



Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2026 – 07:02 PM JST

PDB ID : 9X4U / pdb_00009x4u
Title : Crystal structure of Fgm3 in complex with PLP
Authors : Zhang, H.; Xia, M.; Fang, P.; Liu, W.
Deposited on : 2025-10-11
Resolution : 1.67 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	:	1.8.5 (274361), CSD as541be (2020)
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

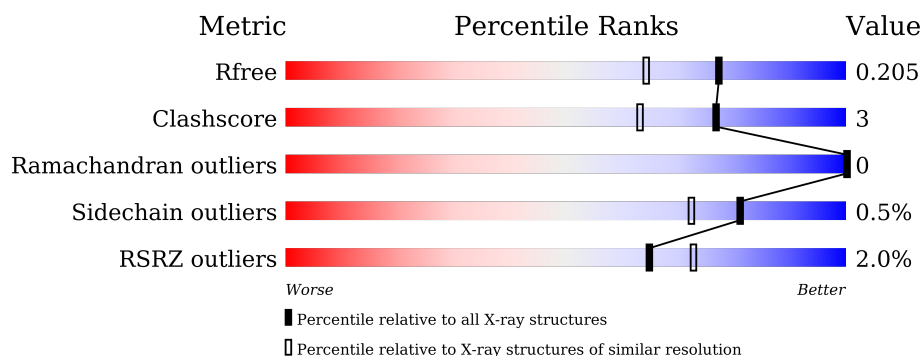
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	408	
1	B	408	
1	C	408	
1	D	408	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14586 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-like protein FGM3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	P	S	0	2	0
			3094	1974	518	596	1	5			
1	B	399	Total	C	N	O	P	S	0	2	0
			3110	1983	522	599	1	5			
1	C	397	Total	C	N	O	P	S	0	2	0
			3094	1974	518	596	1	5			
1	D	399	Total	C	N	O	P	S	0	2	0
			3110	1983	522	599	1	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	SER	ARG	conflict	UNP A0A1C3YKE0
A	?	-	GLN	deletion	UNP A0A1C3YKE0
A	?	-	LEU	deletion	UNP A0A1C3YKE0
A	?	-	SER	deletion	UNP A0A1C3YKE0
A	?	-	PRO	deletion	UNP A0A1C3YKE0
A	399	LEU	-	expression tag	UNP A0A1C3YKE0
A	400	GLU	-	expression tag	UNP A0A1C3YKE0
A	401	HIS	-	expression tag	UNP A0A1C3YKE0
A	402	HIS	-	expression tag	UNP A0A1C3YKE0
A	403	HIS	-	expression tag	UNP A0A1C3YKE0
A	404	HIS	-	expression tag	UNP A0A1C3YKE0
A	405	HIS	-	expression tag	UNP A0A1C3YKE0
A	406	HIS	-	expression tag	UNP A0A1C3YKE0
A	407	HIS	-	expression tag	UNP A0A1C3YKE0
A	408	HIS	-	expression tag	UNP A0A1C3YKE0
B	40	SER	ARG	conflict	UNP A0A1C3YKE0
B	?	-	GLN	deletion	UNP A0A1C3YKE0
B	?	-	LEU	deletion	UNP A0A1C3YKE0
B	?	-	SER	deletion	UNP A0A1C3YKE0
B	?	-	PRO	deletion	UNP A0A1C3YKE0
B	399	LEU	-	expression tag	UNP A0A1C3YKE0

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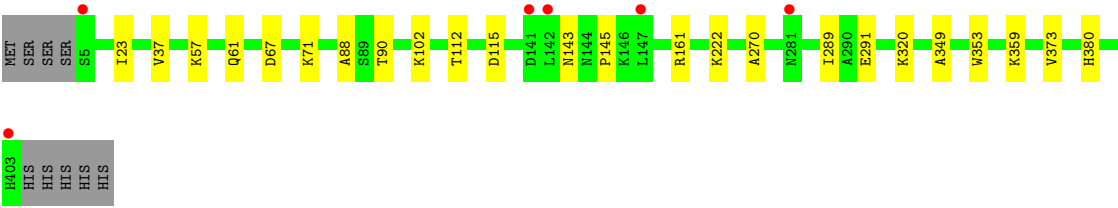
Chain	Residue	Modelled	Actual	Comment	Reference
B	400	GLU	-	expression tag	UNP A0A1C3YKE0
B	401	HIS	-	expression tag	UNP A0A1C3YKE0
B	402	HIS	-	expression tag	UNP A0A1C3YKE0
B	403	HIS	-	expression tag	UNP A0A1C3YKE0
B	404	HIS	-	expression tag	UNP A0A1C3YKE0
B	405	HIS	-	expression tag	UNP A0A1C3YKE0
B	406	HIS	-	expression tag	UNP A0A1C3YKE0
B	407	HIS	-	expression tag	UNP A0A1C3YKE0
B	408	HIS	-	expression tag	UNP A0A1C3YKE0
C	40	SER	ARG	conflict	UNP A0A1C3YKE0
C	?	-	GLN	deletion	UNP A0A1C3YKE0
C	?	-	LEU	deletion	UNP A0A1C3YKE0
C	?	-	SER	deletion	UNP A0A1C3YKE0
C	?	-	PRO	deletion	UNP A0A1C3YKE0
C	399	LEU	-	expression tag	UNP A0A1C3YKE0
C	400	GLU	-	expression tag	UNP A0A1C3YKE0
C	401	HIS	-	expression tag	UNP A0A1C3YKE0
C	402	HIS	-	expression tag	UNP A0A1C3YKE0
C	403	HIS	-	expression tag	UNP A0A1C3YKE0
C	404	HIS	-	expression tag	UNP A0A1C3YKE0
C	405	HIS	-	expression tag	UNP A0A1C3YKE0
C	406	HIS	-	expression tag	UNP A0A1C3YKE0
C	407	HIS	-	expression tag	UNP A0A1C3YKE0
C	408	HIS	-	expression tag	UNP A0A1C3YKE0
D	40	SER	ARG	conflict	UNP A0A1C3YKE0
D	?	-	GLN	deletion	UNP A0A1C3YKE0
D	?	-	LEU	deletion	UNP A0A1C3YKE0
D	?	-	SER	deletion	UNP A0A1C3YKE0
D	?	-	PRO	deletion	UNP A0A1C3YKE0
D	399	LEU	-	expression tag	UNP A0A1C3YKE0
D	400	GLU	-	expression tag	UNP A0A1C3YKE0
D	401	HIS	-	expression tag	UNP A0A1C3YKE0
D	402	HIS	-	expression tag	UNP A0A1C3YKE0
D	403	HIS	-	expression tag	UNP A0A1C3YKE0
D	404	HIS	-	expression tag	UNP A0A1C3YKE0
D	405	HIS	-	expression tag	UNP A0A1C3YKE0
D	406	HIS	-	expression tag	UNP A0A1C3YKE0
D	407	HIS	-	expression tag	UNP A0A1C3YKE0
D	408	HIS	-	expression tag	UNP A0A1C3YKE0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Na 1	0	0
2	B	1	Total 1	Na 1	0	0
2	C	1	Total 1	Na 1	0	0
2	D	1	Total 1	Na 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	519	Total 519	O 519	0	0
3	B	577	Total 577	O 577	0	0
3	C	524	Total 524	O 524	0	0
3	D	554	Total 554	O 554	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.80Å 97.69Å 124.68Å 90.00° 93.72° 90.00°	Depositor
Resolution (Å)	21.90 – 1.67 21.90 – 1.67	Depositor EDS
% Data completeness (in resolution range)	98.9 (21.90-1.67) 98.9 (21.90-1.67)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.65 (at 1.67Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.178 , 0.203 0.180 , 0.205	Depositor DCC
R_{free} test set	9492 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.7	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	0.96	EDS
Total number of atoms	14586	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 87.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0489e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NA, 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	0.28	0/3141	0.53	0/4281
1	B	0.30	0/3158	0.54	0/4304
1	C	0.33	0/3141	0.58	1/4281 (0.0%)
1	D	0.30	0/3158	0.53	0/4304
All	All	0.30	0/12598	0.55	1/17170 (0.0%)

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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	GLU	N-CA-C	6.66	118.62	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	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	3094	0	3065	22	0
1	B	3110	0	3077	16	0
1	C	3094	0	3065	22	0
1	D	3110	0	3077	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	519	0	0	7	0
3	B	577	0	0	7	0
3	C	524	0	0	6	0
3	D	554	0	0	3	0
All	All	14586	0	12284	72	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 3.

All (72) 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:21:ARG:HB3	3:A:601:HOH:O	1.75	0.85
1:A:21:ARG:C	3:A:601:HOH:O	2.23	0.80
1:B:359:LYS:HE2	3:B:793:HOH:O	1.91	0.70
1:B:359:LYS:NZ	3:B:601:HOH:O	2.28	0.66
1:C:385:GLU:HG3	3:C:855:HOH:O	1.98	0.62
1:B:67:ASP:O	1:B:71:LYS:HG3	2.00	0.61
1:B:57:LYS:HE2	1:B:61:GLN:HE22	1.67	0.60
1:A:179:LYS:HD2	1:A:210:GLU:O	2.02	0.59
1:A:22:GLN:N	3:A:601:HOH:O	2.35	0.57
1:C:67:ASP:O	1:C:71:LYS:HG3	2.03	0.57
1:B:400:GLU:HG2	3:B:690:HOH:O	2.05	0.57
1:C:37:VAL:HG13	1:C:270:ALA:HB1	1.87	0.55
1:B:298:THR:O	1:B:302:GLU:HG3	2.08	0.54
1:A:81:ILE:HD12	1:A:82:ASP:N	2.22	0.53
1:C:141:ASP:OD1	1:C:142:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:LEU:HG	3:C:689:HOH:O	2.06	0.53
1:C:9:GLU:H	1:C:9:GLU:CD	2.17	0.52
1:D:161:ARG:NE	3:D:613:HOH:O	2.42	0.52
1:C:104:GLN:HG3	1:C:107:ASP:CG	2.34	0.52
1:C:102:LYS:HA	3:C:871:HOH:O	2.10	0.50
1:C:298:THR:O	1:C:302:GLU:HG3	2.11	0.50
1:B:332:GLU:HG2	3:B:945:HOH:O	2.12	0.50
1:B:23:ILE:HB	1:B:349:ALA:HA	1.93	0.49
1:A:283:LYS:HE2	3:A:938:HOH:O	2.12	0.49
1:B:57:LYS:HE2	1:B:61:GLN:NE2	2.27	0.49
1:C:289:ILE:HG23	1:C:380:HIS:HB3	1.96	0.48
1:A:21:ARG:NH2	3:A:607:HOH:O	2.45	0.48
1:A:385:GLU:O	1:A:389:GLN:HG3	2.13	0.48
1:D:102:LYS:O	1:D:161:ARG:NH1	2.47	0.48
1:A:23:ILE:HB	1:A:349:ALA:HA	1.96	0.48
1:B:150:GLU:OE2	1:B:153:ARG:NH1	2.47	0.47
1:A:37:VAL:HG13	1:A:270:ALA:HB1	1.97	0.47
1:C:9:GLU:HA	3:C:988:HOH:O	2.13	0.47
1:C:19:GLU:HA	1:C:19:GLU:OE1	2.15	0.47
1:A:298:THR:O	1:A:302:GLU:HG3	2.14	0.47
1:B:37:VAL:HG13	1:B:270:ALA:HB1	1.97	0.47
1:A:21:ARG:CB	3:A:601:HOH:O	2.48	0.46
1:C:23:ILE:HB	1:C:349:ALA:HA	1.98	0.46
1:D:57:LYS:HE2	1:D:61:GLN:HE22	1.81	0.45
1:D:23:ILE:HB	1:D:349:ALA:HA	1.98	0.45
1:A:153:ARG:HA	1:A:156:LEU:HD12	1.99	0.44
1:A:102:LYS:O	1:A:161:ARG:NH1	2.51	0.44
1:C:104:GLN:HG3	1:C:107:ASP:OD2	2.17	0.44
1:C:143:ASN:C	1:C:145:PRO:HD3	2.43	0.44
1:B:42:THR:HG22	3:B:867:HOH:O	2.17	0.44
1:C:109:LEU:HB2	1:C:134:ILE:HD13	2.00	0.43
1:B:90[B]:THR:HG22	3:B:881:HOH:O	2.18	0.43
1:D:37:VAL:HG13	1:D:270:ALA:HB1	2.00	0.43
1:C:88:ALA:HB2	1:D:88:ALA:HB2	1.99	0.43
1:D:291:GLU:OE2	1:D:320:LYS:HE3	2.18	0.43
1:C:201:ALA:HB2	1:C:206:ILE:HD11	2.01	0.43
1:A:289:ILE:HG23	1:A:380:HIS:HB3	2.01	0.43
1:D:90[B]:THR:HG22	3:D:850:HOH:O	2.19	0.43
1:C:107:ASP:CG	1:C:161:ARG:HG3	2.43	0.42
1:D:57:LYS:HE2	1:D:61:GLN:NE2	2.34	0.42
1:B:385:GLU:HG3	3:B:846:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASP:CG	1:A:161:ARG:HG3	2.45	0.42
1:A:196:ASP:OD2	1:A:222:LLP:N1	2.53	0.41
1:C:159:LYS:NZ	3:C:619:HOH:O	2.52	0.41
1:A:88:ALA:HB2	1:B:88:ALA:HB2	2.01	0.41
1:D:143:ASN:C	1:D:145:PRO:HD3	2.46	0.41
1:C:90[B]:THR:HG22	3:C:850:HOH:O	2.21	0.41
1:D:289:ILE:HG23	1:D:380:HIS:HB3	2.02	0.41
1:D:353:TRP:HA	1:D:373:VAL:O	2.20	0.41
1:D:359:LYS:HE2	3:D:748:HOH:O	2.20	0.41
1:C:196:ASP:OD2	1:C:222:LLP:N1	2.53	0.41
1:B:289:ILE:HG23	1:B:380:HIS:HB3	2.03	0.41
1:D:67:ASP:O	1:D:71:LYS:HG3	2.20	0.41
1:A:104:GLN:HA	1:A:104:GLN:HE21	1.86	0.41
1:A:353:TRP:HA	1:A:373:VAL:O	2.21	0.41
1:A:143:ASN:C	1:A:145:PRO:HD3	2.46	0.40
1:A:90[B]:THR:HG22	3:A:838:HOH:O	2.22	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	396/408 (97%)	385 (97%)	11 (3%)	0	100	100
1	B	398/408 (98%)	386 (97%)	12 (3%)	0	100	100
1	C	396/408 (97%)	384 (97%)	12 (3%)	0	100	100
1	D	398/408 (98%)	386 (97%)	12 (3%)	0	100	100
All	All	1588/1632 (97%)	1541 (97%)	47 (3%)	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	332/341 (97%)	330 (99%)	2 (1%)	78	67
1	B	334/341 (98%)	333 (100%)	1 (0%)	86	81
1	C	332/341 (97%)	330 (99%)	2 (1%)	78	67
1	D	334/341 (98%)	332 (99%)	2 (1%)	78	67
All	All	1332/1364 (98%)	1325 (100%)	7 (0%)	81	72

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

Mol	Chain	Res	Type
1	A	112	THR
1	A	115	ASP
1	B	112	THR
1	C	112	THR
1	C	322	VAL
1	D	112	THR
1	D	115	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	130	ASN
1	A	151	GLN
1	B	61	GLN
1	C	10	ASN
1	C	144	ASN
1	C	151	GLN
1	C	284	GLN
1	C	401	HIS
1	C	402	HIS
1	D	10	ASN
1	D	61	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	222	1	23,24,25	1.53	4 (17%)	25,32,34	1.04	3 (12%)
1	LLP	D	222	1	23,24,25	1.42	3 (13%)	25,32,34	1.06	2 (8%)
1	LLP	C	222	1	23,24,25	1.47	3 (13%)	25,32,34	1.44	4 (16%)
1	LLP	A	222	1	23,24,25	1.50	3 (13%)	25,32,34	1.19	3 (12%)

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	222	1	-	1/16/17/19	0/1/1/1
1	LLP	D	222	1	-	2/16/17/19	0/1/1/1
1	LLP	C	222	1	-	2/16/17/19	0/1/1/1
1	LLP	A	222	1	-	1/16/17/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	LLP	C4'-NZ	5.00	1.44	1.27
1	A	222	LLP	C4'-NZ	4.92	1.43	1.27
1	C	222	LLP	C4'-NZ	4.91	1.43	1.27
1	D	222	LLP	C4'-NZ	4.86	1.43	1.27
1	B	222	LLP	C4-C4'	2.75	1.51	1.46
1	D	222	LLP	C4-C4'	2.52	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	LLP	C2-N1	2.24	1.38	1.33
1	C	222	LLP	C4-C4'	2.21	1.50	1.46
1	A	222	LLP	C2-N1	2.18	1.38	1.33
1	D	222	LLP	C2-N1	2.17	1.38	1.33
1	C	222	LLP	C2-N1	2.16	1.37	1.33
1	A	222	LLP	C4-C4'	2.11	1.50	1.46
1	B	222	LLP	CE-NZ	2.00	1.51	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	LLP	CE-NZ-C4'	3.83	130.67	118.90
1	C	222	LLP	C2'-C2-C3	2.88	124.45	120.89
1	B	222	LLP	CE-NZ-C4'	2.83	127.60	118.90
1	D	222	LLP	CE-NZ-C4'	2.75	127.35	118.90
1	A	222	LLP	CE-NZ-C4'	2.69	127.15	118.90
1	C	222	LLP	C5-C6-N1	-2.65	119.41	123.82
1	A	222	LLP	C5-C6-N1	-2.62	119.46	123.82
1	B	222	LLP	C5-C6-N1	-2.37	119.88	123.82
1	C	222	LLP	O3-C3-C2	2.36	122.63	117.49
1	D	222	LLP	C5-C6-N1	-2.24	120.09	123.82
1	A	222	LLP	O3-C3-C2	2.20	122.28	117.49
1	B	222	LLP	O3-C3-C2	2.06	121.98	117.49

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	222	LLP	C4-C4'-NZ-CE
1	C	222	LLP	C4-C4'-NZ-CE
1	D	222	LLP	C4-C4'-NZ-CE
1	A	222	LLP	C4-C4'-NZ-CE
1	D	222	LLP	C4-C5-C5'-OP4
1	C	222	LLP	C3-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	222	LLP	1	0
1	A	222	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	396/408 (97%)	-0.07	11 (2%) 55 62	3, 12, 27, 40	2 (0%)
1	B	398/408 (97%)	-0.27	6 (1%) 72 80	3, 10, 27, 47	2 (0%)
1	C	396/408 (97%)	-0.10	9 (2%) 61 68	3, 12, 28, 45	2 (0%)
1	D	398/408 (97%)	-0.25	6 (1%) 72 80	3, 10, 27, 49	2 (0%)
All	All	1588/1632 (97%)	-0.17	32 (2%) 65 73	3, 11, 27, 49	8 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	LEU	5.1
1	A	142	LEU	4.3
1	A	140	SER	4.1
1	B	403	HIS	3.6
1	B	142	LEU	3.3
1	A	141	ASP	3.3
1	C	104	GLN	3.2
1	D	5	SER	3.1
1	C	6	PHE	3.1
1	C	140	SER	3.0
1	C	141	ASP	2.9
1	B	5	SER	2.8
1	D	142	LEU	2.8
1	A	147	LEU	2.8
1	A	281	ASN	2.8
1	C	147	LEU	2.8
1	C	402	HIS	2.6
1	D	403	HIS	2.6
1	D	141	ASP	2.5
1	D	147	LEU	2.5
1	D	281	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	402	HIS	2.3
1	B	158	ASN	2.3
1	B	140	SER	2.3
1	A	6	PHE	2.3
1	A	401	HIS	2.2
1	B	283	LYS	2.2
1	C	284	GLN	2.1
1	C	291	GLU	2.1
1	A	9	GLU	2.0
1	A	104	GLN	2.0
1	A	187	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	222	24/25	0.95	0.07	3,10,12,15	0
1	LLP	C	222	24/25	0.95	0.07	4,9,12,15	0
1	LLP	B	222	24/25	0.96	0.07	3,9,12,13	0
1	LLP	D	222	24/25	0.96	0.07	4,9,12,14	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
2	NA	C	501	1/1	0.87	0.09	22,22,22,22	0
2	NA	A	501	1/1	0.90	0.11	21,21,21,21	0
2	NA	D	501	1/1	0.92	0.12	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	B	501	1/1	0.93	0.10	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.