



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:31 AM UTC

PDB ID : 3FD0 / pdb_00003fd0
Title : Crystal structure of putative cystathionine beta-lyase involved in aluminum resistance (NP_470671.1) from LISTERIA INNOCUA at 2.12 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2008-11-24
Resolution : 2.12 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 ⓘ 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

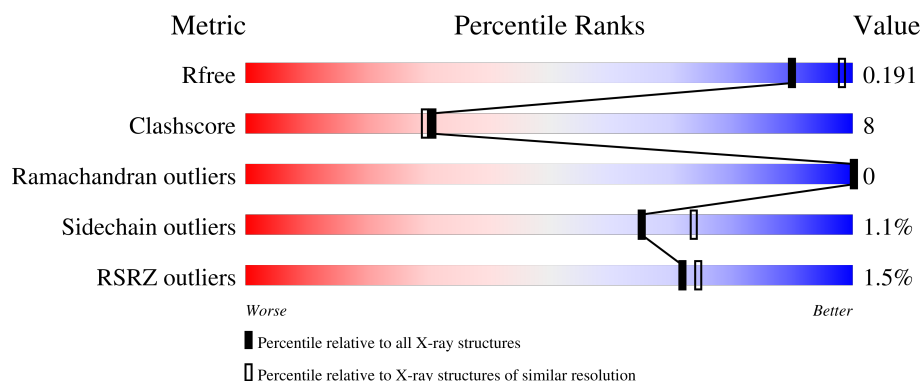
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

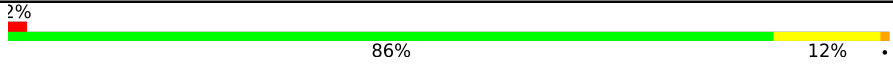
The reported resolution of this entry is 2.12 Å.

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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	409	
1	B	409	

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	414	-	-	X	-
3	EDO	A	424	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6992 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 putative cystathionine beta-lyase involved in aluminum resistance.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	P	S	Se	0	5	0
			3163	2017	520	615	1	2	8			
1	B	408	Total	C	N	O	P	S	Se	0	4	0
			3163	2018	520	614	1	2	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q92C56
B	0	GLY	-	expression tag	UNP Q92C56

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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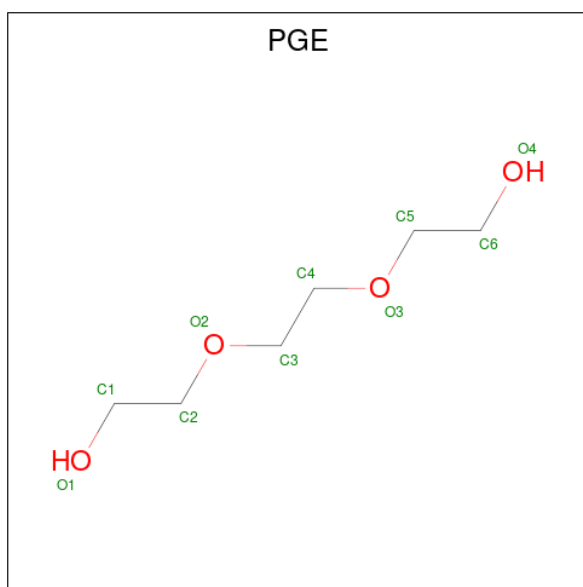
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	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 DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		

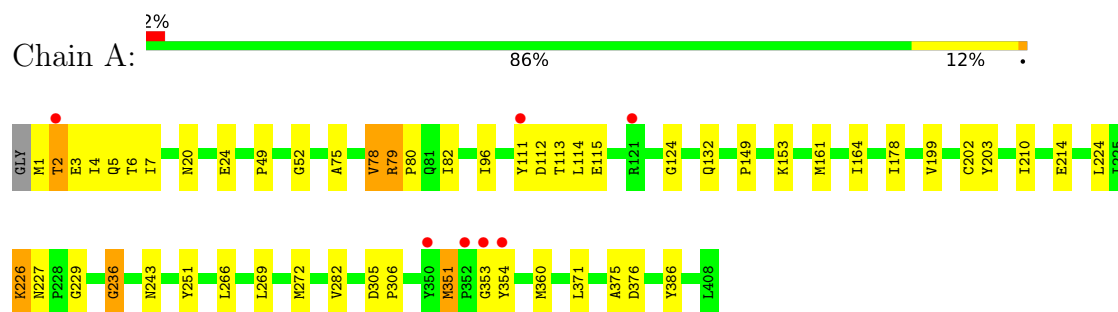
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	283	Total	O	0	10
			293	293		
6	B	214	Total	O	0	5
			219	219		

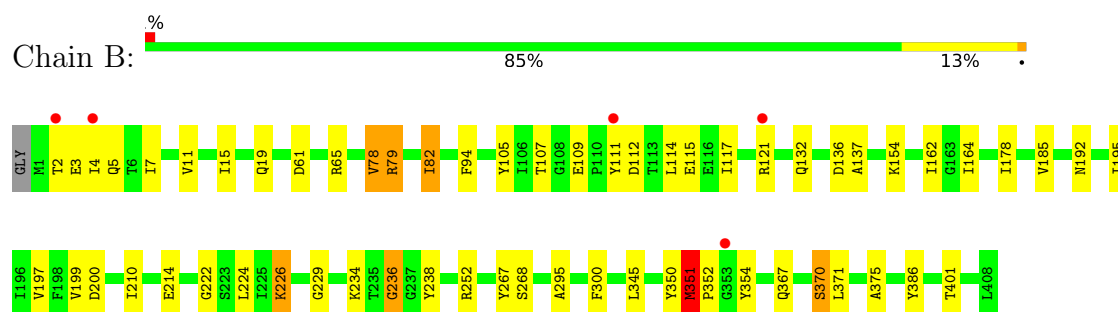
3 Residue-property plots [i](#)

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: putative cystathionine beta-lyase involved in aluminum resistance



- Molecule 1: putative cystathionine beta-lyase involved in aluminum resistance



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.89Å 131.89Å 116.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.18 – 2.12 29.18 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.18-2.12) 99.9 (29.18-2.12)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.4.0067, PHENIX	Depositor
R, R_{free}	0.152 , 0.188 0.155 , 0.191	Depositor DCC
R_{free} test set	3382 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6992	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 3.12% 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: PEG, EDO, CA, PGE, LLP

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	0.89	1/3208 (0.0%)	1.07	7/4341 (0.2%)
1	B	0.85	0/3205	1.08	12/4337 (0.3%)
All	All	0.87	1/6413 (0.0%)	1.08	19/8678 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	MSE	SE-CE	-5.66	1.78	1.95

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	CA-C-N	7.06	127.05	119.28
1	A	79	ARG	C-N-CA	7.06	127.05	119.28
1	B	236	GLY	N-CA-C	6.82	120.42	111.70
1	A	79	ARG	N-CA-C	6.66	114.22	108.22
1	B	79	ARG	CB-CA-C	-6.44	99.99	109.97
1	B	370	SER	CB-CA-C	-6.37	98.68	109.38
1	B	371	LEU	N-CA-C	-5.96	105.50	112.89
1	B	351	MSE	CA-C-N	5.62	126.50	119.98
1	B	351	MSE	C-N-CA	5.62	126.50	119.98
1	A	236	GLY	N-CA-C	5.60	118.87	111.70
1	B	82	ILE	N-CA-C	-5.59	99.18	107.51
1	B	109	GLU	CA-C-N	-5.47	115.13	120.98
1	B	109	GLU	C-N-CA	-5.47	115.13	120.98
1	A	78	VAL	CB-CA-C	5.38	116.55	110.41
1	A	371	LEU	N-CA-C	-5.36	105.48	112.23
1	A	269	LEU	N-CA-C	5.24	116.67	111.07
1	B	345	LEU	CA-C-N	-5.16	114.64	119.85
1	B	345	LEU	C-N-CA	-5.16	114.64	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ASP	N-CA-C	5.03	118.19	111.75

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	3163	0	3121	51	0
1	B	3163	0	3121	49	0
2	A	1	0	0	0	0
3	A	68	0	102	12	0
3	B	44	0	66	1	0
4	A	14	0	20	2	0
4	B	7	0	10	1	0
5	A	10	0	14	1	0
5	B	10	0	14	1	0
6	A	293	0	0	0	0
6	B	219	0	0	2	0
All	All	6992	0	6468	107	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 8.

All (107) 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:2:THR:HG22	1:A:5:GLN:CD	1.64	1.20
1:A:2:THR:CG2	1:A:5:GLN:HG3	1.90	1.00
1:A:2:THR:HG23	1:A:5:GLN:HG3	1.41	0.98
3:A:414:EDO:H22	3:A:424:EDO:H12	1.42	0.97
1:A:2:THR:CG2	1:A:5:GLN:CG	2.45	0.93
3:A:414:EDO:H22	3:A:424:EDO:C1	1.98	0.93
3:A:414:EDO:H22	3:A:424:EDO:H22	1.48	0.92
1:A:2:THR:CG2	1:A:5:GLN:CD	2.41	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:THR:HG23	1:A:5:GLN:CG	2.00	0.91
3:A:414:EDO:H22	3:A:424:EDO:C2	2.01	0.89
1:A:112:ASP:O	1:A:115:GLU:HG3	1.78	0.82
1:B:226:LLP:H4'1	1:B:226:LLP:OP4	1.79	0.81
1:A:351:MSE:HG2	1:A:354:TYR:HD2	1.46	0.79
1:A:178:ILE:HG21	1:A:210[B]:ILE:CD1	2.15	0.77
3:A:414:EDO:C2	3:A:424:EDO:H12	2.14	0.76
3:A:423:EDO:O1	3:A:424:EDO:H21	1.84	0.75
1:B:351:MSE:HG2	1:B:354:TYR:HD2	1.50	0.75
1:B:4:ILE:HD13	1:B:401:THR:HG23	1.69	0.72
1:B:2:THR:OG1	1:B:3:GLU:N	2.22	0.72
3:A:423:EDO:O1	3:A:424:EDO:C2	2.37	0.71
1:A:82:ILE:O	1:A:236:GLY:HA2	1.90	0.71
1:A:1:MSE:HE3	1:A:6:THR:OG1	1.93	0.69
1:A:2:THR:HG22	1:A:5:GLN:OE1	1.91	0.69
1:B:351:MSE:HG2	1:B:354:TYR:CD2	2.28	0.68
1:A:351:MSE:HG2	1:A:354:TYR:CD2	2.29	0.67
3:A:414:EDO:C2	3:A:424:EDO:H22	2.25	0.65
1:B:226:LLP:OP4	1:B:226:LLP:C4'	2.44	0.65
1:A:251:TYR:CZ	3:A:425:EDO:H22	2.32	0.65
1:A:132[B]:GLN:OE1	1:B:132[B]:GLN:NE2	2.28	0.64
1:B:162:ILE:HG12	1:B:195[A]:ILE:CD1	2.29	0.62
1:B:115:GLU:HB3	1:B:121:ARG:HB2	1.81	0.62
1:B:375:ALA:HA	1:B:386:TYR:O	2.00	0.61
1:A:79:ARG:HB2	1:A:80:PRO:HD2	1.82	0.61
1:A:111:TYR:CE2	1:A:113:THR:HB	2.35	0.61
1:B:162:ILE:HG12	1:B:195[A]:ILE:HD11	1.83	0.60
1:A:178:ILE:HG21	1:A:210[B]:ILE:HG13	1.83	0.60
1:A:353:GLY:O	1:A:354:TYR:CD1	2.55	0.59
1:A:226:LLP:OP4	1:A:226:LLP:H4'1	2.04	0.57
1:A:251:TYR:CE1	3:A:425:EDO:H22	2.39	0.57
1:A:210[A]:ILE:HD11	4:A:427:PEG:H31	1.87	0.57
1:B:185:VAL:HG22	1:B:197:VAL:HG11	1.87	0.56
1:B:268:SER:HB2	6:B:561:HOH:O	2.04	0.56
1:B:136:ASP:OD2	1:B:154:LYS:NZ	2.34	0.56
1:B:82:ILE:O	1:B:236:GLY:HA2	2.05	0.56
1:A:2:THR:OG1	1:A:3:GLU:N	2.38	0.55
1:B:11:VAL:HG13	1:B:295:ALA:HB1	1.89	0.55
1:A:2:THR:N	1:A:5:GLN:OE1	2.34	0.55
1:A:178:ILE:HG21	1:A:210[B]:ILE:CG1	2.36	0.55
1:B:111:TYR:CE1	1:B:114:LEU:HG	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:414:EDO:C1	3:A:424:EDO:H12	2.37	0.54
1:B:2:THR:HG23	1:B:5:GLN:CB	2.39	0.53
1:A:178:ILE:HG21	1:A:210[B]:ILE:HD11	1.90	0.53
1:A:111:TYR:CE1	1:A:226:LLP:H6	2.45	0.52
1:A:79:ARG:HB2	1:A:80:PRO:CD	2.40	0.52
1:A:96:ILE:HB	1:A:161:MSE:HE1	1.92	0.51
1:B:4:ILE:HD13	1:B:401:THR:CG2	2.40	0.51
1:A:49:PRO:HB3	1:A:266:LEU:O	2.11	0.50
1:A:75:ALA:HB2	1:A:243[B]:ASN:OD1	2.11	0.50
1:B:4:ILE:CD1	1:B:401:THR:HG23	2.38	0.50
1:B:2:THR:CG2	1:B:5:GLN:CB	2.90	0.49
1:A:202:CYS:O	1:A:203:TYR:HB2	2.13	0.48
1:B:4:ILE:HA	1:B:7:ILE:HD12	1.94	0.47
1:B:7:ILE:HD13	1:B:300:PHE:CZ	2.49	0.47
1:B:115:GLU:OE1	1:B:121:ARG:CZ	2.63	0.47
1:A:224:LEU:O	1:A:229:GLY:HA3	2.14	0.47
1:B:15:ILE:O	1:B:19:GLN:HG2	2.14	0.47
1:A:2:THR:HG22	1:A:5:GLN:NE2	2.24	0.47
1:A:2:THR:HG23	1:A:5:GLN:CB	2.44	0.46
1:B:61:ASP:O	1:B:65:ARG:HG3	2.16	0.46
1:B:224:LEU:O	1:B:229:GLY:HA3	2.16	0.46
1:A:282:VAL:HG22	3:A:418:EDO:H11	1.98	0.46
1:B:192:ASN:O	1:B:195[A]:ILE:HG22	2.16	0.45
1:B:351:MSE:HA	1:B:352:PRO:HD2	1.79	0.45
1:B:115:GLU:OE1	1:B:121:ARG:NH1	2.50	0.45
1:A:210[A]:ILE:HG23	1:A:214:GLU:HB2	1.98	0.45
1:A:79:ARG:CB	1:A:80:PRO:CD	2.95	0.45
1:A:375:ALA:HA	1:A:386:TYR:O	2.16	0.44
1:B:226:LLP:HG3	1:B:370:SER:HB2	1.98	0.44
1:B:210[A]:ILE:HD11	4:B:420:PEG:H31	1.99	0.44
1:A:360:MSE:HG2	1:A:376:ASP:HB2	2.00	0.44
1:A:149:PRO:O	1:A:153:LYS:HG2	2.18	0.44
1:A:124:GLY:HA2	6:B:551:HOH:O	2.18	0.43
1:B:111:TYR:CZ	1:B:226:LLP:H6	2.53	0.43
1:B:234:LYS:HE2	5:B:421:PGE:C6	2.48	0.43
1:B:78:VAL:HG23	1:B:224:LEU:HD11	2.00	0.43
1:A:20:ASN:O	1:A:24[A]:GLU:HG3	2.19	0.43
1:A:210[A]:ILE:HD11	4:A:427:PEG:C3	2.48	0.43
1:B:105:TYR:O	1:B:137:ALA:HA	2.19	0.43
1:B:178:ILE:HG21	1:B:210[B]:ILE:HG13	2.00	0.43
1:A:52:GLY:HA3	1:B:367:GLN:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ILE:HB	1:B:199:VAL:HG22	2.00	0.42
1:B:351:MSE:HG3	1:B:352:PRO:HD2	2.01	0.42
1:A:178:ILE:CG2	1:A:210[B]:ILE:CD1	2.93	0.42
1:B:222:GLY:HA3	1:B:238:TYR:CE1	2.54	0.42
1:B:210[A]:ILE:CG2	1:B:214:GLU:HB2	2.50	0.42
1:A:178:ILE:CG2	1:A:210[B]:ILE:HD11	2.50	0.42
1:B:200:ASP:OD2	1:B:226:LLP:N1	2.53	0.42
1:B:350:TYR:OH	1:B:352:PRO:HA	2.20	0.41
1:B:114:LEU:HD23	1:B:117:ILE:HD12	2.01	0.41
1:B:107:THR:HG21	1:B:164:ILE:HG23	2.02	0.41
1:A:4:ILE:HA	1:A:7:ILE:HD12	2.03	0.41
1:B:94:PHE:HB3	1:B:252:ARG:HE	1.86	0.41
5:A:429:PGE:H32	1:B:267:TYR:CE2	2.56	0.40
1:B:367:GLN:HB2	3:B:417:EDO:H22	2.03	0.40
1:A:111:TYR:CE1	1:A:114:LEU:HG	2.56	0.40
1:A:164:ILE:HB	1:A:199:VAL:HG22	2.04	0.40
1:A:305:ASP:HA	1:A:306:PRO:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	410/409 (100%)	400 (98%)	10 (2%)	0	100	100
1	B	409/409 (100%)	395 (97%)	14 (3%)	0	100	100
All	All	819/818 (100%)	795 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	330/323 (102%)	326 (99%)	4 (1%)	63	71
1	B	329/323 (102%)	326 (99%)	3 (1%)	70	78
All	All	659/646 (102%)	652 (99%)	7 (1%)	65	74

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	78	VAL
1	A	227	ASN
1	A	351	MSE
1	B	78	VAL
1	B	79	ARG
1	B	351	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	ASN
1	B	14	GLN
1	B	406	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](#)

2 non-standard protein/DNA/RNA residues 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
1	LLP	B	226	1	23,24,25	1.62	3 (13%)	25,32,34	1.58	5 (20%)
1	LLP	A	226	1	23,24,25	1.66	3 (13%)	25,32,34	1.78	5 (20%)

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
1	LLP	B	226	1	-	5/16/17/19	0/1/1/1
1	LLP	A	226	1	-	4/16/17/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	LLP	O3-C3	-5.56	1.24	1.36
1	B	226	LLP	O3-C3	-5.41	1.24	1.36
1	A	226	LLP	C4-C4'	2.89	1.52	1.46
1	B	226	LLP	C4-C4'	2.87	1.52	1.46
1	A	226	LLP	C4'-NZ	2.23	1.34	1.27
1	B	226	LLP	C4'-NZ	2.10	1.34	1.27

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	LLP	OP2-P-OP4	-5.23	93.03	106.67
1	B	226	LLP	OP4-C5'-C5	3.20	115.36	109.36
1	A	226	LLP	OP4-C5'-C5	3.12	115.20	109.36
1	B	226	LLP	OP4-P-OP1	-3.11	98.04	106.44
1	B	226	LLP	C4-C4'-NZ	-2.98	110.28	124.04
1	A	226	LLP	OP3-P-OP2	2.81	118.35	107.80
1	B	226	LLP	C5-C4-C4'	-2.57	117.51	121.47
1	A	226	LLP	C2'-C2-C3	2.51	123.74	120.80
1	A	226	LLP	C4-C4'-NZ	-2.38	113.06	124.04
1	B	226	LLP	C2'-C2-C3	2.18	123.34	120.80

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	226	LLP	C4-C5-C5'-OP4
1	A	226	LLP	C6-C5-C5'-OP4
1	B	226	LLP	C4-C5-C5'-OP4
1	B	226	LLP	C6-C5-C5'-OP4
1	A	226	LLP	C4-C4'-NZ-CE
1	B	226	LLP	C4-C4'-NZ-CE
1	B	226	LLP	C5'-OP4-P-OP2
1	B	226	LLP	C5'-OP4-P-OP1
1	A	226	LLP	C3-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	226	LLP	5	0
1	A	226	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 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	$\# Z > 2$
4	PEG	A	427	-	6,6,6	0.52	0	5,5,5	0.48	0
3	EDO	B	418	-	3,3,3	0.55	0	2,2,2	0.34	0
5	PGE	B	421	-	9,9,9	0.60	0	8,8,8	0.73	0
3	EDO	B	411	-	3,3,3	0.40	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	415	-	3,3,3	0.45	0	2,2,2	0.59	0
3	EDO	A	425	-	3,3,3	0.42	0	2,2,2	0.27	0
3	EDO	A	426	-	3,3,3	0.38	0	2,2,2	0.53	0
3	EDO	A	412	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	A	417	-	3,3,3	0.36	0	2,2,2	0.47	0
3	EDO	A	411	-	3,3,3	0.38	0	2,2,2	0.24	0
3	EDO	B	417	-	3,3,3	0.28	0	2,2,2	0.95	0
3	EDO	A	415	-	3,3,3	0.38	0	2,2,2	0.61	0
3	EDO	A	418	-	3,3,3	0.52	0	2,2,2	0.38	0
3	EDO	A	424	-	3,3,3	0.44	0	2,2,2	0.57	0
3	EDO	B	416	-	3,3,3	0.48	0	2,2,2	0.32	0
4	PEG	B	420	-	6,6,6	0.49	0	5,5,5	0.34	0
3	EDO	A	421	-	3,3,3	0.36	0	2,2,2	0.63	0
3	EDO	B	412	-	3,3,3	0.39	0	2,2,2	0.64	0
3	EDO	A	423	-	3,3,3	0.29	0	2,2,2	0.75	0
3	EDO	A	410	-	3,3,3	0.49	0	2,2,2	0.52	0
3	EDO	B	414	-	3,3,3	0.37	0	2,2,2	0.64	0
3	EDO	B	410	-	3,3,3	0.45	0	2,2,2	0.41	0
3	EDO	B	409	-	3,3,3	0.41	0	2,2,2	0.49	0
5	PGE	A	429	-	9,9,9	0.58	0	8,8,8	0.42	0
3	EDO	A	420	-	3,3,3	0.37	0	2,2,2	0.57	0
3	EDO	A	422	-	3,3,3	0.26	0	2,2,2	0.74	0
3	EDO	A	414	-	3,3,3	0.45	0	2,2,2	0.18	0
3	EDO	B	413	-	3,3,3	0.32	0	2,2,2	0.43	0
3	EDO	A	413	-	3,3,3	0.21	0	2,2,2	0.54	0
3	EDO	A	416	-	3,3,3	0.48	0	2,2,2	0.25	0
3	EDO	A	419	-	3,3,3	0.62	0	2,2,2	0.04	0
3	EDO	B	419	-	3,3,3	0.58	0	2,2,2	0.21	0
4	PEG	A	428	-	6,6,6	0.51	0	5,5,5	0.29	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
4	PEG	A	427	-	-	2/4/4/4	-
3	EDO	B	418	-	-	1/1/1/1	-
5	PGE	B	421	-	-	2/7/7/7	-
3	EDO	B	411	-	-	1/1/1/1	-
3	EDO	B	415	-	-	0/1/1/1	-
3	EDO	A	425	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	426	-	-	1/1/1/1	-
3	EDO	A	412	-	-	0/1/1/1	-
3	EDO	A	417	-	-	0/1/1/1	-
3	EDO	A	411	-	-	1/1/1/1	-
3	EDO	B	417	-	-	1/1/1/1	-
3	EDO	A	415	-	-	1/1/1/1	-
3	EDO	A	418	-	-	1/1/1/1	-
3	EDO	A	424	-	-	1/1/1/1	-
3	EDO	B	416	-	-	1/1/1/1	-
4	PEG	B	420	-	-	2/4/4/4	-
3	EDO	A	421	-	-	1/1/1/1	-
3	EDO	B	412	-	-	1/1/1/1	-
3	EDO	A	423	-	-	1/1/1/1	-
3	EDO	A	410	-	-	0/1/1/1	-
3	EDO	B	414	-	-	1/1/1/1	-
3	EDO	B	410	-	-	1/1/1/1	-
3	EDO	B	409	-	-	0/1/1/1	-
5	PGE	A	429	-	-	7/7/7/7	-
3	EDO	A	420	-	-	1/1/1/1	-
3	EDO	A	422	-	-	0/1/1/1	-
3	EDO	A	414	-	-	0/1/1/1	-
3	EDO	B	413	-	-	1/1/1/1	-
3	EDO	A	413	-	-	0/1/1/1	-
3	EDO	A	416	-	-	1/1/1/1	-
3	EDO	A	419	-	-	0/1/1/1	-
3	EDO	B	419	-	-	0/1/1/1	-
4	PEG	A	428	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	421	PGE	O2-C3-C4-O3
5	A	429	PGE	O3-C5-C6-O4
4	B	420	PEG	C1-C2-O2-C3
4	A	428	PEG	O1-C1-C2-O2
4	A	427	PEG	O2-C3-C4-O4
5	A	429	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	423	EDO	O1-C1-C2-O2
3	B	412	EDO	O1-C1-C2-O2
5	B	421	PGE	O3-C5-C6-O4
4	A	427	PEG	O1-C1-C2-O2
4	B	420	PEG	O2-C3-C4-O4
3	A	418	EDO	O1-C1-C2-O2
3	A	424	EDO	O1-C1-C2-O2
3	B	417	EDO	O1-C1-C2-O2
3	B	414	EDO	O1-C1-C2-O2
3	B	413	EDO	O1-C1-C2-O2
5	A	429	PGE	C3-C4-O3-C5
4	A	428	PEG	O2-C3-C4-O4
4	A	428	PEG	C1-C2-O2-C3
5	A	429	PGE	C6-C5-O3-C4
4	A	428	PEG	C4-C3-O2-C2
3	A	421	EDO	O1-C1-C2-O2
3	A	426	EDO	O1-C1-C2-O2
3	B	416	EDO	O1-C1-C2-O2
3	A	415	EDO	O1-C1-C2-O2
5	A	429	PGE	C4-C3-O2-C2
3	A	420	EDO	O1-C1-C2-O2
3	B	410	EDO	O1-C1-C2-O2
5	A	429	PGE	C1-C2-O2-C3
3	A	416	EDO	O1-C1-C2-O2
3	B	411	EDO	O1-C1-C2-O2
3	B	418	EDO	O1-C1-C2-O2
3	A	411	EDO	O1-C1-C2-O2
5	A	429	PGE	O2-C3-C4-O3

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	427	PEG	2	0
5	B	421	PGE	1	0
3	A	425	EDO	2	0
3	B	417	EDO	1	0
3	A	418	EDO	1	0
3	A	424	EDO	9	0
4	B	420	PEG	1	0
3	A	423	EDO	2	0
5	A	429	PGE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	414	EDO	7	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	399/409 (97%)	-0.12	7 (1%) 67 70	18, 30, 49, 83	5 (1%)
1	B	399/409 (97%)	-0.10	5 (1%) 75 77	19, 31, 48, 81	4 (1%)
All	All	798/818 (97%)	-0.11	12 (1%) 72 74	18, 31, 48, 83	9 (1%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	TYR	4.9
1	A	111	TYR	4.0
1	A	353	GLY	3.8
1	B	2	THR	3.3
1	A	350	TYR	3.2
1	B	4	ILE	3.2
1	A	2	THR	2.6
1	B	111	TYR	2.4
1	A	352	PRO	2.3
1	B	121	ARG	2.2
1	B	353	GLY	2.2
1	A	121	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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(Å ²)	Q<0.9
1	LLP	B	226	24/25	0.92	0.11	27,41,50,53	0
1	LLP	A	226	24/25	0.95	0.09	26,37,46,49	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
3	EDO	A	414	4/4	0.57	0.25	70,71,75,76	0
3	EDO	A	426	4/4	0.64	0.20	86,90,90,91	0
3	EDO	B	412	4/4	0.68	0.25	62,64,66,67	0
3	EDO	B	414	4/4	0.78	0.22	55,61,61,62	0
5	PGE	B	421	10/10	0.78	0.18	44,51,57,57	10
4	PEG	B	420	7/7	0.79	0.18	57,65,75,76	0
3	EDO	B	415	4/4	0.80	0.19	64,69,69,73	0
4	PEG	A	428	7/7	0.81	0.18	47,57,64,68	0
3	EDO	A	417	4/4	0.83	0.18	53,61,61,62	0
3	EDO	A	424	4/4	0.84	0.19	59,61,64,64	0
3	EDO	A	420	4/4	0.84	0.20	63,66,68,71	0
3	EDO	A	423	4/4	0.85	0.16	60,60,63,65	0
3	EDO	A	415	4/4	0.85	0.16	47,50,53,58	0
4	PEG	A	427	7/7	0.85	0.15	46,54,56,58	0
3	EDO	B	417	4/4	0.86	0.16	45,45,49,52	0
5	PGE	A	429	10/10	0.87	0.17	53,57,59,60	10
3	EDO	B	416	4/4	0.87	0.17	38,53,53,54	0
3	EDO	A	421	4/4	0.89	0.13	41,48,49,55	0
3	EDO	B	410	4/4	0.89	0.15	43,43,45,46	0
3	EDO	A	422	4/4	0.89	0.17	57,58,59,62	0
3	EDO	B	418	4/4	0.90	0.14	45,48,56,57	0
3	EDO	A	412	4/4	0.90	0.12	46,46,52,53	0
3	EDO	A	418	4/4	0.90	0.12	19,32,34,45	4
3	EDO	A	425	4/4	0.91	0.20	32,40,45,50	0
3	EDO	B	409	4/4	0.92	0.12	38,46,48,51	0
3	EDO	A	419	4/4	0.93	0.14	39,44,45,46	0
3	EDO	B	413	4/4	0.93	0.15	46,49,50,54	0
3	EDO	B	411	4/4	0.93	0.13	50,51,54,59	0
3	EDO	A	410	4/4	0.94	0.10	29,34,41,42	0
3	EDO	A	416	4/4	0.95	0.13	37,42,46,54	0
3	EDO	A	411	4/4	0.95	0.15	45,46,49,57	0
3	EDO	B	419	4/4	0.96	0.10	31,35,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	413	4/4	0.97	0.08	25,29,30,31	0
2	CA	A	409	1/1	0.99	0.08	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.