



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:03 AM GMT

PDB ID : 2P6G
Title : Crystal structures of *Saccharomyces cerevisiae* N-myristoyltransferase with bound myristoyl-CoA and inhibitors
Authors : Wu, J.; Ding, J.
Deposited on : 2007-03-18
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

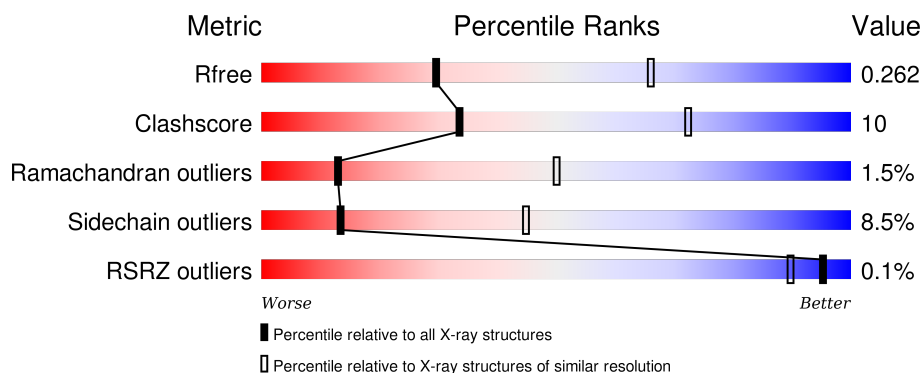
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	455	 71% 22% . .
1	B	455	 69% 23% . .
1	C	455	 66% 26% . .
1	D	455	 70% 23% . .
1	E	455	 68% 23% . .

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Mol	Chain	Length	Quality of chain
1	F	455	 69% 22% . .

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	MYA	A	601	X	-	-	-
2	MYA	B	602	X	-	-	-
2	MYA	C	603	X	-	-	-
2	MYA	D	604	X	-	-	-
2	MYA	E	605	X	-	-	-
2	MYA	F	606	X	-	-	-
3	3LP	C	703	-	-	-	X
3	3LP	F	706	-	-	X	X

2 Entry composition [i](#)

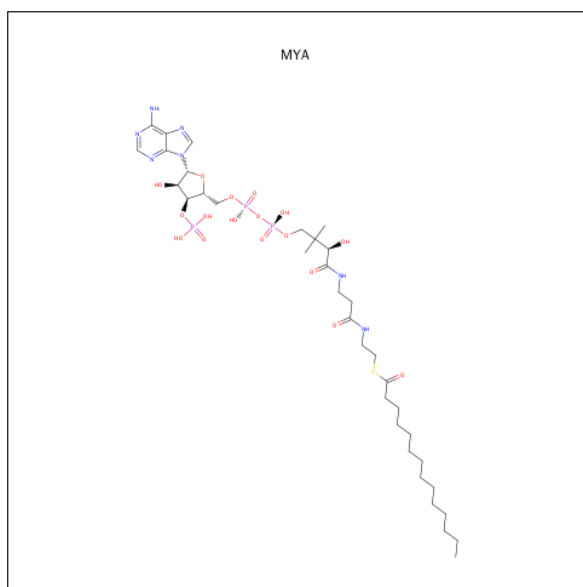
There are 3 unique types of molecules in this entry. The entry contains 21848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycylpeptide N-tetradecanoyltransferase.

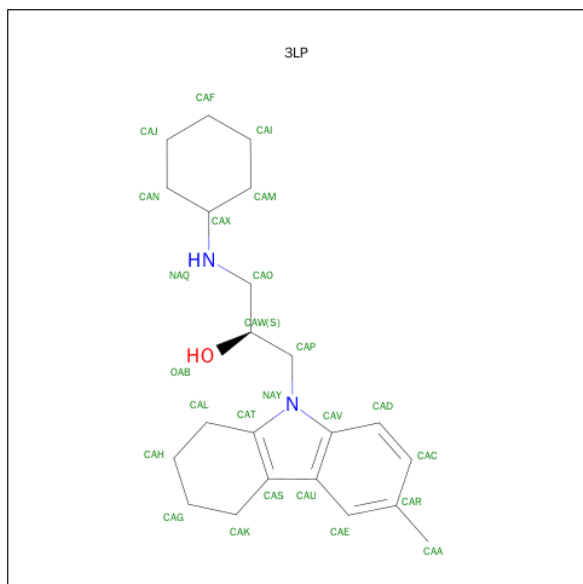
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			
1	B	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			
1	C	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			
1	D	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			
1	E	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			
1	F	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			

- Molecule 2 is TETRADECANOYL-COA (three-letter code: MYA) (formula: $C_{35}H_{62}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

- Molecule 3 is 1-(CYCLOHEXYLAMINO)-3-(6-METHYL-3,4-DIHYDRO-1H-CARBAZOL-9(2H)-YL)PROPAN-2-OL (three-letter code: 3LP) (formula: C₂₂H₃₂N₂O).

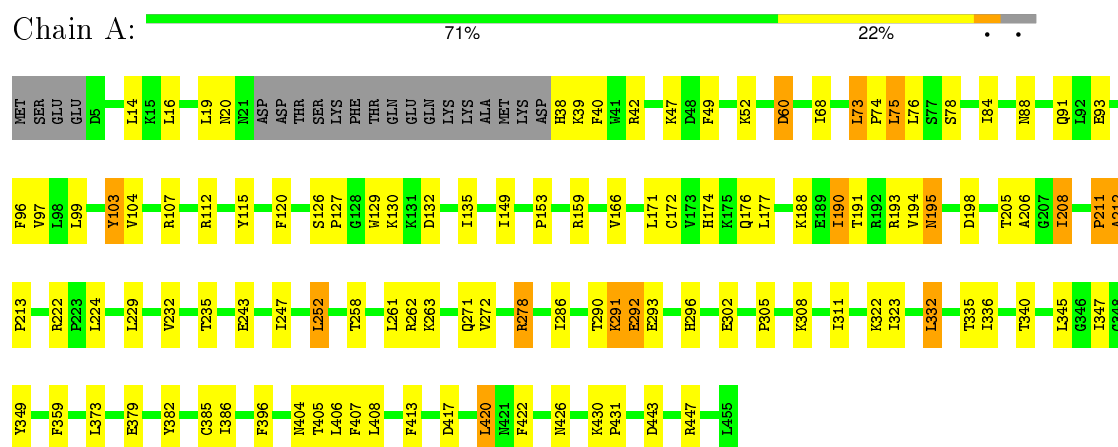


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			25	22	2	1		
3	F	1	Total	C	N	O	0	0
			25	22	2	1		

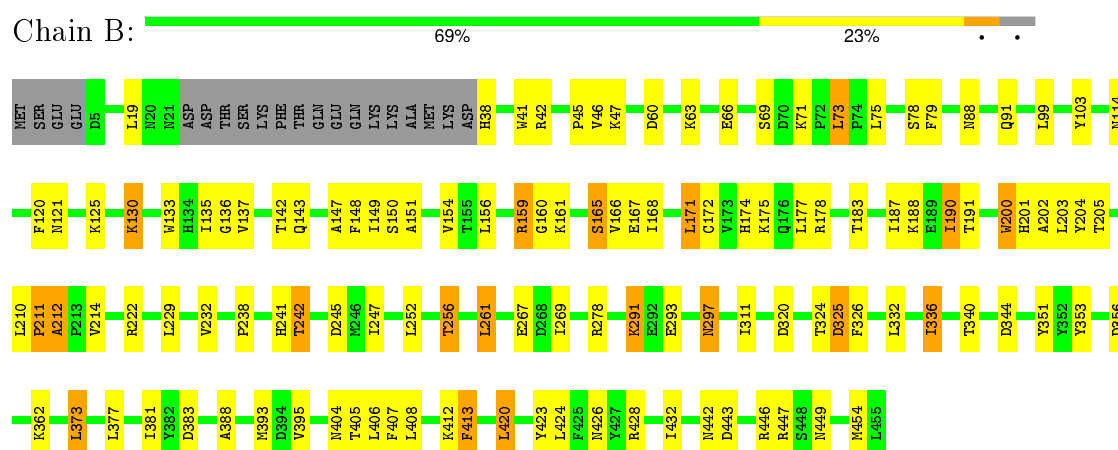
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

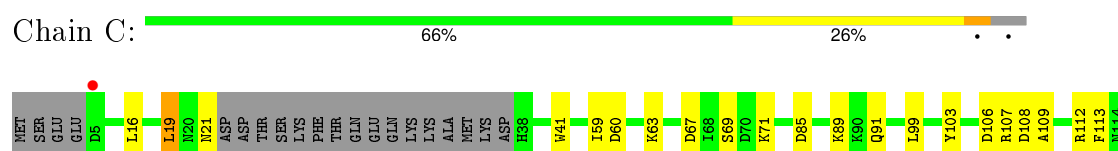
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

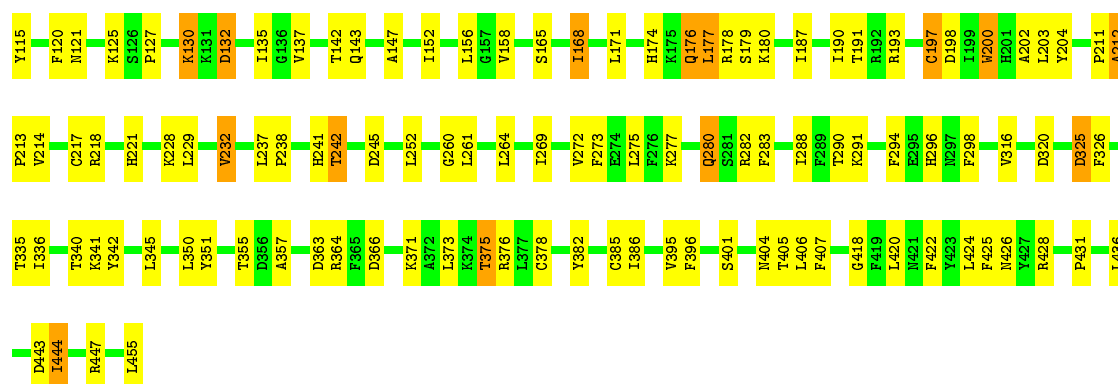


• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



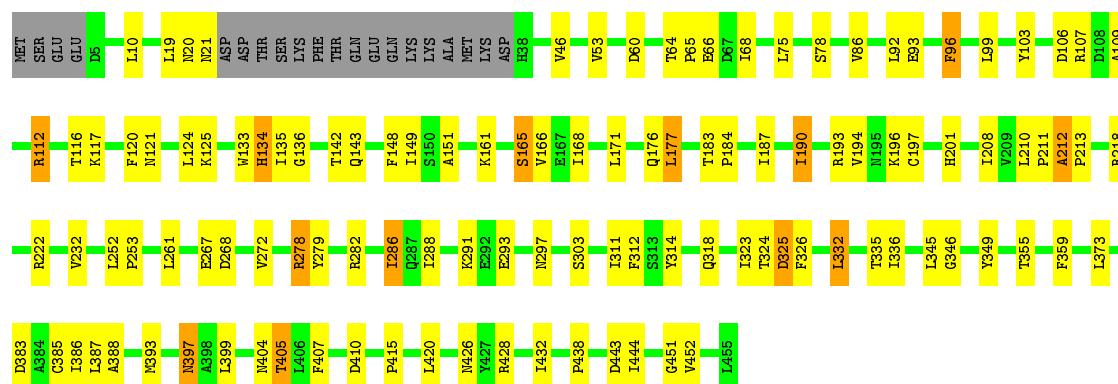
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase





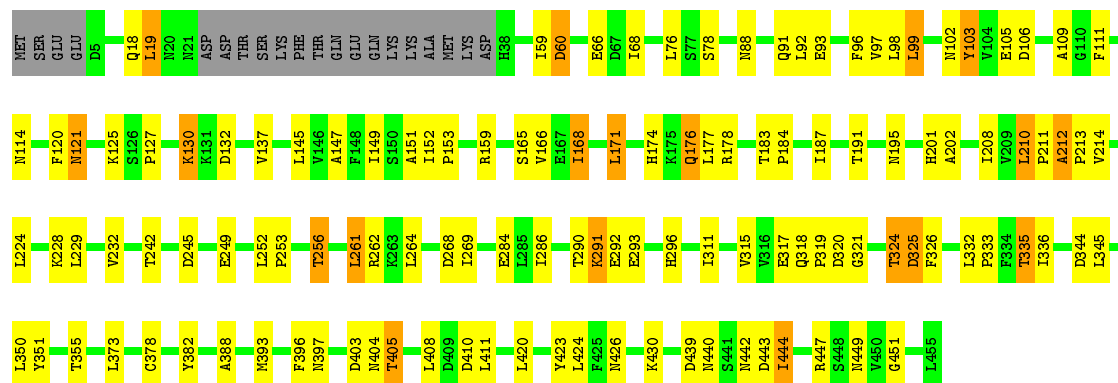
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain D: 70% 23%



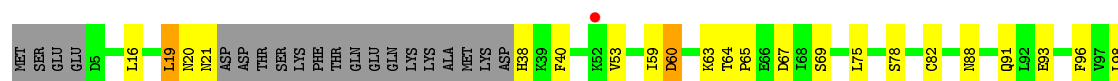
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain E: 68% 23%



• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain F: 69% 22%



D356	L229	L99	D357	V232	Y103	D358	L237	Y104	E105	R112	K117	N121	K130	L145	F148	I152	L156	G157	V158	R159	G160	S165	L171	H174	K175	Q176	L177	K180	T183	K188	E189	I190	V194	N200	L203	Y204	T205	P211	A212	Y219	R222	P223	L224	Y351																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
R364	L238	L239	E241	G240	H241	L252	R262	V272	R278	R282	L285	L286	Q287	L288	K291	E292	E293	N297	E301	L304	P305	K308	I311	V315	V316	E317	K322	I323	T324	K325	F326	P333	T340	K341	L345	G346	I347																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
T375	C378	Y382	C385	I386	N392	F396	Q402	D403	N404	T405	L406	F407	K412	D417	G418	F419	L420	N421	N426	Y427	R428	N442	G451	V452	L455																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.85Å 151.30Å 134.19Å 90.00° 107.64° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 14.98 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-3.00) 97.7 (14.98-2.99)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.260 , 0.318 0.262 , 0.262	Depositor DCC
R_{free} test set	3526 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 16.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	4 of 70172 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	21848	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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 43.51 % 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 1.7446e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MYA, 3LP

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	0.34	0/3658	0.54	0/4946
1	B	0.34	0/3658	0.53	0/4946
1	C	0.34	0/3658	0.52	0/4946
1	D	0.34	0/3658	0.52	0/4946
1	E	0.34	0/3658	0.53	0/4946
1	F	0.34	0/3658	0.53	0/4946
All	All	0.34	0/21948	0.53	0/29676

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	PRO	Peptide

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	3570	0	3569	68	0
1	B	3570	0	3569	79	0
1	C	3570	0	3569	75	0
1	D	3570	0	3569	70	0
1	E	3570	0	3569	80	0
1	F	3570	0	3569	81	0
2	A	63	0	58	3	0
2	B	63	0	58	11	0
2	C	63	0	58	5	0
2	D	63	0	58	3	0
2	E	63	0	58	9	0
2	F	63	0	58	4	0
3	C	25	0	32	4	0
3	F	25	0	32	10	0
All	All	21848	0	21826	447	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 10.

The worst 5 of 447 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:112:ARG:HH11	1:D:112:ARG:HG2	1.09	1.11
1:D:212:ALA:H	1:D:213:PRO:HD3	1.18	1.02
1:D:60:ASP:H	1:D:426:ASN:HD21	1.21	0.87
1:A:127:PRO:HG2	1:A:293:GLU:HA	1.56	0.85
1:D:212:ALA:N	1:D:213:PRO:HD3	1.89	0.85

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	431/455 (95%)	381 (88%)	45 (10%)	5 (1%)	16	56
1	B	431/455 (95%)	399 (93%)	23 (5%)	9 (2%)	9	40
1	C	431/455 (95%)	378 (88%)	47 (11%)	6 (1%)	14	51
1	D	431/455 (95%)	384 (89%)	41 (10%)	6 (1%)	14	51
1	E	431/455 (95%)	380 (88%)	44 (10%)	7 (2%)	12	48
1	F	431/455 (95%)	387 (90%)	39 (9%)	5 (1%)	16	56
All	All	2586/2730 (95%)	2309 (89%)	239 (9%)	38 (2%)	13	50

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ALA
1	D	212	ALA
1	E	78	SER
1	E	212	ALA
1	F	69	SER

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	393/413 (95%)	362 (92%)	31 (8%)	15	48
1	B	393/413 (95%)	359 (91%)	34 (9%)	13	43
1	C	393/413 (95%)	363 (92%)	30 (8%)	16	51
1	D	393/413 (95%)	357 (91%)	36 (9%)	11	40
1	E	393/413 (95%)	356 (91%)	37 (9%)	11	39
1	F	393/413 (95%)	361 (92%)	32 (8%)	15	47
All	All	2358/2478 (95%)	2158 (92%)	200 (8%)	13	45

5 of 200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	351	TYR

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Mol	Chain	Res	Type
1	D	208	ILE
1	F	291	LYS
1	C	420	LEU
1	D	112	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	114	ASN
1	D	18	GLN
1	F	404	ASN
1	C	397	ASN
1	D	176	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	MYA	A	601	-	53,65,65	0.75	2 (3%)	65,91,91	1.92	7 (10%)
2	MYA	B	602	-	53,65,65	0.71	1 (1%)	65,91,91	1.84	10 (15%)
2	MYA	C	603	-	53,65,65	0.71	1 (1%)	65,91,91	1.86	10 (15%)
3	3LP	C	703	-	25,28,28	0.78	0	25,39,39	1.25	5 (20%)
2	MYA	D	604	-	53,65,65	0.73	1 (1%)	65,91,91	1.93	9 (13%)
2	MYA	E	605	-	53,65,65	0.71	1 (1%)	65,91,91	1.84	7 (10%)
2	MYA	F	606	-	53,65,65	0.73	2 (3%)	65,91,91	1.93	8 (12%)
3	3LP	F	706	-	25,28,28	0.81	1 (4%)	25,39,39	1.38	6 (24%)

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	MYA	A	601	-	1/1/12/14	0/59/80/80	0/3/3/3
2	MYA	B	602	-	1/1/12/14	0/59/80/80	0/3/3/3
2	MYA	C	603	-	1/1/12/14	0/59/80/80	0/3/3/3
3	3LP	C	703	-	-	0/7/24/24	0/4/4/4
2	MYA	D	604	-	1/1/12/14	0/59/80/80	0/3/3/3
2	MYA	E	605	-	1/1/12/14	0/59/80/80	0/3/3/3
2	MYA	F	606	-	1/1/12/14	0/59/80/80	0/3/3/3
3	3LP	F	706	-	-	0/7/24/24	0/4/4/4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	MYA	C2-S1	-3.57	1.76	1.81
2	E	605	MYA	C2-S1	-3.45	1.76	1.81
2	D	604	MYA	C2-S1	-3.43	1.76	1.81
2	F	606	MYA	C2-S1	-3.23	1.77	1.81
2	C	603	MYA	C2-S1	-3.20	1.77	1.81

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	606	MYA	N3A-C2A-N1A	-10.45	120.89	128.89
2	A	601	MYA	N3A-C2A-N1A	-10.40	120.93	128.89
2	E	605	MYA	N3A-C2A-N1A	-10.30	121.00	128.89
2	C	603	MYA	N3A-C2A-N1A	-10.28	121.02	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	MYA	N3A-C2A-N1A	-10.03	121.22	128.89

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	604	MYA	C10
2	C	603	MYA	C10
2	A	601	MYA	C10
2	F	606	MYA	C10
2	E	605	MYA	C10

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	MYA	3	0
2	B	602	MYA	11	0
2	C	603	MYA	5	0
3	C	703	3LP	4	0
2	D	604	MYA	3	0
2	E	605	MYA	9	0
2	F	606	MYA	4	0
3	F	706	3LP	10	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	435/455 (95%)	-0.61	0	100	100	11, 30, 58, 80	0
1	B	435/455 (95%)	-0.68	0	100	100	11, 24, 47, 81	0
1	C	435/455 (95%)	-0.40	1 (0%)	95	87	13, 40, 77, 95	0
1	D	435/455 (95%)	-0.58	0	100	100	12, 29, 59, 82	0
1	E	435/455 (95%)	-0.64	0	100	100	11, 26, 54, 79	0
1	F	435/455 (95%)	-0.47	1 (0%)	95	87	11, 36, 77, 93	0
All	All	2610/2730 (95%)	-0.56	2 (0%)	95	90	11, 30, 73, 95	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	ASP	2.5
1	F	52	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	3LP	C	703	25/25	0.74	0.38	6.12	71,72,73,74	0
3	3LP	F	706	25/25	0.73	0.35	4.70	71,72,73,74	0
2	MYA	F	606	63/63	0.91	0.20	-0.14	39,40,51,52	0
2	MYA	E	605	63/63	0.95	0.13	-0.35	16,31,36,36	0
2	MYA	B	602	63/63	0.95	0.14	-0.50	23,26,28,28	0
2	MYA	C	603	63/63	0.93	0.16	-0.55	41,43,49,49	0
2	MYA	A	601	63/63	0.95	0.14	-0.60	25,38,44,44	0
2	MYA	D	604	63/63	0.95	0.13	-0.83	18,30,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.