



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:48 AM UTC

PDB ID : 3DZZ / pdb_00003dzz
Title : CRYSTAL STRUCTURE OF A PUTATIVE PLP-DEPENDENT AMINO-TRANSFERASE (LBUL_1103) FROM LACTOBACILLUS DELBRUECKII SUBSP. AT 1.61 Å RESOLUTION
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2008-07-30
Resolution : 1.61 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

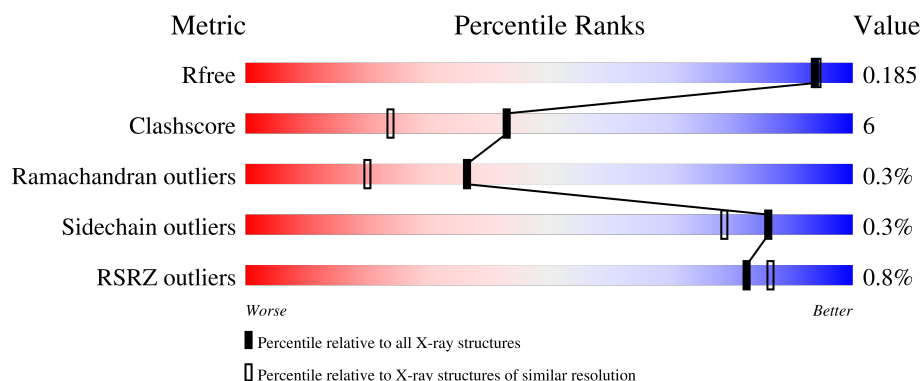
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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	391	89% 9% ..
1	B	391	89% 8% ..

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
5	PEG	A	395	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6796 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 pyridoxal 5'-phosphate-dependent C-S lyase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	P	S	Se	0	11	0
			3079	1983	509	568	1	6	12			
1	B	385	Total	C	N	O	P	S	Se	0	11	0
			3082	1980	509	574	1	7	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q04A76
B	0	GLY	-	expression tag	UNP Q04A76

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

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

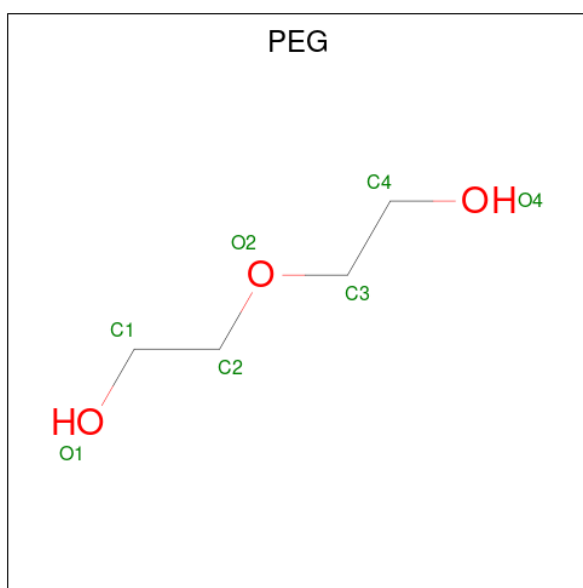
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



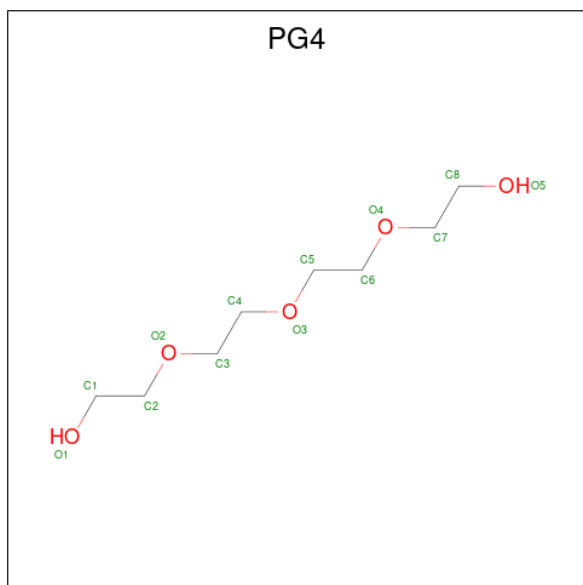
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		

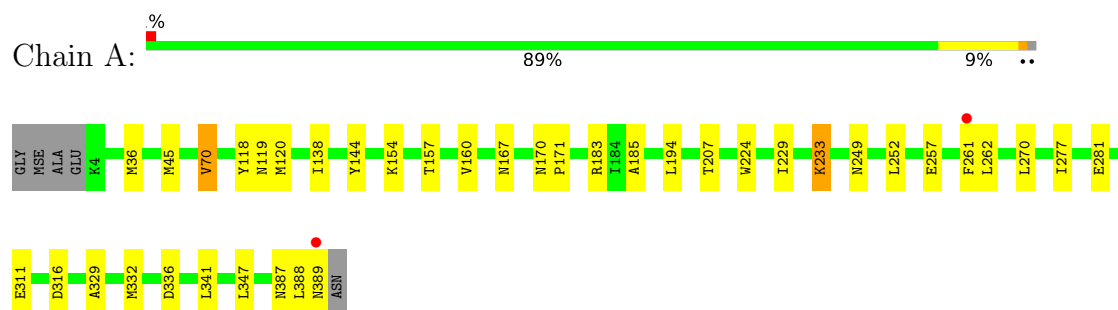
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	301	Total	O	0	0
			301	301		
7	B	274	Total	O	0	0
			274	274		

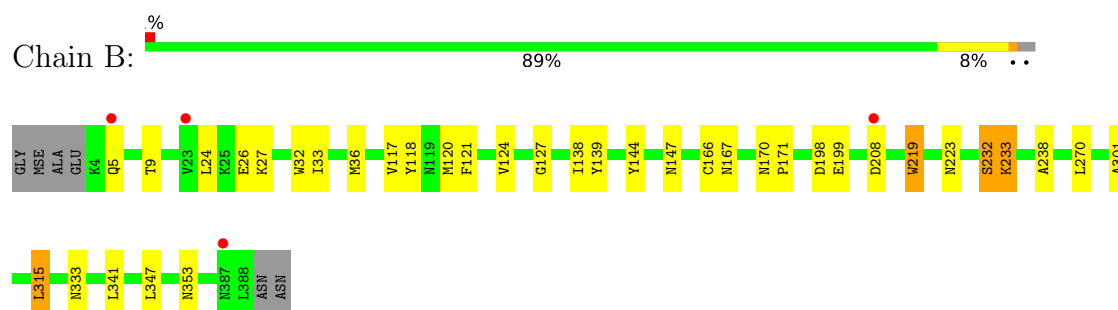
3 Residue-property plots [i](#)

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 pyridoxal 5'-phosphate-dependent C-S lyase



- Molecule 1: putative pyridoxal 5'-phosphate-dependent C-S lyase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.80Å 94.80Å 84.60Å 90.00° 127.13° 90.00°	Depositor
Resolution (Å)	38.78 – 1.61 38.78 – 1.61	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.78-1.61) 98.9 (38.78-1.61)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.4.0067, PHENIX	Depositor
R, R_{free}	0.144 , 0.175 0.161 , 0.185	Depositor DCC
R_{free} test set	4663 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6796	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: CA, ACT, PG4, PEG, LLP, CL

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	1.02	2/3119 (0.1%)	0.98	2/4234 (0.0%)
1	B	1.06	1/3121 (0.0%)	0.98	2/4233 (0.0%)
All	All	1.04	3/6240 (0.0%)	0.98	4/8467 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	ASN	C-O	-6.06	1.17	1.24
1	A	185	ALA	CA-CB	5.27	1.61	1.53
1	B	301	ALA	CA-CB	5.03	1.61	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	TRP	N-CA-C	-6.71	101.03	110.50
1	B	208	ASP	N-CA-C	-5.80	106.16	113.18
1	A	316	ASP	N-CA-C	-5.61	101.55	109.96
1	A	70	VAL	N-CA-C	-5.05	105.57	110.42

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	3079	0	2944	34	0
1	B	3082	0	2943	34	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	1	0
5	A	21	0	30	7	0
5	B	14	0	20	4	0
6	B	13	0	18	0	0
7	A	301	0	0	5	0
7	B	274	0	0	12	0
All	All	6796	0	5961	76	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 (76) 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:121:PHE:CE2	1:B:166[B]:CYS:SG	2.34	1.19
1:B:121:PHE:HE2	1:B:166[B]:CYS:SG	1.65	1.17
1:A:387:ASN:C	1:A:389:ASN:H	1.81	0.87
5:B:395:PEG:H22	7:B:405:HOH:O	1.73	0.86
1:B:333:ASN:HD21	1:B:353:ASN:HD21	1.19	0.86
5:A:397:PEG:H32	7:A:513:HOH:O	1.77	0.85
1:A:154:LYS:O	1:A:157[B]:THR:HG22	1.77	0.84
1:B:117:VAL:CG2	1:B:166[B]:CYS:SG	2.74	0.76
5:A:395:PEG:H42	7:A:553:HOH:O	1.87	0.73
1:B:233:LLP:H5'2	7:B:633:HOH:O	1.87	0.72
1:A:157[B]:THR:HG23	1:A:160:VAL:HG23	1.72	0.71
1:A:332:MSE:HE2	1:A:336:ASP:HB3	1.72	0.70
1:A:157[B]:THR:CG2	1:A:160:VAL:HG23	2.23	0.69
1:B:26:GLU:O	1:B:27:LYS:CB	2.42	0.68
1:A:387:ASN:C	1:A:389:ASN:N	2.45	0.67
5:B:395:PEG:H42	7:B:405:HOH:O	1.97	0.64
1:B:138:ILE:HD11	1:B:147:ASN:HB2	1.80	0.64
1:A:249[B]:ASN:ND2	5:A:395:PEG:H22	2.15	0.62
1:A:277:ILE:O	1:A:281[B]:GLU:HG3	2.00	0.61
1:A:257:GLU:O	1:A:261:PHE:HD1	1.83	0.61
1:B:117:VAL:HG21	1:B:166[B]:CYS:SG	2.41	0.61
1:B:333:ASN:ND2	1:B:353:ASN:HD21	1.95	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:TYR:CE2	1:A:120[A]:MSE:HB2	2.36	0.60
1:B:233:LLP:HE2	7:B:569:HOH:O	2.03	0.59
1:A:257:GLU:O	1:A:261:PHE:CD1	2.56	0.59
5:A:397:PEG:C3	7:A:513:HOH:O	2.44	0.58
1:A:341:LEU:HD21	1:A:347:LEU:HD23	1.85	0.57
1:B:333:ASN:HD21	1:B:353:ASN:ND2	1.97	0.57
1:A:45[A]:MSE:HA	1:A:45[A]:MSE:HE2	1.86	0.56
1:A:207:THR:HG22	5:A:397:PEG:H22	1.87	0.54
1:B:120[B]:MSE:O	1:B:124[B]:VAL:HG23	2.07	0.54
5:A:395:PEG:C4	7:A:553:HOH:O	2.51	0.52
1:B:9[A]:THR:HG23	7:B:564:HOH:O	2.09	0.52
1:A:261:PHE:CD1	1:A:261:PHE:N	2.78	0.52
1:A:138:ILE:O	1:A:144:TYR:HA	2.10	0.52
1:A:157[B]:THR:CG2	1:A:160:VAL:CG2	2.88	0.51
1:A:183:ARG:NE	7:A:629:HOH:O	2.43	0.51
1:B:232[A]:SER:HB2	1:B:238:ALA:HA	1.93	0.50
5:B:394:PEG:H42	7:B:579:HOH:O	2.10	0.50
1:A:332:MSE:CE	1:A:336:ASP:HB3	2.41	0.49
1:B:24:LEU:HD21	7:B:522:HOH:O	2.13	0.48
1:B:170[A]:ASN:OD1	1:B:171:PRO:HA	2.12	0.48
1:A:70:VAL:HG13	1:A:229:ILE:HD11	1.95	0.48
1:B:36:MSE:HE3	1:B:233:LLP:O	2.13	0.48
1:A:194[B]:LEU:HD11	1:A:252:LEU:HD21	1.96	0.48
1:A:194[B]:LEU:CD1	1:A:252:LEU:HD21	2.45	0.47
1:B:118:TYR:CE2	1:B:120[B]:MSE:HB2	2.50	0.47
1:B:270[A]:LEU:O	1:B:270[A]:LEU:HD12	2.14	0.47
1:A:233:LLP:HE2	7:B:519:HOH:O	2.15	0.47
1:B:170[B]:ASN:OD1	1:B:171:PRO:HA	2.15	0.47
1:B:198:ASP:OD2	1:B:233:LLP:N1	2.48	0.46
1:B:219:TRP:HZ3	1:B:223:ASN:CG	2.24	0.46
1:B:315[B]:LEU:HG	7:B:607:HOH:O	2.16	0.46
1:A:170[B]:ASN:OD1	1:A:171:PRO:HA	2.16	0.45
1:B:32:TRP:CG	1:B:33:ILE:H	2.34	0.45
1:B:138:ILE:O	1:B:144:TYR:HA	2.16	0.45
1:B:5:GLN:NE2	7:B:610:HOH:O	2.32	0.45
4:B:392:ACT:O	7:B:597:HOH:O	2.21	0.45
1:A:194[B]:LEU:HD12	1:A:224:TRP:O	2.16	0.44
1:B:270[A]:LEU:HD12	1:B:270[A]:LEU:C	2.43	0.43
1:A:249[B]:ASN:HD22	5:A:395:PEG:H22	1.80	0.43
1:A:262:LEU:HD21	1:B:127:GLY:HA3	2.01	0.43
1:A:120[B]:MSE:HE3	1:A:120[B]:MSE:HB3	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:LEU:HD21	1:B:347:LEU:HD23	2.00	0.42
5:B:395:PEG:H42	7:B:617:HOH:O	2.19	0.42
1:A:36:MSE:HE3	1:A:233:LLP:O	2.19	0.42
1:B:120[B]:MSE:HA	1:B:120[B]:MSE:HE2	2.02	0.42
1:B:219:TRP:HZ3	1:B:223:ASN:OD1	2.02	0.42
1:B:139:TYR:CE1	1:B:315[A]:LEU:HD21	2.55	0.41
1:A:119:ASN:ND2	1:A:120[A]:MSE:CE	2.83	0.41
1:A:311:GLU:O	1:A:329:ALA:HB3	2.21	0.41
1:B:117:VAL:HG22	1:B:166[B]:CYS:SG	2.60	0.41
1:A:261:PHE:HD1	1:A:261:PHE:N	2.18	0.41
1:A:249[B]:ASN:OD1	1:A:249[B]:ASN:C	2.63	0.40
1:B:167:ASN:O	1:B:199:GLU:HA	2.20	0.40
1:A:261:PHE:HD1	1:A:261:PHE:H	1.68	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	394/391 (101%)	383 (97%)	10 (2%)	1 (0%)	36	20
1	B	393/391 (100%)	382 (97%)	9 (2%)	2 (0%)	24	10
All	All	787/782 (101%)	765 (97%)	19 (2%)	3 (0%)	36	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	232[A]	SER
1	B	232[B]	SER
1	A	388	LEU

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	307/316 (97%)	306 (100%)	1 (0%)	86	79
1	B	311/316 (98%)	309 (99%)	2 (1%)	78	66
All	All	618/632 (98%)	615 (100%)	3 (0%)	86	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	LEU
1	B	315[A]	LEU
1	B	315[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	103	GLN
1	B	114	GLN
1	B	192	GLN
1	B	292	GLN
1	B	333	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	A	233	1	23,24,25	1.94	6 (26%)	25,32,34	2.41	8 (32%)
1	LLP	B	233	1	23,24,25	1.68	7 (30%)	25,32,34	2.56	10 (40%)

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	A	233	1	-	5/16/17/19	0/1/1/1
1	LLP	B	233	1	-	3/16/17/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	LLP	O3-C3	-5.45	1.24	1.36
1	B	233	LLP	O3-C3	-3.61	1.28	1.36
1	A	233	LLP	C2-N1	3.57	1.40	1.33
1	A	233	LLP	P-OP2	3.18	1.66	1.54
1	B	233	LLP	P-OP2	3.07	1.66	1.54
1	B	233	LLP	C2-N1	3.06	1.39	1.33
1	A	233	LLP	C4-C4'	2.68	1.52	1.46
1	B	233	LLP	C4-C4'	2.67	1.52	1.46
1	A	233	LLP	C5'-C5	2.47	1.57	1.50
1	B	233	LLP	C6-N1	2.30	1.39	1.34
1	B	233	LLP	P-OP4	2.23	1.67	1.60
1	B	233	LLP	C4'-NZ	2.03	1.34	1.27
1	A	233	LLP	C2'-C2	2.02	1.53	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LLP	OP3-P-OP4	-5.71	91.78	106.67
1	B	233	LLP	OP4-P-OP1	-5.43	91.76	106.44
1	A	233	LLP	OP3-P-OP2	5.30	127.66	107.80
1	B	233	LLP	OP4-C5'-C5	5.29	119.27	109.36
1	A	233	LLP	OP4-C5'-C5	4.67	118.11	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	LLP	OP3-P-OP4	-4.40	95.19	106.67
1	A	233	LLP	OP4-P-OP1	-4.07	95.44	106.44
1	B	233	LLP	OP3-P-OP2	3.83	122.16	107.80
1	B	233	LLP	C4-C4'-NZ	-3.49	107.94	124.04
1	A	233	LLP	C5-C4-C4'	-3.41	116.22	121.47
1	B	233	LLP	C4-C3-C2	-2.97	118.47	120.14
1	B	233	LLP	OP2-P-OP4	2.90	114.23	106.67
1	A	233	LLP	C4-C4'-NZ	-2.80	111.13	124.04
1	B	233	LLP	C2'-C2-C3	2.69	123.94	120.80
1	B	233	LLP	C5-C6-N1	-2.67	119.49	123.83
1	A	233	LLP	O3-C3-C2	2.58	122.94	117.58
1	B	233	LLP	C5-C4-C4'	-2.44	117.70	121.47
1	A	233	LLP	C3-C4-C4'	2.11	124.21	120.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	233	LLP	C5'-OP4-P-OP2
1	B	233	LLP	C5'-OP4-P-OP2
1	A	233	LLP	C4-C4'-NZ-CE
1	B	233	LLP	C4-C4'-NZ-CE
1	A	233	LLP	C3-C4-C4'-NZ
1	B	233	LLP	C3-C4-C4'-NZ
1	A	233	LLP	CA-CB-CG-CD
1	A	233	LLP	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	233	LLP	2	0
1	B	233	LLP	4	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
5	PEG	A	395	-	6,6,6	0.44	0	5,5,5	0.40	0
4	ACT	A	394	-	3,3,3	0.93	0	3,3,3	1.77	1 (33%)
5	PEG	A	396	-	6,6,6	0.39	0	5,5,5	0.73	0
4	ACT	B	392	-	3,3,3	1.59	1 (33%)	3,3,3	1.50	0
5	PEG	A	397	-	6,6,6	0.44	0	5,5,5	0.68	0
6	PG4	B	393	-	12,12,12	0.81	0	11,11,11	0.91	1 (9%)
5	PEG	B	395	-	6,6,6	0.48	0	5,5,5	1.19	0
5	PEG	B	394	-	6,6,6	0.55	0	5,5,5	0.69	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
5	PEG	A	395	-	-	2/4/4/4	-
5	PEG	A	396	-	-	4/4/4/4	-
5	PEG	A	397	-	-	3/4/4/4	-
6	PG4	B	393	-	-	3/10/10/10	-
5	PEG	B	395	-	-	2/4/4/4	-
5	PEG	B	394	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	392	ACT	OXT-C	-2.74	1.18	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	394	ACT	OXT-C-O	-2.51	112.72	122.03
6	B	393	PG4	C7-O4-C6	2.03	122.16	113.26

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	395	PEG	C4-C3-O2-C2
5	B	394	PEG	O1-C1-C2-O2
5	B	395	PEG	O2-C3-C4-O4
5	A	395	PEG	O2-C3-C4-O4
5	B	394	PEG	O2-C3-C4-O4
5	A	397	PEG	C4-C3-O2-C2
5	A	396	PEG	C4-C3-O2-C2
6	B	393	PG4	O1-C1-C2-O2
6	B	393	PG4	C3-C4-O3-C5
5	A	396	PEG	O1-C1-C2-O2
5	A	396	PEG	O2-C3-C4-O4
6	B	393	PG4	C6-C5-O3-C4
5	B	394	PEG	C4-C3-O2-C2
5	A	396	PEG	C1-C2-O2-C3
5	A	395	PEG	O1-C1-C2-O2
5	A	397	PEG	O1-C1-C2-O2
5	A	397	PEG	O2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	395	PEG	4	0
4	B	392	ACT	1	0
5	A	397	PEG	3	0
5	B	395	PEG	3	0
5	B	394	PEG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	375/391 (95%)	-0.26	2 (0%) 87 90	7, 18, 29, 51	9 (2%)
1	B	374/391 (95%)	-0.06	4 (1%) 78 82	7, 18, 32, 49	10 (2%)
All	All	749/782 (95%)	-0.16	6 (0%) 82 86	7, 18, 30, 51	19 (2%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	PHE	4.9
1	B	23	VAL	3.7
1	A	389	ASN	3.3
1	B	208	ASP	2.4
1	B	5	GLN	2.2
1	B	387	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	B	233	24/25	0.84	0.13	16,23,52,63	0
1	LLP	A	233	24/25	0.92	0.10	16,21,53,69	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	B	394	7/7	0.67	0.19	38,44,58,61	0
6	PG4	B	393	13/13	0.82	0.14	30,34,44,44	0
5	PEG	A	396	7/7	0.83	0.13	38,43,48,53	0
5	PEG	B	395	7/7	0.85	0.11	34,42,47,53	0
5	PEG	A	395	7/7	0.85	0.13	32,44,50,60	0
5	PEG	A	397	7/7	0.86	0.14	31,37,45,55	0
3	CL	B	391	1/1	0.87	0.13	60,60,60,60	0
3	CL	A	393	1/1	0.89	0.11	57,57,57,57	0
4	ACT	A	394	4/4	0.89	0.15	23,27,31,40	0
4	ACT	B	392	4/4	0.89	0.11	25,36,36,42	0
2	CA	A	392	1/1	0.92	0.16	29,29,29,29	1
2	CA	A	391	1/1	0.99	0.12	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.