



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2026 – 09:21 PM JST

PDB ID : 9WPK / pdb_00009wpk
Title : structure of Mycoplasma hyopneumoniae Leucine aminopeptidase
Authors : Rong, C.; Ke, M.; Zehou, L.; Shuijun, Z.; Zhixin, F.
Deposited on : 2025-09-09
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 : 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

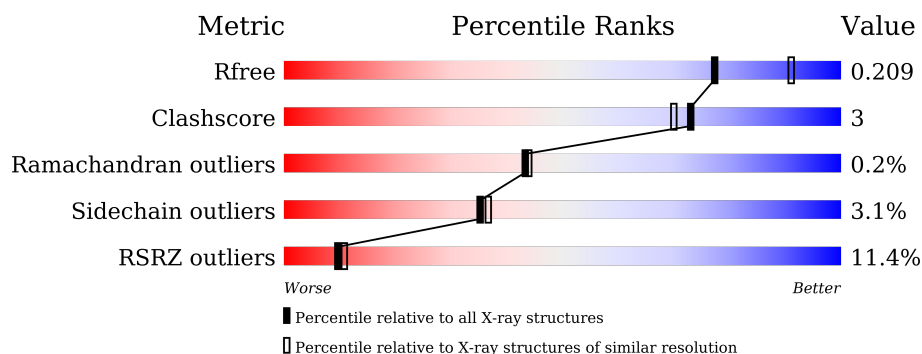
1 Overall quality at a glance

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	467	7% 87% 7% 5%
1	B	467	9% 84% 9% 6%
1	C	467	16% 82% 10% 6%

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
2	FMT	A	604	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10623 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 Probable cytosol aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3487	2223	596	654	14			
1	B	440	Total	C	N	O	S	0	0	0
			3474	2216	593	651	14			
1	C	437	Total	C	N	O	S	0	0	0
			3446	2199	587	647	13			

There are 24 discrepancies between the modelled and reference sequences:

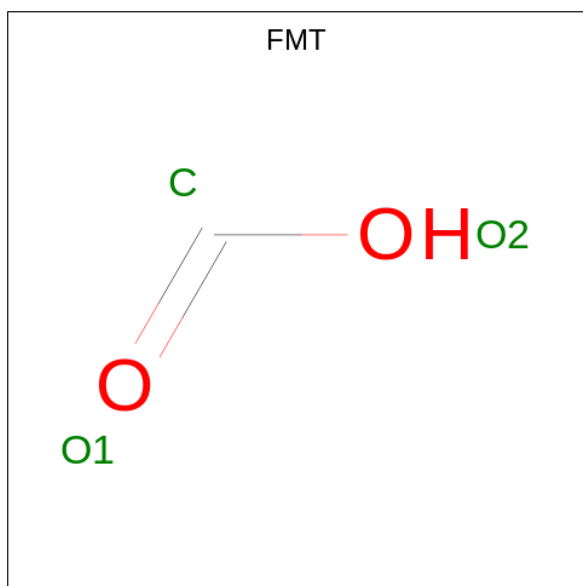
Chain	Residue	Modelled	Actual	Comment	Reference
A	460	LEU	-	expression tag	UNP E4QTC1
A	461	GLU	-	expression tag	UNP E4QTC1
A	462	HIS	-	expression tag	UNP E4QTC1
A	463	HIS	-	expression tag	UNP E4QTC1
A	464	HIS	-	expression tag	UNP E4QTC1
A	465	HIS	-	expression tag	UNP E4QTC1
A	466	HIS	-	expression tag	UNP E4QTC1
A	467	HIS	-	expression tag	UNP E4QTC1
B	460	LEU	-	expression tag	UNP E4QTC1
B	461	GLU	-	expression tag	UNP E4QTC1
B	462	HIS	-	expression tag	UNP E4QTC1
B	463	HIS	-	expression tag	UNP E4QTC1
B	464	HIS	-	expression tag	UNP E4QTC1
B	465	HIS	-	expression tag	UNP E4QTC1
B	466	HIS	-	expression tag	UNP E4QTC1
B	467	HIS	-	expression tag	UNP E4QTC1
C	460	LEU	-	expression tag	UNP E4QTC1
C	461	GLU	-	expression tag	UNP E4QTC1
C	462	HIS	-	expression tag	UNP E4QTC1
C	463	HIS	-	expression tag	UNP E4QTC1
C	464	HIS	-	expression tag	UNP E4QTC1
C	465	HIS	-	expression tag	UNP E4QTC1
C	466	HIS	-	expression tag	UNP E4QTC1

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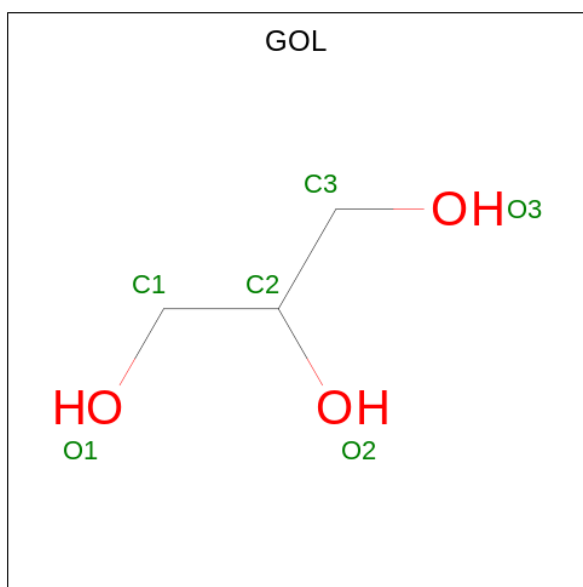
Chain	Residue	Modelled	Actual	Comment	Reference
C	467	HIS	-	expression tag	UNP E4QTC1

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		

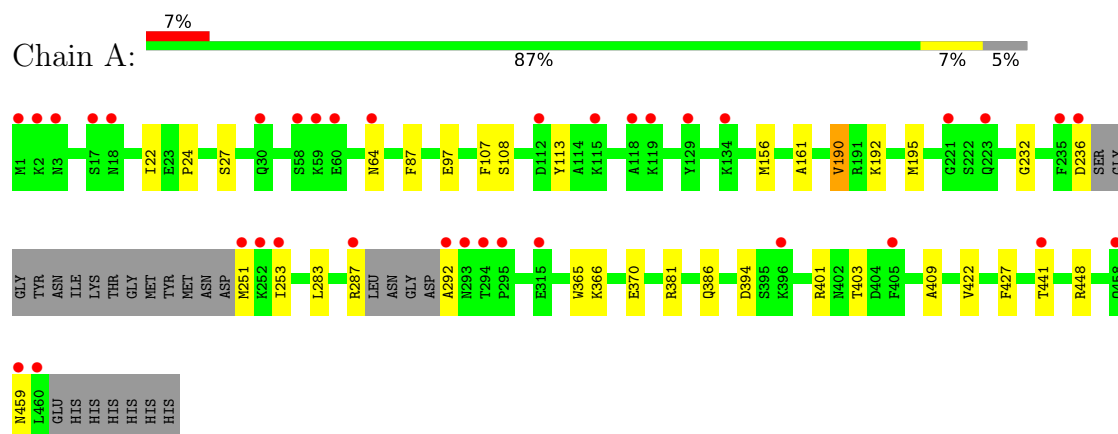
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total	O	0	0
			97	97		
4	B	57	Total	O	0	0
			57	57		
4	C	26	Total	O	0	0
			26	26		

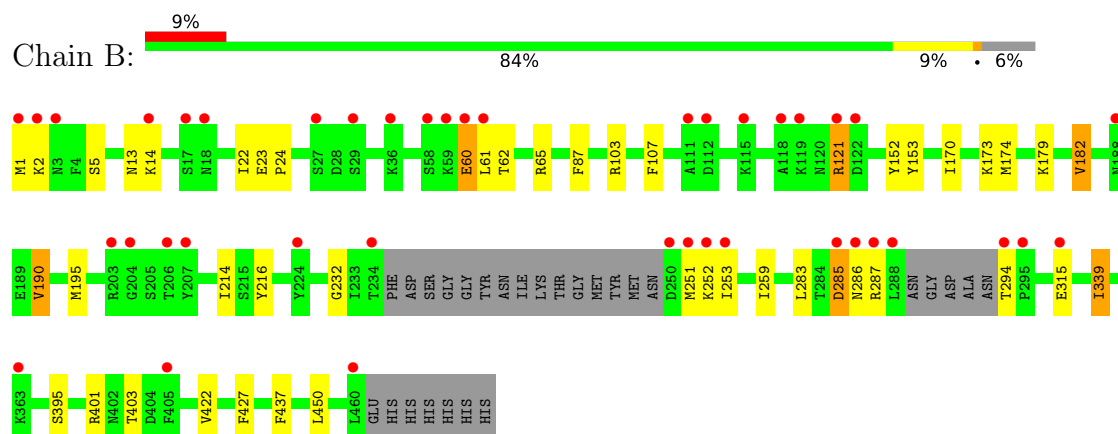
3 Residue-property plots [i](#)

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.

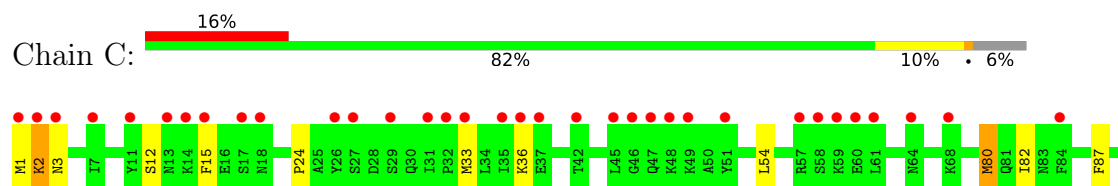
- Molecule 1: Probable cytosol aminopeptidase

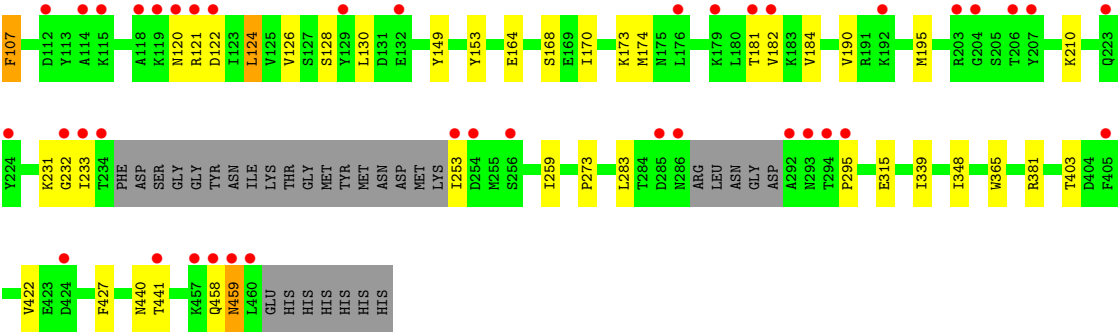


- Molecule 1: Probable cytosol aminopeptidase



- Molecule 1: Probable cytosol aminopeptidase





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	218.72Å 218.72Å 301.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.78 – 2.15 48.78 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.78-2.15) 100.0 (48.78-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.190 , 0.207 0.191 , 0.209	Depositor DCC
R_{free} test set	9798 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.010 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10623	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: FMT, GOL

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	0.14	0/3547	0.35	0/4788
1	B	0.15	0/3534	0.38	0/4770
1	C	0.11	0/3506	0.33	0/4735
All	All	0.14	0/10587	0.36	0/14293

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	287	ARG	Sidechain

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	3487	0	3537	18	0
1	B	3474	0	3526	26	0
1	C	3446	0	3496	26	0
2	A	15	0	5	2	0
2	B	12	0	4	0	0
2	C	3	0	1	0	0
3	C	6	0	8	0	0
4	A	97	0	0	0	0
4	B	57	0	0	0	0
4	C	26	0	0	0	0
All	All	10623	0	10577	68	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 (68) 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:251:MET:HE1	1:C:295:PRO:HD2	1.75	0.69
1:C:315:GLU:OE1	1:C:315:GLU:N	2.21	0.68
1:A:386:GLN:HG2	2:A:604:FMT:H	1.76	0.68
1:B:251:MET:HG2	1:B:252:LYS:H	1.59	0.67
1:A:190:VAL:HG13	1:A:195:MET:HB2	1.75	0.67
1:C:190:VAL:HG13	1:C:195:MET:HB2	1.81	0.63
1:C:15:PHE:CZ	1:C:126:VAL:HG21	2.36	0.61
1:C:2:LYS:HD3	1:C:3:ASN:H	1.69	0.57
1:B:174:MET:HB2	1:B:182:VAL:HG21	1.85	0.57
1:B:190:VAL:HG13	1:B:195:MET:HB2	1.87	0.57
1:B:315:GLU:OE1	1:B:315:GLU:N	2.30	0.57
1:B:285:ASP:OD1	1:B:285:ASP:N	2.39	0.56
1:A:287:ARG:HH12	1:A:292:ALA:HB2	1.73	0.54
1:A:156:MET:HE2	1:A:161:ALA:HB2	1.91	0.52
1:B:232:GLY:HA3	1:B:283:LEU:HD23	1.91	0.51
1:C:232:GLY:HA3	1:C:283:LEU:HD23	1.93	0.51
1:B:13:ASN:OD1	1:B:14:LYS:HE3	2.11	0.50
1:B:286:ASN:HB2	1:B:315:GLU:HG3	1.93	0.50
1:C:149:TYR:CE1	1:C:173:LYS:HG3	2.46	0.49
1:B:24:PRO:HD3	1:B:87:PHE:CE1	2.47	0.49
1:B:395:SER:HB2	1:B:401:ARG:HG3	1.96	0.48
1:C:12:SER:O	1:C:126:VAL:HA	2.14	0.48
1:B:182:VAL:HG13	1:B:214:ILE:HG12	1.96	0.48
1:C:1:MET:SD	1:C:107:PHE:HA	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:SER:HB3	1:C:124:LEU:HD11	1.96	0.47
1:C:459:ASN:OD1	1:C:459:ASN:N	2.48	0.47
1:B:179:LYS:HE3	1:B:216:TYR:HE1	1.79	0.47
1:C:24:PRO:HD3	1:C:87:PHE:CE2	2.49	0.47
1:B:170:ILE:O	1:B:174:MET:HG2	2.15	0.47
1:A:156:MET:HE2	1:A:156:MET:HB3	1.81	0.47
1:B:2:LYS:HE3	1:B:173:LYS:HD3	1.97	0.46
1:A:108:SER:HB3	1:A:113:TYR:CG	2.51	0.46
1:C:121:ARG:HD3	1:C:122:ASP:N	2.31	0.46
1:A:251:MET:HG2	1:A:253:ILE:HG12	1.97	0.45
1:C:231:LYS:HE3	1:C:233:ILE:HG13	1.98	0.45
1:B:60:GLU:HG2	1:B:62:THR:HG22	1.97	0.45
1:B:251:MET:O	1:B:252:LYS:HB3	2.17	0.45
1:C:153:TYR:HB2	1:C:259:ILE:HG12	1.99	0.45
1:A:97:GLU:HG3	1:A:448:ARG:HH21	1.83	0.44
1:C:273:PRO:HA	1:C:458:GLN:OE1	2.17	0.44
1:A:365:TRP:CH2	1:A:381:ARG:HB2	2.52	0.44
1:A:409:ALA:HA	1:C:348:ILE:O	2.18	0.44
1:A:192:LYS:HE3	1:A:192:LYS:HB2	1.61	0.44
1:A:287:ARG:NH1	1:A:292:ALA:HB2	2.32	0.44
1:B:61:LEU:HD23	1:B:65:ARG:HG2	1.99	0.44
1:A:386:GLN:H	2:A:604:FMT:C	2.31	0.43
1:B:339:ILE:HD11	1:B:450:LEU:HD21	2.00	0.43
1:C:33:MET:HE3	1:C:33:MET:HB2	1.81	0.43
1:B:23:GLU:HG2	1:B:24:PRO:HD2	2.00	0.43
1:B:253:ILE:HG21	1:B:437:PHE:HB2	2.00	0.43
1:C:82:ILE:O	1:C:126:VAL:HG22	2.20	0.42
1:B:60:GLU:O	1:B:61:LEU:HB2	2.19	0.42
1:B:1:MET:HE2	1:B:152:TYR:OH	2.19	0.42
1:C:80:MET:HE3	1:C:80:MET:HB3	1.90	0.42
1:C:164:GLU:HG2	1:C:210:LYS:HE3	2.01	0.42
1:B:422:VAL:HG11	1:B:427:PHE:CG	2.55	0.42
1:A:394:ASP:O	1:A:401:ARG:NH1	2.53	0.42
1:C:365:TRP:CH2	1:C:381:ARG:HB2	2.55	0.42
1:C:36:LYS:HB2	1:C:36:LYS:HE2	1.81	0.42
1:A:24:PRO:HD3	1:A:87:PHE:CE1	2.55	0.41
1:B:153:TYR:HB2	1:B:259:ILE:HG12	2.03	0.41
1:C:170:ILE:O	1:C:174:MET:HG2	2.20	0.41
1:A:422:VAL:HG11	1:A:427:PHE:CG	2.56	0.41
1:B:103:ARG:NH1	1:B:121:ARG:O	2.54	0.41
1:C:2:LYS:HD3	1:C:3:ASN:N	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:VAL:HG11	1:C:427:PHE:CG	2.56	0.41
1:A:232:GLY:HA3	1:A:283:LEU:HD23	2.03	0.41
1:A:366:LYS:NZ	1:A:370:GLU:OE2	2.54	0.41

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	436/467 (93%)	425 (98%)	10 (2%)	1 (0%)	43	44
1	B	434/467 (93%)	416 (96%)	17 (4%)	1 (0%)	43	44
1	C	431/467 (92%)	415 (96%)	15 (4%)	1 (0%)	43	44
All	All	1301/1401 (93%)	1256 (96%)	42 (3%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	PHE
1	B	107	PHE
1	C	107	PHE

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	375/397 (94%)	367 (98%)	8 (2%)	47	52
1	B	374/397 (94%)	364 (97%)	10 (3%)	39	41
1	C	371/397 (94%)	354 (95%)	17 (5%)	24	22
All	All	1120/1191 (94%)	1085 (97%)	35 (3%)	35	37

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	27	SER
1	A	64	ASN
1	A	190	VAL
1	A	236	ASP
1	A	403	THR
1	A	441	THR
1	A	459	ASN
1	B	5	SER
1	B	22	ILE
1	B	60	GLU
1	B	121	ARG
1	B	182	VAL
1	B	190	VAL
1	B	285	ASP
1	B	294	THR
1	B	339	ILE
1	B	403	THR
1	C	2	LYS
1	C	54	LEU
1	C	80	MET
1	C	120	ASN
1	C	124	LEU
1	C	128	SER
1	C	130	LEU
1	C	168	SER
1	C	181	THR
1	C	182	VAL
1	C	184	VAL
1	C	253	ILE
1	C	339	ILE
1	C	403	THR
1	C	440	ASN
1	C	441	THR

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Mol	Chain	Res	Type
1	C	459	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	202	ASN
1	A	458	GLN
1	B	47	GLN
1	C	120	ASN
1	C	202	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
3	GOL	C	601	-	5,5,5	0.92	0	5,5,5	0.98	0
2	FMT	B	601	-	2,2,2	0.71	0	1,1,1	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMT	C	602	-	2,2,2	0.74	0	1,1,1	0.25	0
2	FMT	B	603	-	2,2,2	0.71	0	1,1,1	0.22	0
2	FMT	A	603	-	2,2,2	0.71	0	1,1,1	0.23	0
2	FMT	A	604	-	2,2,2	0.73	0	1,1,1	0.22	0
2	FMT	A	601	-	2,2,2	0.71	0	1,1,1	0.23	0
2	FMT	B	602	-	2,2,2	0.73	0	1,1,1	0.24	0
2	FMT	B	604	-	2,2,2	0.72	0	1,1,1	0.23	0
2	FMT	A	602	-	2,2,2	0.72	0	1,1,1	0.22	0
2	FMT	A	605	-	2,2,2	0.73	0	1,1,1	0.25	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
3	GOL	C	601	-	-	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
3	C	601	GOL	O1-C1-C2-C3
3	C	601	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	FMT	2	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

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	442/467 (94%)	0.29	35 (7%)	18 20	44, 56, 92, 125	0
1	B	440/467 (94%)	0.41	41 (9%)	14 16	45, 61, 97, 141	0
1	C	437/467 (93%)	0.91	74 (16%)	4 5	45, 70, 119, 142	0
All	All	1319/1401 (94%)	0.54	150 (11%)	10 11	44, 62, 107, 142	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	LEU	14.6
1	C	405	PHE	10.2
1	C	460	LEU	9.4
1	C	292	ALA	9.2
1	B	460	LEU	8.1
1	A	251	MET	7.7
1	C	1	MET	7.6
1	C	253	ILE	7.6
1	A	235	PHE	7.3
1	A	460	LEU	7.1
1	A	292	ALA	6.8
1	C	2	LYS	6.7
1	A	287	ARG	6.7
1	B	294	THR	6.6
1	B	251	MET	6.5
1	A	1	MET	6.3
1	C	32	PRO	6.2
1	C	293	ASN	6.1
1	B	287	ARG	6.0
1	B	3	ASN	5.9
1	C	59	LYS	5.9
1	A	294	THR	5.7
1	C	206	THR	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	5.6
1	A	293	ASN	5.5
1	B	250	ASP	5.4
1	B	253	ILE	5.1
1	C	203	ARG	5.0
1	C	14	LYS	4.9
1	A	2	LYS	4.7
1	B	2	LYS	4.6
1	C	207	TYR	4.5
1	C	234	THR	4.5
1	C	3	ASN	4.5
1	C	36	LYS	4.3
1	A	295	PRO	4.2
1	C	18	ASN	4.2
1	B	121	ARG	4.1
1	C	286	ASN	4.0
1	C	33	MET	4.0
1	C	17	SER	4.0
1	A	223	GLN	4.0
1	B	252	LYS	4.0
1	A	221	GLY	3.9
1	B	18	ASN	3.9
1	A	236	ASP	3.8
1	C	60	GLU	3.8
1	C	46	GLY	3.7
1	C	224	TYR	3.7
1	B	405	PHE	3.7
1	C	121	ARG	3.6
1	B	122	ASP	3.5
1	C	129	TYR	3.5
1	A	60	GLU	3.5
1	C	51	TYR	3.5
1	C	115	LYS	3.5
1	C	285	ASP	3.4
1	C	223	GLN	3.4
1	C	27	SER	3.4
1	A	112	ASP	3.4
1	C	294	THR	3.4
1	B	286	ASN	3.3
1	B	59	LYS	3.3
1	C	49	LYS	3.2
1	A	405	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	181	THR	3.1
1	A	118	ALA	3.1
1	C	15	PHE	3.1
1	C	295	PRO	3.1
1	C	459	ASN	3.1
1	A	315	GLU	3.1
1	B	285	ASP	3.0
1	C	31	ILE	3.0
1	A	3	ASN	3.0
1	A	17	SER	3.0
1	A	459	ASN	3.0
1	B	234	THR	3.0
1	B	363	LYS	3.0
1	B	203	ARG	2.9
1	C	192	LYS	2.9
1	C	26	TYR	2.9
1	C	119	LYS	2.9
1	C	68	LYS	2.8
1	C	64	ASN	2.8
1	B	111	ALA	2.8
1	A	253	ILE	2.8
1	B	27	SER	2.8
1	C	120	ASN	2.8
1	A	115	LYS	2.8
1	C	424	ASP	2.8
1	A	441	THR	2.8
1	C	61	LEU	2.7
1	B	17	SER	2.7
1	C	233	ILE	2.7
1	C	112	ASP	2.7
1	C	179	LYS	2.7
1	B	207	TYR	2.7
1	C	58	SER	2.7
1	C	256	SER	2.7
1	A	252	LYS	2.6
1	C	118	ALA	2.6
1	B	115	LYS	2.6
1	A	119	LYS	2.6
1	A	58	SER	2.6
1	B	118	ALA	2.6
1	C	441	THR	2.6
1	B	60	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	315	GLU	2.5
1	A	458	GLN	2.5
1	C	458	GLN	2.5
1	A	18	ASN	2.5
1	C	42	THR	2.5
1	C	45	LEU	2.5
1	C	7	ILE	2.5
1	A	396	LYS	2.4
1	C	254	ASP	2.4
1	B	112	ASP	2.4
1	C	48	LYS	2.4
1	A	129	TYR	2.4
1	C	11	TYR	2.4
1	B	295	PRO	2.4
1	C	13	ASN	2.3
1	C	35	ILE	2.3
1	B	224	TYR	2.3
1	B	14	LYS	2.3
1	B	119	LYS	2.3
1	B	204	GLY	2.3
1	A	64	ASN	2.3
1	C	182	VAL	2.2
1	B	61	LEU	2.2
1	C	122	ASP	2.2
1	A	30	GLN	2.2
1	C	29	SER	2.2
1	A	59	LYS	2.2
1	C	47	GLN	2.1
1	B	188	ASN	2.1
1	C	232	GLY	2.1
1	C	457	LYS	2.1
1	C	57	ARG	2.1
1	C	204	GLY	2.1
1	C	84	PHE	2.1
1	A	134	LYS	2.1
1	B	36	LYS	2.1
1	C	114	ALA	2.1
1	B	58	SER	2.1
1	C	176	LEU	2.1
1	B	29	SER	2.1
1	B	206	THR	2.0
1	C	37	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	132	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
3	GOL	C	601	6/6	0.80	0.27	92,98,108,108	0
2	FMT	B	602	3/3	0.82	0.25	93,93,94,100	0
2	FMT	B	603	3/3	0.83	0.28	68,68,89,93	0
2	FMT	B	601	3/3	0.85	0.22	58,58,63,71	0
2	FMT	A	605	3/3	0.86	0.23	67,67,81,95	0
2	FMT	A	602	3/3	0.88	0.22	71,71,78,79	0
2	FMT	A	601	3/3	0.89	0.18	56,56,64,70	0
2	FMT	A	603	3/3	0.90	0.19	74,74,87,88	0
2	FMT	C	602	3/3	0.94	0.15	65,65,70,79	0
2	FMT	A	604	3/3	0.95	0.16	68,68,73,80	0
2	FMT	B	604	3/3	0.95	0.16	57,57,64,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.