Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2024 – 12:27 PM JST

PDB ID	:	9JXU
Title	:	Crystal structure of cysteine synthase A from Limosilactobacillus reuteri LR1 in its apo form
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Deposited on	:	2024-10-11
Resolution	:	2.20 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:

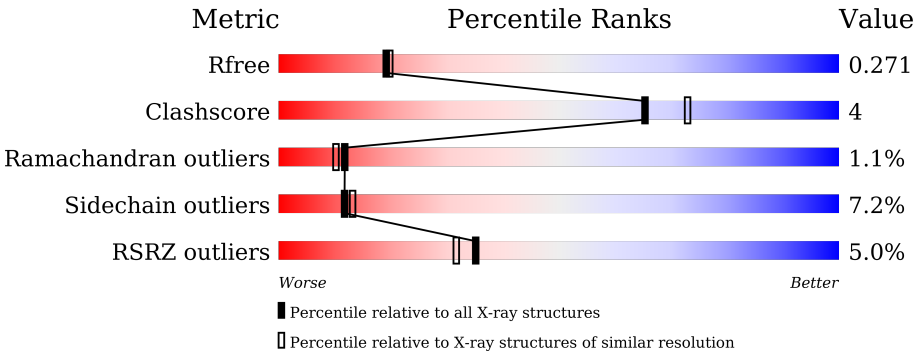
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.20 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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	313	5% 71% 12% • • 12%
1	B	313	4% 76% 11% • 10%

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	EDO	A	402	-	X	-	-
4	PEG	A	403	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4121 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.

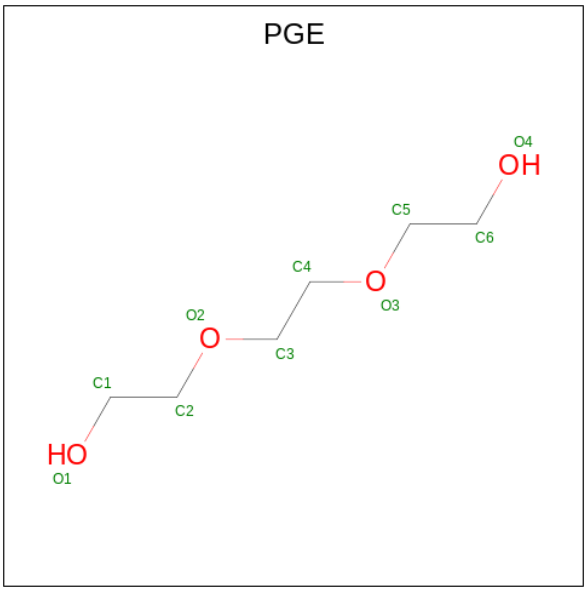
- Molecule 1 is a protein called Cysteine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	3	0
			1973	1256	325	383	9			
1	B	281	Total	C	N	O	S	0	1	0
			2001	1274	327	392	8			

There are 14 discrepancies between the modelled and reference sequences:

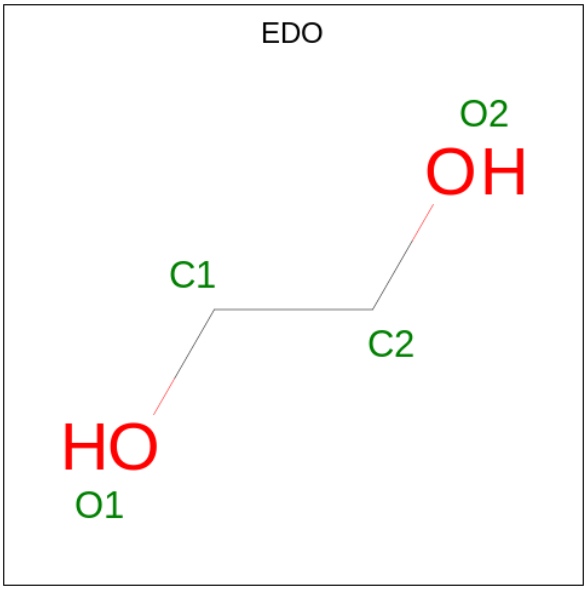
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A1S9AE02
A	2	HIS	-	expression tag	UNP A0A1S9AE02
A	3	HIS	-	expression tag	UNP A0A1S9AE02
A	4	HIS	-	expression tag	UNP A0A1S9AE02
A	5	HIS	-	expression tag	UNP A0A1S9AE02
A	6	HIS	-	expression tag	UNP A0A1S9AE02
A	7	HIS	-	expression tag	UNP A0A1S9AE02
B	1	MET	-	initiating methionine	UNP A0A1S9AE02
B	2	HIS	-	expression tag	UNP A0A1S9AE02
B	3	HIS	-	expression tag	UNP A0A1S9AE02
B	4	HIS	-	expression tag	UNP A0A1S9AE02
B	5	HIS	-	expression tag	UNP A0A1S9AE02
B	6	HIS	-	expression tag	UNP A0A1S9AE02
B	7	HIS	-	expression tag	UNP A0A1S9AE02

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0

- 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

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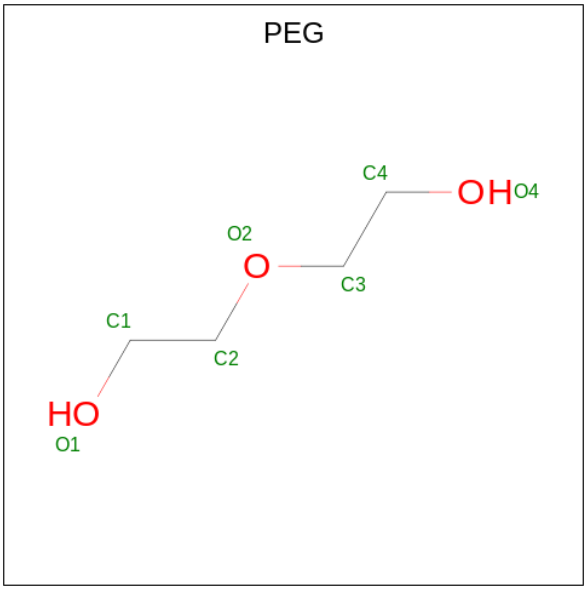
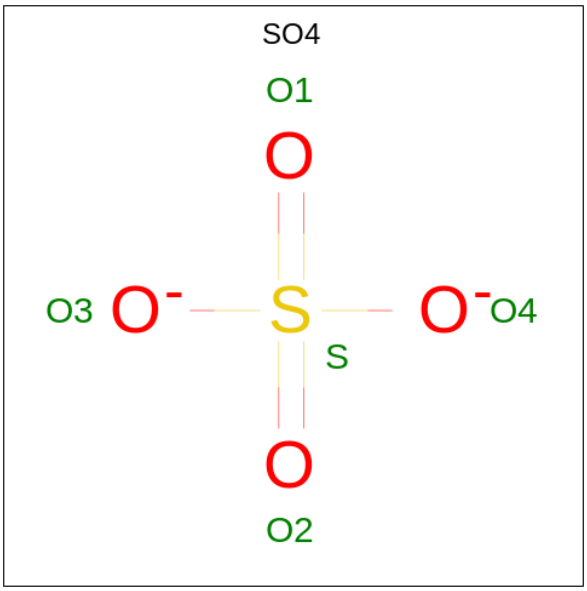
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	1
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

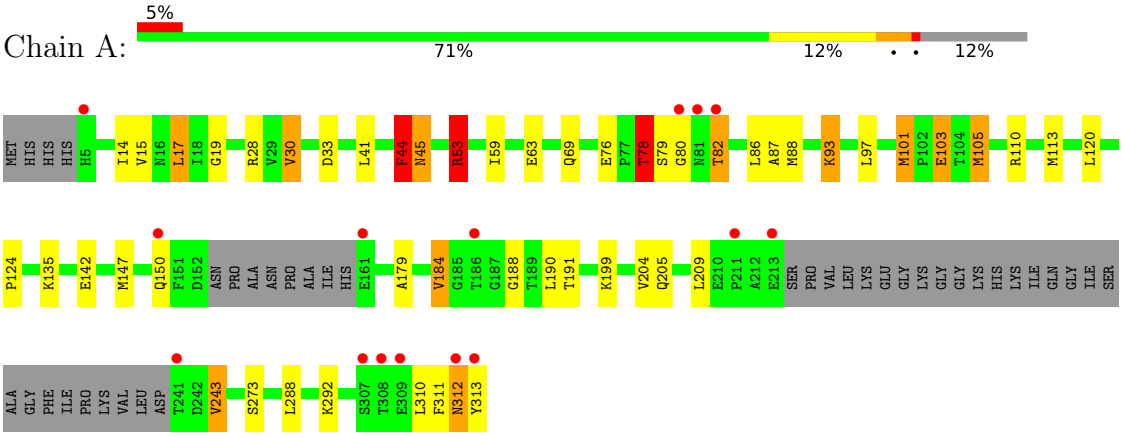
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	39	Total O 39 39	0	1
6	B	47	Total O 47 47	0	1

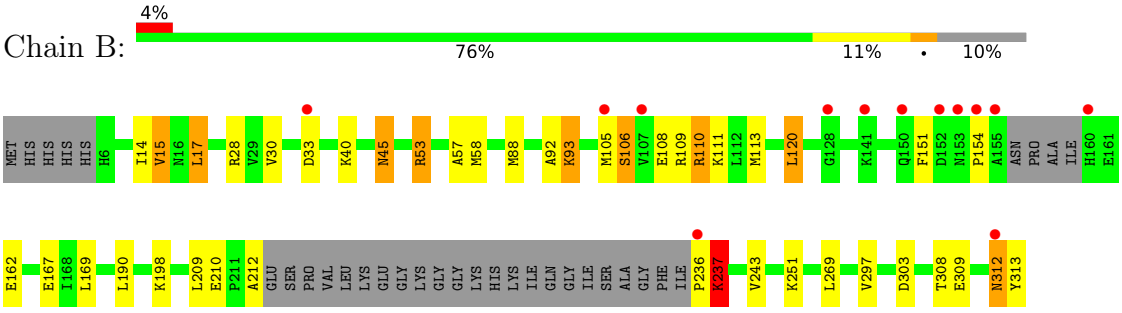
3 Residue-property plots (i)

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: Cysteine synthase



• Molecule 1: Cysteine synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.64Å 101.29Å 63.53Å 90.00° 107.33° 90.00°	Depositor
Resolution (Å)	20.40 – 2.20 20.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.40-2.20) 98.6 (20.40-2.20)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.212 , 0.271 0.212 , 0.271	Depositor DCC
R_{free} test set	1583 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4121	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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: SO4, PGE, PEG, 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	0.75	0/2011	1.53	29/2726 (1.1%)
1	B	0.73	0/2034	1.51	29/2763 (1.0%)
All	All	0.74	0/4045	1.52	58/5489 (1.1%)

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	ARG	NE-CZ-NH1	12.57	126.58	120.30
1	A	101	MET	CG-SD-CE	-10.94	82.70	100.20
1	B	53	ARG	CD-NE-CZ	10.01	137.61	123.60
1	B	17	LEU	CB-CG-CD2	9.31	126.82	111.00
1	B	120	LEU	CB-CG-CD1	-9.27	95.25	111.00
1	A	113	MET	CG-SD-CE	8.51	113.82	100.20
1	A	120	LEU	CB-CG-CD1	8.40	125.28	111.00
1	B	58	MET	CG-SD-CE	7.84	112.75	100.20
1	A	86	LEU	CB-CG-CD1	7.41	123.60	111.00
1	A	45	ASN	CB-CA-C	7.24	124.87	110.40
1	B	45	ASN	CB-CA-C	7.23	124.86	110.40
1	B	198	LYS	CB-CG-CD	7.15	130.19	111.60
1	B	237	LYS	N-CA-CB	7.07	123.32	110.60
1	B	210	GLU	CB-CA-C	6.84	124.07	110.40
1	A	93	LYS	CD-CE-NZ	-6.63	96.44	111.70
1	B	53	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	93	LYS	CB-CG-CD	-6.58	94.50	111.60
1	A	44	PHE	CB-CA-C	-6.43	97.53	110.40
1	A	53	ARG	CD-NE-CZ	6.43	132.60	123.60
1	A	78	THR	OG1-CB-CG2	6.38	124.67	110.00
1	B	169	LEU	CB-CG-CD1	6.37	121.84	111.00
1	B	312	ASN	CB-CA-C	6.34	123.08	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	147	MET	CG-SD-CE	6.26	110.22	100.20
1	A	292	LYS	CB-CG-CD	6.21	127.74	111.60
1	A	312	ASN	CB-CA-C	6.16	122.71	110.40
1	B	28	ARG	CD-NE-CZ	6.15	132.21	123.60
1	A	288	LEU	CB-CG-CD1	-6.09	100.64	111.00
1	A	28	ARG	CD-NE-CZ	6.08	132.11	123.60
1	A	199	LYS	CB-CG-CD	6.01	127.22	111.60
1	A	199	LYS	CA-CB-CG	5.86	126.29	113.40
1	B	120	LEU	CB-CG-CD2	5.85	120.95	111.00
1	A	190	LEU	CB-CG-CD1	5.81	120.88	111.00
1	B	105	MET	CG-SD-CE	5.81	109.50	100.20
1	A	17	LEU	CB-CG-CD1	-5.79	101.15	111.00
1	A	313	TYR	N-CA-CB	5.79	121.01	110.60
1	A	204	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	B	198	LYS	N-CA-CB	5.72	120.90	110.60
1	A	292	LYS	CA-CB-CG	5.69	125.93	113.40
1	B	190	LEU	CB-CG-CD1	5.66	120.62	111.00
1	B	237	LYS	CB-CG-CD	5.56	126.06	111.60
1	B	53	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	313	TYR	N-CA-CB	5.48	120.47	110.60
1	A	273	SER	CB-CA-C	5.43	120.42	110.10
1	A	78	THR	CA-CB-OG1	-5.43	97.59	109.00
1	A	30	VAL	N-CA-CB	5.39	123.35	111.50
1	B	113	MET	CG-SD-CE	5.38	108.80	100.20
1	A	184	VAL	N-CA-CB	5.36	123.30	111.50
1	B	309	GLU	CB-CA-C	5.35	121.10	110.40
1	B	88	MET	CG-SD-CE	-5.34	91.66	100.20
1	A	311	PHE	CB-CA-C	5.33	121.05	110.40
1	B	198	LYS	CD-CE-NZ	5.30	123.90	111.70
1	B	236	PRO	CB-CA-C	5.30	125.26	112.00
1	B	110	ARG	CD-NE-CZ	5.25	130.95	123.60
1	B	93	LYS	CG-CD-CE	5.25	127.64	111.90
1	B	151	PHE	CB-CA-C	5.22	120.83	110.40
1	A	310	LEU	CB-CG-CD1	5.12	119.70	111.00
1	B	269	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	A	93	LYS	CB-CA-C	5.00	120.40	110.40

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	A	1973	0	1916	19	0
1	B	2001	0	1943	10	0
2	A	10	0	14	0	0
3	A	20	0	30	1	0
3	B	4	0	6	0	0
4	A	7	0	10	6	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
6	A	39	0	0	0	0
6	B	47	0	0	1	0
All	All	4121	0	3919	29	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 (29) 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:B:110:ARG:HB2	1:B:120:LEU:HD11	1.72	0.70
1:B:106:SER:HB3	1:B:109:ARG:HB3	1.73	0.69
1:A:79:SER:O	1:A:82:THR:HG22	1.96	0.65
1:B:14:ILE:HD12	1:B:17:LEU:HD12	1.79	0.65
1:B:108:GLU:HA	1:B:111:LYS:HG3	1.88	0.55
1:A:103[A]:GLU:OE2	4:A:403:PEG:H12	2.08	0.53
1:B:40:LYS:HB3	1:B:297:VAL:HG12	1.90	0.53
1:A:124:PRO:HB3	4:A:403:PEG:H11	1.91	0.52
1:A:124:PRO:CA	4:A:403:PEG:H11	2.40	0.51
1:A:124:PRO:HA	4:A:403:PEG:H11	1.93	0.51
1:B:57:ALA:HB2	1:B:167:GLU:HG3	1.93	0.49
1:A:59:ILE:O	1:A:63:GLU:HG3	2.13	0.48
1:A:14:ILE:HD12	1:A:17:LEU:HD12	1.94	0.48
1:A:124:PRO:HB3	4:A:403:PEG:C1	2.43	0.48
1:B:212:ALA:HB2	1:B:251:LYS:HA	1.96	0.48
1:A:80:GLY:N	1:A:105:MET:HE1	2.31	0.45
1:A:124:PRO:CB	4:A:403:PEG:H11	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLU:HB3	6:B:545:HOH:O	2.18	0.43
1:A:135:LYS:HB2	3:A:405:EDO:H21	2.01	0.43
1:A:191:THR:HA	1:A:243:VAL:HG11	2.01	0.43
1:A:41:LEU:O	1:A:44:PHE:HB2	2.19	0.42
1:B:15:VAL:HG12	1:B:92:ALA:HB1	2.01	0.42
1:A:87:ALA:HA	1:A:97:LEU:CD2	2.49	0.42
1:A:19:GLY:HA3	1:A:53:ARG:HB2	2.02	0.42
1:A:76:GLU:OE2	1:A:150:GLN:HB2	2.19	0.42
1:A:78:THR:HG22	1:A:101:MET:HB3	2.01	0.41
1:A:179:ALA:HA	1:A:205:GLN:O	2.20	0.41
1:B:53:ARG:HG2	1:B:167:GLU:HB3	2.03	0.41
1:A:105:MET:HB3	1:A:110:ARG:HD2	2.02	0.41

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	271/313 (87%)	261 (96%)	6 (2%)	4 (2%)	8 6
1	B	276/313 (88%)	264 (96%)	9 (3%)	3 (1%)	12 10
All	All	547/626 (87%)	525 (96%)	15 (3%)	7 (1%)	12 8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	LYS
1	A	312	ASN
1	A	103[A]	GLU
1	A	103[B]	GLU
1	B	154	PRO
1	B	312	ASN

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Mol	Chain	Res	Type
1	A	188	GLY

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	A	187/241 (78%)	171 (91%)	16 (9%)	8 9
1	B	191/241 (79%)	180 (94%)	11 (6%)	17 20
All	All	378/482 (78%)	351 (93%)	27 (7%)	12 13

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	30	VAL
1	A	33	ASP
1	A	44	PHE
1	A	45	ASN
1	A	53	ARG
1	A	69	GLN
1	A	78	THR
1	A	82	THR
1	A	88	MET
1	A	93	LYS
1	A	105	MET
1	A	142	GLU
1	A	184	VAL
1	A	209	LEU
1	A	243	VAL
1	B	15	VAL
1	B	30	VAL
1	B	33	ASP
1	B	45	ASN
1	B	93	LYS
1	B	106	SER

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Mol	Chain	Res	Type
1	B	209	LEU
1	B	237	LYS
1	B	243	VAL
1	B	303	ASP
1	B	308	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	12	ASN

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)

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	$\#\|Z\| > 2$
5	SO4	A	409	-	4,4,4	0.28	0	6,6,6	0.30	0
5	SO4	B	402	-	4,4,4	0.37	0	6,6,6	0.22	0
3	EDO	A	405	-	3,3,3	0.99	0	2,2,2	1.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	A	406	-	3,3,3	0.41	0	2,2,2	0.89	0
3	EDO	B	401	-	3,3,3	0.48	0	2,2,2	0.80	0
5	SO4	A	410	-	4,4,4	0.30	0	6,6,6	0.29	0
2	PGE	A	401	-	9,9,9	0.65	0	8,8,8	0.62	0
3	EDO	A	404	-	3,3,3	0.15	0	2,2,2	0.39	0
5	SO4	A	408	-	4,4,4	0.40	0	6,6,6	0.20	0
3	EDO	A	407[B]	-	3,3,3	0.11	0	2,2,2	0.88	0
4	PEG	A	403	-	6,6,6	0.77	0	5,5,5	1.06	1 (20%)
3	EDO	A	402	-	3,3,3	2.15	2 (66%)	2,2,2	2.51	2 (100%)

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	405	-	-	1/1/1/1	-
3	EDO	A	406	-	-	1/1/1/1	-
3	EDO	B	401	-	-	0/1/1/1	-
2	PGE	A	401	-	-	6/7/7/7	-
3	EDO	A	404	-	-	0/1/1/1	-
3	EDO	A	407[B]	-	-	1/1/1/1	-
4	PEG	A	403	-	-	1/4/4/4	-
3	EDO	A	402	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	EDO	O1-C1	2.62	1.55	1.42
3	A	402	EDO	O2-C2	2.48	1.54	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	EDO	O1-C1-C2	2.68	131.22	111.91
3	A	402	EDO	O2-C2-C1	2.32	128.59	111.91
4	A	403	PEG	O1-C1-C2	2.13	124.19	111.81

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	EDO	O1-C1-C2-O2
4	A	403	PEG	O2-C3-C4-O4
2	A	401	PGE	O1-C1-C2-O2
3	A	406	EDO	O1-C1-C2-O2
2	A	401	PGE	C6-C5-O3-C4
2	A	401	PGE	O3-C5-C6-O4
2	A	401	PGE	C3-C4-O3-C5
2	A	401	PGE	C4-C3-O2-C2
2	A	401	PGE	C1-C2-O2-C3
3	A	407[B]	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	EDO	1	0
4	A	403	PEG	6	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	274/313 (87%)	-0.32	15 (5%)	32	28	12, 25, 71, 101	3 (1%)
1	B	281/313 (89%)	-0.03	13 (4%)	38	35	11, 32, 76, 109	1 (0%)
All	All	555/626 (88%)	-0.17	28 (5%)	35	32	11, 28, 73, 109	4 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	ASP	4.5
1	B	155	ALA	4.1
1	A	81	ASN	3.9
1	B	107	VAL	3.9
1	B	105	MET	3.7
1	A	241	THR	3.7
1	A	80	GLY	3.6
1	B	153	ASN	3.4
1	A	309	GLU	3.4
1	B	312	ASN	3.2
1	B	160	HIS	3.1
1	B	128	GLY	3.0
1	A	150	GLN	2.9
1	B	33	ASP	2.8
1	A	307	SER	2.8
1	A	5	HIS	2.6
1	B	154	PRO	2.5
1	A	186	THR	2.5
1	A	211	PRO	2.5
1	A	308	THR	2.4
1	A	161	GLU	2.4
1	A	312	ASN	2.3
1	A	313	TYR	2.2
1	B	141	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	236	PRO	2.2
1	A	82	THR	2.1
1	A	213	GLU	2.1
1	B	150	GLN	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	402	4/4	0.75	0.16	3,3,4,4	4
3	EDO	A	407[B]	4/4	0.80	0.25	19,22,22,23	4
3	EDO	B	401	4/4	0.85	0.16	45,54,55,60	0
2	PGE	A	401	10/10	0.86	0.15	27,69,84,87	0
3	EDO	A	405	4/4	0.86	0.15	37,40,47,55	0
5	SO4	A	409	5/5	0.88	0.13	58,62,66,92	0
4	PEG	A	403	7/7	0.89	0.14	35,48,66,67	0
5	SO4	A	410	5/5	0.89	0.15	53,76,83,91	0
5	SO4	B	402	5/5	0.90	0.09	41,50,52,63	0
3	EDO	A	406	4/4	0.92	0.10	39,43,45,51	0
3	EDO	A	404	4/4	0.93	0.10	38,40,40,43	0
5	SO4	A	408	5/5	0.94	0.09	53,55,58,62	0

6.5 Other polymers (i)

There are no such residues in this entry.