



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:17 am BST

PDB ID : 4I0X  
Title : Crystal structure of the Mycobacterium abscessus EsxEF (Mab\_3112-Mab\_3113) complex  
Authors : Arbing, M.A.; Chan, S.; Lu, J.; Kuo, E.; Harris, L.; Eisenberg, D.; Integrated Center for Structure and Function Innovation (ISFI); TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2012-11-19  
Resolution : 1.96 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 : 2.11  
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

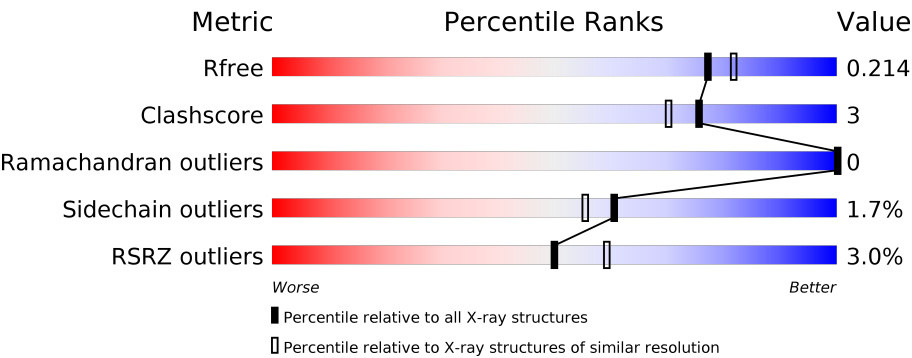
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	94	<div><div>3%</div><div><div></div><div>76%</div><div></div><div>20%</div></div><div></div></div>
1	C	94	<div><div>2%</div><div><div></div><div>78%</div><div></div><div>20%</div></div><div></div></div>
1	E	94	<div><div>%</div><div><div></div><div>67%</div><div></div><div>29%</div></div><div></div></div>
1	G	94	<div><div>%</div><div><div></div><div>68%</div><div></div><div>28%</div></div><div></div></div>
1	I	94	<div><div>3%</div><div><div></div><div>78%</div><div></div><div>19%</div></div><div></div></div>
1	K	94	<div><div>3%</div><div><div></div><div>74%</div><div>7%</div><div>18%</div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	B	103	<div><div><div></div><div></div><div></div></div><div>2%71%10%19%</div></div>
2	D	103	<div><div><div></div><div></div><div></div></div><div>2%75%6%19%</div></div>
2	F	103	<div><div><div></div><div></div><div></div></div><div>5%73%9%17%</div></div>
2	H	103	<div><div><div></div><div></div><div></div></div><div>3%68%6%26%</div></div>
2	J	103	<div><div><div></div><div></div><div></div></div><div>2%64%10%26%</div></div>
2	L	103	<div><div><div></div><div></div><div></div></div><div>%78%20%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14032 atoms, of which 6636 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 ESAT-6-like protein MAB\_3112.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	75	Total	C	H	N	O	S	0	0	0
			1070	341	517	96	114	2			
1	C	75	Total	C	H	N	O	S	0	0	0
			1070	341	517	96	114	2			
1	E	67	Total	C	H	N	O	S	0	0	0
			976	310	475	87	102	2			
1	G	68	Total	C	H	N	O	S	0	0	0
			988	314	479	88	105	2			
1	I	76	Total	C	H	N	O	S	0	0	0
			1090	347	529	97	115	2			
1	K	77	Total	C	H	N	O	S	0	0	0
			1098	350	530	100	116	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP B1MD68
A	23	ASN	SER	engineered mutation	UNP B1MD68
A	37	LYS	ARG	engineered mutation	UNP B1MD68
A	75	ALA	VAL	engineered mutation	UNP B1MD68
A	93	ASP	GLY	engineered mutation	UNP B1MD68
C	0	SER	-	EXPRESSION TAG	UNP B1MD68
C	23	ASN	SER	engineered mutation	UNP B1MD68
C	37	LYS	ARG	engineered mutation	UNP B1MD68
C	75	ALA	VAL	engineered mutation	UNP B1MD68
C	93	ASP	GLY	engineered mutation	UNP B1MD68
E	0	SER	-	EXPRESSION TAG	UNP B1MD68
E	23	ASN	SER	engineered mutation	UNP B1MD68
E	37	LYS	ARG	engineered mutation	UNP B1MD68
E	75	ALA	VAL	engineered mutation	UNP B1MD68
E	93	ASP	GLY	engineered mutation	UNP B1MD68
G	0	SER	-	EXPRESSION TAG	UNP B1MD68
G	23	ASN	SER	engineered mutation	UNP B1MD68

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Chain	Residue	Modelled	Actual	Comment	Reference
G	37	LYS	ARG	engineered mutation	UNP B1MD68
G	75	ALA	VAL	engineered mutation	UNP B1MD68
G	93	ASP	GLY	engineered mutation	UNP B1MD68
I	0	SER	-	EXPRESSION TAG	UNP B1MD68
I	23	ASN	SER	engineered mutation	UNP B1MD68
I	37	LYS	ARG	engineered mutation	UNP B1MD68
I	75	ALA	VAL	engineered mutation	UNP B1MD68
I	93	ASP	GLY	engineered mutation	UNP B1MD68
K	0	SER	-	EXPRESSION TAG	UNP B1MD68
K	23	ASN	SER	engineered mutation	UNP B1MD68
K	37	LYS	ARG	engineered mutation	UNP B1MD68
K	75	ALA	VAL	engineered mutation	UNP B1MD68
K	93	ASP	GLY	engineered mutation	UNP B1MD68

- Molecule 2 is a protein called ESAT-6-like protein MAB\_3113.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	83	Total	C	H	N	O	S	0	0	0
			1264	404	611	117	130	2			
2	D	83	Total	C	H	N	O	S	0	0	0
			1260	402	610	117	129	2			
2	F	85	Total	C	H	N	O	S	0	0	0
			1278	405	618	117	136	2			
2	H	76	Total	C	H	N	O	S	0	0	0
			1161	364	566	110	119	2			
2	J	76	Total	C	H	N	O	S	0	0	0
			1162	368	565	109	118	2			
2	L	82	Total	C	H	N	O	S	0	0	0
			1249	399	605	116	127	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ALA	PRO	engineered mutation	UNP B1MD69
B	51	ALA	THR	engineered mutation	UNP B1MD69
B	60	GLN	GLU	engineered mutation	UNP B1MD69
B	77	SER	ASN	engineered mutation	UNP B1MD69
D	2	ALA	PRO	engineered mutation	UNP B1MD69
D	51	ALA	THR	engineered mutation	UNP B1MD69
D	60	GLN	GLU	engineered mutation	UNP B1MD69
D	77	SER	ASN	engineered mutation	UNP B1MD69
F	2	ALA	PRO	engineered mutation	UNP B1MD69

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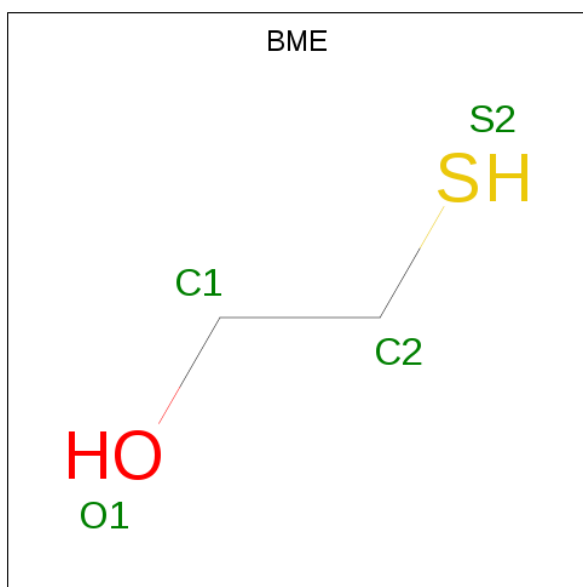
Chain	Residue	Modelled	Actual	Comment	Reference
F	51	ALA	THR	engineered mutation	UNP B1MD69
F	60	GLN	GLU	engineered mutation	UNP B1MD69
F	77	SER	ASN	engineered mutation	UNP B1MD69
H	2	ALA	PRO	engineered mutation	UNP B1MD69
H	51	ALA	THR	engineered mutation	UNP B1MD69
H	60	GLN	GLU	engineered mutation	UNP B1MD69
H	77	SER	ASN	engineered mutation	UNP B1MD69
J	2	ALA	PRO	engineered mutation	UNP B1MD69
J	51	ALA	THR	engineered mutation	UNP B1MD69
J	60	GLN	GLU	engineered mutation	UNP B1MD69
J	77	SER	ASN	engineered mutation	UNP B1MD69
L	2	ALA	PRO	engineered mutation	UNP B1MD69
L	51	ALA	THR	engineered mutation	UNP B1MD69
L	60	GLN	GLU	engineered mutation	UNP B1MD69
L	77	SER	ASN	engineered mutation	UNP B1MD69

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is water.

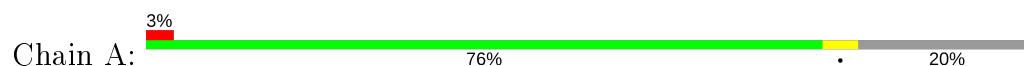
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	34	Total 34	O 34	0	0
6	B	32	Total 32	O 32	0	0
6	C	34	Total 34	O 34	0	0
6	D	40	Total 40	O 40	0	0
6	E	23	Total 23	O 23	0	0
6	F	22	Total 22	O 22	0	0
6	G	25	Total 25	O 25	0	0
6	H	23	Total 23	O 23	0	0
6	I	30	Total 30	O 30	0	0
6	J	18	Total 18	O 18	0	0
6	K	30	Total 30	O 30	0	0
6	L	26	Total 26	O 26	0	0



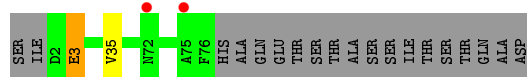
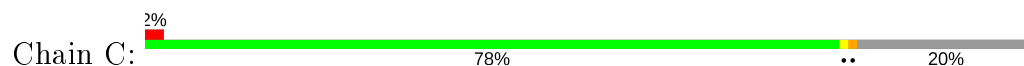
### 3 Residue-property plots [i](#)

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.

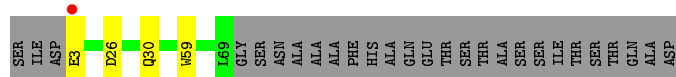
- Molecule 1: ESAT-6-like protein MAB\_3112



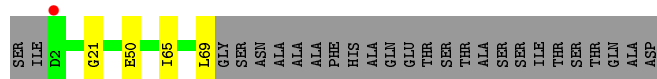
- Molecule 1: ESAT-6-like protein MAB\_3112



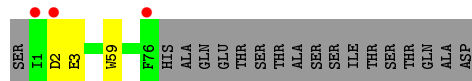
- Molecule 1: ESAT-6-like protein MAB\_3112



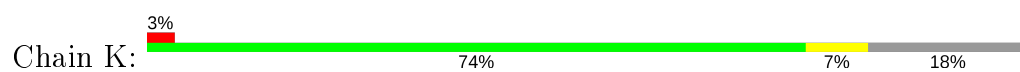
- Molecule 1: ESAT-6-like protein MAB\_3112



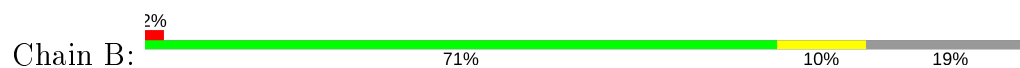
- Molecule 1: ESAT-6-like protein MAB\_3112



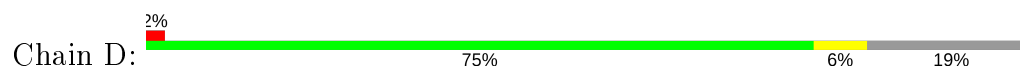
- Molecule 1: ESAT-6-like protein MAB\_3112



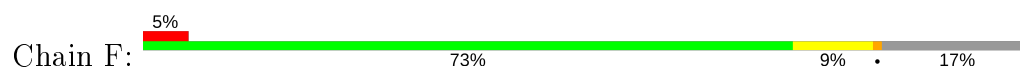
- Molecule 2: ESAT-6-like protein MAB\_3113



- Molecule 2: ESAT-6-like protein MAB\_3113



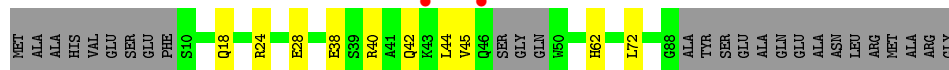
- Molecule 2: ESAT-6-like protein MAB\_3113



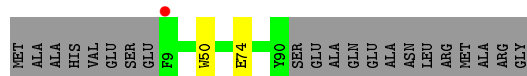
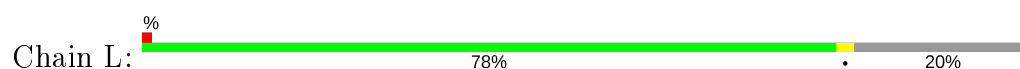
- Molecule 2: ESAT-6-like protein MAB\_3113



- Molecule 2: ESAT-6-like protein MAB\_3113



- Molecule 2: ESAT-6-like protein MAB\_3113



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.60 Å 74.06 Å 84.42 Å 114.57° 103.28° 95.52°	Depositor
Resolution (Å)	20.00 – 1.96 20.00 – 1.96	Depositor EDS
% Data completeness (in resolution range)	93.4 (20.00-1.96) 93.4 (20.00-1.96)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.96 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.159 , 0.213 0.161 , 0.214	Depositor DCC
$R_{free}$ test set	6711 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.51 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,h+k+l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.79% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, BME

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	0.61	0/562	0.62	0/760
1	C	0.63	0/562	0.64	0/760
1	E	0.58	0/509	0.61	0/688
1	G	0.52	0/517	0.59	0/699
1	I	0.56	0/570	0.58	0/771
1	K	0.60	0/578	0.63	0/782
2	B	0.65	0/665	0.66	0/895
2	D	0.62	0/662	0.61	0/891
2	F	0.55	0/669	0.61	0/898
2	H	0.54	0/604	0.62	0/813
2	J	0.61	0/606	0.64	0/814
2	L	0.59	0/656	0.58	0/883
All	All	0.59	0/7160	0.62	0/9654

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

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	553	517	517	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	553	517	517	4	0
1	E	501	475	475	1	0
1	G	509	479	479	6	0
1	I	561	529	531	2	0
1	K	568	530	529	6	0
2	B	653	611	608	7	0
2	D	650	610	607	6	0
2	F	660	618	613	6	0
2	H	595	566	562	6	0
2	J	597	565	562	7	1
2	L	644	605	602	1	0
3	B	5	0	0	0	0
4	B	4	6	6	1	0
5	C	6	8	8	0	0
6	A	34	0	0	1	0
6	B	32	0	0	0	0
6	C	34	0	0	0	0
6	D	40	0	0	1	0
6	E	23	0	0	0	0
6	F	22	0	0	1	0
6	G	25	0	0	0	0
6	H	23	0	0	0	0
6	I	30	0	0	0	0
6	J	18	0	0	1	0
6	K	30	0	0	0	0
6	L	26	0	0	0	0
All	All	7396	6636	6616	42	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (42) 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:C:35:VAL:CG2	2:D:12:ASP:OD1	2.50	0.60
2:B:88:GLY:HA3	1:G:21:GLY:HA2	1.84	0.59
1:I:3:GLU:CB	2:J:44:LEU:HD21	2.33	0.58
2:H:67:ASP:OD1	2:H:70:ARG:NH2	2.37	0.58
1:I:3:GLU:HB3	2:J:44:LEU:HD21	1.86	0.58
2:J:38:GLU:OE1	2:J:62:HIS:CD2	2.58	0.56
1:C:35:VAL:HG21	2:D:12:ASP:OD1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:GLU:CD	1:C:3:GLU:H	2.11	0.54
1:G:50:GLU:HG3	2:H:71:GLU:HG2	1.90	0.54
2:B:90:TYR:O	4:B:202:BME:S2	2.67	0.53
2:J:40:ARG:NH1	6:J:204:HOH:O	2.40	0.53
2:F:96:ALA:CB	1:K:2:ASP:HB2	2.39	0.52
1:A:35:VAL:HG22	6:A:119:HOH:O	2.11	0.51
1:K:7:LEU:HD23	1:K:69:LEU:CD1	2.40	0.51
2:D:18:GLN:OE1	2:D:22:ARG:NH2	2.44	0.50
1:K:26:ASP:O	1:K:30:GLN:HG2	2.11	0.50
2:F:7:SER:HB3	6:F:219:HOH:O	2.12	0.48
1:C:35:VAL:HG23	2:D:12:ASP:OD1	2.13	0.48
1:K:7:LEU:HD23	1:K:69:LEU:HD13	1.96	0.48
1:A:53:ASP:OD2	1:A:57:LYS:HE3	2.14	0.48
2:J:24:ARG:O	2:J:28:GLU:HG2	2.16	0.46
1:G:65:ILE:HD13	2:H:58:TYR:HA	1.98	0.46
2:B:69:ALA:O	2:B:73:VAL:HG13	2.16	0.46
2:B:70:ARG:O	2:B:73:VAL:HG22	2.16	0.45
1:G:65:ILE:HG13	1:G:69:LEU:HD22	1.97	0.45
2:D:62:HIS:HD2	6:D:201:HOH:O	1.99	0.44
1:A:9:LYS:NZ	2:F:60:GLN:OE1	2.40	0.44
2:J:72:LEU:HD23	2:J:72:LEU:C	2.38	0.44
2:B:9:PHE:CZ	2:B:87:HIS:ND1	2.86	0.43
2:F:27:LYS:O	2:F:31:THR:HG23	2.17	0.43
2:J:42:GLN:O	2:J:45:VAL:HG12	2.18	0.43
1:G:65:ILE:CD1	2:H:58:TYR:HA	2.50	0.41
1:E:26:ASP:O	1:E:30:GLN:HG2	2.21	0.41
2:B:9:PHE:HZ	2:B:87:HIS:ND1	2.18	0.41
2:F:72:LEU:HD23	2:F:72:LEU:C	2.40	0.41
2:B:72:LEU:HD23	2:B:72:LEU:C	2.42	0.40
2:D:72:LEU:C	2:D:72:LEU:HD23	2.41	0.40
1:G:50:GLU:CG	2:H:71:GLU:HG2	2.52	0.40
2:F:81:GLU:OE1	2:F:94:GLN:OE1	2.40	0.40
2:H:34:LEU:O	2:H:38:GLU:HG3	2.22	0.40
1:K:35:VAL:O	1:K:35:VAL:HG22	2.20	0.40
1:K:50:GLU:OE2	2:L:74:GLU:OE1	2.39	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:18:GLN:HE22	2:J:45:VAL:O[1_655]	1.52	0.08

## 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	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
1	C	73/94 (78%)	73 (100%)	0	0	100	100
1	E	65/94 (69%)	65 (100%)	0	0	100	100
1	G	66/94 (70%)	66 (100%)	0	0	100	100
1	I	74/94 (79%)	74 (100%)	0	0	100	100
1	K	75/94 (80%)	75 (100%)	0	0	100	100
2	B	81/103 (79%)	80 (99%)	1 (1%)	0	100	100
2	D	81/103 (79%)	78 (96%)	3 (4%)	0	100	100
2	F	81/103 (79%)	80 (99%)	1 (1%)	0	100	100
2	H	74/103 (72%)	74 (100%)	0	0	100	100
2	J	72/103 (70%)	71 (99%)	1 (1%)	0	100	100
2	L	80/103 (78%)	80 (100%)	0	0	100	100
All	All	895/1182 (76%)	888 (99%)	7 (1%)	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	54/70 (77%)	54 (100%)	0	100	100
1	C	54/70 (77%)	53 (98%)	1 (2%)	57	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	50/70 (71%)	48 (96%)	2 (4%)	31	19
1	G	51/70 (73%)	51 (100%)	0	100	100
1	I	55/70 (79%)	53 (96%)	2 (4%)	35	23
1	K	55/70 (79%)	55 (100%)	0	100	100
2	B	63/77 (82%)	61 (97%)	2 (3%)	39	27
2	D	63/77 (82%)	62 (98%)	1 (2%)	62	58
2	F	64/77 (83%)	61 (95%)	3 (5%)	26	13
2	H	58/77 (75%)	58 (100%)	0	100	100
2	J	58/77 (75%)	58 (100%)	0	100	100
2	L	62/77 (80%)	61 (98%)	1 (2%)	62	58
All	All	687/882 (78%)	675 (98%)	12 (2%)	60	55

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	27	LYS
2	B	42	GLN
1	C	3	GLU
2	D	27	LYS
1	E	3	GLU
1	E	59	TRP
2	F	7	SER
2	F	63	LYS
2	F	77	SER
1	I	2	ASP
1	I	59	TRP
2	L	50	TRP

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

Mol	Chain	Res	Type
2	D	62	HIS
2	D	87	HIS
2	J	87	HIS
2	L	62	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 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	$\# Z  > 2$
4	BME	B	202	-	3,3,3	0.25	0	1,2,2	0.43	0
3	SO4	B	201	-	4,4,4	0.17	0	6,6,6	0.28	0
5	GOL	C	101	-	5,5,5	0.41	0	5,5,5	0.30	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
4	BME	B	202	-	-	0/1/1/1	-
5	GOL	C	101	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	101	GOL	O1-C1-C2-O2
5	C	101	GOL	O1-C1-C2-C3
5	C	101	GOL	C1-C2-C3-O3
5	C	101	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	BME	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	75/94 (79%)	-0.01	3 (4%) 38 48	12, 18, 40, 52	0
1	C	75/94 (79%)	0.00	2 (2%) 54 63	11, 19, 38, 45	0
1	E	67/94 (71%)	0.07	1 (1%) 73 81	11, 21, 33, 50	0
1	G	68/94 (72%)	-0.19	1 (1%) 73 81	14, 24, 38, 46	0
1	I	76/94 (80%)	0.09	3 (3%) 39 49	12, 20, 43, 59	0
1	K	77/94 (81%)	-0.04	3 (3%) 39 49	12, 21, 42, 57	0
2	B	83/103 (80%)	0.00	2 (2%) 59 68	11, 22, 36, 53	0
2	D	83/103 (80%)	0.01	2 (2%) 59 68	13, 21, 39, 44	0
2	F	85/103 (82%)	0.33	5 (5%) 22 30	13, 26, 47, 58	0
2	H	76/103 (73%)	0.17	3 (3%) 39 49	17, 31, 47, 58	0
2	J	76/103 (73%)	0.19	2 (2%) 56 65	14, 26, 53, 66	0
2	L	82/103 (79%)	-0.12	1 (1%) 79 84	14, 23, 34, 44	0
All	All	923/1182 (78%)	0.05	28 (3%) 50 59	11, 23, 43, 66	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	76	PHE	6.4
2	F	96	ALA	4.4
1	K	72	ASN	4.1
1	C	75	ALA	4.1
2	J	43	LYS	3.9
1	I	1	ILE	3.8
2	H	14	ASP	3.8
1	A	74	ALA	3.6
2	F	43	LYS	3.6
1	K	73	ALA	3.5
1	A	75	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	J	46	GLN	3.4
1	C	72	ASN	3.3
2	B	8	GLU	3.2
2	F	95	GLU	3.2
2	L	9	PHE	3.2
1	G	2	ASP	3.0
1	E	3	GLU	2.9
1	A	2	ASP	2.9
2	D	90	TYR	2.8
1	K	2	ASP	2.8
2	H	13	LEU	2.7
1	I	2	ASP	2.6
2	F	51	ALA	2.6
2	D	10	SER	2.5
2	B	46	GLN	2.4
2	F	45	VAL	2.3
2	H	47	SER	2.3

## 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 ⓘ

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. 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
4	BME	B	202	4/4	0.80	0.23	33,39,71,85	0
5	GOL	C	101	6/6	0.87	0.23	37,44,51,53	0
3	SO4	B	201	5/5	0.98	0.08	36,39,42,50	0

## 6.5 Other polymers

There are no such residues in this entry.