



# wwPDB X-ray Structure Validation Summary Report

Sep 1, 2014 – 11:12 AM EDT

PDB ID : 4MFP  
Title : The crystal structure of acyltransferase in complex with decanoyl-CoA and Tei pseudoaglycone  
Authors : Lyu, S.Y.; Liu, Y.C.; Chang, C.Y.; Huang, C.J.; Li, T.L.  
Deposited on : 2013-08-28  
Resolution : 2.15 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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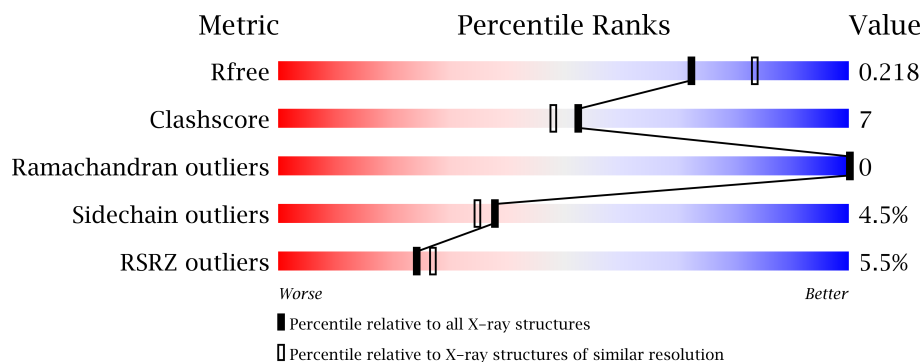
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1094 (2.18-2.14)
Clashscore	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)
RSRZ outliers	66119	1094 (2.18-2.14)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	345	
2	B	7	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	B	501	-	X
8	DKA	B	504	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3143 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Putative uncharacterized protein tcp24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	11	0
			2699	1720	492	479	8			

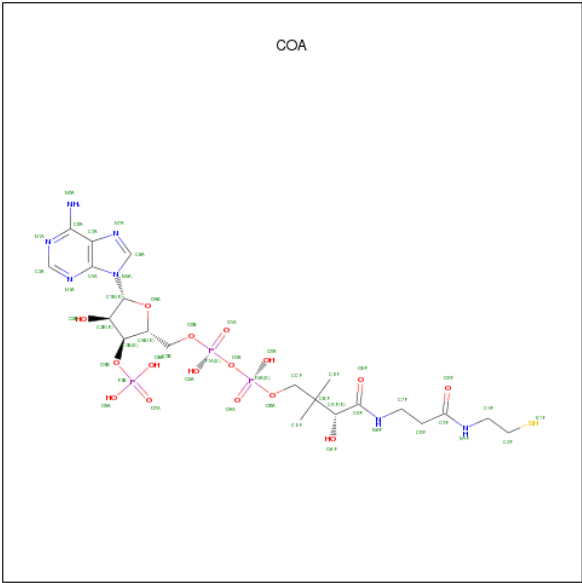
There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP Q70AY4
A	-20	GLY	-	EXPRESSION TAG	UNP Q70AY4
A	-19	SER	-	EXPRESSION TAG	UNP Q70AY4
A	-18	SER	-	EXPRESSION TAG	UNP Q70AY4
A	-17	HIS	-	EXPRESSION TAG	UNP Q70AY4
A	-16	HIS	-	EXPRESSION TAG	UNP Q70AY4
A	-15	HIS	-	EXPRESSION TAG	UNP Q70AY4
A	-14	HIS	-	EXPRESSION TAG	UNP Q70AY4
A	-13	HIS	-	EXPRESSION TAG	UNP Q70AY4
A	-12	HIS	-	EXPRESSION TAG	UNP Q70AY4
A	-11	SER	-	EXPRESSION TAG	UNP Q70AY4
A	-10	SER	-	EXPRESSION TAG	UNP Q70AY4
A	-9	GLY	-	EXPRESSION TAG	UNP Q70AY4
A	-8	LEU	-	EXPRESSION TAG	UNP Q70AY4
A	-7	VAL	-	EXPRESSION TAG	UNP Q70AY4
A	-6	PRO	-	EXPRESSION TAG	UNP Q70AY4
A	-5	ARG	-	EXPRESSION TAG	UNP Q70AY4
A	-4	GLY	-	EXPRESSION TAG	UNP Q70AY4
A	-3	SER	-	EXPRESSION TAG	UNP Q70AY4
A	-2	HIS	-	EXPRESSION TAG	UNP Q70AY4
A	-1	MET	-	EXPRESSION TAG	UNP Q70AY4
A	0	MET	-	EXPRESSION TAG	UNP Q70AY4
A	196	ALA	HIS	ENGINEERED MUTATION	UNP Q70AY4

- Molecule 2 is a protein called Teicoplanin pseudoaglycone.

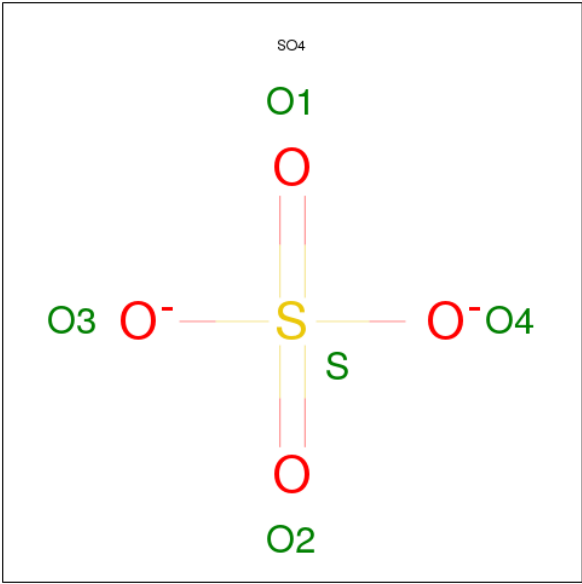
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



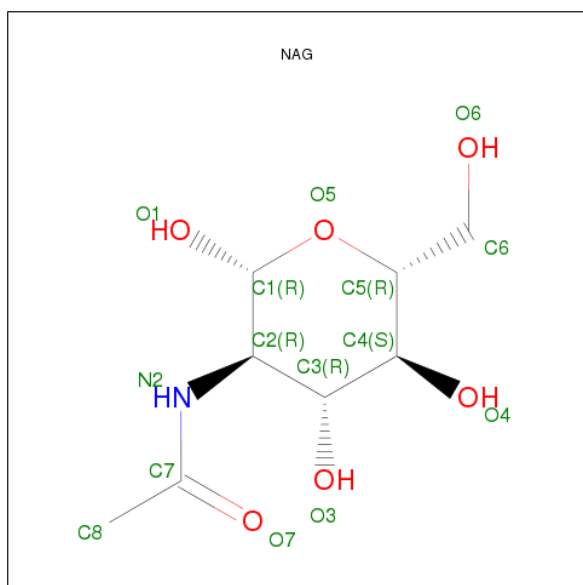
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



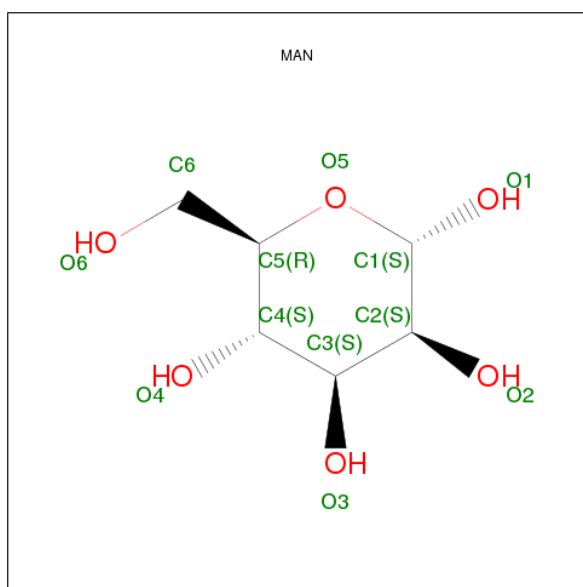
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



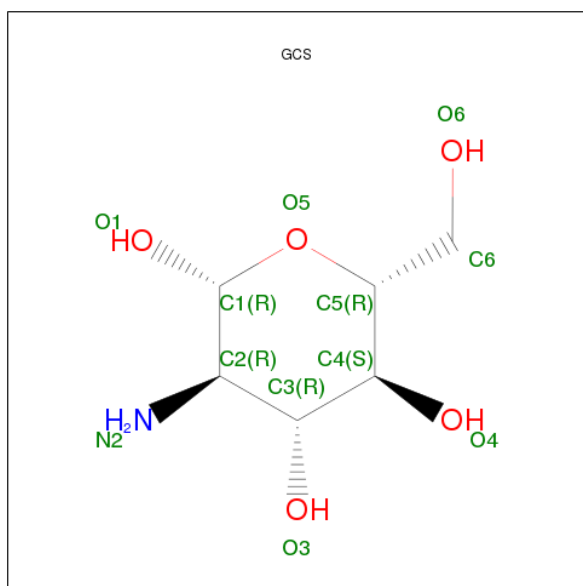
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



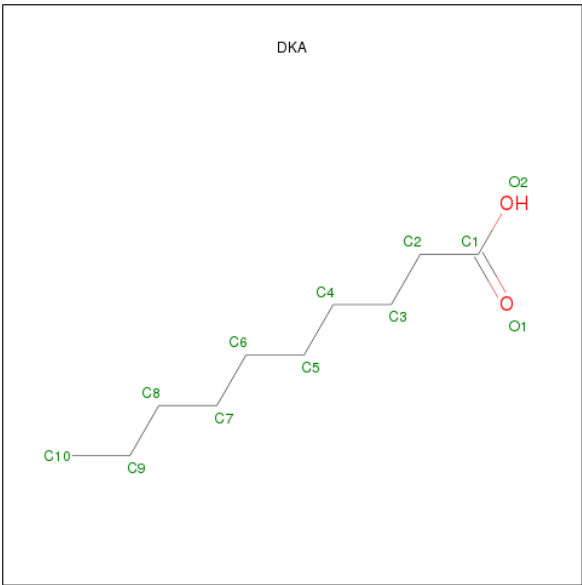
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is SUGAR (D-GLUCOSAMINE) (three-letter code: GCS) (formula:  $C_6H_{13}NO_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 8 is DECANOIC ACID (three-letter code: DKA) (formula:  $C_{10}H_{20}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			11	10	1		

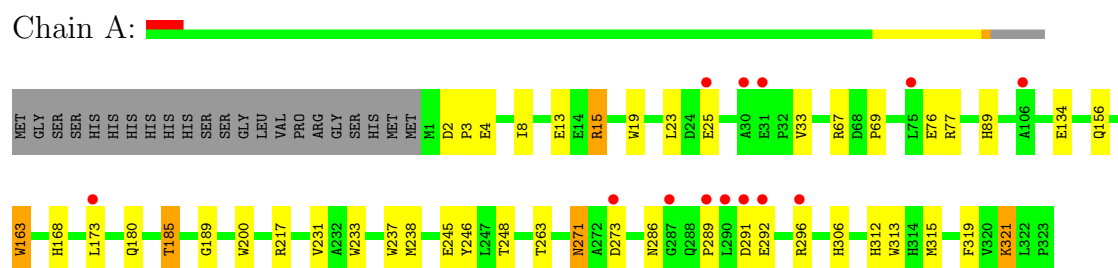
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	245	Total	O	0	0
			245	245		
9	B	9	Total	O	0	0
			9	9		

### 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: Putative uncharacterized protein tcp24



- Molecule 2: Teicoplanin pseudoaglycone





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.11Å 134.11Å 49.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.15 26.99 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.15) 100.0 (26.99-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.80 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.177 , 0.217 0.177 , 0.218	Depositor DCC
$R_{free}$ test set	1395 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.7	EDS
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 27789 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GHP, NAG, 3MY, COA, GCS, SO4, DKA, 3FG, OMY, MAN

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	0.78	5/2787 (0.2%)	0.75	0/3794

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
2	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	TRP	CD2-CE2	5.70	1.48	1.41
1	A	19	TRP	CD2-CE2	5.62	1.48	1.41
1	A	237	TRP	CD2-CE2	5.37	1.47	1.41
1	A	313	TRP	CD2-CE2	5.29	1.47	1.41
1	A	163	TRP	CD2-CE2	5.21	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	399	3FG	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2699	0	2613	32	0
2	B	85	0	32	4	0
3	A	48	0	32	3	0
4	A	10	0	0	0	0
5	B	14	0	13	2	0
6	B	11	0	10	1	0
7	B	11	0	11	1	0
8	B	11	0	19	4	0
9	A	245	0	0	6	0
9	B	9	0	0	0	0
All	All	3143	0	2730	38	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 38 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:B:503:GCS:HN22	8:B:504:DKA:C1	1.26	1.48
3:A:401:COA:S1P	8:B:504:DKA:C1	2.31	1.18
1:A:286:ASN:HB3	9:A:615:HOH:O	1.77	0.82
1:A:15:ARG:HH11	1:A:15:ARG:HG2	1.45	0.81
1:A:163:TRP:HD1	9:A:517:HOH:O	1.72	0.72

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/345 (96%)	324 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/283 (97%)	262 (95%)	13 (5%)	36	33

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185[A]	THR
1	A	185[B]	THR
1	A	291	ASP
1	A	168	HIS
1	A	273	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	242	GLN
1	A	271	ASN
1	A	306	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GHP	B	397	2	11,11,12	5.78	3 (27%)	12,14,16	9.81	1 (8%)
2	3MY	B	398	2	13,13,14	5.79	4 (30%)	15,17,19	3.71	2 (13%)
2	3FG	B	399	2	12,12,13	5.49	3 (25%)	14,16,18	0.97	0
2	GHP	B	400	2,7	11,11,12	4.86	2 (18%)	12,14,16	3.56	4 (33%)
2	GHP	B	401	2	11,11,12	6.76	3 (27%)	12,14,16	13.59	1 (8%)
2	OMY	B	402	2,5	14,14,15	5.12	4 (28%)	17,19,21	1.77	4 (23%)
2	3FG	B	403	2,6	13,13,13	1.23	2 (15%)	18,18,18	1.64	4 (22%)

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	GHP	B	397	2	-	0/4/6/8	0/1/1/1
2	3MY	B	398	2	-	0/4/6/8	0/1/1/1
2	3FG	B	399	2	-	0/4/6/8	0/1/1/1
2	GHP	B	400	2,7	-	0/4/6/8	0/1/1/1
2	GHP	B	401	2	-	0/4/6/8	0/1/1/1
2	OMY	B	402	2,5	-	0/8/10/12	0/1/1/1
2	3FG	B	403	2,6	-	0/8/8/8	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	GHP	O-C	20.24	1.25	1.11
2	B	398	3MY	O-C	18.78	1.24	1.11
2	B	399	3FG	O-C	17.96	1.23	1.11
2	B	397	GHP	O-C	17.61	1.23	1.11
2	B	402	OMY	O-C	16.88	1.23	1.11

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GHP	C-CA-N	-46.91	107.95	113.27
2	B	397	GHP	C-CA-N	-33.82	109.44	113.27
2	B	398	3MY	C-CA-N	13.96	127.77	113.83
2	B	400	GHP	C-CA-N	9.82	114.38	113.27
2	B	402	OMY	ODE-CB-CA	5.45	118.12	107.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
3	COA	A	401	-	50,50,50	1.79	13 (26%)	75,75,75	1.60	8 (10%)
4	SO4	A	402	-	4,4,4	0.50	0	6,6,6	0.16	0
4	SO4	A	403	-	4,4,4	0.66	0	6,6,6	0.26	0
5	NAG	B	501	2	12,14,15	0.80	0	15,19,21	2.10	3 (20%)
6	MAN	B	502	2	10,11,12	0.76	1 (10%)	11,15,17	1.38	1 (9%)
7	GCS	B	503	8,2	9,11,12	1.46	1 (11%)	11,15,17	1.06	1 (9%)
8	DKA	B	504	7	10,10,11	5.16	1 (10%)	7,9,11	0.65	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	COA	A	401	-	-	0/48/64/64	0/3/3/3
4	SO4	A	402	-	-	0/0/0/0	0/0/0/0
4	SO4	A	403	-	-	0/0/0/0	0/0/0/0
5	NAG	B	501	2	-	0/6/23/26	0/1/1/1
6	MAN	B	502	2	-	0/2/19/22	0/1/1/1
7	GCS	B	503	8,2	-	0/2/19/22	0/1/1/1
8	DKA	B	504	7	-	0/7/8/9	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	504	DKA	O1-C1	16.29	1.22	1.11
3	A	401	COA	C4A-N9A	-4.88	1.30	1.37
7	B	503	GCS	O5-C5	-3.75	1.39	1.45
3	A	401	COA	P2A-O5A	-3.42	1.40	1.55
3	A	401	COA	CBP-CAP	-3.25	1.53	1.55

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	COA	C5A-C4A-N3A	-7.20	118.96	125.98
5	B	501	NAG	O5-C5-C6	6.60	113.91	106.98
3	A	401	COA	N3A-C2A-N1A	-5.42	124.12	128.89
3	A	401	COA	N3A-C4A-N9A	5.20	134.32	125.39
3	A	401	COA	C4A-C5A-N7A	-3.69	105.84	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	323/345 (93%)	0.00	13 (4%) 36 40	20, 34, 67, 95	0
2	B	7/7 (100%)	4.79	5 (71%) 0 0	74, 82, 102, 118	0
All	All	330/352 (93%)	0.10	18 (5%) 24 27	20, 35, 71, 118	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	397	GHP	15.0
2	B	401	GHP	6.5
1	A	289	PRO	3.9
2	B	402	OMY	3.5
1	A	292	GLU	3.3

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

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	3MY	B	398	13/14	0.24	7.73	84,91,98,102	0
2	GHP	B	401	11/12	0.27	3.58	75,81,85,86	0
2	OMY	B	402	14/15	0.22	2.95	64,75,81,94	0
2	GHP	B	400	11/12	0.16	2.35	66,72,77,87	0
2	GHP	B	397	11/12	0.48	2.19	104,119,126,129	0
2	3FG	B	403	13/13	0.42	-	82,101,108,109	0
2	3FG	B	399	12/13	0.40	-	86,100,108,115	0



### 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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	501	14/15	0.23	2.38	54,72,82,83	0
8	DKA	B	504	11/12	0.18	2.20	33,38,43,43	0
4	SO4	A	403	5/5	0.22	1.41	72,79,84,88	0
4	SO4	A	402	5/5	0.12	0.52	95,97,98,103	0
7	GCS	B	503	11/12	0.13	-0.27	42,49,53,55	0
3	COA	A	401	48/48	0.07	-0.71	29,34,49,53	0
6	MAN	B	502	11/12	0.38	-	101,117,123,128	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.