



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2026 – 12:34 PM EDT

PDB ID : 9YYS / pdb_00009yys
Title : Crystal Structure of the Poly(Hexamethylene Adipamide) (Nylon66) Hydro-
lase Nyl10 at Cryo Temperature
Authors : Capra, N.; Meilleur, F.
Deposited on : 2025-10-29
Resolution : 1.30 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

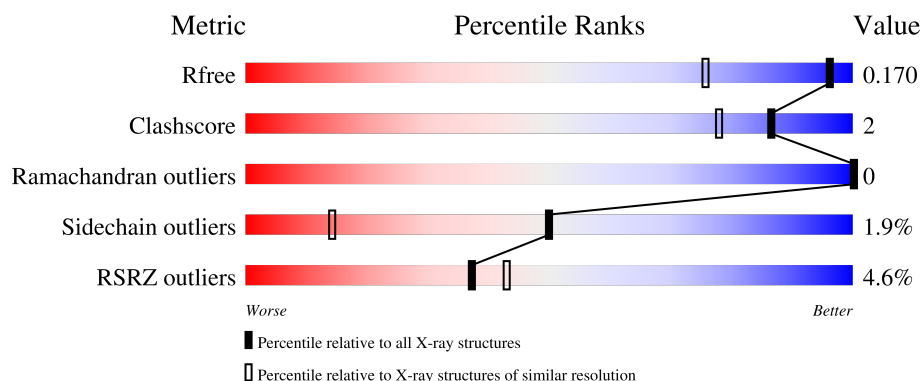
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	285	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>••</div> </div> </div>
1	B	285	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>••</div> </div> </div>
1	C	285	<div> <div>8%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
1	D	285	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>••</div> </div> </div>
1	E	285	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	285	

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	PYR	D	301	-	X	-	-

2 Entry composition [i](#)

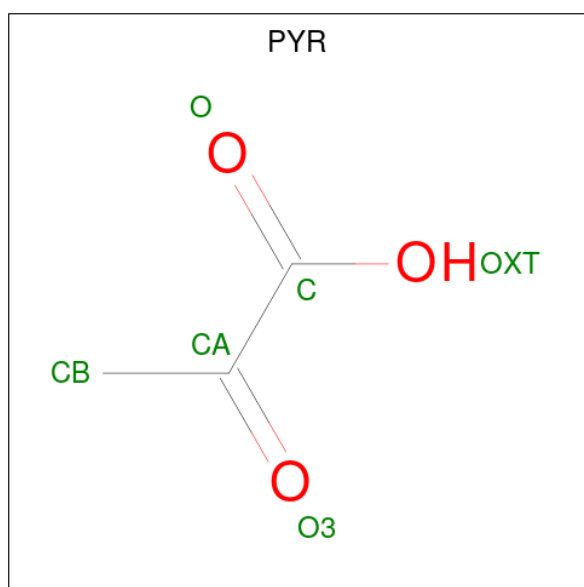
There are 5 unique types of molecules in this entry. The entry contains 12497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-aminopeptidase/D-esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	3	0
			1958	1207	367	378	6			
1	B	273	Total	C	N	O	S	0	3	0
			1952	1205	366	375	6			
1	C	272	Total	C	N	O	S	0	0	0
			1920	1185	359	371	5			
1	D	274	Total	C	N	O	S	0	1	0
			1944	1200	365	374	5			
1	E	273	Total	C	N	O	S	0	3	0
			1946	1202	363	375	6			
1	F	273	Total	C	N	O	S	0	2	0
			1944	1199	365	374	6			

- Molecule 2 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).



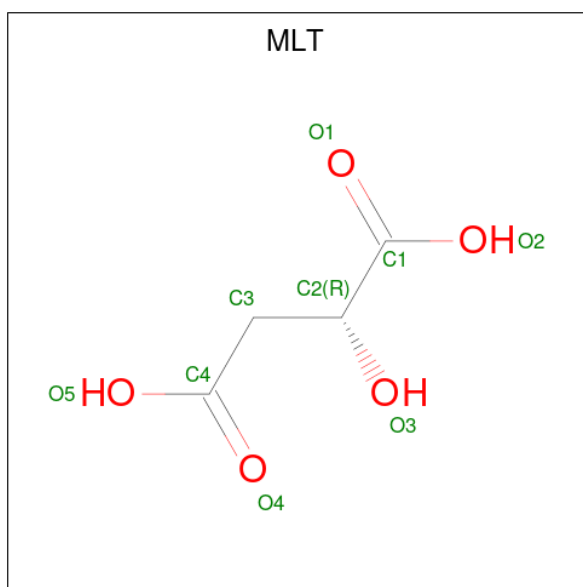
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is D-MALATE (CCD ID: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			9	4	5		

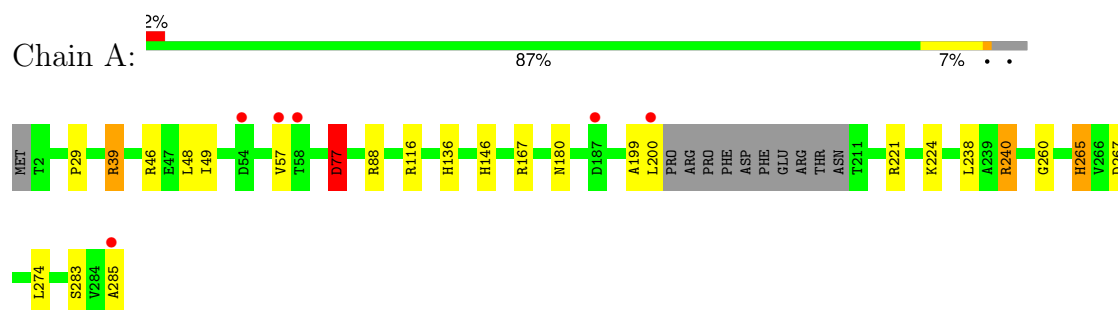
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total	O	0	3
			175	175		
5	B	183	Total	O	0	5
			188	188		
5	C	71	Total	O	0	1
			73	73		
5	D	116	Total	O	0	1
			117	117		
5	E	143	Total	O	0	1
			144	144		
5	F	90	Total	O	0	1
			91	91		

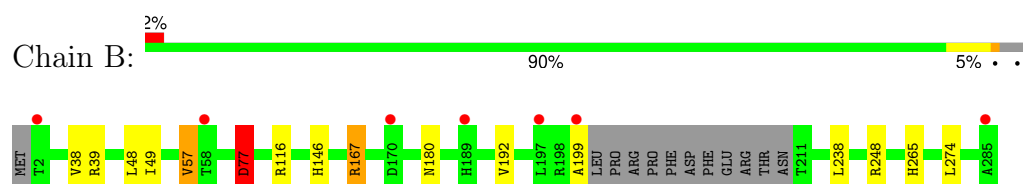
3 Residue-property plots [i](#)

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.

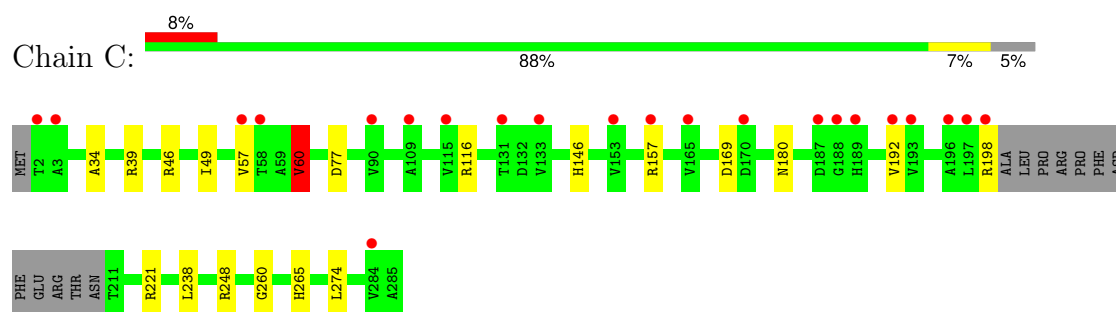
- Molecule 1: L-aminopeptidase/D-esterase



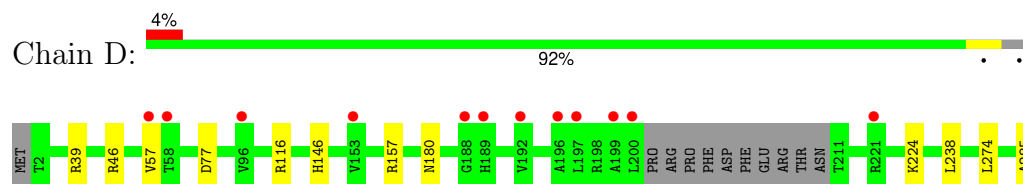
- Molecule 1: L-aminopeptidase/D-esterase



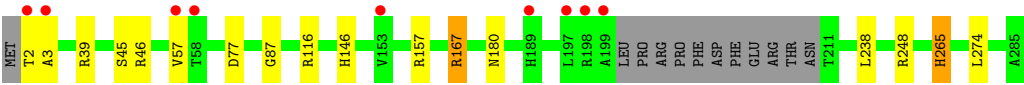
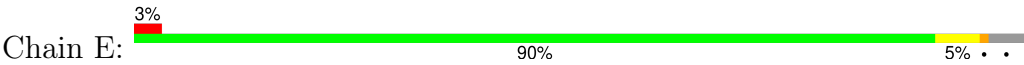
- Molecule 1: L-aminopeptidase/D-esterase



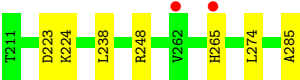
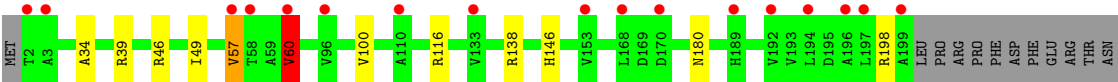
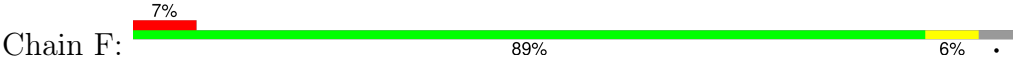
- Molecule 1: L-aminopeptidase/D-esterase



- Molecule 1: L-aminopeptidase/D-esterase



● Molecule 1: L-aminopeptidase/D-esterase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.13Å 120.19Å 148.31Å 90.00° 92.99° 90.00°	Depositor
Resolution (Å)	68.40 – 1.30 68.40 – 1.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (68.40-1.30) 98.0 (68.40-1.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.142 , 0.170 0.143 , 0.170	Depositor DCC
R_{free} test set	17757 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12497	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: PYR, MLT, 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	1.00	2/1987 (0.1%)	1.09	4/2714 (0.1%)
1	B	0.82	1/1981 (0.1%)	1.03	4/2705 (0.1%)
1	C	0.64	0/1949	0.91	4/2663 (0.2%)
1	D	0.67	0/1973	0.89	2/2695 (0.1%)
1	E	0.79	0/1974	1.02	4/2695 (0.1%)
1	F	0.66	0/1973	0.93	4/2694 (0.1%)
All	All	0.77	3/11837 (0.0%)	0.98	22/16166 (0.1%)

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	2
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
All	All	0	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	HIS	CD2-NE2	-6.35	1.30	1.37
1	B	57	VAL	C-O	-5.54	1.18	1.24
1	A	39	ARG	NE-CZ	5.38	1.39	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ASP	CA-CB-CG	10.00	122.60	112.60
1	A	77	ASP	CA-CB-CG	9.67	122.27	112.60
1	A	285	ALA	CA-C-O	-9.13	105.28	120.80
1	D	285	ALA	CA-C-O	-7.61	107.87	120.80
1	F	285	ALA	CA-C-O	-7.50	108.05	120.80
1	E	77	ASP	CA-CB-CG	6.55	119.15	112.60
1	D	77	ASP	CA-CB-CG	6.51	119.11	112.60
1	E	46	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	B	265	HIS	CB-CG-CD2	-6.17	123.19	131.20
1	B	199	ALA	CA-C-O	-5.90	110.77	120.80
1	A	240	ARG	CD-NE-CZ	5.86	132.61	124.40
1	A	240	ARG	CB-CG-CD	-5.83	97.90	111.30
1	F	60	VAL	CB-CA-C	5.57	119.27	110.81
1	C	77	ASP	CB-CA-C	5.56	120.02	110.79
1	C	265	HIS	CB-CG-ND1	5.53	130.99	122.70
1	F	265	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	B	265	HIS	CB-CG-ND1	5.45	130.88	122.70
1	C	265	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	F	223	ASP	CA-CB-CG	5.23	117.83	112.60
1	E	265	HIS	CB-CG-ND1	5.11	130.36	122.70
1	C	60	VAL	CB-CA-C	5.08	118.53	110.81
1	E	167	ARG	CD-NE-CZ	5.07	131.50	124.40

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	ARG	Sidechain
1	A	88	ARG	Sidechain
1	B	167	ARG	Sidechain
1	B	248	ARG	Sidechain
1	B	39	ARG	Sidechain
1	C	157	ARG	Sidechain
1	C	248	ARG	Sidechain
1	C	39	ARG	Sidechain
1	D	157	ARG	Sidechain
1	D	39	ARG	Sidechain
1	D	46[A]	ARG	Sidechain
1	E	157	ARG	Sidechain
1	E	248	ARG	Sidechain
1	E	39	ARG	Sidechain
1	F	138	ARG	Sidechain
1	F	248	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	39	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	1958	0	1938	16	0
1	B	1952	0	1940	9	0
1	C	1920	0	1905	8	0
1	D	1944	0	1933	4	0
1	E	1946	0	1933	8	0
1	F	1944	0	1930	11	0
2	A	6	0	0	1	0
2	D	6	0	0	1	0
2	F	6	0	0	2	0
3	A	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
4	B	9	0	4	0	0
5	A	175	0	0	3	0
5	B	188	0	0	1	0
5	C	73	0	0	1	0
5	D	117	0	0	1	0
5	E	144	0	0	3	0
5	F	91	0	0	2	0
All	All	12497	0	11607	50	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 2.

All (50) 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:D:224:LYS:HE3	5:D:492[B]:HOH:O	1.64	0.97
1:A:265:HIS:HD2	1:A:267:ASP:H	1.14	0.92
1:A:240:ARG:HD2	5:A:510:HOH:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:THR:HG21	5:E:477:HOH:O	1.86	0.76
1:F:224:LYS:HE3	5:F:416:HOH:O	1.87	0.73
1:A:265:HIS:CD2	1:A:267:ASP:H	2.05	0.64
2:A:301:PYR:CB	1:B:49:ILE:H	2.12	0.63
1:E:265:HIS:HB2	5:E:530:HOH:O	1.99	0.62
1:C:49:ILE:H	2:D:301:PYR:CB	2.14	0.60
1:F:224:LYS:CE	5:F:416:HOH:O	2.47	0.58
1:A:49:ILE:HD12	1:B:48:LEU:HD12	1.85	0.57
1:F:49:ILE:H	2:F:301:PYR:CB	2.18	0.56
1:A:49:ILE:HG21	1:B:38:VAL:HG21	1.88	0.55
1:A:199:ALA:O	1:A:200:LEU:CB	2.56	0.52
1:A:224:LYS:HE3	5:A:431:HOH:O	2.12	0.50
1:E:3:ALA:HB1	5:E:528:HOH:O	2.12	0.49
1:B:238:LEU:C	1:B:238:LEU:HD23	2.37	0.49
1:C:192:VAL:HG23	5:C:362:HOH:O	2.12	0.49
1:E:238:LEU:C	1:E:238:LEU:HD23	2.37	0.49
1:F:34:ALA:HB3	1:F:60:VAL:HG13	1.94	0.48
1:A:29:PRO:HB3	1:E:87:GLY:HA3	1.94	0.48
1:F:238:LEU:C	1:F:238:LEU:HD23	2.38	0.48
1:C:169:ASP:OD2	1:F:198:ARG:NH1	2.42	0.48
1:C:238:LEU:C	1:C:238:LEU:HD23	2.39	0.47
1:D:238:LEU:C	1:D:238:LEU:HD23	2.38	0.47
1:F:34:ALA:HB3	1:F:60:VAL:CG1	2.44	0.46
1:A:48:LEU:HD12	1:B:49:ILE:HD12	1.98	0.46
1:A:146:HIS:O	1:A:180:ASN:HA	2.16	0.45
1:C:274:LEU:C	1:C:274:LEU:HD23	2.42	0.45
1:C:146:HIS:O	1:C:180:ASN:HA	2.17	0.44
1:A:167:ARG:NH2	5:A:403:HOH:O	2.42	0.43
1:D:146:HIS:O	1:D:180:ASN:HA	2.19	0.43
1:B:192:VAL:HG23	5:B:552:HOH:O	2.17	0.43
1:A:136:HIS:HE1	1:A:283:SER:O	2.00	0.43
1:D:274:LEU:HD23	1:D:274:LEU:C	2.44	0.43
1:E:274:LEU:C	1:E:274:LEU:HD23	2.43	0.43
1:A:221:ARG:HA	1:A:260:GLY:HA2	2.00	0.43
1:B:274:LEU:C	1:B:274:LEU:HD23	2.44	0.43
1:F:146:HIS:O	1:F:180:ASN:HA	2.19	0.43
1:A:238:LEU:C	1:A:238:LEU:HD23	2.43	0.42
1:F:57:VAL:O	1:F:224:LYS:NZ	2.47	0.42
1:B:146:HIS:O	1:B:180:ASN:HA	2.18	0.42
1:C:34:ALA:HB3	1:C:60:VAL:CG1	2.50	0.42
1:E:146:HIS:O	1:E:180:ASN:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:LEU:C	1:F:274:LEU:HD23	2.46	0.41
1:E:45:SER:OG	2:F:301:PYP:CB	2.68	0.41
1:A:274:LEU:C	1:A:274:LEU:HD23	2.46	0.41
1:F:46[B]:ARG:NH1	1:F:100:VAL:O	2.54	0.40
1:A:77:ASP:OD2	1:B:77:ASP:OD2	2.39	0.40
1:C:221:ARG:HA	1:C:260:GLY:HA2	2.03	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	273/285 (96%)	267 (98%)	6 (2%)	0	100	100
1	B	272/285 (95%)	266 (98%)	6 (2%)	0	100	100
1	C	268/285 (94%)	261 (97%)	7 (3%)	0	100	100
1	D	271/285 (95%)	265 (98%)	6 (2%)	0	100	100
1	E	271/285 (95%)	265 (98%)	6 (2%)	0	100	100
1	F	271/285 (95%)	265 (98%)	6 (2%)	0	100	100
All	All	1626/1710 (95%)	1589 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	189/198 (96%)	184 (97%)	5 (3%)	40	7
1	B	189/198 (96%)	185 (98%)	4 (2%)	47	11
1	C	186/198 (94%)	181 (97%)	5 (3%)	39	7
1	D	188/198 (95%)	186 (99%)	2 (1%)	65	33
1	E	188/198 (95%)	185 (98%)	3 (2%)	55	19
1	F	188/198 (95%)	185 (98%)	3 (2%)	55	19
All	All	1128/1188 (95%)	1106 (98%)	22 (2%)	50	12

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46[A]	ARG
1	A	46[B]	ARG
1	A	57	VAL
1	A	77	ASP
1	A	116	ARG
1	B	57	VAL
1	B	77	ASP
1	B	116	ARG
1	B	167	ARG
1	C	46	ARG
1	C	57	VAL
1	C	60	VAL
1	C	116	ARG
1	C	198	ARG
1	D	57	VAL
1	D	116	ARG
1	E	57	VAL
1	E	116	ARG
1	E	167	ARG
1	F	57	VAL
1	F	60	VAL
1	F	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
1	A	189	HIS
1	A	265	HIS

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Mol	Chain	Res	Type
1	C	136	HIS
1	C	146	HIS
1	C	189	HIS
1	D	136	HIS

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](#)

7 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	PYR	A	301	-	5,5,5	3.79	3 (60%)	3,6,6	0.94	0
3	GOL	E	301	-	5,5,5	0.21	0	5,5,5	1.32	1 (20%)
2	PYR	F	301	-	5,5,5	4.19	2 (40%)	3,6,6	0.52	0
3	GOL	A	302	-	5,5,5	0.13	0	5,5,5	0.25	0
4	MLT	B	301	-	8,8,8	1.37	1 (12%)	10,10,10	1.65	3 (30%)
3	GOL	D	302	-	5,5,5	0.17	0	5,5,5	0.53	0
2	PYR	D	301	-	5,5,5	4.08	3 (60%)	3,6,6	1.54	1 (33%)

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	PYR	A	301	-	-	1/4/4/4	-
3	GOL	E	301	-	-	3/4/4/4	-
2	PYR	F	301	-	-	0/4/4/4	-
3	GOL	A	302	-	-	0/4/4/4	-
4	MLT	B	301	-	-	6/8/8/8	-
3	GOL	D	302	-	-	0/4/4/4	-
2	PYR	D	301	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	PYR	CA-C	-8.11	1.27	1.54
2	D	301	PYR	CA-C	-8.02	1.27	1.54
2	A	301	PYR	CA-C	-6.44	1.33	1.54
2	A	301	PYR	OXT-C	-4.60	1.18	1.30
2	F	301	PYR	OXT-C	-4.24	1.19	1.30
2	D	301	PYR	OXT-C	-3.76	1.20	1.30
2	A	301	PYR	O3-CA	-2.79	1.16	1.23
4	B	301	MLT	O3-C2	-2.35	1.37	1.42
2	D	301	PYR	O3-CA	-2.06	1.18	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	MLT	O5-C4-C3	2.68	122.34	114.00
4	B	301	MLT	O4-C4-C3	-2.64	114.72	122.84
4	B	301	MLT	O1-C1-C2	-2.27	118.05	122.60
3	E	301	GOL	O1-C1-C2	2.21	120.33	110.38
2	D	301	PYR	OXT-C-CA	2.10	119.40	113.59

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	PYR	O-C-CA-CB
3	E	301	GOL	O2-C2-C3-O3
3	E	301	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	301	MLT	O1-C1-C2-C3
4	B	301	MLT	O2-C1-C2-C3
3	E	301	GOL	O1-C1-C2-O2
2	D	301	PYR	O-C-CA-CB
2	D	301	PYR	OXT-C-CA-CB
4	B	301	MLT	C2-C3-C4-O4
4	B	301	MLT	O2-C1-C2-O3
4	B	301	MLT	C2-C3-C4-O5
4	B	301	MLT	O1-C1-C2-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PYR	1	0
2	F	301	PYR	2	0
2	D	301	PYR	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 ⓘ

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	274/285 (96%)	-0.20	6 (2%)	62	67	7, 15, 30, 49	3 (1%)
1	B	273/285 (95%)	-0.22	7 (2%)	57	63	7, 15, 30, 47	3 (1%)
1	C	272/285 (95%)	0.76	22 (8%)	18	20	19, 29, 48, 66	0
1	D	274/285 (96%)	0.31	12 (4%)	39	44	13, 23, 39, 60	1 (0%)
1	E	273/285 (95%)	-0.10	9 (3%)	49	55	9, 18, 34, 60	3 (1%)
1	F	273/285 (95%)	0.56	19 (6%)	22	26	11, 25, 42, 58	2 (0%)
All	All	1639/1710 (95%)	0.18	75 (4%)	37	43	7, 21, 41, 66	12 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	THR	6.2
1	F	2	THR	5.7
1	C	197	LEU	4.5
1	C	192	VAL	4.5
1	A	200	LEU	4.4
1	F	199	ALA	4.4
1	C	153	VAL	4.3
1	E	2	THR	4.1
1	C	193	VAL	4.0
1	B	58	THR	4.0
1	E	199	ALA	3.8
1	D	200	LEU	3.6
1	C	188	GLY	3.6
1	D	188	GLY	3.5
1	C	196	ALA	3.5
1	F	196	ALA	3.5
1	A	57	VAL	3.3
1	C	3	ALA	3.2
1	D	199	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	189	HIS	3.2
1	D	58	THR	3.1
1	F	153	VAL	3.1
1	D	197	LEU	3.1
1	C	198	ARG	3.1
1	C	131	THR	3.0
1	C	133	VAL	3.0
1	D	189	HIS	3.0
1	A	187	ASP	3.0
1	B	285	ALA	2.9
1	E	197	LEU	2.9
1	A	58	THR	2.9
1	D	153	VAL	2.8
1	A	54	ASP	2.8
1	E	189	HIS	2.7
1	F	57	VAL	2.7
1	F	192	VAL	2.7
1	F	189	HIS	2.7
1	B	199	ALA	2.6
1	F	58	THR	2.6
1	F	197	LEU	2.6
1	F	170	ASP	2.5
1	B	2	THR	2.5
1	C	58	THR	2.5
1	C	170	ASP	2.5
1	C	189	HIS	2.5
1	E	198	ARG	2.5
1	F	262	VAL	2.5
1	D	196	ALA	2.4
1	E	3	ALA	2.4
1	C	187	ASP	2.4
1	B	197	LEU	2.3
1	C	57	VAL	2.3
1	F	96	VAL	2.3
1	F	133	VAL	2.3
1	C	109	ALA	2.3
1	C	115	VAL	2.2
1	C	165	VAL	2.2
1	D	57	VAL	2.2
1	E	153	VAL	2.2
1	F	60	VAL	2.2
1	C	90	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	170	ASP	2.1
1	C	284	VAL	2.1
1	F	168	LEU	2.1
1	E	58	THR	2.1
1	F	110	ALA	2.1
1	E	57	VAL	2.1
1	C	157	ARG	2.1
1	F	194	LEU	2.1
1	F	265	HIS	2.1
1	A	285	ALA	2.1
1	F	3	ALA	2.1
1	D	96	VAL	2.1
1	D	221	ARG	2.0
1	D	192	VAL	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(\AA^2)	Q<0.9
3	GOL	A	302	6/6	0.92	0.11	33,38,42,45	0
2	PYR	D	301	6/6	0.93	0.09	28,31,34,39	0
3	GOL	D	302	6/6	0.93	0.10	22,31,33,39	0
3	GOL	E	301	6/6	0.93	0.11	17,28,33,44	0
2	PYR	F	301	6/6	0.96	0.09	25,30,31,36	0
2	PYR	A	301	6/6	0.97	0.06	17,21,25,28	0
4	MLT	B	301	9/9	0.97	0.06	17,20,25,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.