



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:30 PM GMT

PDB ID : 4IHH  
Title : Chasing Acyl Carrier Protein Through a Catalytic Cycle of Lipid A Production  
Authors : Masoudi, A.; Raetz, C.R.H.; Pemble, C.W.  
Deposited on : 2012-12-18  
Resolution : 2.13 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](mailto: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.

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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 : 1.7 (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

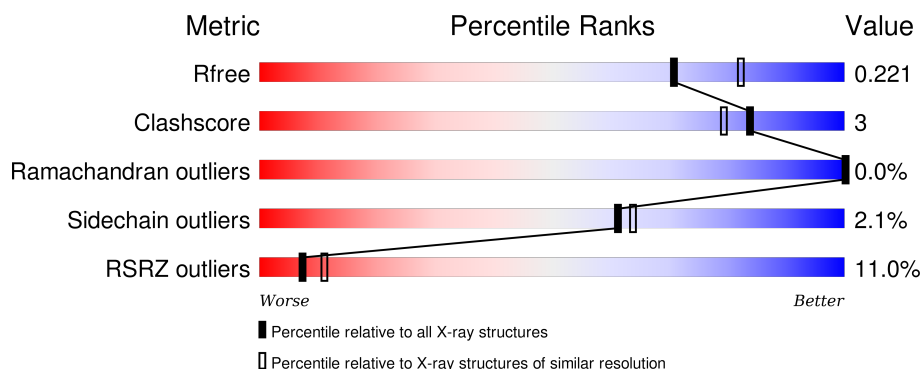
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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. 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	348	<div> <div>4%</div> <div>93%</div> <div>6%</div> <div>• •</div> </div>
1	B	348	<div> <div>3%</div> <div>90%</div> <div>6%</div> <div>•</div> </div>
1	C	348	<div> <div>4%</div> <div>89%</div> <div>8%</div> <div>•</div> </div>
1	D	348	<div> <div>2%</div> <div>91%</div> <div>5%</div> <div>•</div> </div>
1	E	348	<div> <div>6%</div> <div>91%</div> <div>7%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	348	
2	G	80	
2	H	80	
2	I	80	
2	J	80	
2	K	80	
2	L	80	

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
3	MES	A	402	-	-	-	X
3	MES	C	401	-	-	-	X
3	MES	D	401	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18447 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 UDP-3-O-(3-hydroxymyristoyl)glucosamine N-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	1	0
			2488	1553	442	474	19			
1	B	335	Total	C	N	O	S	1	1	0
			2476	1546	441	470	19			
1	C	337	Total	C	N	O	S	1	0	0
			2481	1548	441	473	19			
1	D	335	Total	C	N	O	S	0	0	0
			2468	1541	438	470	19			
1	E	340	Total	C	N	O	S	0	0	0
			2510	1565	449	477	19			
1	F	338	Total	C	N	O	S	0	0	0
			2491	1554	444	474	19			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP P21645
A	-6	GLY	-	EXPRESSION TAG	UNP P21645
A	-5	HIS	-	EXPRESSION TAG	UNP P21645
A	-4	HIS	-	EXPRESSION TAG	UNP P21645
A	-3	HIS	-	EXPRESSION TAG	UNP P21645
A	-2	HIS	-	EXPRESSION TAG	UNP P21645
A	-1	HIS	-	EXPRESSION TAG	UNP P21645
A	0	HIS	-	EXPRESSION TAG	UNP P21645
A	2	ALA	-	EXPRESSION TAG	UNP P21645
B	-6	MET	-	EXPRESSION TAG	UNP P21645
B	-5	GLY	-	EXPRESSION TAG	UNP P21645
B	-4	HIS	-	EXPRESSION TAG	UNP P21645
B	-3	HIS	-	EXPRESSION TAG	UNP P21645
B	-2	HIS	-	EXPRESSION TAG	UNP P21645
B	-1	HIS	-	EXPRESSION TAG	UNP P21645
B	0	HIS	-	EXPRESSION TAG	UNP P21645
B	1	HIS	-	EXPRESSION TAG	UNP P21645

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ALA	-	EXPRESSION TAG	UNP P21645
C	-6	MET	-	EXPRESSION TAG	UNP P21645
C	-5	GLY	-	EXPRESSION TAG	UNP P21645
C	-4	HIS	-	EXPRESSION TAG	UNP P21645
C	-3	HIS	-	EXPRESSION TAG	UNP P21645
C	-2	HIS	-	EXPRESSION TAG	UNP P21645
C	-1	HIS	-	EXPRESSION TAG	UNP P21645
C	0	HIS	-	EXPRESSION TAG	UNP P21645
C	1	HIS	-	EXPRESSION TAG	UNP P21645
C	2	ALA	-	EXPRESSION TAG	UNP P21645
D	-6	MET	-	EXPRESSION TAG	UNP P21645
D	-5	GLY	-	EXPRESSION TAG	UNP P21645
D	-4	HIS	-	EXPRESSION TAG	UNP P21645
D	-3	HIS	-	EXPRESSION TAG	UNP P21645
D	-2	HIS	-	EXPRESSION TAG	UNP P21645
D	-1	HIS	-	EXPRESSION TAG	UNP P21645
D	0	HIS	-	EXPRESSION TAG	UNP P21645
D	1	HIS	-	EXPRESSION TAG	UNP P21645
D	2	ALA	-	EXPRESSION TAG	UNP P21645
E	-7	MET	-	EXPRESSION TAG	UNP P21645
E	-6	GLY	-	EXPRESSION TAG	UNP P21645
E	-5	HIS	-	EXPRESSION TAG	UNP P21645
E	-4	HIS	-	EXPRESSION TAG	UNP P21645
E	-3	HIS	-	EXPRESSION TAG	UNP P21645
E	-2	HIS	-	EXPRESSION TAG	UNP P21645
E	-1	HIS	-	EXPRESSION TAG	UNP P21645
E	0	HIS	-	EXPRESSION TAG	UNP P21645
E	2	ALA	-	EXPRESSION TAG	UNP P21645
F	-7	MET	-	EXPRESSION TAG	UNP P21645
F	-6	GLY	-	EXPRESSION TAG	UNP P21645
F	-5	HIS	-	EXPRESSION TAG	UNP P21645
F	-4	HIS	-	EXPRESSION TAG	UNP P21645
F	-3	HIS	-	EXPRESSION TAG	UNP P21645
F	-2	HIS	-	EXPRESSION TAG	UNP P21645
F	-1	HIS	-	EXPRESSION TAG	UNP P21645
F	0	HIS	-	EXPRESSION TAG	UNP P21645
F	2	ALA	-	EXPRESSION TAG	UNP P21645

- Molecule 2 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	70	Total	C	N	O	S	0	0	0
			547	339	83	124	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	10	Total	C	N	O	S	0	0	0
			76	47	10	18	1			
2	I	75	Total	C	N	O	S	0	0	0
			580	359	88	131	2			
2	J	76	Total	C	N	O	S	0	0	0
			590	365	91	132	2			
2	K	73	Total	C	N	O	S	1	0	0
			569	353	88	127	1			
2	L	10	Total	C	N	O	S	0	0	0
			76	47	10	18	1			

There are 12 discrepancies between the modelled and reference sequences:

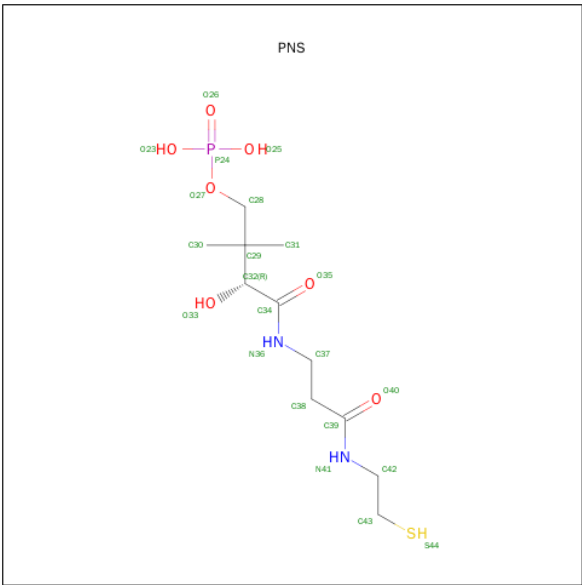
Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	SER	-	EXPRESSION TAG	UNP G7RM21
G	-1	HIS	-	EXPRESSION TAG	UNP G7RM21
H	-2	SER	-	EXPRESSION TAG	UNP G7RM21
H	-1	HIS	-	EXPRESSION TAG	UNP G7RM21
I	-2	SER	-	EXPRESSION TAG	UNP G7RM21
I	-1	HIS	-	EXPRESSION TAG	UNP G7RM21
J	-2	SER	-	EXPRESSION TAG	UNP G7RM21
J	-1	HIS	-	EXPRESSION TAG	UNP G7RM21
K	-2	SER	-	EXPRESSION TAG	UNP G7RM21
K	-1	HIS	-	EXPRESSION TAG	UNP G7RM21
L	-2	SER	-	EXPRESSION TAG	UNP G7RM21
L	-1	HIS	-	EXPRESSION TAG	UNP G7RM21

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	G	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	H	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	I	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	J	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	K	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	L	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total	O	0	0
			136	136		
5	B	154	Total	O	0	0
			154	154		
5	C	137	Total	O	0	0
			137	137		
5	D	137	Total	O	0	0
			137	137		
5	E	139	Total	O	0	0
			139	139		
5	F	164	Total	O	0	0
			164	164		

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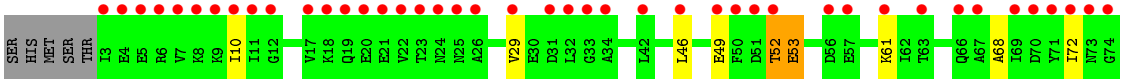
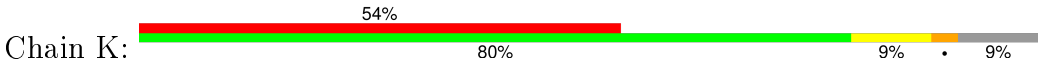
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	2	Total 2	O 2	0	0
5	H	2	Total 2	O 2	0	0
5	I	3	Total 3	O 3	0	0
5	J	3	Total 3	O 3	0	0
5	K	6	Total 6	O 6	0	0
5	L	2	Total 2	O 2	0	0



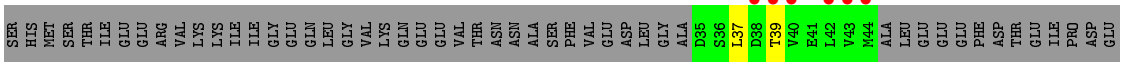




• Molecule 2: Acyl carrier protein



• Molecule 2: Acyl carrier protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.47Å 93.22Å 114.30Å 75.93° 73.81° 58.95°	Depositor
Resolution (Å)	35.89 – 2.13 42.13 – 2.13	Depositor EDS
% Data completeness (in resolution range)	95.0 (35.89-2.13) 92.0 (42.13-2.13)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.177 , 0.216 0.183 , 0.221	Depositor DCC
$R_{free}$ test set	8042 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 160058 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>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: PNS, MES

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	0.36	0/2525	0.52	0/3425
1	B	0.39	0/2512	0.52	0/3406
1	C	0.38	0/2514	0.52	0/3410
1	D	0.39	0/2501	0.53	0/3392
1	E	0.37	0/2545	0.52	0/3452
1	F	0.40	0/2525	0.53	0/3425
2	G	0.27	0/550	0.45	0/744
2	H	0.29	0/75	0.49	0/101
2	I	0.28	0/583	0.45	0/788
2	J	0.28	0/594	0.47	0/803
2	K	0.28	0/573	0.46	0/775
2	L	0.27	0/75	0.53	0/101
All	All	0.37	0/17572	0.52	0/23822

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2488	0	2530	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2476	0	2524	23	0
1	C	2481	0	2522	22	0
1	D	2468	0	2511	13	0
1	E	2510	0	2547	14	0
1	F	2491	0	2532	11	0
2	G	547	0	524	9	0
2	H	76	0	73	2	0
2	I	580	0	562	5	0
2	J	590	0	569	7	0
2	K	569	0	545	4	0
2	L	76	0	73	0	0
3	A	24	0	24	1	0
3	B	12	0	12	4	0
3	C	12	0	12	1	0
3	D	12	0	12	2	0
3	E	12	0	12	3	0
3	F	12	0	12	0	0
4	G	21	0	21	1	0
4	H	21	0	21	1	0
4	I	21	0	21	0	0
4	J	21	0	21	0	0
4	K	21	0	21	1	0
4	L	21	0	21	1	0
5	A	136	0	0	0	0
5	B	154	0	0	2	0
5	C	137	0	0	1	0
5	D	137	0	0	0	0
5	E	139	0	0	1	0
5	F	164	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
5	I	3	0	0	0	0
5	J	3	0	0	0	0
5	K	6	0	0	0	0
5	L	2	0	0	0	0
All	All	18447	0	17722	105	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.

The worst 5 of 105 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)
2:J:52:THR:OG1	2:J:53:GLU:N	2.10	0.83
1:F:115:ASN:HD22	1:F:133:ASN:HD22	1.32	0.75
1:B:115:ASN:HD22	1:B:133:ASN:HD22	1.33	0.74
1:E:17:LEU:HD21	1:E:21:GLY:HA2	1.75	0.68
1:D:31:MET:HB2	3:D:401:MES:H62	1.75	0.68

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	336/348 (97%)	332 (99%)	4 (1%)	0	100	100
1	B	334/348 (96%)	330 (99%)	4 (1%)	0	100	100
1	C	335/348 (96%)	330 (98%)	5 (2%)	0	100	100
1	D	333/348 (96%)	328 (98%)	5 (2%)	0	100	100
1	E	338/348 (97%)	331 (98%)	7 (2%)	0	100	100
1	F	336/348 (97%)	330 (98%)	5 (2%)	1 (0%)	46	41
2	G	68/80 (85%)	64 (94%)	4 (6%)	0	100	100
2	H	8/80 (10%)	8 (100%)	0	0	100	100
2	I	73/80 (91%)	70 (96%)	3 (4%)	0	100	100
2	J	74/80 (92%)	68 (92%)	6 (8%)	0	100	100
2	K	71/80 (89%)	68 (96%)	3 (4%)	0	100	100
2	L	8/80 (10%)	8 (100%)	0	0	100	100
All	All	2314/2568 (90%)	2267 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	F	336	LYS

### 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	266/275 (97%)	262 (98%)	4 (2%)	72	76
1	B	265/275 (96%)	263 (99%)	2 (1%)	86	91
1	C	265/275 (96%)	264 (100%)	1 (0%)	93	96
1	D	264/275 (96%)	260 (98%)	4 (2%)	72	76
1	E	268/275 (98%)	264 (98%)	4 (2%)	72	76
1	F	266/275 (97%)	261 (98%)	5 (2%)	65	68
2	G	61/69 (88%)	57 (93%)	4 (7%)	21	14
2	H	10/69 (14%)	10 (100%)	0	100	100
2	I	65/69 (94%)	61 (94%)	4 (6%)	23	17
2	J	66/69 (96%)	61 (92%)	5 (8%)	16	10
2	K	63/69 (91%)	59 (94%)	4 (6%)	22	16
2	L	10/69 (14%)	8 (80%)	2 (20%)	1	0
All	All	1869/2064 (91%)	1830 (98%)	39 (2%)	61	64

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	239	HIS
2	G	19	GLN
2	K	61	LYS
1	F	331	LYS
1	F	332	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	173	GLN
1	E	173	GLN
2	J	73	ASN
1	D	310	ASN
1	E	133	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

13 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	MES	A	401	-	11,12,12	0.62	0	14,16,16	2.43	6 (42%)
3	MES	A	402	-	11,12,12	0.64	0	14,16,16	2.65	7 (50%)
3	MES	B	401	-	11,12,12	0.58	0	14,16,16	2.48	6 (42%)
3	MES	C	401	-	11,12,12	0.63	0	14,16,16	2.18	7 (50%)
3	MES	D	401	-	11,12,12	0.62	0	14,16,16	2.27	7 (50%)
3	MES	E	401	-	11,12,12	0.64	0	14,16,16	2.14	5 (35%)
3	MES	F	401	-	11,12,12	0.59	0	14,16,16	2.29	6 (42%)
4	PNS	G	101	2	14,20,21	1.89	3 (21%)	16,26,29	2.27	5 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PNS	H	101	2	14,20,21	1.87	3 (21%)	16,26,29	1.78	3 (18%)
4	PNS	I	101	2	14,20,21	1.76	3 (21%)	16,26,29	1.09	1 (6%)
4	PNS	J	101	2	14,20,21	1.82	3 (21%)	16,26,29	2.43	5 (31%)
4	PNS	K	101	2	14,20,21	1.86	3 (21%)	16,26,29	2.51	7 (43%)
4	PNS	L	101	2	14,20,21	1.85	3 (21%)	16,26,29	1.66	6 (37%)

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	MES	A	401	-	-	0/6/14/14	0/1/1/1
3	MES	A	402	-	-	0/6/14/14	0/1/1/1
3	MES	B	401	-	-	0/6/14/14	0/1/1/1
3	MES	C	401	-	-	0/6/14/14	0/1/1/1
3	MES	D	401	-	-	0/6/14/14	0/1/1/1
3	MES	E	401	-	-	0/6/14/14	0/1/1/1
3	MES	F	401	-	-	0/6/14/14	0/1/1/1
4	PNS	G	101	2	-	0/24/26/27	0/0/0/0
4	PNS	H	101	2	-	0/24/26/27	0/0/0/0
4	PNS	I	101	2	-	0/24/26/27	0/0/0/0
4	PNS	J	101	2	-	0/24/26/27	0/0/0/0
4	PNS	K	101	2	-	0/24/26/27	0/0/0/0
4	PNS	L	101	2	-	0/24/26/27	0/0/0/0

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	101	PNS	C30-C29	-2.54	1.48	1.53
4	L	101	PNS	C30-C29	-2.54	1.48	1.53
4	H	101	PNS	C30-C29	-2.44	1.48	1.53
4	K	101	PNS	C30-C29	-2.43	1.48	1.53
4	I	101	PNS	C30-C29	-2.41	1.48	1.53

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	MES	C6-C5-N4	-3.80	104.37	110.12
3	D	401	MES	C2-C3-N4	-3.56	104.74	110.12
3	F	401	MES	C6-C5-N4	-3.32	105.10	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	MES	C6-C5-N4	-3.17	105.32	110.12
4	K	101	PNS	C42-N41-C39	-2.85	117.19	122.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	MES	1	0
3	B	401	MES	4	0
3	C	401	MES	1	0
3	D	401	MES	2	0
3	E	401	MES	3	0
4	G	101	PNS	1	0
4	H	101	PNS	1	0
4	K	101	PNS	1	0
4	L	101	PNS	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, 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	337/348 (96%)	0.05	14 (4%)	40	49	8, 27, 69, 100	0
1	B	335/348 (96%)	0.09	12 (3%)	46	56	11, 26, 62, 101	0
1	C	337/348 (96%)	0.20	15 (4%)	37	46	12, 28, 64, 100	1 (0%)
1	D	335/348 (96%)	0.05	7 (2%)	67	73	11, 26, 62, 96	0
1	E	340/348 (97%)	0.23	21 (6%)	24	31	8, 27, 68, 105	0
1	F	338/348 (97%)	0.02	13 (3%)	44	54	11, 25, 58, 97	0
2	G	70/80 (87%)	3.25	50 (71%)	0	0	47, 90, 112, 115	0
2	H	10/80 (12%)	2.83	5 (50%)	0	0	59, 73, 81, 82	0
2	I	75/80 (93%)	1.77	26 (34%)	0	1	41, 75, 111, 128	0
2	J	76/80 (95%)	1.95	44 (57%)	0	0	38, 75, 99, 105	0
2	K	73/80 (91%)	2.43	43 (58%)	0	0	42, 77, 106, 121	1 (1%)
2	L	10/80 (12%)	2.98	6 (60%)	0	0	59, 73, 82, 84	0
All	All	2336/2568 (90%)	0.41	256 (10%)	7	11	8, 29, 89, 128	2 (0%)

The worst 5 of 256 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	42	LEU	9.3
2	G	17	VAL	9.1
2	L	42	LEU	9.0
2	G	32	LEU	7.0
2	G	50	PHE	6.9

### 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 [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MES	C	401	12/12	0.84	0.26	3.95	32,43,70,71	12
3	MES	D	401	12/12	0.87	0.20	2.21	38,50,66,67	12
3	MES	A	402	12/12	0.87	0.20	2.14	64,81,99,102	0
3	MES	E	401	12/12	0.88	0.23	1.84	55,64,76,77	12
3	MES	B	401	12/12	0.88	0.21	1.51	36,51,65,71	12
4	PNS	K	101	21/22	0.91	0.14	0.11	28,45,58,60	0
4	PNS	G	101	21/22	0.96	0.14	0.01	45,51,65,74	0
3	MES	A	401	12/12	0.96	0.12	-0.12	42,61,80,82	0
3	MES	F	401	12/12	0.97	0.10	-0.31	29,46,58,58	0
4	PNS	H	101	21/22	0.91	0.14	-0.47	59,65,68,69	0
4	PNS	I	101	21/22	0.93	0.11	-0.63	39,47,55,58	0
4	PNS	J	101	21/22	0.97	0.12	-0.84	37,48,55,58	0
4	PNS	L	101	21/22	0.93	0.12	-0.98	58,62,65,66	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.