



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 04:52 PM BST

PDB ID : 6ML1  
Title : Structure of the USP15 deubiquitinase domain in complex with an affinity-matured inhibitory Ubv  
Authors : Singer, A.U.; Teyra, J.; Boehmelt, G.; Lenter, M.; Sicheri, F.; Sidhu, S.S.  
Deposited on : 2018-09-26  
Resolution : 1.90 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

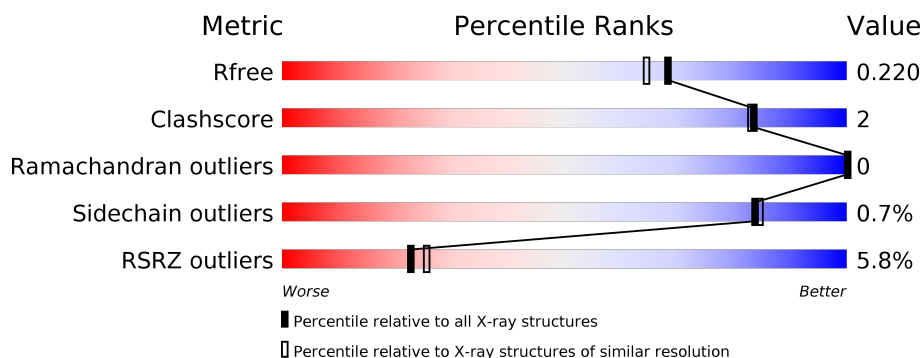
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	349	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>%</span> <span>87%</span> <span>9%</span> </div> </div>
1	B	349	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>%</span> <span>85%</span> <span>7%</span> <span>8%</span> </div> </div>
2	C	92	<div> <div style="width: 23%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>23%</span> <span>92%</span> <span>5%</span> </div> </div>
2	E	92	<div> <div style="width: 16%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>16%</span> <span>82%</span> <span>9%</span> <span>10%</span> </div> </div>
3	G	26	<div> <div style="width: 4%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>4%</span> <span>19%</span> <span>81%</span> </div> </div>

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
9	MES	C	102	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6889 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 Ubiquitin carboxyl-terminal hydrolase 15,Ubiquitin carboxyl-terminal hydrolase 15,Ubiquitin carboxyl-terminal hydrolase 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	2	0
			2547	1646	421	464	16			
1	B	321	Total	C	N	O	S	0	4	0
			2583	1661	425	481	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	SER	-	expression tag	UNP Q9Y4E8
A	271	GLY	-	expression tag	UNP Q9Y4E8
A	272	ALA	-	expression tag	UNP Q9Y4E8
A	273	ALA	-	expression tag	UNP Q9Y4E8
A	274	ALA	-	expression tag	UNP Q9Y4E8
A	872	GLY	-	linker	UNP Q9Y4E8
A	935	SER	-	expression tag	UNP Q9Y4E8
A	936	SER	-	expression tag	UNP Q9Y4E8
A	937	GLY	-	expression tag	UNP Q9Y4E8
B	270	SER	-	expression tag	UNP Q9Y4E8
B	271	GLY	-	expression tag	UNP Q9Y4E8
B	272	ALA	-	expression tag	UNP Q9Y4E8
B	273	ALA	-	expression tag	UNP Q9Y4E8
B	274	ALA	-	expression tag	UNP Q9Y4E8
B	872	GLY	-	linker	UNP Q9Y4E8
B	935	SER	-	expression tag	UNP Q9Y4E8
B	936	SER	-	expression tag	UNP Q9Y4E8
B	937	GLY	-	expression tag	UNP Q9Y4E8

- Molecule 2 is a protein called Ubiquitin variant 15.1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	83	Total 647	C 411	N 111	O 124	S 1	0	0	0
2	C	87	Total 651	C 421	N 107	O 122	S 1	0	1	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ALA	-	insertion	UNP A0A0L7RG06
E	0	ALA	GLY	conflict	UNP A0A0L7RG06
E	2	LEU	GLN	conflict	UNP A0A0L7RG06
E	9	SER	THR	conflict	UNP A0A0L7RG06
E	12	PHE	THR	conflict	UNP A0A0L7RG06
E	14	SER	THR	conflict	UNP A0A0L7RG06
E	19	PRO	ALA	conflict	UNP A0A0L7RG06
E	?	-	ASP	deletion	UNP A0A0L7RG06
E	47	GLY	GLN	conflict	UNP A0A0L7RG06
E	48	LYS	GLN	conflict	UNP A0A0L7RG06
E	51	SER	ILE	conflict	UNP A0A0L7RG06
E	53	TYR	ALA	conflict	UNP A0A0L7RG06
E	54	ARG	GLY	conflict	UNP A0A0L7RG06
E	71	HIS	GLU	conflict	UNP A0A0L7RG06
E	75	GLN	HIS	conflict	UNP A0A0L7RG06
E	77	LEU	VAL	conflict	UNP A0A0L7RG06
E	78	VAL	LEU	conflict	UNP A0A0L7RG06
E	79	ILE	ARG	conflict	UNP A0A0L7RG06
E	80	SER	LEU	conflict	UNP A0A0L7RG06
E	83	ILE	-	expression tag	UNP A0A0L7RG06
E	84	LEU	-	expression tag	UNP A0A0L7RG06
E	85	TYR	-	expression tag	UNP A0A0L7RG06
E	86	GLY	-	expression tag	UNP A0A0L7RG06
E	87	SER	-	expression tag	UNP A0A0L7RG06
E	88	SER	-	expression tag	UNP A0A0L7RG06
E	89	GLY	-	expression tag	UNP A0A0L7RG06
C	-1	ALA	-	insertion	UNP A0A0L7RG06
C	0	ALA	GLY	conflict	UNP A0A0L7RG06
C	2	LEU	GLN	conflict	UNP A0A0L7RG06
C	9	SER	THR	conflict	UNP A0A0L7RG06
C	12	PHE	THR	conflict	UNP A0A0L7RG06
C	14	SER	THR	conflict	UNP A0A0L7RG06
C	19	PRO	ALA	conflict	UNP A0A0L7RG06
C	?	-	ASP	deletion	UNP A0A0L7RG06
C	47	GLY	GLN	conflict	UNP A0A0L7RG06

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Chain	Residue	Modelled	Actual	Comment	Reference
C	48	LYS	GLN	conflict	UNP A0A0L7RG06
C	51	SER	ILE	conflict	UNP A0A0L7RG06
C	53	TYR	ALA	conflict	UNP A0A0L7RG06
C	54	ARG	GLY	conflict	UNP A0A0L7RG06
C	71	HIS	GLU	conflict	UNP A0A0L7RG06
C	75	GLN	HIS	conflict	UNP A0A0L7RG06
C	77	LEU	VAL	conflict	UNP A0A0L7RG06
C	78	VAL	LEU	conflict	UNP A0A0L7RG06
C	79	ILE	ARG	conflict	UNP A0A0L7RG06
C	80	SER	LEU	conflict	UNP A0A0L7RG06
C	83	ILE	-	expression tag	UNP A0A0L7RG06
C	84	LEU	-	expression tag	UNP A0A0L7RG06
C	85	TYR	-	expression tag	UNP A0A0L7RG06
C	86	GLY	-	expression tag	UNP A0A0L7RG06
C	87	SER	-	expression tag	UNP A0A0L7RG06
C	88	SER	-	expression tag	UNP A0A0L7RG06
C	89	GLY	-	expression tag	UNP A0A0L7RG06

- Molecule 3 is a protein called Proteolyzed N-terminal tag of Ubv.15.1a construct.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	5	Total	C	N	O	0	0	0
			40	24	11	5			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	2	Total	Ca	0	0
			2	2		
4	C	1	Total	Ca	0	0
			1	1		

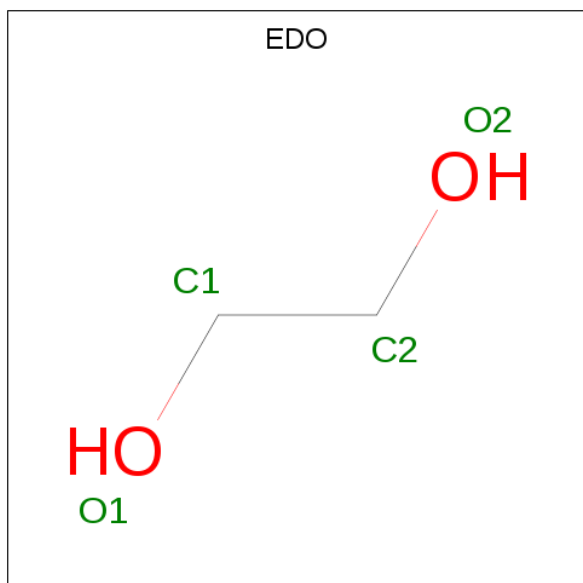
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Na	0	0
			2	2		
6	A	2	Total	Na	0	0
			2	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).

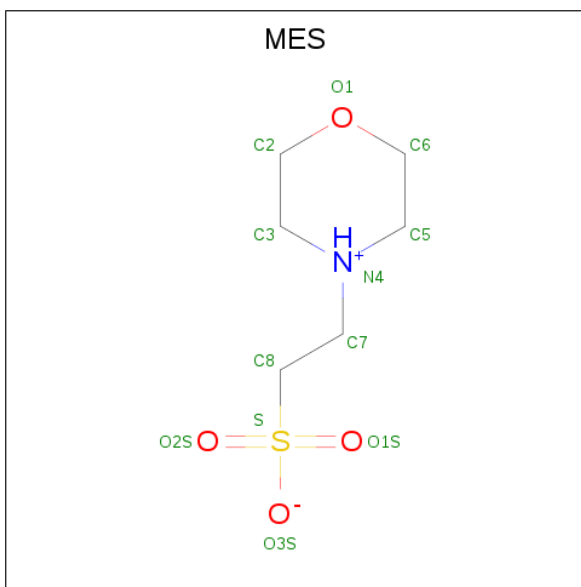


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	1
			2	2		

- Molecule 9 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
9	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is water.

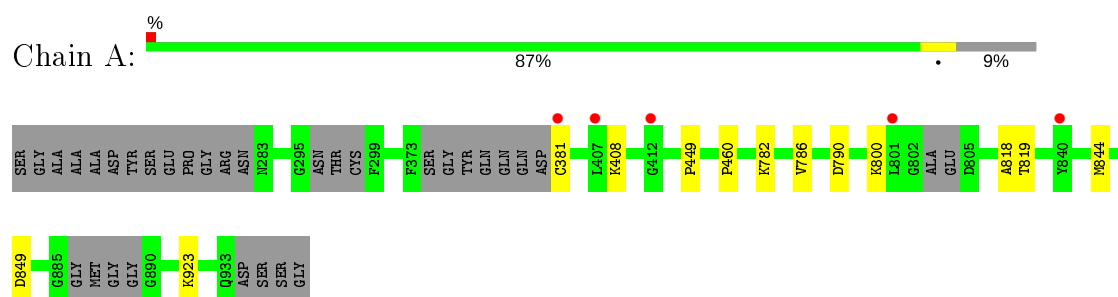
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	155	Total	O	0	2
			157	157		
10	B	175	Total	O	0	2
			177	177		
10	E	33	Total	O	0	0
			33	33		
10	C	23	Total	O	0	0
			23	23		
10	G	3	Total	O	0	0
			3	3		



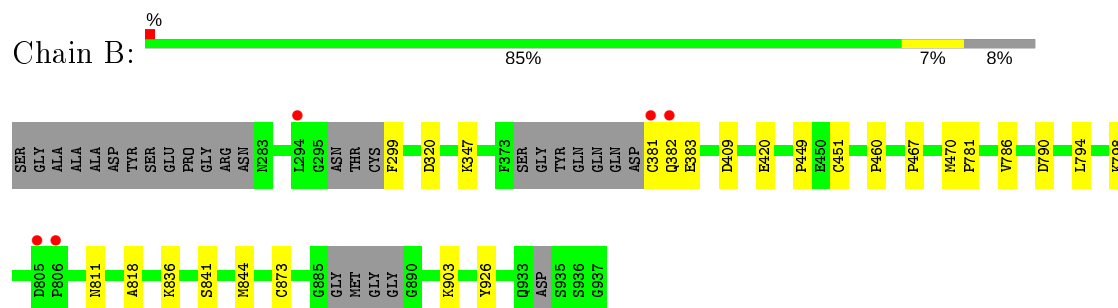
### 3 Residue-property plots [i](#)

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.

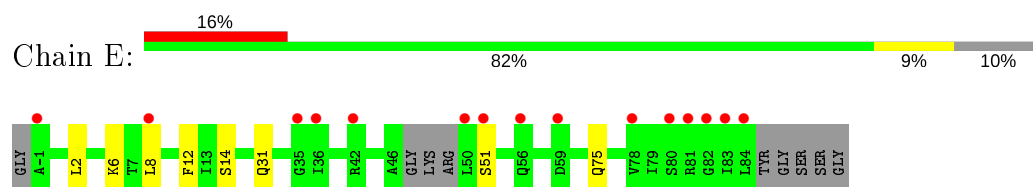
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15,Ubiquitin carboxyl-terminal hydrolase 15,Ubiquitin carboxyl-terminal hydrolase 15



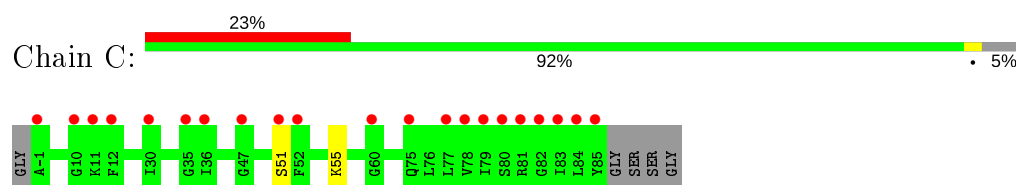
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15,Ubiquitin carboxyl-terminal hydrolase 15,Ubiquitin carboxyl-terminal hydrolase 15



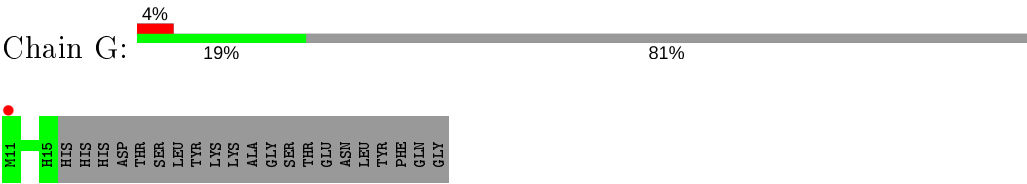
- Molecule 2: Ubiquitin variant 15.1a



- Molecule 2: Ubiquitin variant 15.1a



- Molecule 3: Proteolyzed N-terminal tag of Ubv.15.1a construct



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.77Å 115.29Å 95.32Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	49.32 – 1.90 49.32 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.32-1.90) 98.0 (49.32-1.90)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.189 , 0.220 0.189 , 0.220	Depositor DCC
$R_{free}$ test set	3425 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 59.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: ZN, CL, NA, CA, EDO, 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	0.40	0/2613	0.54	0/3539
1	B	0.40	0/2648	0.55	0/3586
2	C	0.36	0/661	0.49	0/894
2	E	0.32	0/654	0.51	0/880
3	G	0.22	0/42	0.45	0/56
All	All	0.39	0/6618	0.54	0/8955

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	2547	0	2466	7	0
1	B	2583	0	2471	18	0
2	C	651	0	638	1	0
2	E	647	0	660	5	0
3	G	40	0	27	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	B	4	0	6	0	0
8	B	2	0	0	1	0
9	C	12	0	12	0	0
10	A	157	0	0	2	0
10	B	177	0	0	4	0
10	C	23	0	0	0	0
10	E	33	0	0	0	0
10	G	3	0	0	0	0
All	All	6889	0	6280	30	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 2.

All (30) 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:420:GLU:OE1	10:B:1101:HOH:O	1.97	0.82
1:B:460:PRO:O	2:E:51:SER:HB2	1.91	0.69
2:E:6:LYS:O	2:E:75:GLN:NE2	2.27	0.68
1:A:449:PRO:HD3	1:A:818:ALA:HA	1.78	0.65
1:A:782:LYS:HE3	1:A:849:ASP:OD1	1.98	0.63
2:E:2:LEU:HD11	2:E:14:SER:HB2	1.81	0.63
1:B:409[B]:ASP:OD1	10:B:1102:HOH:O	2.16	0.61
1:B:381:CYS:SG	1:B:382:GLN:N	2.74	0.61
1:B:299:PHE:CE2	1:B:382:GLN:HA	2.36	0.60
1:B:449:PRO:HD3	1:B:818:ALA:HA	1.85	0.58
1:B:873:CYS:SG	10:B:1263:HOH:O	2.58	0.56
1:B:798:LYS:HD2	1:B:798:LYS:H	1.73	0.54
8:B:1004[A]:CL:CL	10:B:1137:HOH:O	2.56	0.52
1:A:786:VAL:HG22	1:A:790:ASP:HB2	1.93	0.49
1:B:841:SER:H	1:B:844:MET:HE3	1.79	0.47
1:B:382:GLN:HB2	1:B:926:TYR:CE1	2.50	0.46
1:A:460:PRO:O	2:C:51:SER:HB2	2.16	0.46
1:A:800:LYS:HA	1:A:819:THR:HA	1.98	0.45
1:B:841:SER:HB2	1:B:844:MET:HE2	1.98	0.45
1:B:786:VAL:HG22	1:B:790:ASP:HB2	1.97	0.45
1:A:923:LYS:NZ	10:A:1104:HOH:O	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ASP:OD1	1:B:347:LYS:NZ	2.33	0.44
1:A:844:MET:HA	10:A:1128:HOH:O	2.18	0.42
1:B:467:PRO:HG2	1:B:794:LEU:HB3	2.01	0.42
1:B:451:CYS:SG	1:B:811:ASN:ND2	2.82	0.42
1:B:470:MET:HA	1:B:781:PRO:C	2.39	0.42
1:B:383:GLU:HG2	1:B:383:GLU:H	1.68	0.42
2:E:8:LEU:HA	2:E:8:LEU:HD23	1.76	0.41
1:B:903:LYS:HB3	1:B:903:LYS:HE2	1.78	0.41
2:E:6:LYS:HD2	2:E:12:PHE:CZ	2.56	0.40

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	308/349 (88%)	305 (99%)	3 (1%)	0	100	100
1	B	315/349 (90%)	307 (98%)	8 (2%)	0	100	100
2	C	86/92 (94%)	84 (98%)	2 (2%)	0	100	100
2	E	79/92 (86%)	79 (100%)	0	0	100	100
3	G	3/26 (12%)	3 (100%)	0	0	100	100
All	All	791/908 (87%)	778 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	276/306 (90%)	274 (99%)	2 (1%)	84	84
1	B	279/306 (91%)	278 (100%)	1 (0%)	91	91
2	C	66/80 (82%)	65 (98%)	1 (2%)	65	62
2	E	71/80 (89%)	70 (99%)	1 (1%)	67	65
3	G	3/22 (14%)	3 (100%)	0	100	100
All	All	695/794 (88%)	690 (99%)	5 (1%)	84	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	CYS
1	A	408	LYS
1	B	836	LYS
2	E	31	GLN
2	C	55	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	883	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	$\# Z  > 2$
7	EDO	B	1003	-	3,3,3	0.51	0	2,2,2	0.48	0
9	MES	C	102	-	12,12,12	2.27	1 (8%)	14,16,16	2.42	6 (42%)

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
7	EDO	B	1003	-	-	0/1/1/1	-
9	MES	C	102	-	-	2/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	102	MES	C8-S	-7.55	1.66	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	102	MES	C5-N4-C3	5.16	120.45	108.83
9	C	102	MES	O3S-S-C8	3.58	111.56	105.77
9	C	102	MES	C7-N4-C3	3.29	119.65	111.23
9	C	102	MES	C7-N4-C5	2.90	118.64	111.23
9	C	102	MES	C6-C5-N4	-2.45	106.39	110.10
9	C	102	MES	C2-C3-N4	-2.43	106.41	110.10

There are no chirality outliers.

All (2) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
9	C	102	MES	N4-C7-C8-S
9	C	102	MES	C8-C7-N4-C3

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	316/349 (90%)	0.09	5 (1%) 72 74	16, 31, 58, 74	0
1	B	321/349 (91%)	0.08	5 (1%) 72 74	17, 31, 57, 77	0
2	C	87/92 (94%)	1.15	21 (24%) 0 0	29, 49, 66, 77	0
2	E	83/92 (90%)	1.02	15 (18%) 1 1	26, 46, 63, 80	0
3	G	5/26 (19%)	1.14	1 (20%) 1 1	41, 43, 47, 63	0
All	All	812/908 (89%)	0.30	47 (5%) 23 25	16, 34, 61, 80	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	85	TYR	6.9
2	C	83	ILE	5.1
2	C	84	LEU	4.8
2	E	81	ARG	4.6
2	E	80	SER	4.3
2	C	52[A]	PHE	4.3
2	E	82	GLY	3.9
1	B	382	GLN	3.6
2	C	36	ILE	3.5
2	E	8	LEU	3.3
2	C	78	VAL	3.3
2	C	30	ILE	3.3
2	E	35	GLY	3.1
1	B	294	LEU	3.0
2	E	83	ILE	3.0
2	E	50	LEU	3.0
2	C	51	SER	2.9
2	C	12	PHE	2.9
2	E	-1	ALA	2.9
2	E	36	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	801	LEU	2.8
1	A	407	LEU	2.7
2	C	47	GLY	2.7
2	E	78	VAL	2.7
2	C	-1	ALA	2.6
1	B	381	CYS	2.6
1	B	806	PRO	2.5
3	G	11	MET	2.4
2	C	77	LEU	2.4
2	C	81	ARG	2.4
2	C	80	SER	2.4
2	C	75	GLN	2.4
2	E	59	ASP	2.3
2	C	82	GLY	2.3
2	E	51	SER	2.3
1	A	840	TYR	2.3
2	C	60	GLY	2.3
1	A	412	GLY	2.2
2	C	35	GLY	2.2
2	C	11	LYS	2.2
2	E	56	GLN	2.2
2	C	79	ILE	2.1
1	B	805	ASP	2.1
2	C	10	GLY	2.1
2	E	84	LEU	2.1
1	A	381	CYS	2.0
2	E	42	ARG	2.0

## 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 monosaccharides 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(Å <sup>2</sup> )	Q<0.9
9	MES	C	102	12/12	0.62	0.42	70,87,99,109	0
8	CL	B	1004[A]	1/1	0.86	0.19	47,47,47,47	1
8	CL	B	1004[B]	1/1	0.86	0.19	37,37,37,37	1
7	EDO	B	1003	4/4	0.88	0.12	45,47,47,52	0
4	CA	B	1001	1/1	0.92	0.05	62,62,62,62	0
6	NA	B	1006	1/1	0.94	0.13	45,45,45,45	0
4	CA	C	101	1/1	0.94	0.11	62,62,62,62	0
6	NA	A	1004	1/1	0.94	0.09	50,50,50,50	0
5	ZN	B	1002	1/1	0.98	0.08	39,39,39,39	0
5	ZN	A	1003	1/1	0.98	0.06	47,47,47,47	0
4	CA	A	1002	1/1	0.99	0.04	31,31,31,31	0
6	NA	A	1005	1/1	0.99	0.08	27,27,27,27	0
4	CA	A	1001	1/1	0.99	0.12	19,19,19,19	0
6	NA	B	1005	1/1	0.99	0.10	28,28,28,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.