



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:46 PM UTC

PDB ID : 3F6T / pdb_00003f6t
Title : Crystal structure of aspartate aminotransferase (E.C. 2.6.1.1) (YP_194538.1)
from *Lactobacillus acidophilus* NCFM at 2.15 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2008-11-06
Resolution : 2.15 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

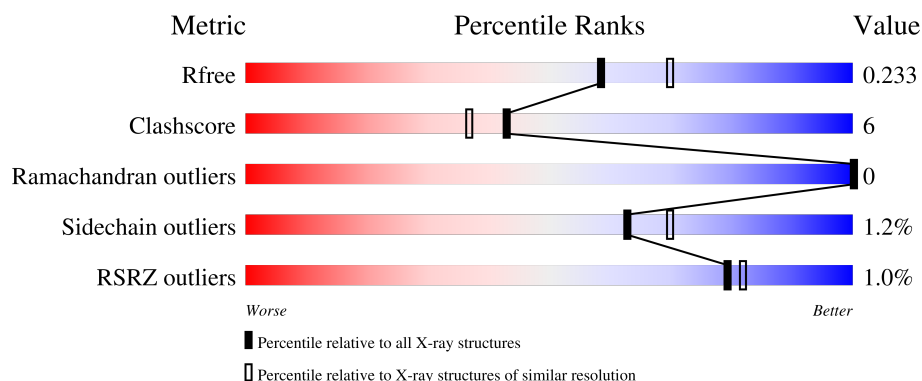
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	533	% 80% 15% ..
1	B	533	% 84% 11% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8986 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 Aspartate aminotransferase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	P	S	Se	0	6	0
			4176	2678	690	795	1	4	8			
1	B	517	Total	C	N	O	P	S	Se	0	13	0
			4219	2701	695	810	1	4	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q5FIG7
B	0	GLY	-	expression tag	UNP Q5FIG7

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



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

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

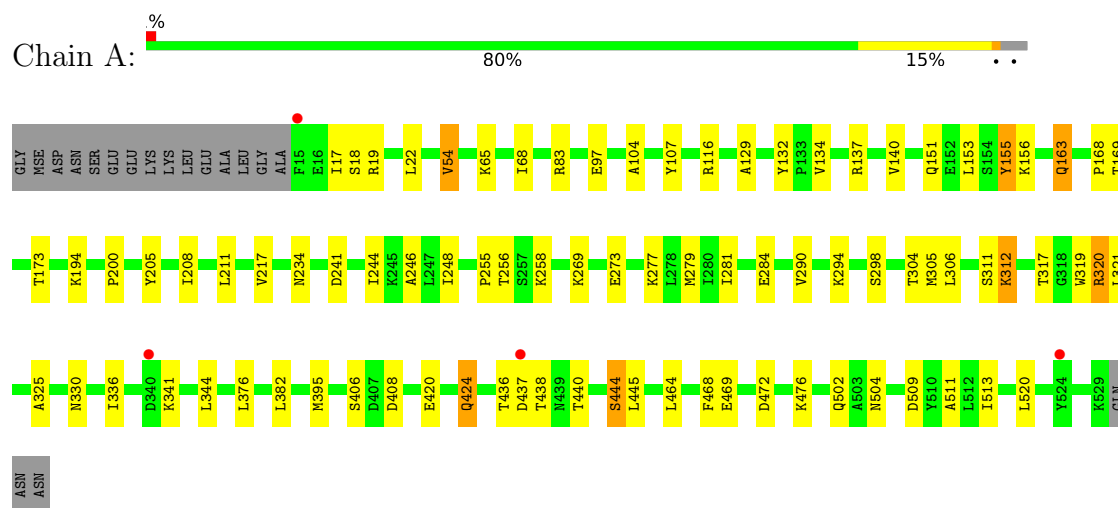
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	290	Total	O	0	5
			295	295		
3	B	273	Total	O	0	3
			276	276		

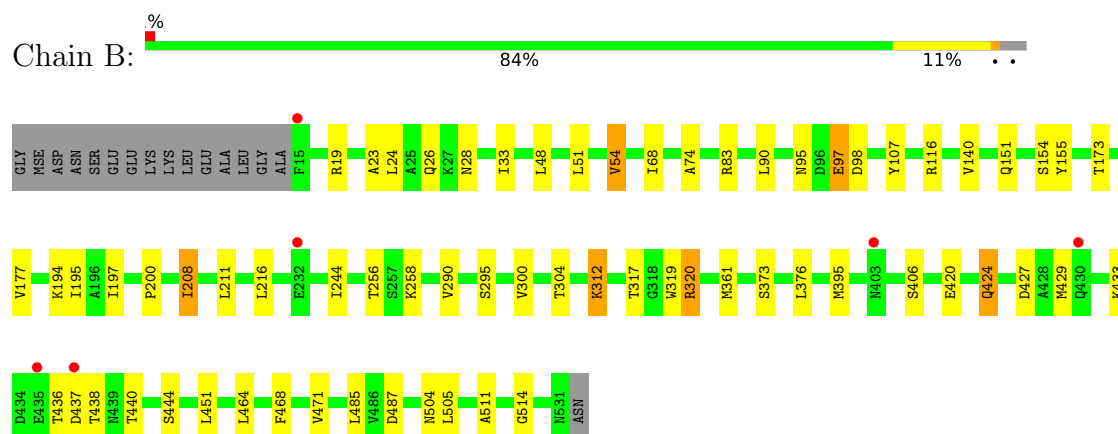
3 Residue-property plots [i](#)

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: Aspartate aminotransferase



• Molecule 1: Aspartate aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.78Å 107.75Å 119.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.15 29.92 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.92-2.15) 99.2 (29.92-2.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.177 , 0.238 0.181 , 0.233	Depositor DCC
R_{free} test set	3199 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.9	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	0.94	EDS
Total number of atoms	8986	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 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	0.95	3/4242 (0.1%)	1.10	14/5740 (0.2%)
1	B	0.91	3/4311 (0.1%)	1.10	9/5834 (0.2%)
All	All	0.93	6/8553 (0.1%)	1.10	23/11574 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	VAL	CA-CB	7.02	1.62	1.54
1	A	305	MSE	SE-CE	-6.08	1.77	1.95
1	B	54	VAL	CA-CB	5.90	1.62	1.54
1	B	361	MSE	SE-CE	-5.59	1.78	1.95
1	B	300	VAL	CA-CB	5.48	1.61	1.54
1	A	134	VAL	CA-C	5.44	1.57	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	GLU	CB-CA-C	-8.71	96.33	110.79
1	B	504	ASN	N-CA-C	7.69	122.97	112.90
1	A	97	GLU	CB-CA-C	-7.51	98.32	110.79
1	B	140[A]	VAL	N-CA-C	7.48	118.25	110.62
1	B	140[B]	VAL	N-CA-C	7.48	118.25	110.62
1	A	408	ASP	N-CA-C	-6.02	102.80	108.22
1	B	208	ILE	N-CA-C	-6.01	103.06	108.95
1	A	504	ASN	N-CA-C	5.85	120.56	112.90
1	A	153	LEU	N-CA-C	5.82	117.62	111.28
1	A	304	THR	N-CA-C	5.80	118.36	108.90
1	A	408	ASP	CB-CA-C	5.71	117.76	110.22
1	A	140[A]	VAL	N-CA-C	5.67	116.45	110.72
1	A	140[B]	VAL	N-CA-C	5.67	116.45	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	ASN	N-CA-C	5.66	117.75	108.52
1	A	406	SER	N-CA-C	5.53	117.31	111.28
1	B	48	LEU	N-CA-C	5.51	116.96	111.07
1	A	163	GLN	CB-CA-C	-5.45	102.24	111.02
1	B	304	THR	N-CA-C	5.36	117.63	108.90
1	A	284	GLU	N-CA-C	5.26	119.01	112.59
1	B	406	SER	N-CA-C	5.17	116.92	111.28
1	A	54	VAL	CB-CA-C	-5.15	105.29	111.88
1	A	97	GLU	CA-CB-CG	5.01	124.13	114.10
1	A	330	ASN	N-CA-C	5.00	116.60	109.14

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	4176	0	4139	59	0
1	B	4219	0	4187	54	0
2	A	16	0	24	2	0
2	B	4	0	6	0	0
3	A	295	0	0	5	0
3	B	276	0	0	3	0
All	All	8986	0	8356	104	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 (104) 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:258:LYS:HZ2	1:A:438:THR:HG23	1.19	1.03
1:A:54:VAL:HG13	1:B:54:VAL:HG13	1.05	1.01
1:A:258:LYS:NZ	1:A:438:THR:HG23	1.74	1.00
1:A:54:VAL:CG1	1:B:54:VAL:HG13	1.92	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:VAL:HG13	1:B:54:VAL:CG1	1.98	0.89
1:B:258:LYS:HZ2	1:B:438[A]:THR:HG23	1.43	0.83
1:B:424:GLN:HG2	3:B:675:HOH:O	1.81	0.78
1:B:436:THR:CG2	1:B:438[A]:THR:HG22	2.21	0.70
1:B:258:LYS:NZ	1:B:438[A]:THR:HG23	2.05	0.70
1:A:68:ILE:HG23	2:A:533:EDO:H21	1.73	0.70
1:A:258:LYS:NZ	1:A:438:THR:CG2	2.54	0.70
1:A:290:VAL:HG13	1:A:440:THR:HG22	1.77	0.66
1:A:436:THR:CG2	1:A:438:THR:HG22	2.26	0.66
1:B:420:GLU:OE2	1:B:424:GLN:NE2	2.29	0.65
1:B:429:MSE:HE2	1:B:514:GLY:HA2	1.78	0.65
1:A:376:LEU:HB3	1:B:173:THR:HG23	1.79	0.65
1:A:200:PRO:HG3	1:A:256:THR:HG23	1.79	0.63
1:B:436:THR:HG22	1:B:438[B]:THR:H	1.64	0.62
1:A:248:ILE:HD12	1:A:281:ILE:HD12	1.81	0.62
1:B:436:THR:HG22	1:B:438[A]:THR:H	1.64	0.61
1:A:173:THR:HG23	1:B:376:LEU:HB3	1.84	0.59
1:A:163:GLN:HG3	3:A:610:HOH:O	2.02	0.58
1:B:194:LYS:HG2	1:B:244:ILE:HD13	1.86	0.57
1:B:208:ILE:HB	1:B:211:LEU:HD13	1.86	0.57
1:B:195:ILE:HG12	1:B:216:LEU:HD23	1.87	0.56
1:A:200:PRO:HG3	1:A:256:THR:CG2	2.34	0.56
1:B:151:GLN:HA	1:B:155:TYR:CG	2.40	0.56
1:A:424:GLN:HG3	1:A:511:ALA:HB2	1.88	0.56
1:B:258:LYS:NZ	1:B:438[A]:THR:CG2	2.69	0.55
1:B:151:GLN:HA	1:B:155:TYR:CD2	2.42	0.55
1:B:436:THR:HG21	1:B:438[A]:THR:HG22	1.89	0.55
1:B:200:PRO:HG3	1:B:256[A]:THR:HG23	1.89	0.54
2:A:536:EDO:H12	3:B:694:HOH:O	2.07	0.53
1:B:107:TYR:CD1	1:B:395:MSE:HE1	2.44	0.53
1:B:424:GLN:HG3	1:B:511:ALA:HB2	1.91	0.53
1:B:83:ARG:HG3	1:B:116:ARG:HB3	1.91	0.52
1:A:65:LYS:NZ	3:A:586:HOH:O	2.43	0.51
1:A:436:THR:HG21	1:A:438:THR:HG22	1.92	0.51
1:A:464:LEU:O	1:A:468:PHE:HB2	2.11	0.51
1:B:23:ALA:O	1:B:26[A]:GLN:HG2	2.11	0.51
1:A:420:GLU:OE2	1:A:424:GLN:NE2	2.43	0.50
1:A:424:GLN:HG2	3:A:685:HOH:O	2.11	0.50
1:B:429:MSE:HG2	1:B:451:LEU:HD21	1.93	0.50
1:A:258:LYS:HZ1	1:A:438:THR:CG2	2.24	0.50
1:B:464:LEU:O	1:B:468:PHE:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ARG:N	1:A:19:ARG:HD2	2.27	0.49
1:A:208[B]:ILE:HB	1:A:211:LEU:HD13	1.95	0.49
1:B:195:ILE:HG13	1:B:197:ILE:HD11	1.93	0.49
1:A:107:TYR:CD1	1:A:395:MSE:HE1	2.47	0.49
1:B:427:ASP:OD1	1:B:433:LYS:CE	2.61	0.49
1:A:83:ARG:HG3	1:A:116:ARG:HB3	1.95	0.48
1:A:312:LLP:H5'2	1:A:312:LLP:NZ	2.28	0.48
1:B:290:VAL:HG13	1:B:440:THR:HG22	1.95	0.48
1:A:319:TRP:HB3	1:A:321:LEU:HG	1.96	0.48
1:B:436:THR:HG22	1:B:437:ASP:N	2.29	0.48
1:A:132:TYR:HB2	1:B:33:ILE:HD13	1.96	0.48
1:A:476:LYS:HB3	1:A:520:LEU:HD21	1.94	0.48
1:B:24:LEU:HD13	1:B:471:VAL:HG13	1.96	0.47
1:A:208[B]:ILE:HG23	1:B:373:SER:HB3	1.96	0.47
1:B:19:ARG:N	1:B:19:ARG:HD2	2.27	0.47
1:B:51:LEU:HB3	1:B:97:GLU:CG	2.44	0.47
1:A:17:ILE:O	1:A:18:SER:C	2.58	0.47
1:B:317:THR:O	1:B:320[B]:ARG:HD2	2.13	0.47
1:B:436:THR:HG22	1:B:438[A]:THR:HG22	1.96	0.46
1:A:241:ASP:HB3	1:A:244:ILE:HG12	1.99	0.45
1:A:269:LYS:O	1:A:273:GLU:HG3	2.16	0.45
1:B:154:SER:HB2	1:B:295:SER:HB2	1.98	0.45
1:A:137:ARG:O	1:A:168:PRO:HD2	2.17	0.45
1:A:311:SER:HB3	1:A:317:THR:HG22	1.98	0.45
1:A:317:THR:O	1:A:320[B]:ARG:HD2	2.17	0.45
1:B:90:LEU:HB3	1:B:98:ASP:HB3	1.99	0.45
1:A:306:LEU:HB3	1:A:325:ALA:HB3	1.99	0.44
1:A:129:ALA:HB3	1:B:319:TRP:CD1	2.52	0.44
1:A:208[A]:ILE:HB	1:A:211:LEU:HD13	2.00	0.44
1:A:132:TYR:HB2	1:B:33:ILE:CD1	2.48	0.44
1:B:28:ASN:HD22	1:B:485:LEU:HB3	1.83	0.43
1:A:205:TYR:O	1:A:208[A]:ILE:HD13	2.17	0.43
1:A:104:ALA:HA	1:A:395:MSE:HE2	2.01	0.43
1:A:151:GLN:HA	1:A:155:TYR:CG	2.54	0.43
1:B:312:LLP:OP1	1:B:320[A]:ARG:NH2	2.52	0.43
1:A:376:LEU:HD12	1:B:177:VAL:HG23	2.00	0.43
1:B:258:LYS:HZ2	1:B:438[A]:THR:CG2	2.22	0.43
1:A:436:THR:HG22	1:A:437:ASP:N	2.33	0.43
3:A:677:HOH:O	1:B:320[A]:ARG:HD3	2.18	0.42
1:A:200:PRO:CG	1:A:256:THR:HG23	2.46	0.42
1:A:169:THR:C	1:A:382:LEU:HD13	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320[A]:ARG:HD3	3:B:577:HOH:O	2.18	0.42
1:A:336:ILE:O	1:A:344:LEU:HD21	2.20	0.42
1:A:156:LYS:NZ	3:A:729:HOH:O	2.44	0.42
1:A:194:LYS:HG2	1:A:244:ILE:HD13	2.01	0.41
1:B:68:ILE:O	1:B:74:ALA:HA	2.19	0.41
1:B:487:ASP:O	1:B:505:LEU:HD21	2.20	0.41
1:A:509:ASP:O	1:A:513:ILE:HG12	2.20	0.41
1:A:246:ALA:HA	1:A:279:MSE:O	2.21	0.41
1:A:294:LYS:HZ2	1:A:298:SER:CB	2.32	0.41
1:B:320[B]:ARG:HA	1:B:320[B]:ARG:NH2	2.35	0.41
1:B:320[B]:ARG:HA	1:B:320[B]:ARG:HH21	1.86	0.41
1:A:194:LYS:HD3	1:A:217:VAL:HG21	2.02	0.41
1:B:427:ASP:OD1	1:B:433:LYS:HE3	2.21	0.41
1:A:469:GLU:HG3	1:A:472:ASP:H	1.86	0.41
1:B:195:ILE:HG13	1:B:197:ILE:CD1	2.51	0.41
1:A:255:PRO:HG2	1:A:445:LEU:HD11	2.03	0.40
1:B:195:ILE:HG12	1:B:216:LEU:CD2	2.51	0.40
1:A:444:SER:HG	1:A:502:GLN:HE22	1.66	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	518/533 (97%)	505 (98%)	13 (2%)	0	100	100
1	B	527/533 (99%)	516 (98%)	11 (2%)	0	100	100
All	All	1045/1066 (98%)	1021 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	453/457 (99%)	444 (98%)	9 (2%)	48	54
1	B	462/457 (101%)	458 (99%)	4 (1%)	70	77
All	All	915/914 (100%)	902 (99%)	13 (1%)	63	66

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

Mol	Chain	Res	Type
1	A	22	LEU
1	A	155	TYR
1	A	234	ASN
1	A	277	LYS
1	A	320[A]	ARG
1	A	320[B]	ARG
1	A	341	LYS
1	A	424	GLN
1	A	444	SER
1	B	320[A]	ARG
1	B	320[B]	ARG
1	B	424	GLN
1	B	444	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	222	HIS
1	A	303	ASN
1	A	467	ASN
1	B	28	ASN
1	B	95	ASN
1	B	378	HIS
1	B	470	GLN
1	B	502	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	312	1	23,24,25	1.69	3 (13%)	25,32,34	2.29	7 (28%)
1	LLP	A	312	1	23,24,25	1.79	4 (17%)	25,32,34	1.91	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	312	1	-	6/16/17/19	0/1/1/1
1	LLP	A	312	1	-	2/16/17/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	LLP	O3-C3	-5.40	1.24	1.36
1	B	312	LLP	O3-C3	-4.95	1.25	1.36
1	B	312	LLP	C6-N1	3.13	1.40	1.34
1	A	312	LLP	C2-N1	2.87	1.39	1.33
1	A	312	LLP	C6-N1	2.84	1.40	1.34
1	B	312	LLP	C2-N1	2.79	1.38	1.33
1	A	312	LLP	CE-NZ	2.63	1.52	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	LLP	C3-C4-C4'	-5.17	111.06	120.40
1	A	312	LLP	C3-C4-C4'	-5.14	111.12	120.40
1	B	312	LLP	CE-NZ-C4'	-4.66	103.79	118.72
1	A	312	LLP	C5-C4-C4'	4.53	128.46	121.47
1	B	312	LLP	C3-C4-C5	4.15	121.61	118.28
1	B	312	LLP	C5-C4-C4'	3.80	127.33	121.47
1	B	312	LLP	OP4-C5'-C5	3.75	116.38	109.36
1	A	312	LLP	C3-C4-C5	2.66	120.41	118.28
1	B	312	LLP	C5'-C5-C6	-2.60	115.12	119.36
1	A	312	LLP	C5'-C5-C6	-2.07	115.98	119.36
1	B	312	LLP	C3-C2-N1	-2.05	118.37	120.96
1	A	312	LLP	OP4-P-OP1	-2.03	100.96	106.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	312	LLP	O-C-CA-CB
1	B	312	LLP	C5'-OP4-P-OP1
1	B	312	LLP	C5'-OP4-P-OP3
1	A	312	LLP	CA-CB-CG-CD
1	B	312	LLP	C4-C5-C5'-OP4
1	B	312	LLP	CA-CB-CG-CD
1	B	312	LLP	C6-C5-C5'-OP4
1	B	312	LLP	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	312	LLP	1	0
1	A	312	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
2	EDO	A	533	-	3,3,3	0.27	0	2,2,2	0.47	0
2	EDO	B	533	-	3,3,3	0.49	0	2,2,2	0.26	0
2	EDO	A	534	-	3,3,3	0.52	0	2,2,2	0.18	0
2	EDO	A	536	-	3,3,3	0.37	0	2,2,2	0.34	0
2	EDO	A	535	-	3,3,3	0.38	0	2,2,2	0.27	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	EDO	A	533	-	-	1/1/1/1	-
2	EDO	B	533	-	-	0/1/1/1	-
2	EDO	A	534	-	-	0/1/1/1	-
2	EDO	A	536	-	-	1/1/1/1	-
2	EDO	A	535	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	533	EDO	O1-C1-C2-O2
2	A	535	EDO	O1-C1-C2-O2
2	A	536	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	533	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	536	EDO	1	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 [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	506/533 (94%)	0.09	4 (0%) 82 84	14, 29, 42, 55	6 (1%)
1	B	508/533 (95%)	-0.06	6 (1%) 76 79	14, 29, 41, 55	13 (2%)
All	All	1014/1066 (95%)	0.02	10 (0%) 79 82	14, 29, 42, 55	19 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	524	TYR	3.7
1	A	15	PHE	3.2
1	B	15	PHE	2.6
1	B	430	GLN	2.4
1	A	340	ASP	2.3
1	A	437	ASP	2.3
1	B	437	ASP	2.2
1	B	403	ASN	2.2
1	B	435	GLU	2.1
1	B	232	GLU	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	A	312	24/25	0.97	0.06	28,31,32,34	0
1	LLP	B	312	24/25	0.97	0.07	28,30,32,33	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($\text{\AA}^2$)	Q<0.9
2	EDO	A	534	4/4	0.81	0.19	39,40,41,42	0
2	EDO	A	536	4/4	0.86	0.24	39,40,42,44	0
2	EDO	B	533	4/4	0.87	0.11	40,41,42,42	0
2	EDO	A	535	4/4	0.90	0.14	31,31,34,37	0
2	EDO	A	533	4/4	0.92	0.12	40,41,42,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.