



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:17 PM UTC

PDB ID : 1RXT / pdb_00001rxt
Title : Crystal structure of human myristoyl-CoA:protein N-myristoyltransferase.
Authors : Yang, J.; Wang, Y.; Frey, G.; Abeles, R.H.; Petsko, G.A.; Ringe, D.
Deposited on : 2003-12-18
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

<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

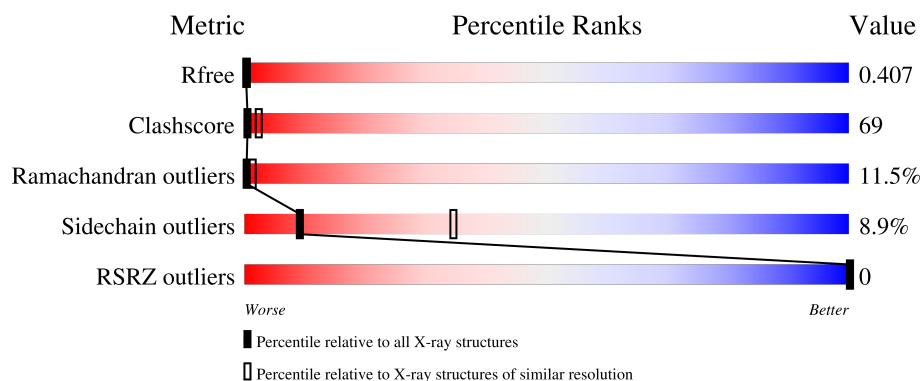
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	496	
1	B	496	
1	C	496	
1	D	496	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10420 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2646	1724	439	471	12			
1	B	342	Total	C	N	O	S	0	0	0
			2640	1718	438	472	12			
1	C	325	Total	C	N	O	S	0	0	0
			2538	1652	424	450	12			
1	D	326	Total	C	N	O	S	0	0	0
			2523	1642	418	451	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	ILE	LEU	conflict	UNP P30419
B	452	ILE	LEU	conflict	UNP P30419
C	452	ILE	LEU	conflict	UNP P30419
D	452	ILE	LEU	conflict	UNP P30419

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Co	0	0
			1	1		

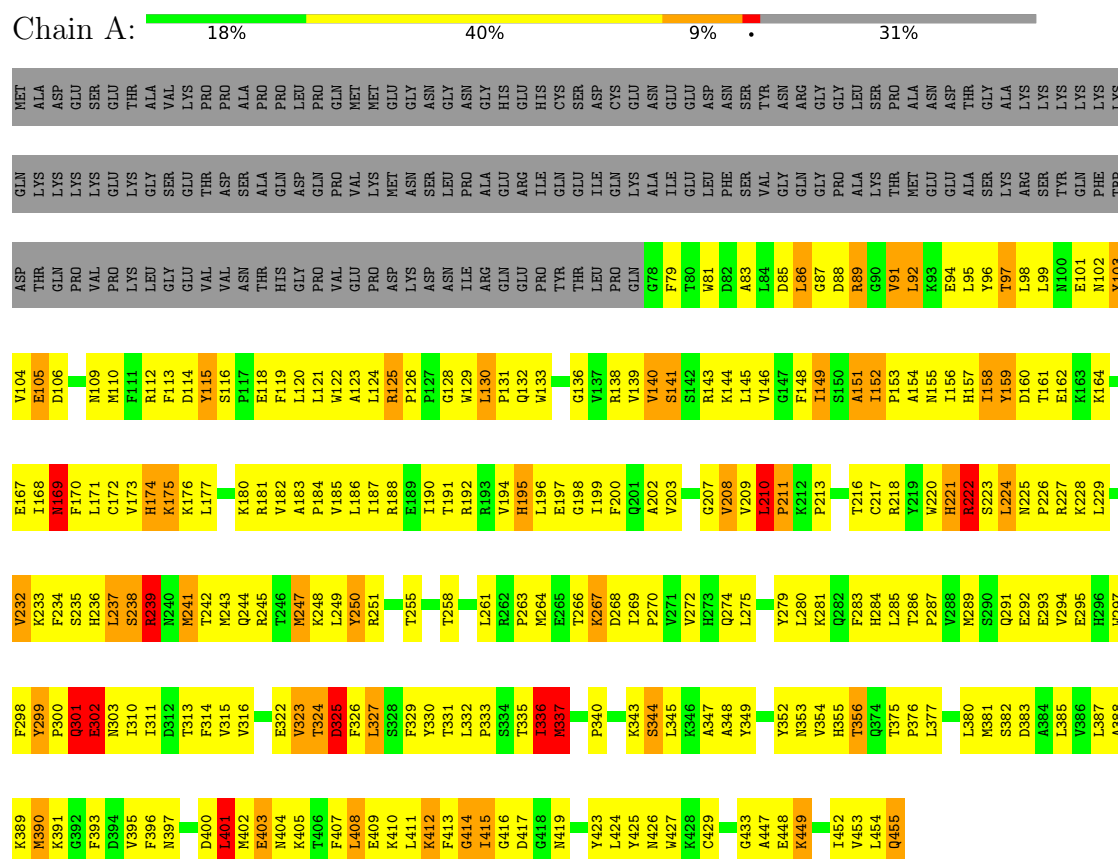
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	13	Total	O	0	0
			13	13		
4	C	10	Total	O	0	0
			10	10		
4	D	16	Total	O	0	0
			16	16		

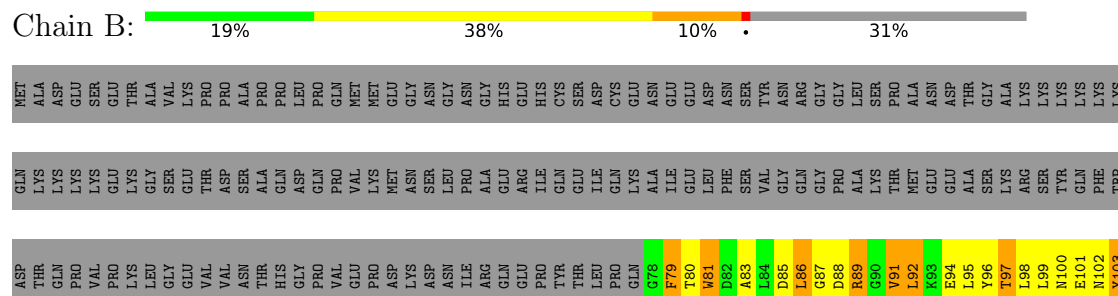
3 Residue-property plots

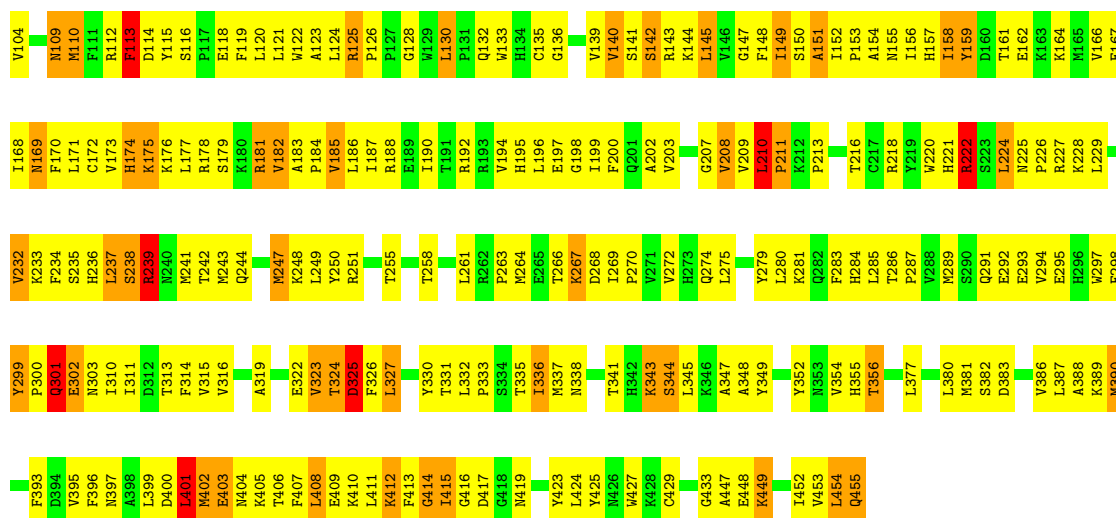
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycylpeptide N-tetradecanoyltransferase 1



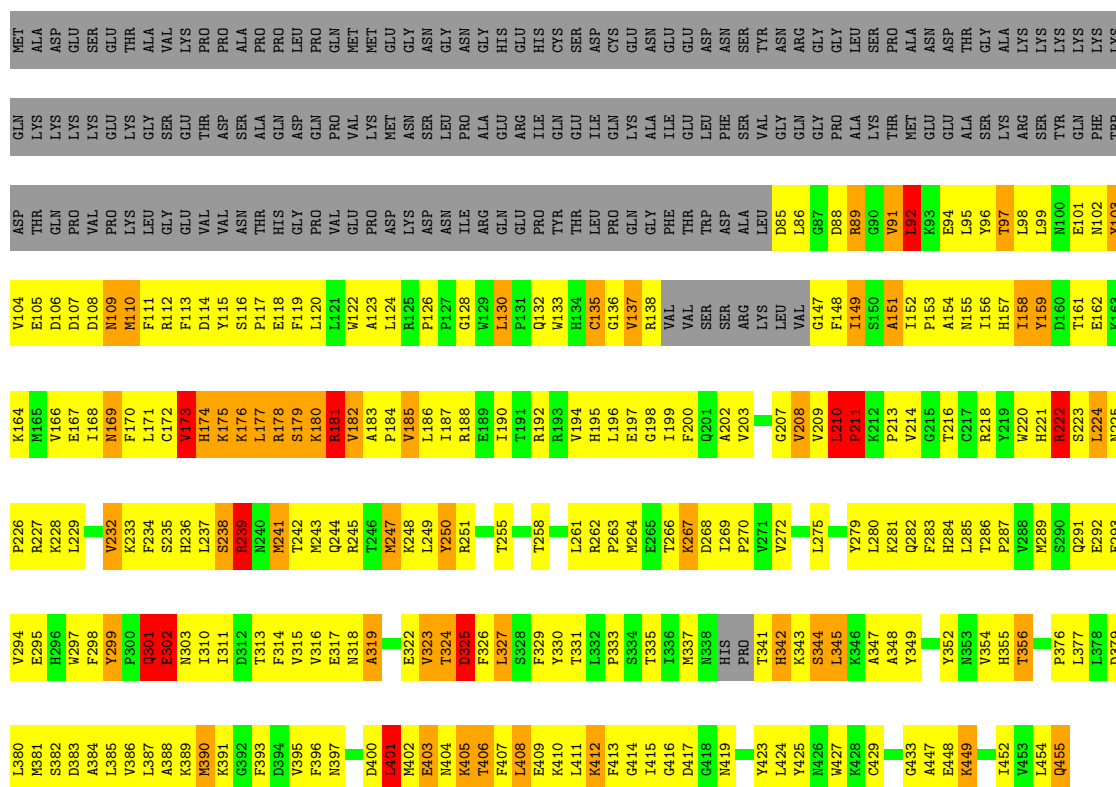
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1





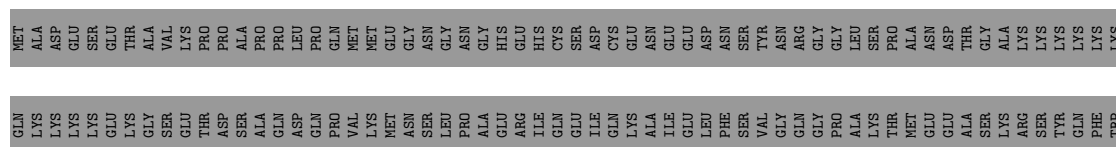
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1

Chain C: 16% 38% 10% 34%



• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1

Chain D: 16% 38% 10% 34%



D379	L380	K381	S382	D383	A384	L385	V386	L387	A388	K389	M390	K391	G392	F393		F396	M397		D400	L401	M402	E403	M404	K405	T406	F407	L408	E409	K410	L411	K412	F413	G414	I415	G416	D417	G418	M419		Y423	L424	Y425	M426	M427	K428	C429		M432	G433	A447	E448	K449		I452	V453	L454	Q455		
E293	V294	E295	H296	V297	F298	Y299	P300	Q301	E302	N303	I310	I311	D312	T313	F314	V315	V316		A319		E322	V323	T324	D325	F326	L327	L408	F329	Y330	T331	L332	P333	S334	T335	I336	M337	K338	H339	P340	T341	K342	K343	S344	L345	F346	A347	A348	Y349		Y352	N353	V354	H355	T356	O374	T375	P376	L377	L378
P226	R227	K228	L229		V232	K233	F234	S235	H236	L237	S238	R239	N240	M241	T242	M243	Q244	R245	T246	M247	K248	L249	Y250	R251		T255		T258		L261	R262	P263	M264	E265	T266	K267	D268	I269	P270	V271	V272	H273	Q274	L275		Y279	L280	K281	Q282	F283	H284	L285	T286	P287	V288	M289	S290	L291	E292
K164	M165	V166	E167	I168	N169	F170	L171	C172	H173	H174	K175	K176	L177	R178	S179	K180	R181	V182	A183	P184	V185	L186	I187	R188	E189	I190	T191	R192	R193	V194	H195	L196	E197	G198	I199	F200	Q201	A202	V203		G207	V208	V209	P211	K212	P213	V214	G215	T216	C217	R218	Y219	W220	H221	R222	S223	L224	N225	
ASP	THR	GLN	PRO	VAL	PRO	LYS	LEU	GLY	GLU	VAL	VAL	ASN	THR	HIS	GLY	PRO	VAL	GLU	PRO	ASP	LYS	ASP	ASN	ILE	ARG	GLN	GLU	PRO	TYR	THR	LEU	PRO	GLY	PHE	THR	TRP	ASP	ALA	LEU	D85	L86	G87	D88	R89	G90	V91	L92	K93	E94	L95	Y96	T97	L98	L99	M100	E101	N102	Y103	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.63Å 116.42Å 90.36Å 90.00° 90.13° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.00) 96.5 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.283 , 0.391 0.337 , 0.407	Depositor DCC
R_{free} test set	1412 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 200.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	0.380 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10420	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 59.63 % 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 1.7162e-05. 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: SO4, CO

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	1.19	3/2718 (0.1%)	1.39	28/3715 (0.8%)
1	B	1.72	4/2712 (0.1%)	1.78	26/3709 (0.7%)
1	C	1.16	3/2605 (0.1%)	1.39	24/3551 (0.7%)
1	D	1.80	4/2592 (0.2%)	1.72	27/3542 (0.8%)
All	All	1.50	14/10627 (0.1%)	1.58	105/14517 (0.7%)

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	3
1	B	0	3
1	C	0	4
1	D	0	3
All	All	0	13

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	401	LEU	C-N	-58.51	0.59	1.33
1	B	401	LEU	C-N	-56.51	0.62	1.33
1	A	401	LEU	C-N	-53.19	0.59	1.33
1	B	402	MET	C-N	49.36	1.99	1.33
1	D	402	MET	C-N	47.77	1.97	1.33

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	301	GLN	O-C-N	-65.60	46.66	123.41
1	B	301	GLN	O-C-N	-61.85	51.04	123.41
1	C	301	GLN	O-C-N	-49.07	63.09	123.44
1	A	301	GLN	O-C-N	-34.83	75.62	123.34
1	D	402	MET	CA-C-N	-30.65	73.61	122.65

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	301	GLN	Mainchain
1	A	401	LEU	Peptide,Mainchain
1	B	301	GLN	Mainchain
1	B	401	LEU	Peptide,Mainchain
1	C	301	GLN	Mainchain

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	2646	0	2523	337	0
1	B	2640	0	2514	357	0
1	C	2538	0	2434	360	1
1	D	2523	0	2395	350	1
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	C	1	0	0	0	0
4	A	13	0	0	3	0
4	B	13	0	0	3	0
4	C	10	0	0	4	0
4	D	16	0	0	2	0
All	All	10420	0	9866	1404	1

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 69.

The worst 5 of 1404 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:302:GLU:C	1:D:303:ASN:CA	2.03	1.32
1:B:302:GLU:CA	1:B:303:ASN:N	1.95	1.29
1:D:302:GLU:CA	1:D:303:ASN:N	1.94	1.29
1:C:302:GLU:O	1:C:303:ASN:N	1.61	1.26
1:B:302:GLU:C	1:B:303:ASN:CA	2.09	1.25

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:O	1:D:196:LEU:O[1_655]	2.17	0.03

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	338/496 (68%)	224 (66%)	80 (24%)	34 (10%)	0	2
1	B	340/496 (68%)	226 (66%)	73 (22%)	41 (12%)	0	1
1	C	317/496 (64%)	212 (67%)	65 (20%)	40 (13%)	0	1
1	D	322/496 (65%)	213 (66%)	73 (23%)	36 (11%)	0	1
All	All	1317/1984 (66%)	875 (66%)	291 (22%)	151 (12%)	0	1

5 of 151 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	SER
1	A	151	ALA
1	A	232	VAL
1	A	238	SER
1	A	239	ARG

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	272/443 (61%)	247 (91%)	25 (9%)	8	33
1	B	271/443 (61%)	247 (91%)	24 (9%)	9	34
1	C	263/443 (59%)	239 (91%)	24 (9%)	9	33
1	D	259/443 (58%)	237 (92%)	22 (8%)	10	36
All	All	1065/1772 (60%)	970 (91%)	95 (9%)	9	34

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	181	ARG
1	C	449	LYS
1	C	210	LEU
1	C	267	LYS
1	D	101	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	426	ASN
1	D	301	GLN
1	C	455	GLN
1	D	201	GLN
1	D	397	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](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	SO4	A	902	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	A	903	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SO4	B	901	-	4,4,4	0.39	0	6,6,6	0.14	0
2	SO4	C	904	-	4,4,4	0.38	0	6,6,6	0.07	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	4

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Mol	Chain	Number of breaks
1	A	4
1	B	4
1	D	4

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	402:MET	C	403:GLU	N	2.12
1	A	402:MET	C	403:GLU	N	2.01
1	B	402:MET	C	403:GLU	N	1.99
1	D	402:MET	C	403:GLU	N	1.97
1	A	302:GLU	C	303:ASN	N	1.15

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	342/496 (68%)	-1.11	0 100 100	0, 32, 106, 190	0
1	B	342/496 (68%)	-1.12	0 100 100	0, 30, 100, 197	0
1	C	325/496 (65%)	-0.96	0 100 100	3, 47, 131, 191	0
1	D	326/496 (65%)	-0.93	0 100 100	1, 50, 129, 197	0
All	All	1335/1984 (67%)	-1.03	0 100 100	0, 39, 122, 197	0

There are no RSRZ outliers to report.

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
2	SO4	A	902	5/5	0.96	0.09	106,108,111,112	0
2	SO4	C	904	5/5	0.96	0.08	104,105,109,112	0
2	SO4	B	901	5/5	0.97	0.05	69,72,75,77	0
2	SO4	A	903	5/5	0.98	0.05	80,84,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CO	C	990	1/1	0.99	0.04	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.