	602	EDO	1	0
3	A	603	SO4	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 [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	A	530/562 (94%)	-0.04	5 (0%) 81 74	49, 80, 140, 204	0
1	B	525/562 (93%)	-0.01	6 (1%) 78 70	48, 81, 140, 199	0
1	C	483/562 (85%)	0.15	12 (2%) 58 48	51, 88, 149, 199	0
1	D	485/562 (86%)	0.11	8 (1%) 70 61	60, 87, 132, 179	0
All	All	2023/2248 (89%)	0.05	31 (1%) 72 63	48, 85, 140, 204	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	439	ALA	4.6
1	C	89	PHE	3.6
1	B	45	LEU	3.5
1	B	72	LEU	3.0
1	D	539	ALA	2.9

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($\text{\AA}^2$)	Q<0.9
2	EDO	C	602	4/4	0.70	0.19	89,90,102,110	0
2	EDO	C	601	4/4	0.75	0.11	113,117,119,128	0
2	EDO	A	602	4/4	0.75	0.13	65,77,78,83	0
2	EDO	D	601	4/4	0.76	0.26	81,87,88,107	0
3	SO4	B	1004	5/5	0.77	0.08	115,119,122,140	0
2	EDO	B	1001	4/4	0.79	0.12	64,72,80,91	0
2	EDO	B	1002	4/4	0.80	0.20	50,59,67,71	0
3	SO4	A	603	5/5	0.82	0.08	109,111,130,142	0
3	SO4	C	604	5/5	0.83	0.14	97,108,124,130	0
2	EDO	C	603	4/4	0.84	0.10	83,109,111,114	0
2	EDO	A	601	4/4	0.87	0.11	79,96,97,107	0
2	EDO	B	1003	4/4	0.92	0.13	69,73,73,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.