Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 03:50 PM EDT

PDB ID	:	8DQO
Title	:	Crystal structure of Arabidopsis thaliana COSY
Authors	:	Kim, C.Y.; Mitchell, A.J.; Gutierrez, M.; Weng, J.K.
Deposited on	:	2022-07-19
Resolution	:	1.90 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

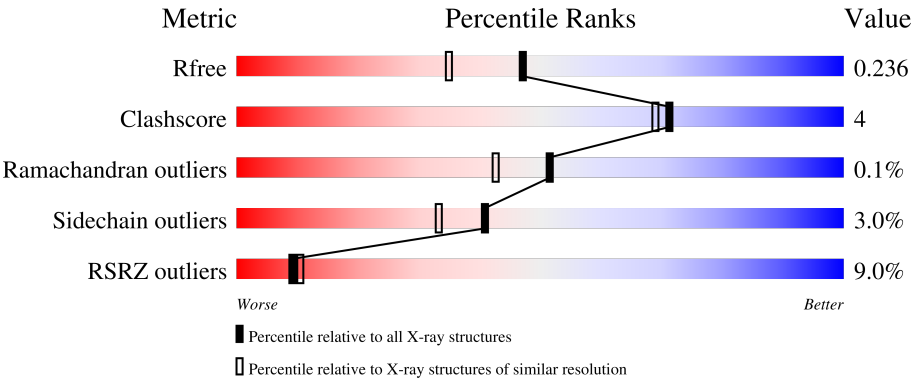
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	451	5% 88% 8%
1	B	451	12% 85% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7232 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.

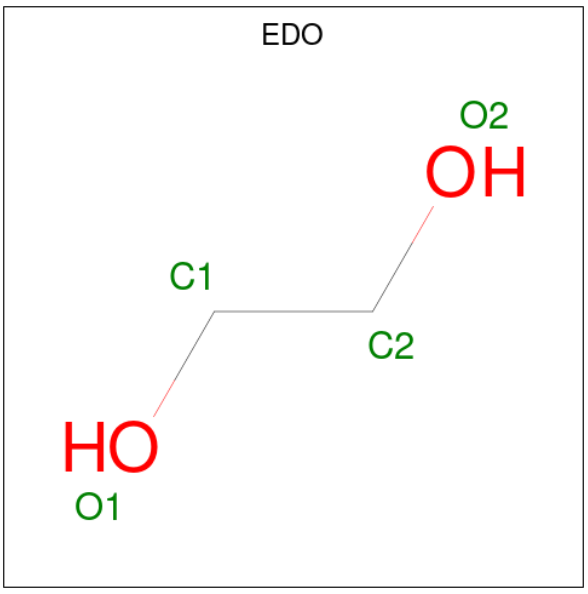
- Molecule 1 is a protein called Coumarin Synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	2	0
			3421	2181	580	644	16			
1	B	437	Total	C	N	O	S	0	1	0
			3414	2177	578	642	17			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

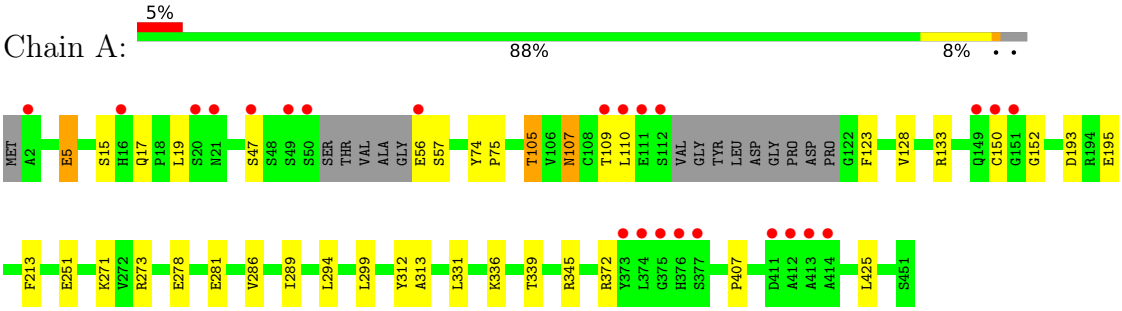
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	228	Total O 228 228	0	0
4	B	123	Total O 123 123	0	0

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.

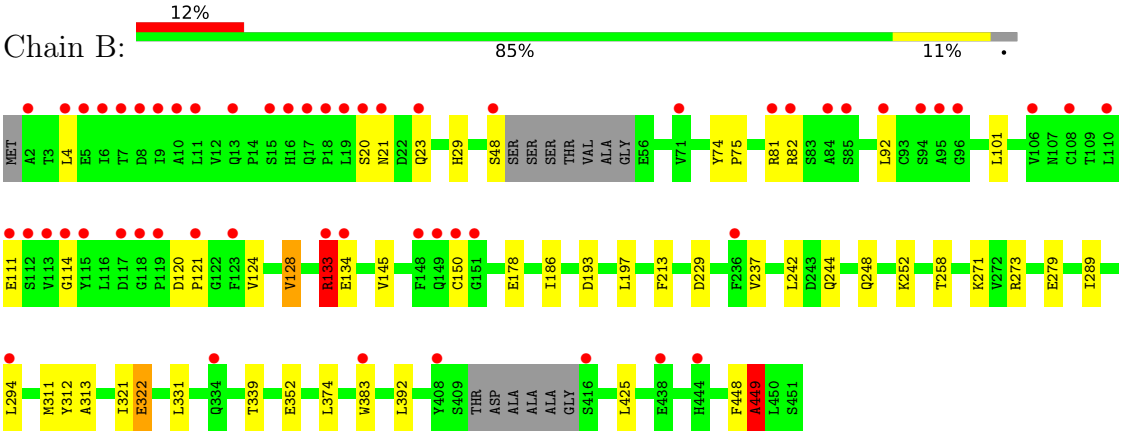
• Molecule 1: Coumarin Synthase

Chain A:



• Molecule 1: Coumarin Synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.41Å 57.90Å 270.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 1.90 48.72 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.76-1.90) 98.5 (48.72-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.190 , 0.230 0.199 , 0.236	Depositor DCC
R_{free} test set	3653 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7232	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, CA

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	0.62	5/3504 (0.1%)	0.73	2/4750 (0.0%)
1	B	0.61	3/3498 (0.1%)	0.66	1/4747 (0.0%)
All	All	0.61	8/7002 (0.1%)	0.70	3/9497 (0.0%)

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	2
1	B	0	3
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	322	GLU	CG-CD	13.55	1.72	1.51
1	B	279	GLU	CD-OE1	-12.05	1.12	1.25
1	A	5	GLU	CD-OE2	-9.22	1.15	1.25
1	B	449	ALA	C-O	8.44	1.39	1.23
1	A	251	GLU	CD-OE2	6.75	1.33	1.25
1	A	105	THR	C-O	-5.90	1.12	1.23
1	A	57	SER	CB-OG	5.23	1.49	1.42
1	A	5	GLU	C-O	5.06	1.32	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	GLU	OE1-CD-OE2	7.62	132.44	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	279	GLU	OE1-CD-OE2	7.48	132.28	123.30
1	A	133	ARG	NE-CZ-NH1	5.70	123.15	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	THR	Mainchain
1	A	273	ARG	Sidechain
1	B	114	GLY	Peptide
1	B	133	ARG	Sidechain
1	B	273	ARG	Sidechain

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	3421	0	3351	24	0
1	B	3414	0	3332	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	36	0	54	2	0
3	B	8	0	12	0	0
4	A	228	0	0	1	0
4	B	123	0	0	0	0
All	All	7232	0	6749	48	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 (48) 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:286:VAL:HG22	1:A:312[B]:TYR:CD1	2.01	0.94
1:A:286:VAL:CG2	1:A:312[B]:TYR:CD1	2.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ARG:HH22	3:A:509:EDO:C2	2.12	0.62
1:B:294:LEU:CD2	1:B:339:THR:HG22	2.31	0.61
1:B:29:HIS:HE1	1:B:352:GLU:OE1	1.83	0.60
1:A:286:VAL:HG21	1:A:312[B]:TYR:CE1	2.37	0.59
1:A:286:VAL:CG2	1:A:312[B]:TYR:CE1	2.87	0.58
1:B:48:SER:OG	1:B:383:TRP:CD1	2.56	0.57
1:A:213[A]:PHE:HB2	1:A:312[A]:TYR:CE1	2.40	0.56
1:B:120:ASP:OD1	1:B:124:VAL:HG23	2.06	0.56
1:B:101:LEU:HD11	1:B:145:VAL:HG23	1.91	0.52
1:B:178:GLU:OE1	1:B:186:ILE:HA	2.10	0.52
1:B:81:ARG:NH2	1:B:92:LEU:HD22	2.27	0.50
1:B:321:ILE:HG13	1:B:322:GLU:HG2	1.93	0.50
1:B:4:LEU:C	1:B:4:LEU:HD23	2.32	0.50
1:B:128:VAL:CG1	1:B:392:LEU:HD12	2.42	0.49
1:A:345:ARG:HH22	3:A:509:EDO:H21	1.78	0.49
1:A:110:LEU:HD11	1:A:152:GLY:HA3	1.94	0.49
1:B:23:GLN:NE2	1:B:74:TYR:OH	2.45	0.49
1:B:237:VAL:HG12	1:B:242:LEU:CD2	2.43	0.48
1:A:195:GLU:HB3	4:A:607:HOH:O	2.12	0.48
1:B:294:LEU:HD22	1:B:339:THR:HG22	1.95	0.48
1:B:425:LEU:C	1:B:425:LEU:HD23	2.34	0.48
1:A:107:ASN:O	1:A:107:ASN:ND2	2.46	0.47
1:A:56:GLU:N	1:A:56:GLU:OE1	2.48	0.47
1:A:109:THR:HA	1:A:150:CYS:HB2	1.97	0.46
1:A:17:GLN:HE21	1:A:19:LEU:H	1.63	0.46
1:A:289:ILE:CD1	1:A:339:THR:HG23	2.45	0.46
1:B:82:ARG:NH2	1:B:133:ARG:HH22	2.14	0.45
1:B:82:ARG:HH21	1:B:133:ARG:HH22	1.65	0.44
1:A:278:GLU:HB2	1:A:281:GLU:HG3	2.00	0.44
1:B:313:ALA:HB1	1:B:331:LEU:HG	2.00	0.44
1:B:29:HIS:CE1	1:B:352:GLU:OE1	2.69	0.43
1:B:289:ILE:HG13	1:B:311:MET:HG2	1.99	0.43
1:A:278:GLU:HB2	1:A:281:GLU:CG	2.49	0.42
1:A:289:ILE:HD11	1:A:339:THR:HG23	2.01	0.41
1:A:372:ARG:HA	1:A:407:PRO:HA	2.01	0.41
1:B:448:PHE:O	1:B:449:ALA:C	2.59	0.41
1:A:425:LEU:C	1:A:425:LEU:HD23	2.40	0.41
1:A:294:LEU:HD22	1:A:339:THR:HG22	2.03	0.41
1:A:313:ALA:HB1	1:A:331:LEU:HG	2.03	0.41
1:A:289:ILE:HD13	1:A:339:THR:CG2	2.50	0.41
1:B:74:TYR:N	1:B:75:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:PRO:HD2	1:B:124:VAL:HG23	2.03	0.41
1:B:213:PHE:HB2	1:B:312:TYR:CE1	2.55	0.41
1:A:5:GLU:OE1	1:B:258:THR:HA	2.21	0.41
1:B:244:GLN:HE21	1:B:248:GLN:HE21	1.69	0.41
1:A:74:TYR:N	1:A:75:PRO:CD	2.85	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	432/451 (96%)	423 (98%)	9 (2%)	0	100 100
1	B	432/451 (96%)	423 (98%)	8 (2%)	1 (0%)	47 38
All	All	864/902 (96%)	846 (98%)	17 (2%)	1 (0%)	51 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	449	ALA

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/380 (98%)	362 (98%)	9 (2%)	49	43
1	B	370/380 (97%)	357 (96%)	13 (4%)	36	27
All	All	741/760 (98%)	719 (97%)	22 (3%)	41	33

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	47	SER
1	A	107	ASN
1	A	123	PHE
1	A	128	VAL
1	A	193	ASP
1	A	271	LYS
1	A	299	LEU
1	A	336	LYS
1	B	20	SER
1	B	21	ASN
1	B	111	GLU
1	B	128	VAL
1	B	133	ARG
1	B	134	GLU
1	B	150	CYS
1	B	193	ASP
1	B	197	LEU
1	B	229	ASP
1	B	252	LYS
1	B	271	LYS
1	B	374	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	17	GLN
1	A	107	ASN
1	A	225	GLN
1	B	21	ASN

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Mol	Chain	Res	Type
1	B	23	GLN
1	B	29	HIS
1	B	149	GLN
1	B	174	ASN
1	B	225	GLN
1	B	244	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	EDO	A	503	-	3,3,3	0.35	0	2,2,2	0.70	0
3	EDO	A	506	-	3,3,3	0.39	0	2,2,2	0.36	0
3	EDO	A	509	-	3,3,3	0.44	0	2,2,2	0.47	0
3	EDO	A	508	-	3,3,3	0.42	0	2,2,2	0.53	0
3	EDO	A	507	-	3,3,3	0.45	0	2,2,2	0.25	0
3	EDO	B	503	-	3,3,3	0.40	0	2,2,2	0.28	0
3	EDO	A	505	-	3,3,3	0.38	0	2,2,2	0.52	0
3	EDO	A	502	-	3,3,3	0.37	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	A	510	-	3,3,3	0.53	0	2,2,2	0.44	0
3	EDO	A	504	-	3,3,3	0.40	0	2,2,2	0.54	0
3	EDO	B	502	-	3,3,3	0.40	0	2,2,2	0.43	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	EDO	A	503	-	-	1/1/1/1	-
3	EDO	A	506	-	-	0/1/1/1	-
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	A	508	-	-	0/1/1/1	-
3	EDO	A	507	-	-	0/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	A	510	-	-	1/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-

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	504	EDO	O1-C1-C2-O2
3	A	503	EDO	O1-C1-C2-O2
3	A	510	EDO	O1-C1-C2-O2
3	B	502	EDO	O1-C1-C2-O2
3	A	509	EDO	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	509	EDO	2	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^{th} 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	436/451 (96%)	0.35	24 (5%) 25 28	14, 24, 49, 76	0
1	B	437/451 (96%)	0.76	55 (12%) 3 4	25, 39, 64, 73	0
All	All	873/902 (96%)	0.56	79 (9%) 9 10	14, 32, 61, 76	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	ASN	7.6
1	B	408	TYR	7.4
1	B	19	LEU	7.3
1	A	375	GLY	6.3
1	B	20	SER	6.3
1	B	150	CYS	5.8
1	B	95	ALA	5.6
1	B	96	GLY	5.4
1	A	20	SER	5.1
1	A	150	CYS	5.1
1	B	16	HIS	5.1
1	A	50	SER	5.0
1	B	123	PHE	4.5
1	B	84	ALA	4.5
1	A	377	SER	4.2
1	A	414	ALA	4.1
1	B	81	ARG	4.0
1	A	413	ALA	4.0
1	A	112	SER	4.0
1	B	48	SER	3.7
1	B	2	ALA	3.7
1	B	111	GLU	3.6
1	B	9	ILE	3.6
1	B	133	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	149	GLN	3.4
1	B	113	VAL	3.4
1	B	236	PHE	3.4
1	A	412	ALA	3.4
1	B	94	SER	3.3
1	B	11	LEU	3.3
1	B	294	LEU	3.3
1	B	110	LEU	3.3
1	B	115	TYR	3.2
1	B	108	CYS	3.2
1	B	10	ALA	3.2
1	A	16	HIS	3.2
1	B	119	PRO	3.1
1	A	110	LEU	3.1
1	B	112	SER	3.1
1	A	374	LEU	3.1
1	A	376	HIS	3.0
1	A	149	GLN	3.0
1	B	85	SER	3.0
1	A	109	THR	2.9
1	B	92	LEU	2.9
1	A	56	GLU	2.9
1	B	151	GLY	2.8
1	B	444	HIS	2.8
1	A	151	GLY	2.7
1	B	121	PRO	2.6
1	A	411	ASP	2.6
1	B	134	GLU	2.6
1	B	416	SER	2.6
1	B	114	GLY	2.6
1	A	49	SER	2.5
1	B	334	GLN	2.5
1	B	148	PHE	2.5
1	B	17	GLN	2.4
1	B	15	SER	2.4
1	B	7	THR	2.4
1	A	47	SER	2.3
1	B	6	ILE	2.3
1	B	106	VAL	2.2
1	B	117	ASP	2.2
1	B	438	GLU	2.2
1	B	71	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	23	GLN	2.2
1	A	2	ALA	2.1
1	A	111	GLU	2.1
1	B	8	ASP	2.1
1	B	18	PRO	2.1
1	A	21	ASN	2.1
1	B	118	GLY	2.1
1	B	13	GLN	2.1
1	B	383	TRP	2.1
1	B	82	ARG	2.0
1	B	4	LEU	2.0
1	A	373	TYR	2.0
1	B	5	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 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^{th} 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^2)	Q<0.9
3	EDO	A	509	4/4	0.77	0.29	55,57,57,59	0
3	EDO	A	503	4/4	0.79	0.37	38,40,41,46	0
3	EDO	B	503	4/4	0.80	0.18	50,50,50,55	0
3	EDO	A	504	4/4	0.83	0.20	31,36,39,46	0
3	EDO	B	502	4/4	0.86	0.21	41,45,46,49	0
3	EDO	A	505	4/4	0.86	0.16	39,39,42,45	0
3	EDO	A	502	4/4	0.88	0.23	29,35,37,44	0
3	EDO	A	510	4/4	0.88	0.23	29,37,38,43	0
3	EDO	A	507	4/4	0.92	0.13	35,37,38,40	0
3	EDO	A	508	4/4	0.92	0.17	36,40,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	506	4/4	0.92	0.15	30,31,33,36	0
2	CA	B	501	1/1	0.97	0.07	28,28,28,28	0
2	CA	A	501	1/1	1.00	0.05	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.