



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:07 am BST

PDB ID : 3HDS  
Title : Crystal structure of 4-methylmuconolactone methylisomerase in complex with MES  
Authors : Marin, M.; Heinz, D.W.; Pieper, D.H.; Klink, B.U.  
Deposited on : 2009-05-07  
Resolution : 1.45 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

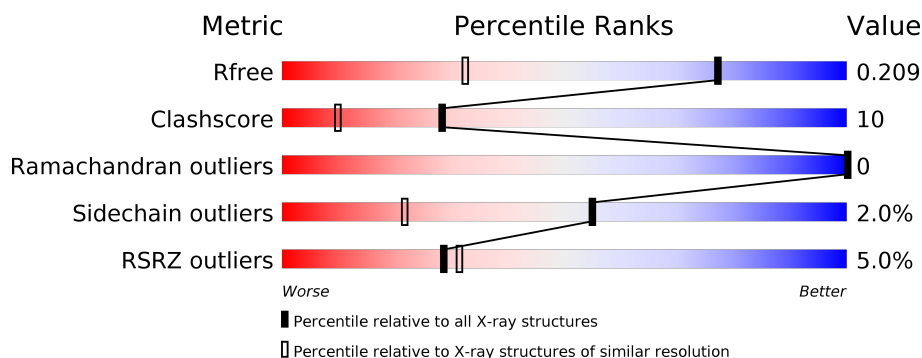
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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))
$R_{free}$	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 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	116	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>.</div> </div> </div>
1	B	116	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>..</div> </div> </div>
1	C	116	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>6%</div> </div> </div>
1	D	116	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>.</div> <div>6%</div> </div> </div>
2	E	5	<div> <div>80%</div> <div> <div></div> <div>60%</div> <div>40%</div> </div> </div>
2	F	5	<div> <div>40%</div> <div> <div></div> <div>60%</div> <div>40%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4561 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 4-methylmuconolactone methylisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	11	0
			1053	680	180	185	8			
1	B	115	Total	C	N	O	S	0	14	0
			1057	688	174	187	8			
1	C	109	Total	C	N	O	S	0	6	0
			947	613	161	166	7			
1	D	109	Total	C	N	O	S	0	8	0
			963	622	165	168	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	PRO	-	EXPRESSION TAG	UNP C5MR76
A	-7	GLN	-	EXPRESSION TAG	UNP C5MR76
A	-6	PHE	-	EXPRESSION TAG	UNP C5MR76
A	-5	GLU	-	EXPRESSION TAG	UNP C5MR76
A	-4	LYS	-	EXPRESSION TAG	UNP C5MR76
A	-3	ILE	-	EXPRESSION TAG	UNP C5MR76
A	-2	GLU	-	EXPRESSION TAG	UNP C5MR76
A	-1	GLY	-	EXPRESSION TAG	UNP C5MR76
A	0	ARG	-	EXPRESSION TAG	UNP C5MR76
B	-8	PRO	-	EXPRESSION TAG	UNP C5MR76
B	-7	GLN	-	EXPRESSION TAG	UNP C5MR76
B	-6	PHE	-	EXPRESSION TAG	UNP C5MR76
B	-5	GLU	-	EXPRESSION TAG	UNP C5MR76
B	-4	LYS	-	EXPRESSION TAG	UNP C5MR76
B	-3	ILE	-	EXPRESSION TAG	UNP C5MR76
B	-2	GLU	-	EXPRESSION TAG	UNP C5MR76
B	-1	GLY	-	EXPRESSION TAG	UNP C5MR76
B	0	ARG	-	EXPRESSION TAG	UNP C5MR76
C	-8	PRO	-	EXPRESSION TAG	UNP C5MR76
C	-7	GLN	-	EXPRESSION TAG	UNP C5MR76
C	-6	PHE	-	EXPRESSION TAG	UNP C5MR76

*Continued on next page...*

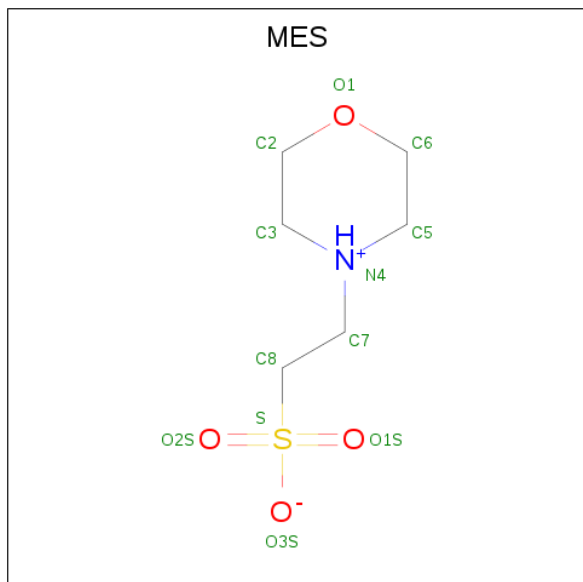
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLU	-	EXPRESSION TAG	UNP C5MR76
C	-4	LYS	-	EXPRESSION TAG	UNP C5MR76
C	-3	ILE	-	EXPRESSION TAG	UNP C5MR76
C	-2	GLU	-	EXPRESSION TAG	UNP C5MR76
C	-1	GLY	-	EXPRESSION TAG	UNP C5MR76
C	0	ARG	-	EXPRESSION TAG	UNP C5MR76
D	-8	PRO	-	EXPRESSION TAG	UNP C5MR76
D	-7	GLN	-	EXPRESSION TAG	UNP C5MR76
D	-6	PHE	-	EXPRESSION TAG	UNP C5MR76
D	-5	GLU	-	EXPRESSION TAG	UNP C5MR76
D	-4	LYS	-	EXPRESSION TAG	UNP C5MR76
D	-3	ILE	-	EXPRESSION TAG	UNP C5MR76
D	-2	GLU	-	EXPRESSION TAG	UNP C5MR76
D	-1	GLY	-	EXPRESSION TAG	UNP C5MR76
D	0	ARG	-	EXPRESSION TAG	UNP C5MR76

- Molecule 2 is a protein called short peptide ASWSA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			36	23	6	7			
2	F	5	Total	C	N	O	0	0	0
			36	23	6	7			

- 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	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	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

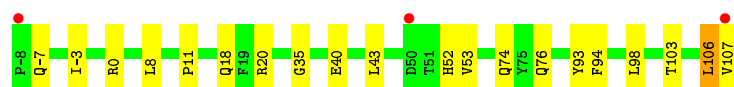
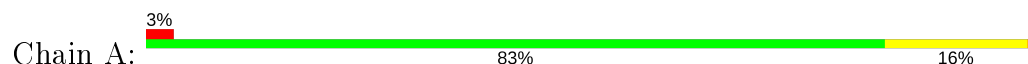
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	107	Total	O	0	0
			107	107		
4	B	115	Total	O	0	0
			115	115		
4	C	104	Total	O	0	0
			104	104		
4	D	92	Total	O	0	0
			92	92		
4	F	3	Total	O	0	0
			3	3		

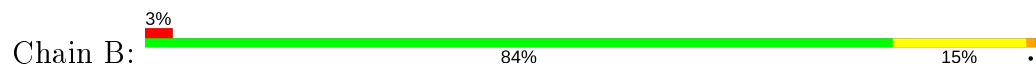
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

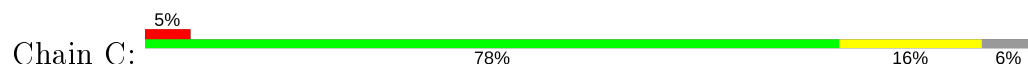
- Molecule 1: 4-methylmuconolactone methylisomerase



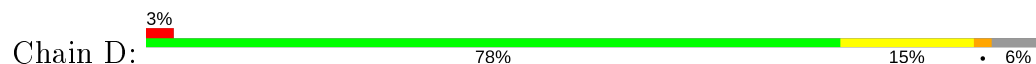
- Molecule 1: 4-methylmuconolactone methylisomerase



- Molecule 1: 4-methylmuconolactone methylisomerase



- Molecule 1: 4-methylmuconolactone methylisomerase



- Molecule 2: short peptide ASWSA



- Molecule 2: short peptide ASWSA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.87Å 84.16Å 150.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.07 – 1.45 42.08 – 1.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.07-1.45) 100.0 (42.08-1.45)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 1.45Å)	Xtriage
Refinement program	REFMAC refmac _5.5.0071	Depositor
R, $R_{free}$	0.185 , 0.209 0.182 , 0.209	Depositor DCC
$R_{free}$ test set	4591 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.088 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4561	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.47% 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, 0.333 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: 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	0.70	0/1087	0.76	0/1462
1	B	0.75	1/1100 (0.1%)	0.79	0/1482
1	C	0.75	0/979	0.85	2/1318 (0.2%)
1	D	0.74	0/998	0.90	3/1343 (0.2%)
2	E	0.87	0/37	0.61	0/50
2	F	1.01	0/37	0.84	0/50
All	All	0.74	1/4238 (0.0%)	0.82	5/5705 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	17	GLU	CD-OE2	-5.03	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	42[A]	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	D	42[B]	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	D	84	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	C	42[A]	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	42[B]	ARG	NE-CZ-NH2	-5.17	117.71	120.30

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	1053	0	1039	22	0
1	B	1057	0	1050	33	0
1	C	947	0	935	18	0
1	D	963	0	952	25	0
2	E	36	0	29	2	0
2	F	36	0	29	3	0
3	B	12	0	13	0	0
3	C	12	0	12	0	0
3	D	24	0	25	0	0
4	A	107	0	0	3	0
4	B	115	0	0	2	0
4	C	104	0	0	4	0
4	D	92	0	0	2	0
4	F	3	0	0	0	0
All	All	4561	0	4084	81	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.

All (81) 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:B:53[B]:VAL:CG1	1:B:54[B]:PRO:HD2	1.61	1.28
1:B:53[B]:VAL:HG12	1:B:54[B]:PRO:HD2	1.30	1.09
1:B:53[B]:VAL:CG1	1:B:54[B]:PRO:CD	2.34	1.06
1:B:53[B]:VAL:HG13	1:B:54[B]:PRO:HD2	1.34	1.04
1:B:53[B]:VAL:HG12	1:B:54[B]:PRO:CD	1.90	1.02
1:D:26:HIS:CD2	1:D:90:HIS:HD2	1.79	1.01
1:D:26:HIS:HD2	1:D:90:HIS:HD2	0.96	0.92
1:D:26:HIS:HD2	1:D:90:HIS:CD2	1.87	0.92
1:B:53[B]:VAL:HG13	1:B:54[B]:PRO:CD	2.03	0.86
1:A:20[B]:ARG:HG3	4:A:135:HOH:O	1.78	0.84
1:B:40[A]:GLU:OE1	4:B:220:HOH:O	1.94	0.84
1:A:20[B]:ARG:HG2	1:A:43:LEU:HD11	1.62	0.81
1:A:8[B]:LEU:HD23	1:A:98:LEU:HD12	1.65	0.77
4:D:255:HOH:O	2:E:6:ALA:HB2	1.85	0.76
1:A:8[B]:LEU:HD23	1:A:98:LEU:CD1	2.16	0.75
1:B:52[A]:HIS:CE1	1:C:92:LYS:HE3	2.23	0.73
1:D:8[B]:LEU:HD23	1:D:98[B]:LEU:HD12	1.71	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53[B]:VAL:HG12	1:B:54[B]:PRO:N	2.03	0.73
1:A:8[B]:LEU:CD2	1:A:98:LEU:CD1	2.66	0.72
1:B:98[B]:LEU:C	1:B:98[B]:LEU:HD23	2.10	0.72
1:B:53[A]:VAL:HB	1:B:54[A]:PRO:HD2	1.71	0.72
1:D:98[A]:LEU:O	1:D:98[A]:LEU:HD12	1.91	0.70
1:A:103:THR:CB	1:D:42[A]:ARG:HD3	2.23	0.68
1:D:38:LYS:HG3	2:E:4:TRP:O	1.95	0.67
1:B:53[A]:VAL:HB	1:B:54[A]:PRO:CD	2.25	0.67
1:D:76:GLN:HG2	4:D:397:HOH:O	1.94	0.67
1:C:38:LYS:HG3	2:F:4:TRP:O	1.96	0.65
1:D:26:HIS:CD2	1:D:90:HIS:CD2	2.72	0.65
1:B:8[A]:LEU:HD23	1:B:98[A]:LEU:CD1	2.28	0.63
1:B:8[A]:LEU:HD23	1:B:98[A]:LEU:HD12	1.80	0.62
1:B:8[A]:LEU:CD2	1:B:98[A]:LEU:CD1	2.78	0.60
1:D:22:GLU:OE2	1:D:90:HIS:HE1	1.85	0.60
1:A:103:THR:HB	1:D:42[A]:ARG:HD3	1.84	0.60
1:D:98[A]:LEU:C	1:D:98[A]:LEU:HD12	2.22	0.60
1:A:53[B]:VAL:CG1	1:D:92:LYS:HA	2.32	0.59
1:B:16:HIS:HD2	4:B:260:HOH:O	1.85	0.58
1:C:16:HIS:HD2	4:C:237:HOH:O	1.87	0.57
1:B:92:LYS:HE3	1:C:52[B]:HIS:CD2	2.39	0.57
1:A:103:THR:OG1	1:D:42[A]:ARG:HD3	2.06	0.56
1:B:52[A]:HIS:ND1	1:C:92:LYS:HE3	2.21	0.56
1:B:98[B]:LEU:O	1:B:98[B]:LEU:HD23	2.06	0.55
1:B:107:VAL:OXT	2:F:2:ALA:CB	2.55	0.54
1:B:52[A]:HIS:CE1	1:C:88:PHE:HB3	2.43	0.54
1:D:20[A]:ARG:HG3	1:D:43:LEU:HD11	1.90	0.53
1:A:-3:ILE:CD1	1:A:0[A]:ARG:HH11	2.23	0.52
1:D:8[B]:LEU:CD2	1:D:98[B]:LEU:CD1	2.88	0.52
1:B:4[A]:ILE:HD12	1:B:102:VAL:HG22	1.90	0.52
1:A:18[A]:GLN:NE2	1:A:93:TYR:OH	2.42	0.51
1:A:8[B]:LEU:CD2	1:A:98:LEU:HD13	2.40	0.51
1:A:52[B]:HIS:ND1	1:D:92:LYS:HE3	2.26	0.51
1:B:53[A]:VAL:CG1	1:C:92:LYS:HA	2.40	0.51
1:C:82:ASP:OD1	4:C:131:HOH:O	2.20	0.50
1:D:8[B]:LEU:HD23	1:D:98[B]:LEU:CD1	2.40	0.49
1:B:98[B]:LEU:C	1:B:98[B]:LEU:CD2	2.80	0.49
1:C:35:GLY:HA2	1:C:74:GLN:HE21	1.76	0.49
1:B:107:VAL:OXT	2:F:2:ALA:HB1	2.11	0.49
1:C:12:GLU:CG	4:C:402:HOH:O	2.61	0.48
1:B:11:PRO:HD3	1:B:94:PHE:O	2.15	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:GLU:HG3	4:C:402:HOH:O	2.14	0.47
1:B:106:LEU:O	1:B:107:VAL:C	2.53	0.46
1:A:53[B]:VAL:HG12	1:D:92:LYS:HA	1.97	0.46
1:A:52[B]:HIS:CE1	1:D:92:LYS:HE3	2.52	0.45
1:B:52[A]:HIS:ND1	1:C:88:PHE:HB3	2.31	0.45
1:C:36:LEU:HD21	1:C:39:TYR:HB2	1.99	0.45
1:D:50:ASP:N	1:D:50:ASP:OD1	2.45	0.45
1:B:43:LEU:HG	1:C:106:LEU:HD21	1.97	0.45
1:A:76[A]:GLN:HG2	4:A:359:HOH:O	2.17	0.44
1:B:-4:LYS:HZ3	1:B:0:ARG:HH12	1.65	0.44
1:A:40[B]:GLU:OE2	4:A:231:HOH:O	2.20	0.44
1:D:0:ARG:HD3	1:D:70:ALA:O	2.17	0.44
1:A:-3:ILE:HD12	1:A:0[A]:ARG:NH1	2.32	0.44
1:D:11:PRO:HD3	1:D:94:PHE:O	2.18	0.44
1:A:35:GLY:HA2	1:A:74:GLN:NE2	2.33	0.43
1:B:52[A]:HIS:CE1	1:C:92:LYS:CE	2.98	0.43
1:C:98[B]:LEU:N	1:C:98[B]:LEU:HD13	2.33	0.43
1:B:106:LEU:HD21	1:C:43:LEU:HG	2.01	0.43
1:A:106:LEU:O	1:A:107:VAL:C	2.57	0.42
1:D:98[A]:LEU:C	1:D:98[A]:LEU:CD1	2.87	0.42
1:A:106:LEU:HD11	1:D:41:VAL:HG13	2.02	0.41
1:A:11:PRO:HD3	1:A:94:PHE:O	2.21	0.41
1:B:52[A]:HIS:CG	1:C:92:LYS:HE3	2.56	0.41

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	125/116 (108%)	125 (100%)	0	0	100	100
1	B	127/116 (110%)	127 (100%)	0	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	113/116 (97%)	113 (100%)	0	0	100	100
1	D	115/116 (99%)	115 (100%)	0	0	100	100
2	E	3/5 (60%)	3 (100%)	0	0	100	100
2	F	3/5 (60%)	3 (100%)	0	0	100	100
All	All	486/474 (102%)	486 (100%)	0	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	114/103 (111%)	112 (98%)	2 (2%)	59	26
1	B	116/103 (113%)	114 (98%)	2 (2%)	60	28
1	C	102/103 (99%)	99 (97%)	3 (3%)	42	10
1	D	104/103 (101%)	102 (98%)	2 (2%)	57	23
2	E	3/3 (100%)	3 (100%)	0	100	100
2	F	3/3 (100%)	3 (100%)	0	100	100
All	All	442/418 (106%)	433 (98%)	9 (2%)	55	22

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-7	GLN
1	A	106	LEU
1	B	52[A]	HIS
1	B	52[B]	HIS
1	C	5	LEU
1	C	50	ASP
1	C	84	ARG
1	D	0	ARG
1	D	5	LEU

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

Mol	Chain	Res	Type
1	A	74	GLN
1	B	16	HIS
1	C	16	HIS
1	C	74	GLN
1	D	26	HIS
1	D	74	GLN
1	D	90	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	D	108	-	12,12,12	1.91	1 (8%)	14,16,16	2.24	5 (35%)
3	MES	C	201	-	12,12,12	1.97	2 (16%)	14,16,16	1.94	4 (28%)
3	MES	B	201	-	12,12,12	1.59	1 (8%)	14,16,16	1.93	5 (35%)
3	MES	D	201	-	12,12,12	1.67	1 (8%)	14,16,16	2.52	5 (35%)

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	D	108	-	-	3/6/14/14	0/1/1/1
3	MES	C	201	-	-	2/6/14/14	0/1/1/1
3	MES	B	201	-	-	0/6/14/14	0/1/1/1
3	MES	D	201	-	-	0/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	MES	C8-S	5.64	1.85	1.77
3	D	108	MES	C8-S	5.48	1.85	1.77
3	D	201	MES	C8-S	4.50	1.83	1.77
3	B	201	MES	C8-S	4.41	1.83	1.77
3	C	201	MES	O1S-S	2.04	1.51	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	MES	O1S-S-C8	6.58	114.84	106.92
3	B	201	MES	O2S-S-C8	4.94	112.86	106.92
3	D	108	MES	O2S-S-C8	4.31	112.10	106.92
3	D	108	MES	O1-C2-C3	-3.74	103.55	111.80
3	C	201	MES	C7-N4-C3	3.66	120.59	111.23
3	C	201	MES	O3S-S-C8	3.59	111.57	105.77
3	D	201	MES	C7-N4-C5	-3.39	102.57	111.23
3	D	201	MES	O2S-S-C8	-3.24	103.01	106.92
3	D	108	MES	C7-N4-C5	3.18	119.36	111.23
3	D	108	MES	C6-C5-N4	-3.06	105.46	110.10
3	D	201	MES	O3S-S-C8	2.92	110.49	105.77
3	C	201	MES	O1S-S-C8	2.68	110.15	106.92
3	D	108	MES	O3S-S-C8	2.67	110.08	105.77
3	C	201	MES	C7-N4-C5	2.63	117.95	111.23
3	D	201	MES	O3S-S-O1S	-2.59	104.95	111.27
3	B	201	MES	O1-C2-C3	-2.52	106.25	111.80
3	B	201	MES	C7-N4-C3	-2.21	105.57	111.23
3	B	201	MES	O1-C6-C5	-2.19	106.96	111.80
3	B	201	MES	O2S-S-O1S	-2.04	106.91	113.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	108	MES	C7-C8-S-O1S
3	D	108	MES	C7-C8-S-O3S
3	C	201	MES	C7-C8-S-O3S
3	D	108	MES	C7-C8-S-O2S
3	C	201	MES	C7-C8-S-O1S

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](#)

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	116/116 (100%)	-0.05	3 (2%) 56 58	8, 16, 29, 40	0
1	B	115/116 (99%)	-0.08	4 (3%) 44 47	8, 14, 28, 39	0
1	C	109/116 (93%)	-0.21	6 (5%) 25 28	9, 13, 30, 36	0
1	D	109/116 (93%)	-0.13	4 (3%) 41 44	8, 14, 28, 39	0
2	E	5/5 (100%)	2.86	4 (80%) 0 0	22, 23, 30, 32	0
2	F	5/5 (100%)	2.64	2 (40%) 0 0	20, 21, 30, 31	0
All	All	459/474 (96%)	-0.06	23 (5%) 28 31	8, 14, 30, 40	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	VAL	11.6
1	A	107	VAL	10.8
1	D	-1	GLY	6.4
2	F	4	TRP	5.4
2	E	4	TRP	5.3
2	E	5	SER	3.5
1	C	50	ASP	3.3
1	C	0	ARG	3.2
1	D	107	VAL	2.9
1	D	0	ARG	2.9
1	A	-8	PRO	2.8
1	C	-1	GLY	2.8
1	B	106	LEU	2.7
1	C	49	THR	2.6
1	C	107	VAL	2.6
1	B	53[A]	VAL	2.6
2	F	5	SER	2.6
1	A	50	ASP	2.5
2	E	2	ALA	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	50	ASP	2.2
1	B	50	ASP	2.2
1	C	52[A]	HIS	2.1
2	E	6	ALA	2.1

## 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 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MES	D	201	12/12	0.92	0.11	18,20,38,38	0
3	MES	C	201	12/12	0.94	0.09	20,25,34,34	0
3	MES	B	201	12/12	0.94	0.10	19,24,39,39	0
3	MES	D	108	12/12	0.94	0.09	20,24,33,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.