



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:12 PM UTC

PDB ID : 8HQ9 / pdb_00008hq9
Title : Crystal structure of the MlaD domain of the MlaD protein from Escherichia coli (Form II)
Authors : Dutta, A.; Kanaujia, S.P.
Deposited on : 2022-12-13
Resolution : 2.70 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

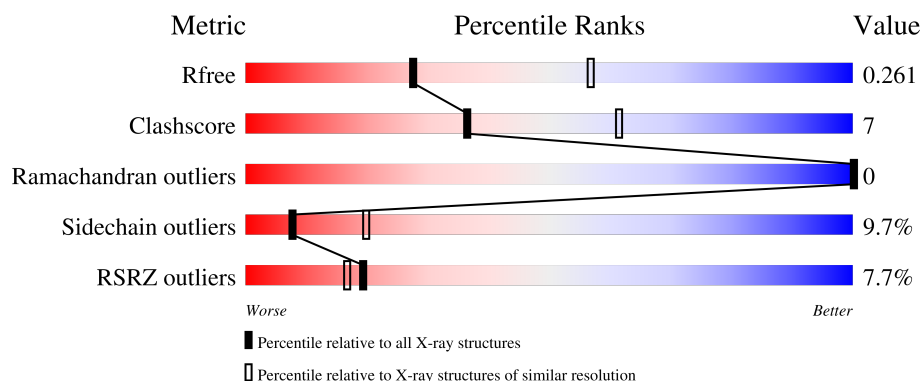
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	162	4% 46% 16% • 36%
1	B	162	6% 49% 14% •• 36%
1	C	162	5% 48% 15% •• 33%
1	D	162	4% 48% 14% • 35%
1	E	162	7% 49% 15% • 33%

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Mol	Chain	Length	Quality of chain
1	F	162	6% 52% 9% 36%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5029 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 Intermembrane phospholipid transport system binding protein MlaD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	0	2	0
			802	506	132	164			
1	B	104	Total	C	N	O	0	1	0
			797	503	131	163			
1	C	108	Total	C	N	O	S	0	0
			824	521	135	167	1		
1	D	105	Total	C	N	O	S	0	0
			800	505	132	162	1		
1	E	108	Total	C	N	O	S	0	1
			829	524	136	168	1		
1	F	104	Total	C	N	O		0	1
			800	504	133	163			0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP P64604
A	23	HIS	-	expression tag	UNP P64604
A	24	HIS	-	expression tag	UNP P64604
A	25	HIS	-	expression tag	UNP P64604
A	26	HIS	-	expression tag	UNP P64604
A	27	HIS	-	expression tag	UNP P64604
A	28	HIS	-	expression tag	UNP P64604
B	22	MET	-	initiating methionine	UNP P64604
B	23	HIS	-	expression tag	UNP P64604
B	24	HIS	-	expression tag	UNP P64604
B	25	HIS	-	expression tag	UNP P64604
B	26	HIS	-	expression tag	UNP P64604
B	27	HIS	-	expression tag	UNP P64604
B	28	HIS	-	expression tag	UNP P64604
C	22	MET	-	initiating methionine	UNP P64604
C	23	HIS	-	expression tag	UNP P64604

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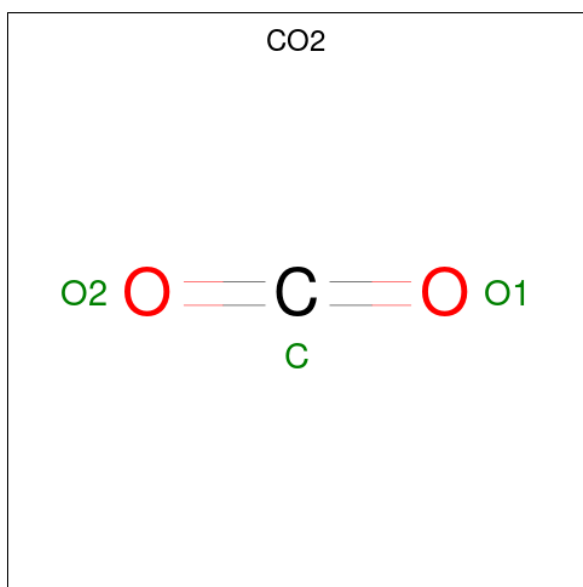
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Chain	Residue	Modelled	Actual	Comment	Reference
C	24	HIS	-	expression tag	UNP P64604
C	25	HIS	-	expression tag	UNP P64604
C	26	HIS	-	expression tag	UNP P64604
C	27	HIS	-	expression tag	UNP P64604
C	28	HIS	-	expression tag	UNP P64604
D	22	MET	-	initiating methionine	UNP P64604
D	23	HIS	-	expression tag	UNP P64604
D	24	HIS	-	expression tag	UNP P64604
D	25	HIS	-	expression tag	UNP P64604
D	26	HIS	-	expression tag	UNP P64604
D	27	HIS	-	expression tag	UNP P64604
D	28	HIS	-	expression tag	UNP P64604
E	22	MET	-	initiating methionine	UNP P64604
E	23	HIS	-	expression tag	UNP P64604
E	24	HIS	-	expression tag	UNP P64604
E	25	HIS	-	expression tag	UNP P64604
E	26	HIS	-	expression tag	UNP P64604
E	27	HIS	-	expression tag	UNP P64604
E	28	HIS	-	expression tag	UNP P64604
F	22	MET	-	initiating methionine	UNP P64604
F	23	HIS	-	expression tag	UNP P64604
F	24	HIS	-	expression tag	UNP P64604
F	25	HIS	-	expression tag	UNP P64604
F	26	HIS	-	expression tag	UNP P64604
F	27	HIS	-	expression tag	UNP P64604
F	28	HIS	-	expression tag	UNP P64604

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is CARBON DIOXIDE (CCD ID: CO2) (formula: CO₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			3	1	2		

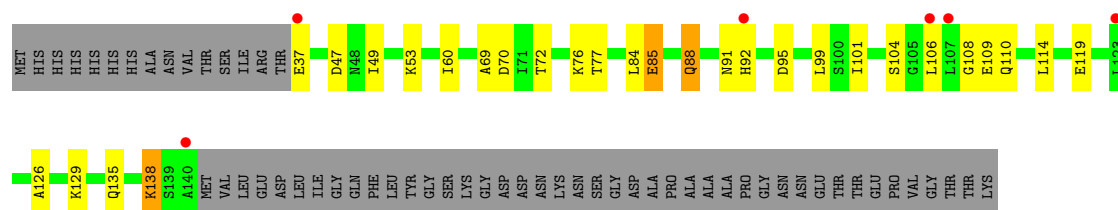
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	20	Total	O	0	0
			20	20		
4	C	50	Total	O	0	0
			50	50		
4	D	29	Total	O	0	0
			29	29		
4	E	16	Total	O	0	0
			16	16		
4	F	26	Total	O	0	0
			26	26		

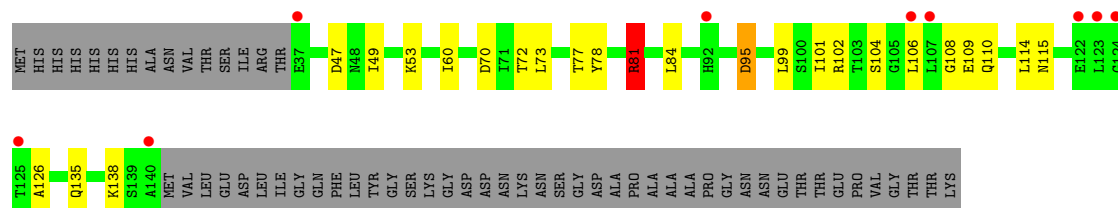
3 Residue-property plots [i](#)

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.

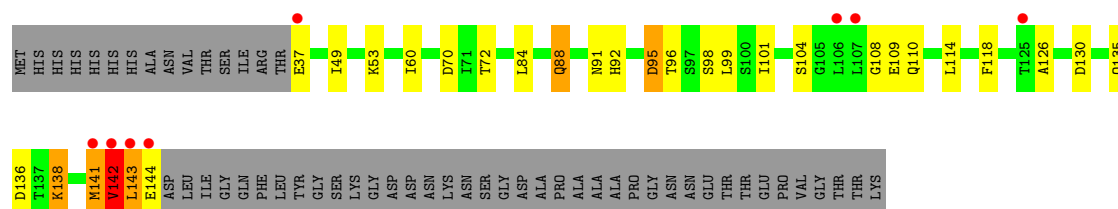
- Molecule 1: Intermembrane phospholipid transport system binding protein MlaD



- Molecule 1: Intermembrane phospholipid transport system binding protein MlaD

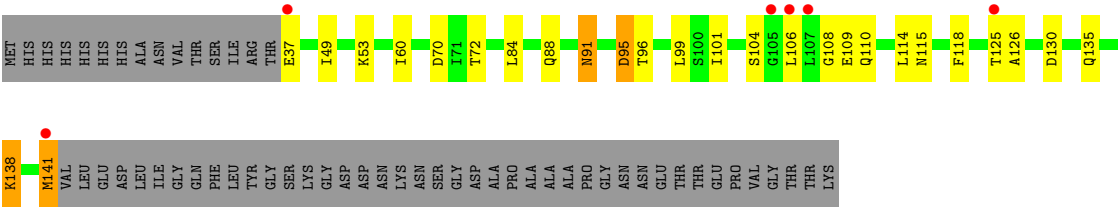


- Molecule 1: Intermembrane phospholipid transport system binding protein MlaD

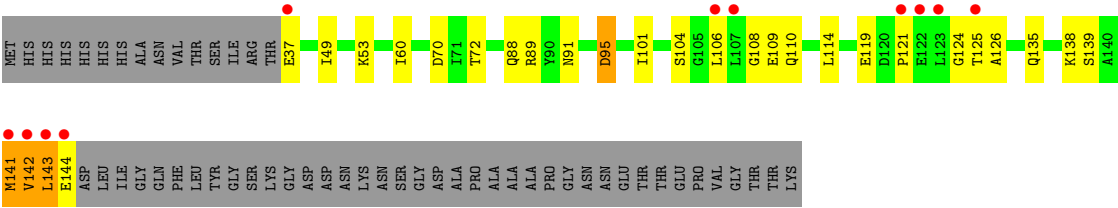


- Molecule 1: Intermembrane phospholipid transport system binding protein MlaD

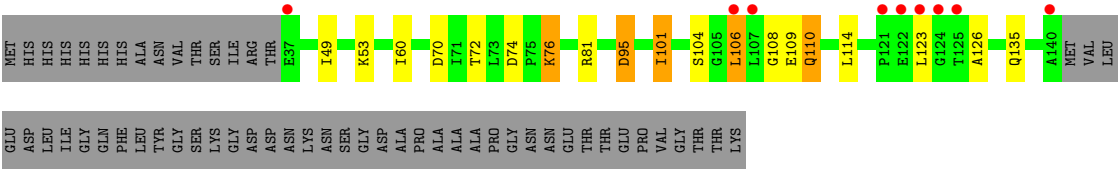




● Molecule 1: Intermembrane phospholipid transport system binding protein MlaD



● Molecule 1: Intermembrane phospholipid transport system binding protein MlaD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	60.42Å 106.95Å 117.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.98 – 2.70 78.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (78.98-2.70) 100.0 (78.98-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.204 , 0.261 0.206 , 0.261	Depositor DCC
R_{free} test set	1037 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtrriage
Anisotropy	0.839	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5029	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2531e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, CO2

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	1.10	1/821 (0.1%)	1.39	2/1119 (0.2%)
1	B	1.03	0/813	1.38	2/1108 (0.2%)
1	C	1.09	2/837 (0.2%)	1.48	5/1140 (0.4%)
1	D	1.04	0/813	1.45	4/1107 (0.4%)
1	E	1.03	0/845	1.43	6/1151 (0.5%)
1	F	1.07	0/813	1.35	2/1108 (0.2%)
All	All	1.06	3/4942 (0.1%)	1.41	21/6733 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	92	HIS	CE1-NE2	5.85	1.38	1.32
1	A	85	GLU	CD-OE2	5.74	1.36	1.25
1	C	118	PHE	C-O	5.00	1.30	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	142	VAL	CB-CA-C	9.11	126.23	111.29
1	A	85	GLU	CB-CG-CD	8.82	127.59	112.60
1	C	142	VAL	CB-CA-C	7.88	124.21	111.29
1	C	130	ASP	CA-CB-CG	7.83	120.42	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	ARG	CG-CD-NE	7.58	128.67	112.00
1	D	95	ASP	CB-CA-C	-6.51	97.84	110.46
1	C	95	ASP	CB-CA-C	-6.41	98.03	110.46
1	B	95	ASP	CB-CA-C	-6.39	98.06	110.46
1	E	95	ASP	CB-CA-C	-6.38	98.09	110.46
1	D	130	ASP	CA-CB-CG	6.27	118.87	112.60
1	F	95	ASP	CB-CA-C	-6.12	98.58	110.46
1	A	92	HIS	CA-CB-CG	5.87	119.67	113.80
1	E	121	PRO	CA-C-N	5.65	128.41	120.28
1	E	121	PRO	C-N-CA	5.65	128.41	120.28
1	E	143	LEU	N-CA-C	-5.54	98.99	110.80
1	C	109	GLU	N-CA-CB	-5.52	101.90	110.29
1	C	88	GLN	CB-CG-CD	5.23	121.49	112.60
1	D	115	ASN	CA-CB-CG	-5.13	107.47	112.60
1	D	91	ASN	CA-C-O	-5.03	113.34	119.03
1	F	101	ILE	CB-CA-C	5.01	116.94	111.08
1	E	141	MET	CB-CA-C	-5.01	102.08	110.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	124	GLY	Peptide

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	802	0	803	14	0
1	B	797	0	797	15	0
1	C	824	0	828	16	0
1	D	800	0	802	16	0
1	E	829	0	834	8	0
1	F	800	0	798	12	0
2	D	1	0	0	0	0
3	D	3	0	0	0	0
4	A	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	0	0	0	0
4	C	50	0	0	1	0
4	D	29	0	0	0	0
4	E	16	0	0	1	0
4	F	26	0	0	3	0
All	All	5029	0	4862	70	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 7.

All (70) 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:47:ASP:OD2	1:D:138:LYS:HE2	1.47	1.13
1:F:110:GLN:HG3	4:F:219:HOH:O	1.83	0.78
1:A:106:LEU:HD12	1:D:106:LEU:HD22	1.66	0.76
1:B:77:THR:HG22	1:D:96:THR:HG21	1.72	0.71
1:F:81:ARG:HD2	4:F:214:HOH:O	1.94	0.67
1:C:142:VAL:HG12	1:C:143:LEU:HD23	1.75	0.66
1:B:47:ASP:OD2	1:D:138:LYS:CE	2.37	0.65
1:F:70:ASP:OD2	1:F:72:THR:HG23	1.97	0.64
1:B:70[A]:ASP:OD2	1:B:72:THR:HG23	1.97	0.64
1:D:70:ASP:OD2	1:D:72:THR:HG23	1.98	0.64
1:E:70:ASP:OD2	1:E:72:THR:HG23	1.98	0.63
1:C:70:ASP:OD2	1:C:72:THR:HG23	1.99	0.63
1:A:70[A]:ASP:OD2	1:A:72:THR:HG23	1.98	0.62
1:A:47:ASP:OD2	1:C:138:LYS:HE3	2.03	0.59
1:F:74:ASP:OD1	1:F:76:LYS:CG	2.51	0.59
1:B:95:ASP:OD2	1:B:126:ALA:HB1	2.05	0.57
1:D:49:ILE:HA	1:D:101:ILE:CD1	2.36	0.56
1:C:49:ILE:HA	1:C:101:ILE:CD1	2.36	0.55
1:C:95:ASP:OD2	1:C:126:ALA:HB1	2.06	0.55
1:C:143:LEU:O	1:C:144:GLU:HB2	2.07	0.55
1:E:49:ILE:HA	1:E:101:ILE:CD1	2.37	0.54
1:A:49:ILE:HA	1:A:101:ILE:CD1	2.38	0.54
1:F:49:ILE:HA	1:F:101:ILE:CD1	2.38	0.54
1:B:102:ARG:HD2	1:C:142:VAL:HG11	1.88	0.54
1:B:78:TYR:HD2	1:D:118:PHE:CE2	2.26	0.53
1:A:138:LYS:HD2	4:C:225:HOH:O	2.07	0.53
1:F:110:GLN:CG	4:F:219:HOH:O	2.50	0.53
1:B:49:ILE:HA	1:B:101:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:MET:HE2	1:C:141:MET:HA	1.92	0.52
1:B:78:TYR:CD2	1:D:118:PHE:CE2	2.98	0.52
1:B:77:THR:HG22	1:D:96:THR:CG2	2.38	0.51
1:F:95:ASP:OD2	1:F:126:ALA:HB1	2.09	0.51
1:D:84:LEU:HD11	1:D:99:LEU:HD11	1.92	0.51
1:A:84:LEU:HD11	1:A:99:LEU:HD11	1.93	0.51
1:A:77:THR:HG22	1:C:96:THR:HG21	1.93	0.49
1:D:104:SER:O	1:D:108:GLY:HA3	2.12	0.49
1:A:104:SER:O	1:A:108:GLY:HA3	2.12	0.49
1:A:69:ALA:HB2	1:A:85:GLU:HG2	1.94	0.49
1:D:88:GLN:O	1:D:91:ASN:HB3	2.13	0.49
1:F:74:ASP:OD1	1:F:76:LYS:HG2	2.12	0.49
1:F:104:SER:O	1:F:108:GLY:HA3	2.13	0.48
1:A:95:ASP:OD2	1:A:126:ALA:HB1	2.13	0.48
1:C:104:SER:O	1:C:108:GLY:HA3	2.13	0.48
1:E:95:ASP:OD2	1:E:126:ALA:HB1	2.13	0.48
1:B:104:SER:O	1:B:108:GLY:HA3	2.14	0.48
1:C:84:LEU:HD11	1:C:99:LEU:HD11	1.96	0.47
1:D:141:MET:O	1:D:141:MET:HG2	2.14	0.47
1:E:104:SER:O	1:E:108:GLY:HA3	2.13	0.47
1:C:88:GLN:O	1:C:91:ASN:HB3	2.15	0.47
1:F:60:ILE:HG12	1:F:114:LEU:HB3	1.97	0.47
1:E:139:SER:OG	4:E:201:HOH:O	2.19	0.46
1:D:95:ASP:OD2	1:D:126:ALA:HB1	2.15	0.46
1:A:106:LEU:HD22	1:F:106:LEU:CD1	2.46	0.46
1:F:74:ASP:OD1	1:F:76:LYS:HG3	2.16	0.45
1:B:60:ILE:HG12	1:B:114:LEU:HB3	1.98	0.45
1:C:60:ILE:HG12	1:C:114:LEU:HB3	1.99	0.45
1:A:119:GLU:OE2	1:A:126:ALA:HB3	2.17	0.44
1:A:88:GLN:O	1:A:91:ASN:HB3	2.18	0.44
1:C:142:VAL:HG12	1:C:143:LEU:CD2	2.47	0.43
1:B:106:LEU:HD23	1:B:106:LEU:HA	1.93	0.43
1:E:60:ILE:HG12	1:E:114:LEU:HB3	2.01	0.43
1:B:81:ARG:HH21	1:B:81:ARG:HG3	1.84	0.43
1:C:98:SER:HA	1:C:136:ASP:O	2.19	0.43
1:E:88:GLN:O	1:E:91:ASN:HB3	2.19	0.43
1:E:119:GLU:OE2	1:E:125:THR:HB	2.19	0.43
1:C:49:ILE:HA	1:C:101:ILE:HD13	2.02	0.42
1:B:84:LEU:HD11	1:B:99:LEU:HD11	2.02	0.41
1:D:60:ILE:HG12	1:D:114:LEU:HB3	2.02	0.41
1:D:49:ILE:HA	1:D:101:ILE:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:HG12	1:A:114:LEU:HB3	2.03	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	104/162 (64%)	103 (99%)	1 (1%)	0	100	100
1	B	103/162 (64%)	102 (99%)	1 (1%)	0	100	100
1	C	106/162 (65%)	103 (97%)	3 (3%)	0	100	100
1	D	103/162 (64%)	100 (97%)	3 (3%)	0	100	100
1	E	107/162 (66%)	104 (97%)	3 (3%)	0	100	100
1	F	103/162 (64%)	102 (99%)	1 (1%)	0	100	100
All	All	626/972 (64%)	614 (98%)	12 (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	90/135 (67%)	81 (90%)	9 (10%)	7	19
1	B	89/135 (66%)	81 (91%)	8 (9%)	9	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	92/135 (68%)	84 (91%)	8 (9%)	9	24
1	D	89/135 (66%)	81 (91%)	8 (9%)	9	23
1	E	93/135 (69%)	81 (87%)	12 (13%)	4	10
1	F	89/135 (66%)	82 (92%)	7 (8%)	11	28
All	All	542/810 (67%)	490 (90%)	52 (10%)	8	20

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	53	LYS
1	A	76	LYS
1	A	88	GLN
1	A	109	GLU
1	A	110	GLN
1	A	129	LYS
1	A	135	GLN
1	A	138	LYS
1	B	53	LYS
1	B	73	LEU
1	B	81	ARG
1	B	109	GLU
1	B	110	GLN
1	B	115	ASN
1	B	135	GLN
1	B	138	LYS
1	C	37	GLU
1	C	53	LYS
1	C	110	GLN
1	C	135	GLN
1	C	138	LYS
1	C	141	MET
1	C	142	VAL
1	C	143	LEU
1	D	37	GLU
1	D	53	LYS
1	D	109	GLU
1	D	110	GLN
1	D	125	THR
1	D	135	GLN
1	D	138	LYS

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Mol	Chain	Res	Type
1	D	141	MET
1	E	37	GLU
1	E	53	LYS
1	E	89	ARG
1	E	106	LEU
1	E	109	GLU
1	E	110	GLN
1	E	135	GLN
1	E	138	LYS
1	E	141	MET
1	E	142	VAL
1	E	143	LEU
1	E	144	GLU
1	F	53	LYS
1	F	76	LYS
1	F	106	LEU
1	F	109	GLU
1	F	110	GLN
1	F	123	LEU
1	F	135	GLN

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

Mol	Chain	Res	Type
1	B	115	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
3	CO2	D	202	-	2,2,2	0.17	0	1,1,1	0.88	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 95th 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 ²)	Q<0.9
1	A	104/162 (64%)	0.01	6 (5%)	29 25	17, 31, 82, 106	2 (1%)
1	B	104/162 (64%)	0.23	9 (8%)	16 13	22, 37, 85, 109	1 (0%)
1	C	108/162 (66%)	0.11	8 (7%)	20 18	18, 31, 71, 118	0
1	D	105/162 (64%)	0.04	6 (5%)	29 26	23, 37, 79, 98	0
1	E	108/162 (66%)	0.36	11 (10%)	12 10	17, 41, 103, 124	1 (0%)
1	F	104/162 (64%)	0.30	9 (8%)	16 13	13, 36, 84, 106	1 (0%)
All	All	633/972 (65%)	0.17	49 (7%)	19 17	13, 36, 89, 124	5 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	VAL	5.5
1	E	142	VAL	5.4
1	C	143	LEU	5.4
1	E	143	LEU	5.2
1	E	123	LEU	4.4
1	B	122	GLU	4.0
1	C	141	MET	3.9
1	C	144	GLU	3.8
1	E	106	LEU	3.7
1	B	92	HIS	3.7
1	C	107	LEU	3.7
1	F	123	LEU	3.6
1	F	106	LEU	3.4
1	D	107	LEU	3.4
1	A	107	LEU	3.3
1	A	123	LEU	3.2
1	D	106	LEU	3.2
1	F	121	PRO	3.2
1	F	125	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	106	LEU	3.1
1	E	144	GLU	3.1
1	F	122	GLU	3.1
1	F	140	ALA	3.1
1	B	106	LEU	3.0
1	C	106	LEU	3.0
1	E	141	MET	2.9
1	E	122	GLU	2.9
1	E	121	PRO	2.9
1	B	140	ALA	2.8
1	D	105	GLY	2.8
1	C	37	GLU	2.6
1	C	125	THR	2.4
1	B	123	LEU	2.4
1	E	107	LEU	2.4
1	E	125	THR	2.4
1	D	37	GLU	2.4
1	B	125	THR	2.3
1	B	124	GLY	2.3
1	F	124	GLY	2.3
1	A	92	HIS	2.3
1	A	37	GLU	2.3
1	B	37	GLU	2.3
1	E	37	GLU	2.2
1	F	37	GLU	2.2
1	B	107	LEU	2.2
1	D	141	MET	2.1
1	D	125	THR	2.1
1	A	140	ALA	2.0
1	F	107	LEU	2.0

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
2	MG	D	201	1/1	0.88	0.12	39,39,39,39	0
3	CO2	D	202	3/3	0.90	0.14	51,51,55,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.