



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 11:36 AM EDT

PDB ID : 5TMA
Title : Zymomonas mobilis pyruvate decarboxylase mutant PDC-2.3
Authors : Alahuhta, P.M.; Lunin, V.V.
Deposited on : unknown
Resolution : 1.67 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

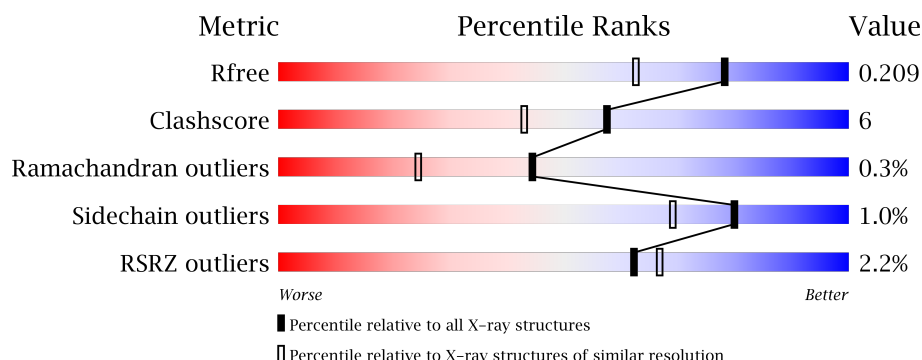
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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}	100719	5252 (1.70-1.66)
Clashscore	112137	5803 (1.70-1.66)
Ramachandran outliers	110173	5704 (1.70-1.66)
Sidechain outliers	110143	5703 (1.70-1.66)
RSRZ outliers	101464	5298 (1.70-1.66)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	576	<div> <div>3%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	B	576	<div> <div>%</div> <div>91%</div> <div>6%</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
4	SO4	A	606	-	-	X	-
4	SO4	A	607[B]	-	-	X	-
4	SO4	B	606[B]	-	-	X	-
4	SO4	B	607[A]	-	-	-	X
4	SO4	B	607[B]	-	-	-	X
4	SO4	B	610	-	-	-	X
4	SO4	B	611	-	-	-	X
5	EDO	A	609	-	-	-	X
5	EDO	A	612	-	-	-	X
5	EDO	A	613	-	-	-	X
5	EDO	A	615	-	-	X	X
5	EDO	A	616[B]	-	-	-	X
5	EDO	A	617	-	-	X	X
5	EDO	B	614	-	-	-	X
5	EDO	B	616	-	-	-	X
5	EDO	B	617	-	-	-	X
5	EDO	B	619	-	-	-	X
5	EDO	B	620	-	-	-	X
5	EDO	B	621	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10255 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 Pyruvate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	567	Total	C	N	O	S	0	29	0
			4560	2886	769	879	26			
1	B	561	Total	C	N	O	S	0	21	0
			4442	2816	751	849	26			

There are 48 discrepancies between the modelled and reference sequences:

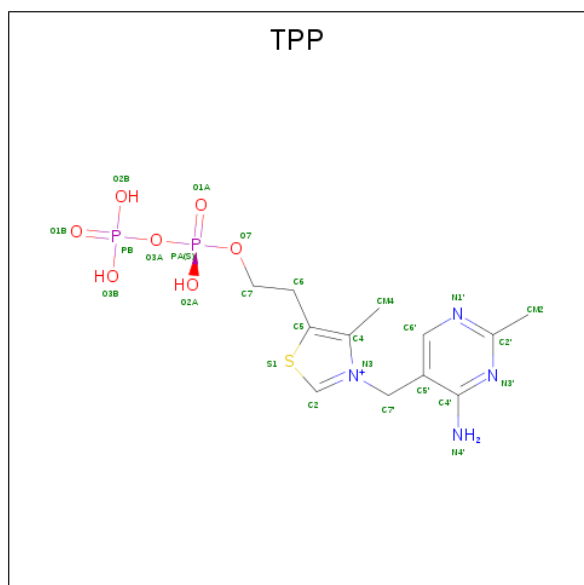
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	SER	engineered mutation	UNP P06672
A	38	ASP	LEU	engineered mutation	UNP P06672
A	109	ALA	GLY	engineered mutation	UNP P06672
A	207	GLU	ALA	engineered mutation	UNP P06672
A	224	ALA	GLY	engineered mutation	UNP P06672
A	333	GLU	GLN	engineered mutation	UNP P06672
A	357	ASP	ALA	engineered mutation	UNP P06672
A	374	ILE	VAL	engineered mutation	UNP P06672
A	376	ASP	ALA	engineered mutation	UNP P06672
A	491	ALA	GLY	engineered mutation	UNP P06672
A	515	ALA	GLY	engineered mutation	UNP P06672
A	516	ALA	GLY	engineered mutation	UNP P06672
A	519	GLU	ALA	engineered mutation	UNP P06672
A	527	ASP	ALA	engineered mutation	UNP P06672
A	540	ALA	GLY	engineered mutation	UNP P06672
A	553	GLU	LYS	engineered mutation	UNP P06672
A	569	LEU	-	expression tag	UNP P06672
A	570	GLU	-	expression tag	UNP P06672
A	571	HIS	-	expression tag	UNP P06672
A	572	HIS	-	expression tag	UNP P06672
A	573	HIS	-	expression tag	UNP P06672
A	574	HIS	-	expression tag	UNP P06672
A	575	HIS	-	expression tag	UNP P06672
A	576	HIS	-	expression tag	UNP P06672
B	2	ASP	SER	engineered mutation	UNP P06672

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	38	ASP	LEU	engineered mutation	UNP P06672
B	109	ALA	GLY	engineered mutation	UNP P06672
B	207	GLU	ALA	engineered mutation	UNP P06672
B	224	ALA	GLY	engineered mutation	UNP P06672
B	333	GLU	GLN	engineered mutation	UNP P06672
B	357	ASP	ALA	engineered mutation	UNP P06672
B	374	ILE	VAL	engineered mutation	UNP P06672
B	376	ASP	ALA	engineered mutation	UNP P06672
B	491	ALA	GLY	engineered mutation	UNP P06672
B	515	ALA	GLY	engineered mutation	UNP P06672
B	516	ALA	GLY	engineered mutation	UNP P06672
B	519	GLU	ALA	engineered mutation	UNP P06672
B	527	ASP	ALA	engineered mutation	UNP P06672
B	540	ALA	GLY	engineered mutation	UNP P06672
B	553	GLU	LYS	engineered mutation	UNP P06672
B	569	LEU	-	expression tag	UNP P06672
B	570	GLU	-	expression tag	UNP P06672
B	571	HIS	-	expression tag	UNP P06672
B	572	HIS	-	expression tag	UNP P06672
B	573	HIS	-	expression tag	UNP P06672
B	574	HIS	-	expression tag	UNP P06672
B	575	HIS	-	expression tag	UNP P06672
B	576	HIS	-	expression tag	UNP P06672

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).

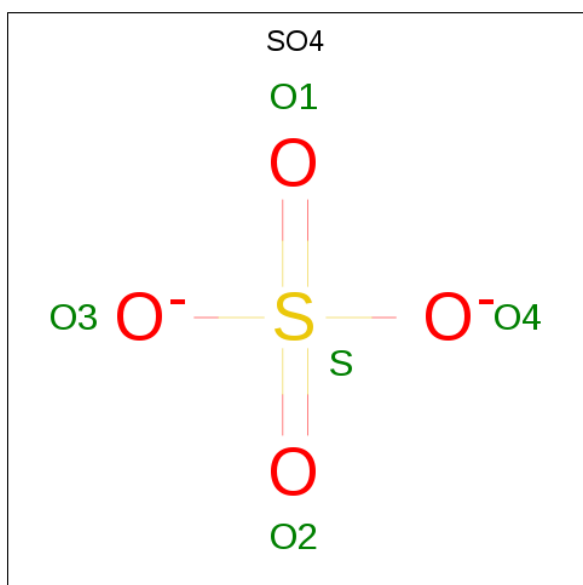


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
2	B	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



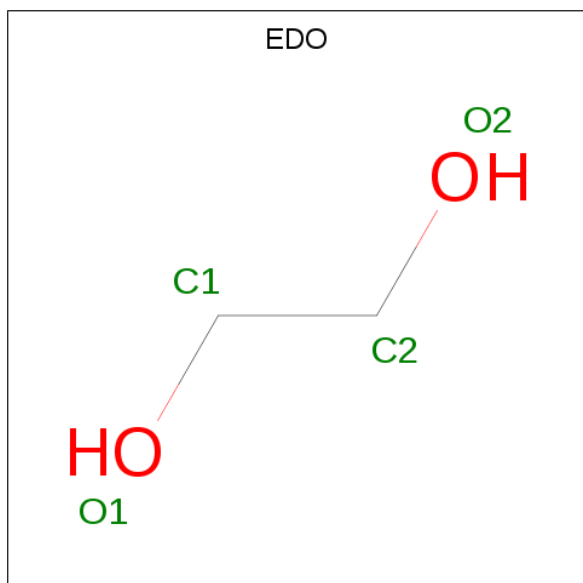
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	1
			10	8	2		
4	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	1
			10	8	2		
4	B	1	Total	O	S	0	1
			10	8	2		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 8 4 4	0	1
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

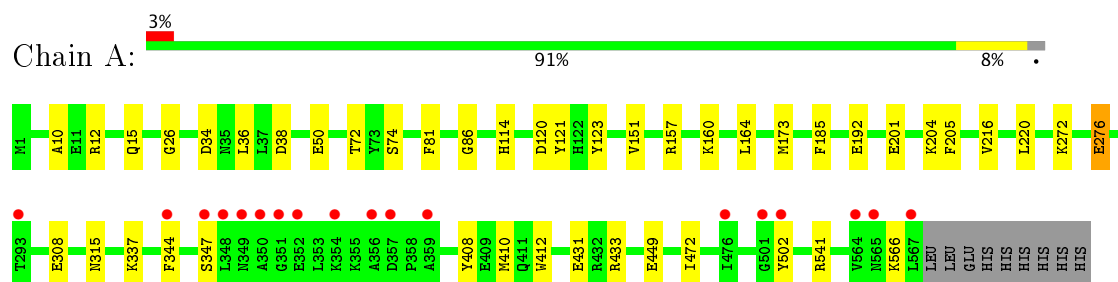
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	507	Total O 520 520	0	13
6	B	497	Total O 508 508	0	11

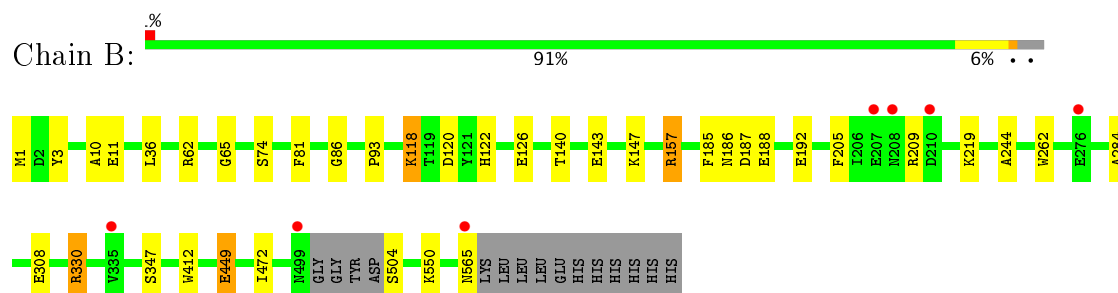
3 Residue-property plots [i](#)

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: Pyruvate decarboxylase



- Molecule 1: Pyruvate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.44Å 124.44Å 173.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.18 – 1.67 52.53 – 1.67	Depositor EDS
% Data completeness (in resolution range)	99.5 (101.18-1.67) 99.5 (52.53-1.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.170 , 0.203 0.181 , 0.209	Depositor DCC
R_{free} test set	7705 reflections (5.16%)	DCC
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10255	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TPP, EDO, SO4

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	1.06	6/4655 (0.1%)	0.98	10/6322 (0.2%)
1	B	1.03	4/4534 (0.1%)	1.00	14/6157 (0.2%)
All	All	1.04	10/9189 (0.1%)	0.99	24/12479 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	74	SER	CB-OG	-6.88	1.33	1.42
1	B	308	GLU	CG-CD	6.87	1.62	1.51
1	B	120	ASP	CB-CG	6.42	1.65	1.51
1	A	50	GLU	CD-OE1	6.37	1.32	1.25
1	B	118	LYS	C-O	6.07	1.34	1.23
1	A	50	GLU	CD-OE2	5.77	1.31	1.25
1	A	431	GLU	CD-OE1	-5.64	1.19	1.25
1	A	308	GLU	CD-OE1	5.45	1.31	1.25
1	A	431	GLU	CB-CG	5.38	1.62	1.52
1	A	308	GLU	CG-CD	5.35	1.59	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157[A]	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	B	157[B]	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	B	62	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	B	308	GLU	OE1-CD-OE2	-7.78	113.96	123.30
1	B	157[A]	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	B	157[B]	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	157[A]	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	157[B]	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	308	GLU	OE1-CD-OE2	-6.44	115.58	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A	433	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	449	GLU	OE1-CD-OE2	-6.18	115.88	123.30
1	B	330[A]	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	330[B]	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	187	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	123	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	B	308	GLU	CG-CD-OE1	5.35	128.99	118.30
1	A	541	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	308	GLU	CG-CD-OE1	5.17	128.65	118.30
1	A	34	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	81	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	B	81	PHE	CB-CG-CD1	5.12	124.38	120.80
1	B	209	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	121	TYR	CB-CG-CD1	-5.05	117.97	121.00

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	4560	0	4460	47	0
1	B	4442	0	4371	33	0
2	A	26	0	16	2	0
2	B	26	0	16	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	35	0	0	5	0
4	B	60	0	0	6	0
5	A	40	0	57	19	0
5	B	36	0	54	9	0
6	A	520	0	0	28	0
6	B	508	0	0	20	0
All	All	10255	0	8974	102	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 6.

All (102) 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)
5:A:616[B]:EDO:H12	6:A:741:HOH:O	1.21	1.30
1:A:114[A]:HIS:HD2	6:A:735:HOH:O	1.19	1.25
4:B:611:SO4:O1	6:B:708:HOH:O	1.57	1.20
4:B:606[B]:SO4:O4	6:B:709:HOH:O	1.58	1.18
4:A:606:SO4:O1	6:A:710:HOH:O	1.56	1.17
4:B:606[B]:SO4:O2	6:B:710:HOH:O	1.63	1.12
1:A:160[B]:LYS:NZ	6:A:712:HOH:O	1.80	1.12
1:A:192[A]:GLU:OE2	5:A:609:EDO:O2	1.69	1.10
4:A:607[B]:SO4:S	6:A:715:HOH:O	2.09	1.08
1:A:38[A]:ASP:OD1	6:A:711[A]:HOH:O	1.70	1.07
1:A:204[A]:LYS:NZ	6:A:713:HOH:O	1.81	1.06
1:A:566[B]:LYS:HA	1:A:566[B]:LYS:HE3	1.37	1.02
1:B:126[B]:GLU:OE1	6:B:711:HOH:O	1.83	0.96
5:B:620:EDO:O1	6:B:712:HOH:O	1.85	0.95
1:A:114[A]:HIS:CD2	6:A:735:HOH:O	2.01	0.94
1:A:566[B]:LYS:HA	1:A:566[B]:LYS:CE	2.02	0.89
5:A:616[B]:EDO:O1	6:A:714:HOH:O	1.92	0.87
1:A:566[B]:LYS:HE3	1:A:566[B]:LYS:CA	1.98	0.86
4:A:607[B]:SO4:O3	6:A:715:HOH:O	1.93	0.83
1:B:185[B]:PHE:O	6:B:713:HOH:O	1.98	0.82
1:A:192[A]:GLU:OE2	5:A:609:EDO:C2	2.29	0.80
1:A:272[B]:LYS:HD2	6:A:1080:HOH:O	1.81	0.79
1:A:204[A]:LYS:HD2	6:A:713:HOH:O	1.84	0.76
1:A:204[A]:LYS:CD	6:A:713:HOH:O	2.31	0.76
1:A:276[A]:GLU:HG3	6:A:840:HOH:O	1.86	0.73
5:B:621:EDO:C1	6:B:1119:HOH:O	2.37	0.72
1:A:38[A]:ASP:OD2	6:A:717:HOH:O	2.09	0.71
1:B:472:ILE:HG21	2:B:601:TPP:S1	2.30	0.71
1:B:118:LYS:O	6:B:715:HOH:O	2.09	0.71
1:B:11[A]:GLU:OE1	6:B:714:HOH:O	2.09	0.70
1:B:143[A]:GLU:HG3	1:B:147[A]:LYS:HD2	1.74	0.69
5:B:617:EDO:O1	6:B:701:HOH:O	0.70	0.69
5:B:621:EDO:C2	6:B:1119:HOH:O	2.39	0.69
1:A:272[B]:LYS:CD	6:A:1080:HOH:O	2.40	0.69
4:A:607[B]:SO4:O4	6:A:715:HOH:O	2.02	0.69
1:B:126[B]:GLU:OE1	6:B:716:HOH:O	2.11	0.68
1:B:122[B]:HIS:HE1	1:B:126[B]:GLU:OE2	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:TYR:CZ	6:A:744:HOH:O	2.44	0.66
5:A:615:EDO:O2	1:B:157[B]:ARG:NE	2.29	0.66
5:A:616[B]:EDO:C1	6:A:741:HOH:O	1.97	0.66
1:B:472:ILE:CG2	2:B:601:TPP:S1	2.86	0.64
1:B:126[B]:GLU:CD	6:B:711:HOH:O	2.33	0.64
5:B:621:EDO:H21	6:B:1119:HOH:O	1.96	0.63
1:A:472:ILE:HG21	2:A:601:TPP:S1	2.39	0.62
5:A:615:EDO:H12	1:B:188:GLU:OE2	1.99	0.62
1:B:192:GLU:OE1	1:B:330[B]:ARG:NH1	2.34	0.60
4:A:606:SO4:S	6:A:710:HOH:O	2.28	0.60
1:B:157[B]:ARG:NH1	6:B:722:HOH:O	2.34	0.60
1:A:408:TYR:HB3	1:A:410[B]:MET:HG3	1.84	0.58
1:A:502:TYR:CE1	6:A:744:HOH:O	2.55	0.58
1:B:122[B]:HIS:CE1	1:B:126[B]:GLU:OE2	2.57	0.57
5:B:621:EDO:H12	6:B:1119:HOH:O	2.01	0.57
1:A:72[B]:THR:HG23	6:A:764:HOH:O	2.04	0.56
5:A:615:EDO:C1	1:B:157[B]:ARG:NH2	2.68	0.56
1:A:205:PHE:CZ	5:A:617:EDO:H22	2.41	0.56
1:A:276[A]:GLU:O	1:A:276[A]:GLU:CG	2.54	0.56
5:B:619:EDO:C2	6:B:755:HOH:O	2.54	0.55
1:A:566[B]:LYS:HA	1:A:566[B]:LYS:NZ	2.22	0.55
1:A:204[A]:LYS:HE2	6:A:1100[A]:HOH:O	2.07	0.55
5:A:609:EDO:C1	6:A:716:HOH:O	2.47	0.54
1:A:26:GLY:HA3	1:A:72[B]:THR:CG2	2.38	0.54
5:A:615:EDO:C1	1:B:188:GLU:OE2	2.56	0.54
1:B:157[B]:ARG:CZ	6:B:722:HOH:O	2.54	0.54
1:A:566[B]:LYS:HA	1:A:566[B]:LYS:HZ2	1.74	0.53
1:A:151:VAL:HG21	1:A:164:LEU:HG	1.91	0.53
1:B:219[A]:LYS:HB2	1:B:284:ALA:HB1	1.91	0.53
1:A:272[B]:LYS:CE	6:A:1080:HOH:O	2.57	0.52
5:A:615:EDO:C2	1:B:157[B]:ARG:CZ	2.86	0.52
1:A:185[B]:PHE:O	5:A:613:EDO:H12	2.10	0.51
1:A:472:ILE:CG2	2:A:601:TPP:S1	2.99	0.51
1:A:86:GLY:HA2	1:A:412:TRP:CG	2.47	0.50
1:A:72[A]:THR:CG2	6:A:735:HOH:O	2.60	0.49
1:A:26:GLY:HA3	1:A:72[B]:THR:HG22	1.94	0.49
1:A:72[A]:THR:HG23	6:A:735:HOH:O	2.13	0.49
2:B:601:TPP:HN42	2:B:601:TPP:C2	2.26	0.49
1:A:205:PHE:CE1	5:A:617:EDO:H22	2.47	0.49
1:B:205:PHE:CE1	5:B:615:EDO:H22	2.48	0.49
1:A:185[B]:PHE:HA	5:A:613:EDO:C1	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:GLY:HA2	1:B:412:TRP:CG	2.48	0.48
1:A:201:GLU:OE1	1:A:315:ASN:ND2	2.45	0.47
1:A:276[A]:GLU:HG2	1:A:344:PHE:CE2	2.49	0.47
1:B:1[B]:MET:HB2	1:B:1[B]:MET:HE2	1.75	0.47
5:A:615:EDO:C2	1:B:157[B]:ARG:NE	2.78	0.46
1:B:122[B]:HIS:CD2	4:B:606[B]:SO4:O1	2.69	0.46
1:B:3:TYR:OH	1:B:11[A]:GLU:OE1	2.27	0.45
1:A:566[B]:LYS:CE	1:A:566[B]:LYS:CA	2.71	0.44
1:A:205:PHE:CE1	5:A:617:EDO:C1	3.01	0.44
1:A:272[B]:LYS:HE3	6:A:1080:HOH:O	2.16	0.43
1:B:122[B]:HIS:HD2	4:B:606[B]:SO4:O1	2.00	0.43
1:B:550:LYS:NZ	6:B:735:HOH:O	2.47	0.43
1:B:140:THR:O	1:B:143[B]:GLU:HG2	2.18	0.43
1:A:10:ALA:HB2	1:A:36:LEU:HD23	2.02	0.42
1:A:185[B]:PHE:HA	5:A:613:EDO:H12	2.00	0.42
1:B:10:ALA:HB2	1:B:36:LEU:HD23	2.01	0.42
1:A:205:PHE:CE1	5:A:617:EDO:H11	2.55	0.41
1:A:12:ARG:HD3	1:A:15:GLN:OE1	2.21	0.41
5:B:616:EDO:C1	6:B:819:HOH:O	2.68	0.41
1:A:216:VAL:HG13	1:A:220:LEU:HD22	2.03	0.41
1:B:244:ALA:HB2	1:B:262:TRP:CD2	2.56	0.40
2:B:601:TPP:H2	2:B:601:TPP:HN42	1.86	0.40
1:B:122[A]:HIS:CD2	4:B:606[A]:SO4:O1	2.75	0.40
1:B:65:GLY:O	1:B:93:PRO:HG2	2.21	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	594/576 (103%)	583 (98%)	9 (2%)	2 (0%)	44 24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	577/576 (100%)	565 (98%)	10 (2%)	2 (0%)	44	24
All	All	1171/1152 (102%)	1148 (98%)	19 (2%)	4 (0%)	44	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	ASN
1	A	74[A]	SER
1	A	74[B]	SER
1	B	347	SER

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	470/450 (104%)	460 (98%)	10 (2%)	59	37
1	B	458/450 (102%)	455 (99%)	3 (1%)	87	79
All	All	928/900 (103%)	915 (99%)	13 (1%)	80	55

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120[A]	ASP
1	A	120[B]	ASP
1	A	173[A]	MET
1	A	173[B]	MET
1	A	276[A]	GLU
1	A	276[B]	GLU
1	A	276[C]	GLU
1	A	337	LYS
1	A	347	SER
1	A	449	GLU
1	B	449	GLU
1	B	504	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	565	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 42 ligands modelled in this entry, 2 are monoatomic - leaving 40 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	$\# Z > 2$
2	TPP	A	601	3	21,27,27	1.34	3 (14%)	25,40,40	1.67	5 (20%)
4	SO4	A	603	-	4,4,4	0.59	0	6,6,6	0.62	0
4	SO4	A	604	-	4,4,4	0.20	0	6,6,6	0.66	0
4	SO4	A	605	-	4,4,4	0.54	0	6,6,6	0.97	0
4	SO4	A	606	-	4,4,4	0.41	0	6,6,6	0.65	0
4	SO4	A	607[A]	-	4,4,4	0.41	0	6,6,6	1.03	1 (16%)
4	SO4	A	607[B]	-	4,4,4	0.44	0	6,6,6	0.47	0
4	SO4	A	608	-	4,4,4	0.46	0	6,6,6	0.22	0
5	EDO	A	609	-	3,3,3	0.35	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	610	-	3,3,3	0.48	0	2,2,2	0.59	0
5	EDO	A	611	-	3,3,3	0.50	0	2,2,2	0.28	0
5	EDO	A	612	-	3,3,3	0.52	0	2,2,2	1.14	0
5	EDO	A	613	-	3,3,3	0.48	0	2,2,2	0.66	0
5	EDO	A	614	-	3,3,3	0.37	0	2,2,2	1.09	0
5	EDO	A	615	-	3,3,3	0.49	0	2,2,2	0.84	0
5	EDO	A	616[A]	-	3,3,3	0.28	0	2,2,2	0.83	0
5	EDO	A	616[B]	-	3,3,3	0.36	0	2,2,2	0.46	0
5	EDO	A	617	-	3,3,3	0.62	0	2,2,2	0.62	0
2	TPP	B	601	3	21,27,27	1.72	4 (19%)	25,40,40	1.84	6 (24%)
4	SO4	B	603	-	4,4,4	0.30	0	6,6,6	1.23	1 (16%)
4	SO4	B	604	-	4,4,4	0.42	0	6,6,6	0.71	0
4	SO4	B	605	-	4,4,4	0.19	0	6,6,6	0.64	0
4	SO4	B	606[A]	-	4,4,4	0.47	0	6,6,6	0.40	0
4	SO4	B	606[B]	-	4,4,4	0.39	0	6,6,6	0.47	0
4	SO4	B	607[A]	-	4,4,4	0.48	0	6,6,6	1.16	0
4	SO4	B	607[B]	-	4,4,4	0.47	0	6,6,6	0.58	0
4	SO4	B	608	-	4,4,4	0.73	0	6,6,6	1.25	1 (16%)
4	SO4	B	609	-	4,4,4	0.46	0	6,6,6	1.20	1 (16%)
4	SO4	B	610	-	4,4,4	0.68	0	6,6,6	0.43	0
4	SO4	B	611	-	4,4,4	0.47	0	6,6,6	0.41	0
4	SO4	B	612	-	4,4,4	0.40	0	6,6,6	0.35	0
5	EDO	B	613	-	3,3,3	0.49	0	2,2,2	0.24	0
5	EDO	B	614	-	3,3,3	0.50	0	2,2,2	0.94	0
5	EDO	B	615	-	3,3,3	0.56	0	2,2,2	0.57	0
5	EDO	B	616	-	3,3,3	0.36	0	2,2,2	0.83	0
5	EDO	B	617	-	3,3,3	0.40	0	2,2,2	0.31	0
5	EDO	B	618	-	3,3,3	0.32	0	2,2,2	0.78	0
5	EDO	B	619	-	3,3,3	0.60	0	2,2,2	0.49	0
5	EDO	B	620	-	3,3,3	0.72	0	2,2,2	0.28	0
5	EDO	B	621	-	3,3,3	0.38	0	2,2,2	0.55	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	TPP	A	601	3	-	0/16/17/17	0/2/2/2
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0
4	SO4	A	604	-	-	0/0/0/0	0/0/0/0
4	SO4	A	605	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	606	-	-	0/0/0/0	0/0/0/0
4	SO4	A	607[A]	-	-	0/0/0/0	0/0/0/0
4	SO4	A	607[B]	-	-	0/0/0/0	0/0/0/0
4	SO4	A	608	-	-	0/0/0/0	0/0/0/0
5	EDO	A	609	-	-	0/1/1/1	0/0/0/0
5	EDO	A	610	-	-	0/1/1/1	0/0/0/0
5	EDO	A	611	-	-	0/1/1/1	0/0/0/0
5	EDO	A	612	-	-	0/1/1/1	0/0/0/0
5	EDO	A	613	-	-	0/1/1/1	0/0/0/0
5	EDO	A	614	-	-	0/1/1/1	0/0/0/0
5	EDO	A	615	-	-	0/1/1/1	0/0/0/0
5	EDO	A	616[A]	-	-	0/1/1/1	0/0/0/0
5	EDO	A	616[B]	-	-	0/1/1/1	0/0/0/0
5	EDO	A	617	-	-	0/1/1/1	0/0/0/0
2	TPP	B	601	3	-	0/16/17/17	0/2/2/2
4	SO4	B	603	-	-	0/0/0/0	0/0/0/0
4	SO4	B	604	-	-	0/0/0/0	0/0/0/0
4	SO4	B	605	-	-	0/0/0/0	0/0/0/0
4	SO4	B	606[A]	-	-	0/0/0/0	0/0/0/0
4	SO4	B	606[B]	-	-	0/0/0/0	0/0/0/0
4	SO4	B	607[A]	-	-	0/0/0/0	0/0/0/0
4	SO4	B	607[B]	-	-	0/0/0/0	0/0/0/0
4	SO4	B	608	-	-	0/0/0/0	0/0/0/0
4	SO4	B	609	-	-	0/0/0/0	0/0/0/0
4	SO4	B	610	-	-	0/0/0/0	0/0/0/0
4	SO4	B	611	-	-	0/0/0/0	0/0/0/0
4	SO4	B	612	-	-	0/0/0/0	0/0/0/0
5	EDO	B	613	-	-	0/1/1/1	0/0/0/0
5	EDO	B	614	-	-	0/1/1/1	0/0/0/0
5	EDO	B	615	-	-	0/1/1/1	0/0/0/0
5	EDO	B	616	-	-	0/1/1/1	0/0/0/0
5	EDO	B	617	-	-	0/1/1/1	0/0/0/0
5	EDO	B	618	-	-	0/1/1/1	0/0/0/0
5	EDO	B	619	-	-	0/1/1/1	0/0/0/0
5	EDO	B	620	-	-	0/1/1/1	0/0/0/0
5	EDO	B	621	-	-	0/1/1/1	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TPP	C4-N3	-3.05	1.37	1.39
2	A	601	TPP	PB-O3A	2.51	1.64	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	TPP	C5'-C4'	2.82	1.49	1.42
2	B	601	TPP	C6'-N1'	2.88	1.40	1.34
2	A	601	TPP	C2'-N1'	2.93	1.39	1.34
2	B	601	TPP	C2'-N1'	3.51	1.40	1.34
2	B	601	TPP	C5'-C4'	3.93	1.52	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	TPP	C5'-C4'-N4'	-3.13	117.66	122.22
2	B	601	TPP	C5'-C6'-N1'	-2.59	119.49	123.87
2	A	601	TPP	CM2-C2'-N1'	-2.37	114.37	117.06
4	A	607[A]	SO4	O4-S-O3	-2.10	99.51	108.96
4	B	609	SO4	O4-S-O1	2.03	120.44	109.26
4	B	603	SO4	O3-S-O1	2.11	120.88	109.26
2	A	601	TPP	C5-C4-N3	2.16	111.89	107.57
4	B	608	SO4	O3-S-O1	2.16	121.17	109.26
2	A	601	TPP	CM2-C2'-N3'	2.26	120.90	117.20
2	A	601	TPP	O3B-PB-O2B	2.33	117.03	107.61
2	B	601	TPP	C5-C4-N3	2.38	112.34	107.57
2	B	601	TPP	C6'-N1'-C2'	2.55	120.28	115.88
2	B	601	TPP	N4'-C4'-N3'	2.66	120.93	117.00
2	A	601	TPP	C6-C5-C4	4.98	131.43	127.43
2	B	601	TPP	C6-C5-C4	5.42	131.78	127.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	TPP	2	0
4	A	606	SO4	2	0
4	A	607[B]	SO4	3	0
5	A	609	EDO	3	0
5	A	613	EDO	3	0
5	A	615	EDO	6	0
5	A	616[B]	EDO	3	0
5	A	617	EDO	4	0
2	B	601	TPP	4	0
4	B	606[A]	SO4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	606[B]	SO4	4	0
4	B	611	SO4	1	0
5	B	615	EDO	1	0
5	B	616	EDO	1	0
5	B	617	EDO	1	0
5	B	619	EDO	1	0
5	B	620	EDO	1	0
5	B	621	EDO	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

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, 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	567/576 (98%)	-0.24	18 (3%) 48 52	11, 21, 44, 69	1 (0%)
1	B	561/576 (97%)	-0.33	7 (1%) 79 83	13, 22, 41, 79	2 (0%)
All	All	1128/1152 (97%)	-0.28	25 (2%) 62 67	11, 21, 42, 79	3 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	502	TYR	7.4
1	A	356	ALA	4.5
1	A	349	ASN	4.2
1	A	501	GLY	4.0
1	A	348	LEU	3.9
1	B	499	ASN	3.8
1	A	350	ALA	3.5
1	A	357	ASP	3.4
1	A	354	LYS	3.4
1	A	344	PHE	3.2
1	A	565	ASN	3.0
1	A	347	SER	2.9
1	B	208	ASN	2.7
1	B	565	ASN	2.6
1	B	335	VAL	2.5
1	A	351	GLY	2.5
1	B	210	ASP	2.5
1	A	567	LEU	2.4
1	A	352	GLU	2.4
1	A	293	THR	2.4
1	A	564	VAL	2.2
1	B	207	GLU	2.2
1	A	476	ILE	2.2
1	B	276	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	359	ALA	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	A	616[B]	4/4	0.86	0.45	34.50	31,32,32,34	4
4	SO4	B	610	5/5	0.89	0.29	22.93	36,45,45,50	5
5	EDO	A	613	4/4	0.86	0.26	8.73	25,32,32,33	4
5	EDO	A	612	4/4	0.90	0.27	7.48	31,34,38,39	4
5	EDO	B	620	4/4	0.63	0.24	7.07	34,36,39,45	4
5	EDO	B	619	4/4	0.77	0.25	6.84	32,33,38,40	4
5	EDO	B	621	4/4	0.95	0.28	5.68	18,19,20,20	4
5	EDO	B	617	4/4	0.94	0.12	5.20	22,26,26,31	4
4	SO4	B	611	5/5	0.95	0.15	4.22	26,26,30,32	5
5	EDO	A	609	4/4	0.80	0.20	3.95	22,23,23,23	4
5	EDO	B	614	4/4	0.91	0.10	3.00	32,33,34,39	0
4	SO4	B	607[B]	5/5	0.97	0.17	2.98	21,30,32,33	5
5	EDO	A	617	4/4	0.90	0.14	2.86	23,30,33,37	4
4	SO4	B	607[A]	5/5	0.97	0.17	2.85	20,21,26,27	5
5	EDO	B	616	4/4	0.90	0.17	2.54	27,31,33,38	4
5	EDO	A	615	4/4	0.88	0.16	2.15	26,27,27,28	4
4	SO4	B	606[A]	5/5	0.95	0.15	1.97	36,43,45,48	5
4	SO4	B	606[B]	5/5	0.95	0.15	1.97	28,31,34,34	5
4	SO4	A	605	5/5	0.97	0.12	1.67	25,25,29,34	5
4	SO4	B	608	5/5	0.95	0.09	1.35	22,25,29,29	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	B	604	5/5	0.93	0.11	1.34	27,32,37,40	5
4	SO4	B	603	5/5	0.99	0.09	1.26	36,39,42,44	0
5	EDO	A	610	4/4	0.94	0.09	1.00	39,41,43,47	0
2	TPP	B	601	26/26	0.96	0.09	0.99	17,23,29,34	26
4	SO4	A	606	5/5	0.98	0.12	0.75	32,36,42,45	5
4	SO4	A	607[A]	5/5	0.97	0.10	0.31	26,29,31,36	5
2	TPP	A	601	26/26	0.96	0.08	0.22	17,25,33,36	0
5	EDO	B	613	4/4	0.97	0.08	0.19	29,31,34,40	0
4	SO4	A	603	5/5	0.96	0.09	0.04	22,27,34,39	5
4	SO4	A	607[B]	5/5	0.97	0.10	-0.03	25,26,27,27	5
5	EDO	A	611	4/4	0.97	0.10	-0.24	25,27,27,27	4
5	EDO	B	615	4/4	0.95	0.09	-0.31	28,36,36,36	0
3	MG	A	602	1/1	1.00	0.06	-0.32	20,20,20,20	0
4	SO4	A	604	5/5	0.97	0.08	-1.21	41,43,49,50	5
3	MG	B	602	1/1	0.99	0.04	-3.27	24,24,24,24	0
5	EDO	A	614	4/4	0.94	0.14	-	28,42,46,47	0
4	SO4	B	612	5/5	0.90	0.24	-	32,37,39,40	5
4	SO4	A	608	5/5	0.93	0.25	-	35,36,39,46	5
4	SO4	B	609	5/5	0.94	0.15	-	29,31,36,39	5
4	SO4	B	605	5/5	0.96	0.11	-	46,50,50,56	5
5	EDO	A	616[A]	4/4	0.86	0.45	-	32,32,32,34	4
5	EDO	B	618	4/4	0.73	0.16	-	35,37,41,44	4

6.5 Other polymers ⓘ

There are no such residues in this entry.