



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:07 AM UTC

PDB ID : 9J32 / pdb_00009j32
Title : Crystal structure of aminotransferase-like protein from *Variovorax paradoxus* mutant N174K
Authors : Ilyasov, I.O.; Minyaev, M.E.; Rakitina, T.V.; Bakunova, A.K.; Matyuta, I.O.; Popov, V.O.; Bezsudnova, E.Y.; Boyko, K.M.
Deposited on : 2024-08-07
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 ⓘ 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

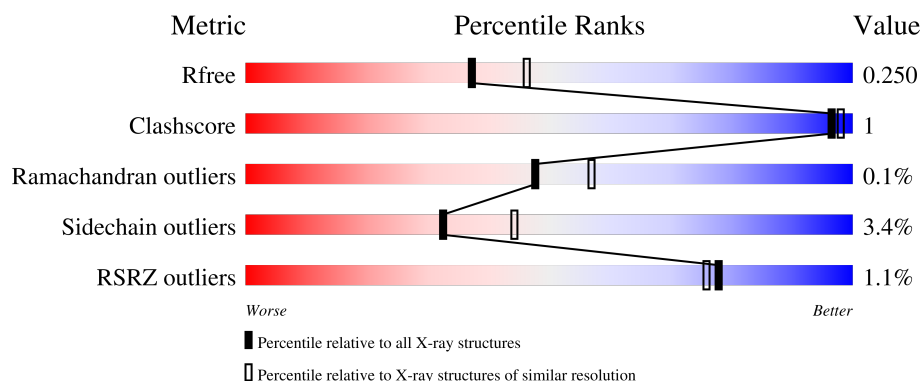
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	317	% 85% 8% • 5%
1	B	317	% 85% 9% • 5%
1	C	317	% 86% 8% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6973 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.

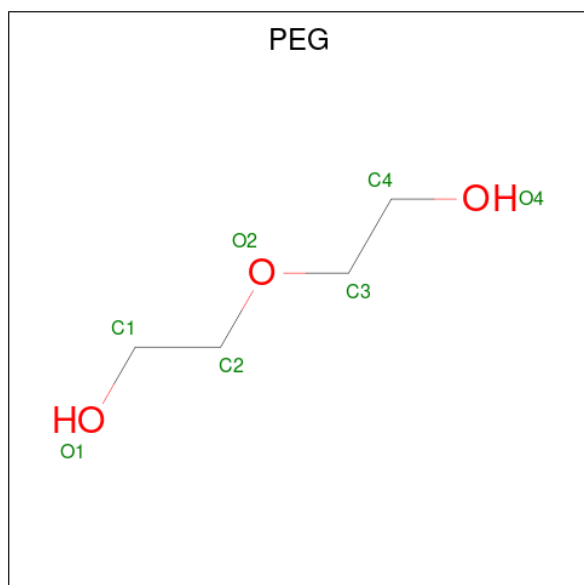
- Molecule 1 is a protein called Aminotransferase, class 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	P	S	0	0	0
			2246	1409	406	420	1	10			
1	B	300	Total	C	N	O	P	S	0	2	0
			2263	1417	413	422	1	10			
1	C	302	Total	C	N	O	P	S	0	0	0
			2254	1413	408	422	1	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	174	LLP	ASN	engineered mutation	UNP T1XIY1
B	174	LLP	ASN	engineered mutation	UNP T1XIY1
C	174	LLP	ASN	engineered mutation	UNP T1XIY1

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

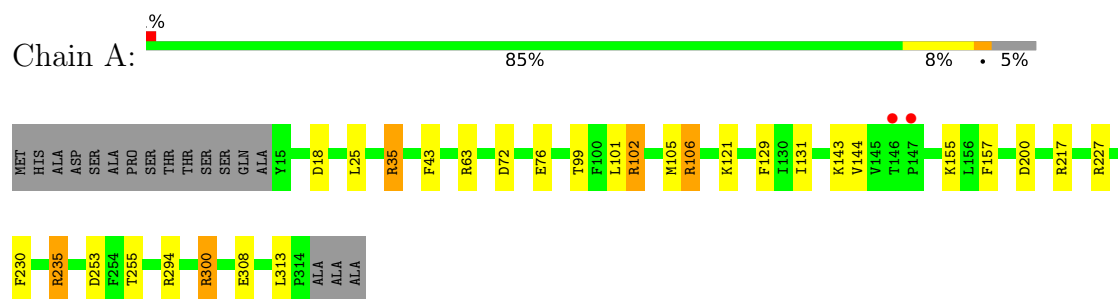
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	83	Total	O		0	0
			83	83			
3	B	64	Total	O		0	0
			64	64			
3	C	56	Total	O		0	0
			56	56			

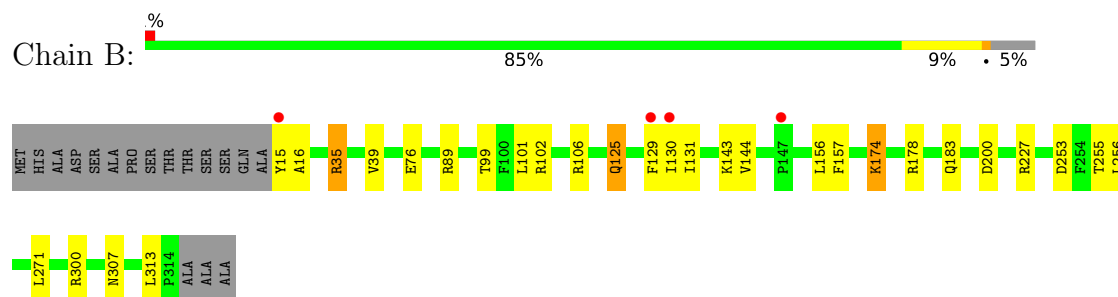
3 Residue-property plots [i](#)

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.

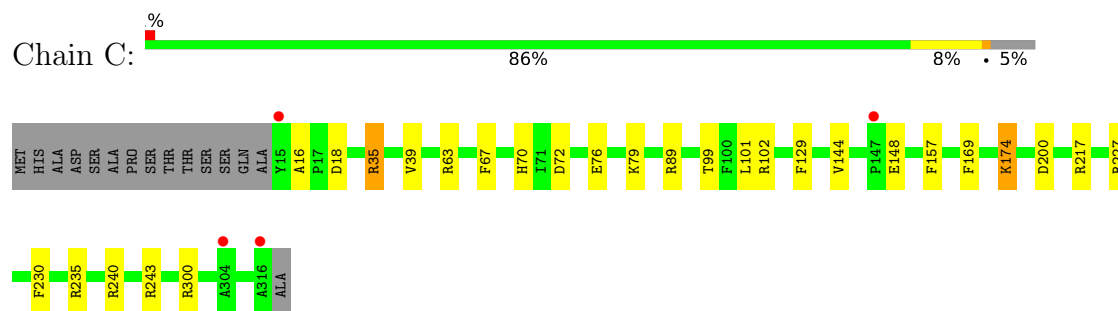
- Molecule 1: Aminotransferase, class 4



- Molecule 1: Aminotransferase, class 4



- Molecule 1: Aminotransferase, class 4



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.25Å 87.34Å 104.66Å 90.00° 99.45° 90.00°	Depositor
Resolution (Å)	21.81 – 2.20 21.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (21.81-2.20) 82.1 (21.81-2.20)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.214 , 0.269 0.200 , 0.250	Depositor DCC
R_{free} test set	2062 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6973	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.49% 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, 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	0.87	0/2261	1.37	17/3077 (0.6%)
1	B	0.80	0/2289	1.36	9/3112 (0.3%)
1	C	0.82	0/2269	1.31	9/3089 (0.3%)
All	All	0.83	0/6819	1.35	35/9278 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	B	0	5
1	C	0	9
All	All	0	24

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	PHE	CB-CA-C	8.44	121.60	111.22
1	A	76	GLU	CB-CA-C	8.31	124.02	110.90
1	B	76	GLU	CB-CA-C	8.11	123.72	110.90
1	A	129	PHE	CB-CA-C	7.93	121.73	111.50
1	C	129	PHE	CB-CA-C	7.39	121.03	111.50
1	B	255	THR	CA-CB-OG1	-7.38	98.53	109.60
1	A	121	LYS	N-CA-CB	7.33	120.90	110.12
1	A	72	ASP	CA-CB-CG	7.05	119.66	112.60
1	C	76	GLU	CB-CA-C	6.89	121.79	110.90
1	A	155	LYS	CB-CG-CD	6.82	126.98	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	PHE	CA-CB-CG	-6.49	107.31	113.80
1	A	99	THR	CA-CB-OG1	-6.30	100.15	109.60
1	C	157	PHE	CA-CB-CG	-6.27	107.53	113.80
1	B	200	ASP	CA-CB-CG	6.19	118.79	112.60
1	B	99	THR	CA-CB-OG1	-6.15	100.37	109.60
1	C	18	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	157	PHE	CA-CB-CG	-6.02	107.78	113.80
1	C	99	THR	CA-CB-OG1	-5.98	100.63	109.60
1	C	200	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	125	GLN	N-CA-CB	5.61	118.78	110.53
1	B	253	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	157	PHE	CA-CB-CG	-5.47	108.33	113.80
1	A	255	THR	CA-CB-OG1	-5.45	101.43	109.60
1	C	148	GLU	CB-CG-CD	5.43	121.84	112.60
1	A	308	GLU	CB-CA-C	5.39	119.71	110.01
1	A	18	ASP	CA-CB-CG	5.31	117.91	112.60
1	C	67	PHE	CA-CB-CG	5.30	119.10	113.80
1	A	200	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	43	PHE	CA-CB-CG	-5.20	108.60	113.80
1	A	253	ASP	CB-CA-C	5.15	118.23	109.84
1	B	256	LEU	CA-C-O	-5.14	115.11	120.55
1	A	235	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	A	143	LYS	CB-CG-CD	5.04	122.88	111.30
1	C	230	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	105	MET	CG-SD-CE	-5.02	89.86	100.90

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	106	ARG	Sidechain
1	A	217	ARG	Sidechain
1	A	227	ARG	Sidechain
1	A	235	ARG	Sidechain
1	A	294	ARG	Sidechain
1	A	300	ARG	Sidechain
1	A	313	LEU	Peptide
1	A	35	ARG	Sidechain
1	A	63	ARG	Sidechain
1	B	15	TYR	Peptide
1	B	16	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	B	227	ARG	Sidechain
1	B	300	ARG	Sidechain
1	B	35	ARG	Sidechain
1	C	16	ALA	Peptide
1	C	217	ARG	Sidechain
1	C	227	ARG	Sidechain
1	C	235	ARG	Sidechain
1	C	240	ARG	Sidechain
1	C	243	ARG	Sidechain
1	C	300	ARG	Sidechain
1	C	35	ARG	Sidechain
1	C	63	ARG	Sidechain

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	2246	0	2203	0	0
1	B	2263	0	2228	9	0
1	C	2254	0	2210	6	0
2	C	7	0	10	2	0
3	A	83	0	0	0	0
3	B	64	0	0	1	0
3	C	56	0	0	1	0
All	All	6973	0	6651	14	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 1.

All (14) 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:106[B]:ARG:HG2	1:B:106[B]:ARG:NH2	1.93	0.84
1:C:169:PHE:HB3	2:C:401:PEG:H32	1.73	0.71
1:B:106[B]:ARG:HH21	1:B:106[B]:ARG:CG	2.11	0.62
1:B:106[B]:ARG:NH2	1:B:106[B]:ARG:CG	2.58	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106[B]:ARG:HG2	1:B:106[B]:ARG:HH21	1.69	0.57
1:C:70:HIS:NE2	3:C:501:HOH:O	2.33	0.57
1:B:143:LYS:HD2	1:B:271:LEU:HD11	1.88	0.55
1:B:183:GLN:NE2	3:B:402:HOH:O	2.41	0.52
1:C:169:PHE:CB	2:C:401:PEG:H32	2.43	0.47
1:C:89:ARG:HH11	1:C:89:ARG:HG3	1.82	0.43
1:C:174:LLP:NZ	1:C:174:LLP:O3	2.48	0.43
1:B:89:ARG:HH11	1:B:89:ARG:HG3	1.86	0.41
1:B:174:LLP:O3	1:B:178:ARG:NH2	2.53	0.41
1:B:39:VAL:HB	1:C:39:VAL:HB	2.04	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	297/317 (94%)	290 (98%)	7 (2%)	0	100	100
1	B	299/317 (94%)	292 (98%)	6 (2%)	1 (0%)	36	42
1	C	299/317 (94%)	291 (97%)	8 (3%)	0	100	100
All	All	895/951 (94%)	873 (98%)	21 (2%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	307	ASN

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	226/247 (92%)	218 (96%)	8 (4%)	32	43
1	B	230/247 (93%)	221 (96%)	9 (4%)	28	39
1	C	226/247 (92%)	220 (97%)	6 (3%)	39	53
All	All	682/741 (92%)	659 (97%)	23 (3%)	32	44

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	35	ARG
1	A	101	LEU
1	A	102	ARG
1	A	106	ARG
1	A	131	ILE
1	A	144	VAL
1	A	300	ARG
1	B	35	ARG
1	B	101	LEU
1	B	102	ARG
1	B	125	GLN
1	B	130	ILE
1	B	131	ILE
1	B	144	VAL
1	B	156	LEU
1	B	313	LEU
1	C	35	ARG
1	C	72	ASP
1	C	79	LYS
1	C	101	LEU
1	C	102	ARG
1	C	144	VAL

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	183	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	174	1	23,24,25	0.65	0	25,32,34	0.86	0
1	LLP	C	174	1	23,24,25	0.93	1 (4%)	25,32,34	1.11	1 (4%)
1	LLP	B	174	1	23,24,25	0.96	1 (4%)	25,32,34	1.07	1 (4%)

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	174	1	-	1/16/17/19	0/1/1/1
1	LLP	C	174	1	-	1/16/17/19	0/1/1/1
1	LLP	B	174	1	-	1/16/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	LLP	C3-C2	2.35	1.43	1.41
1	C	174	LLP	P-OP1	2.31	1.57	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	LLP	OP3-P-OP4	-3.02	98.78	106.67
1	B	174	LLP	OP3-P-OP4	-2.56	99.99	106.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	174	LLP	O-C-CA-CB
1	B	174	LLP	O-C-CA-CB
1	C	174	LLP	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	174	LLP	1	0
1	B	174	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	PEG	C	401	-	6,6,6	0.38	0	5,5,5	0.64	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	PEG	C	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	PEG	O2-C3-C4-O4
2	C	401	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	PEG	2	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	299/317 (94%)	-0.06	2 (0%) 84 82	19, 37, 67, 101	0
1	B	299/317 (94%)	0.01	4 (1%) 75 73	21, 40, 68, 93	2 (0%)
1	C	301/317 (94%)	0.08	4 (1%) 75 73	22, 43, 67, 103	0
All	All	899/951 (94%)	0.01	10 (1%) 78 76	19, 40, 68, 103	2 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	TYR	4.2
1	B	129	PHE	3.8
1	A	147	PRO	3.6
1	C	316	ALA	3.1
1	C	147	PRO	2.7
1	A	146	THR	2.6
1	C	15	TYR	2.6
1	B	147	PRO	2.3
1	B	130	ILE	2.2
1	C	304	ALA	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	174	24/25	0.96	0.06	20,30,33,34	0
1	LLP	C	174	24/25	0.96	0.07	27,30,35,37	0
1	LLP	A	174	24/25	0.97	0.06	19,24,26,27	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	PEG	C	401	7/7	0.91	0.26	43,44,48,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.