



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2023 – 07:03 AM EDT

PDB ID : 3MPW  
Title : Structure of EUTM in 2-D protein membrane  
Authors : Sagermann, M.; Takenoya, M.; Nikolakakis, K.  
Deposited on : 2010-04-27  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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>.

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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 : 2.35  
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) : 2.35

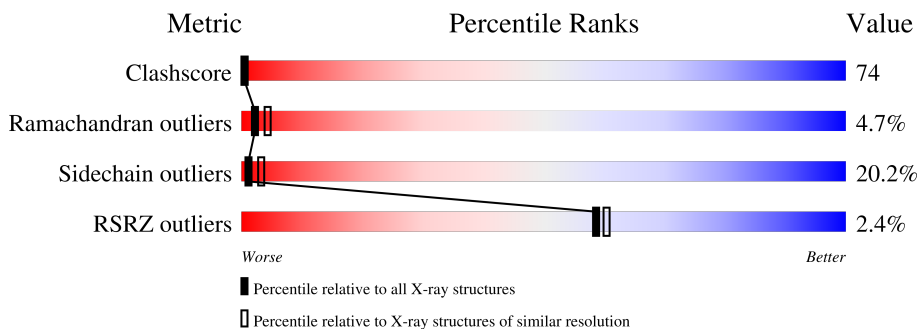
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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  $\geq 3$ , 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	103	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
1	B	103	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 31%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
1	C	103	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
1	D	103	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
1	E	103	<div style="display: flex; align-items: center;"> <div style="width: 22%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 51%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
1	F	103	<div style="display: flex; align-items: center;"> <div style="width: 22%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
1	G	103	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 53%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>

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Mol	Chain	Length	Quality of chain			
1	H	103	29%	47%	12%	13%
1	I	103	19%	54%	14%	13%
1	J	103	34%	40%	13%	13%
1	K	103	25%	51%	9%	13%
1	L	103	34%	41%	13%	13%

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
2	PO4	B	204	-	-	X	-
2	PO4	C	155	-	-	X	-
2	PO4	C	205	-	-	X	-
2	PO4	F	202	-	-	X	-
2	PO4	G	206	-	-	X	-
2	PO4	I	156	-	-	-	X
2	PO4	J	209	-	-	X	-
2	PO4	K	210	-	-	X	-

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7914 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 Ethanolamine utilization protein eutM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	98	698	434	129	130	5	0	0	0
1	H	90	638	400	116	117	5	0	0	0
1	I	90	638	400	116	117	5	0	0	0
1	J	90	638	400	116	117	5	0	0	0
1	K	90	638	400	116	117	5	0	0	0
1	L	90	638	400	116	117	5	0	0	0
1	A	99	708	440	132	131	5	0	0	0
1	B	97	688	428	126	129	5	0	0	0
1	C	91	642	402	117	118	5	0	0	0
1	D	91	642	402	117	118	5	0	0	0
1	E	90	638	400	116	117	5	0	0	0
1	F	90	638	400	116	117	5	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	98	HIS	-	expression tag	UNP P0ABF4
G	99	HIS	-	expression tag	UNP P0ABF4
G	100	HIS	-	expression tag	UNP P0ABF4
G	101	HIS	-	expression tag	UNP P0ABF4
G	102	HIS	-	expression tag	UNP P0ABF4

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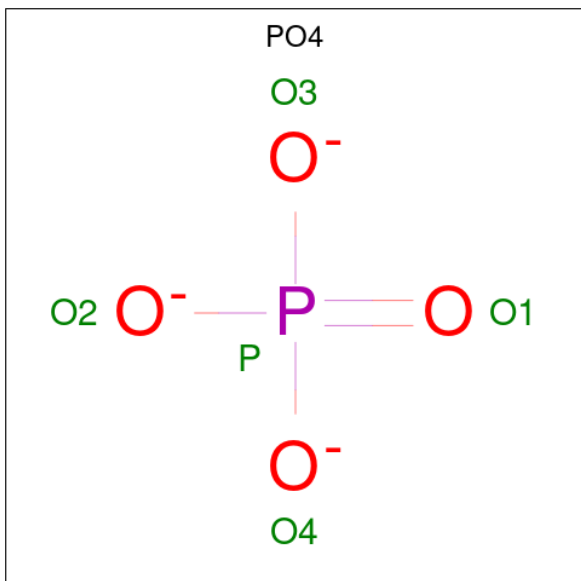
Chain	Residue	Modelled	Actual	Comment	Reference
G	103	HIS	-	expression tag	UNP P0ABF4
H	98	HIS	-	expression tag	UNP P0ABF4
H	99	HIS	-	expression tag	UNP P0ABF4
H	100	HIS	-	expression tag	UNP P0ABF4
H	101	HIS	-	expression tag	UNP P0ABF4
H	102	HIS	-	expression tag	UNP P0ABF4
H	103	HIS	-	expression tag	UNP P0ABF4
I	98	HIS	-	expression tag	UNP P0ABF4
I	99	HIS	-	expression tag	UNP P0ABF4
I	100	HIS	-	expression tag	UNP P0ABF4
I	101	HIS	-	expression tag	UNP P0ABF4
I	102	HIS	-	expression tag	UNP P0ABF4
I	103	HIS	-	expression tag	UNP P0ABF4
J	98	HIS	-	expression tag	UNP P0ABF4
J	99	HIS	-	expression tag	UNP P0ABF4
J	100	HIS	-	expression tag	UNP P0ABF4
J	101	HIS	-	expression tag	UNP P0ABF4
J	102	HIS	-	expression tag	UNP P0ABF4
J	103	HIS	-	expression tag	UNP P0ABF4
K	98	HIS	-	expression tag	UNP P0ABF4
K	99	HIS	-	expression tag	UNP P0ABF4
K	100	HIS	-	expression tag	UNP P0ABF4
K	101	HIS	-	expression tag	UNP P0ABF4
K	102	HIS	-	expression tag	UNP P0ABF4
K	103	HIS	-	expression tag	UNP P0ABF4
L	98	HIS	-	expression tag	UNP P0ABF4
L	99	HIS	-	expression tag	UNP P0ABF4
L	100	HIS	-	expression tag	UNP P0ABF4
L	101	HIS	-	expression tag	UNP P0ABF4
L	102	HIS	-	expression tag	UNP P0ABF4
L	103	HIS	-	expression tag	UNP P0ABF4
A	98	HIS	-	expression tag	UNP P0ABF4
A	99	HIS	-	expression tag	UNP P0ABF4
A	100	HIS	-	expression tag	UNP P0ABF4
A	101	HIS	-	expression tag	UNP P0ABF4
A	102	HIS	-	expression tag	UNP P0ABF4
A	103	HIS	-	expression tag	UNP P0ABF4
B	98	HIS	-	expression tag	UNP P0ABF4
B	99	HIS	-	expression tag	UNP P0ABF4
B	100	HIS	-	expression tag	UNP P0ABF4
B	101	HIS	-	expression tag	UNP P0ABF4
B	102	HIS	-	expression tag	UNP P0ABF4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	103	HIS	-	expression tag	UNP P0ABF4
C	98	HIS	-	expression tag	UNP P0ABF4
C	99	HIS	-	expression tag	UNP P0ABF4
C	100	HIS	-	expression tag	UNP P0ABF4
C	101	HIS	-	expression tag	UNP P0ABF4
C	102	HIS	-	expression tag	UNP P0ABF4
C	103	HIS	-	expression tag	UNP P0ABF4
D	98	HIS	-	expression tag	UNP P0ABF4
D	99	HIS	-	expression tag	UNP P0ABF4
D	100	HIS	-	expression tag	UNP P0ABF4
D	101	HIS	-	expression tag	UNP P0ABF4
D	102	HIS	-	expression tag	UNP P0ABF4
D	103	HIS	-	expression tag	UNP P0ABF4
E	98	HIS	-	expression tag	UNP P0ABF4
E	99	HIS	-	expression tag	UNP P0ABF4
E	100	HIS	-	expression tag	UNP P0ABF4
E	101	HIS	-	expression tag	UNP P0ABF4
E	102	HIS	-	expression tag	UNP P0ABF4
E	103	HIS	-	expression tag	UNP P0ABF4
F	98	HIS	-	expression tag	UNP P0ABF4
F	99	HIS	-	expression tag	UNP P0ABF4
F	100	HIS	-	expression tag	UNP P0ABF4
F	101	HIS	-	expression tag	UNP P0ABF4
F	102	HIS	-	expression tag	UNP P0ABF4
F	103	HIS	-	expression tag	UNP P0ABF4

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

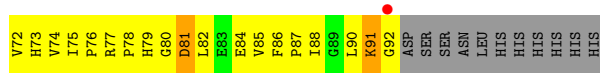


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

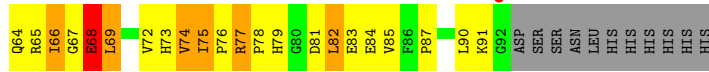
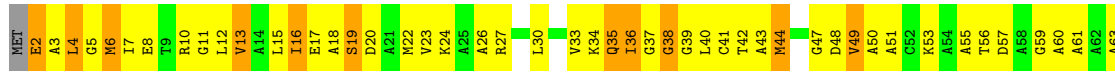
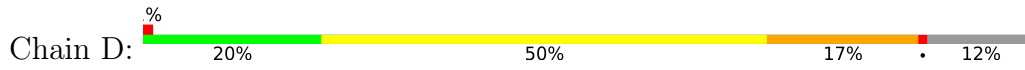




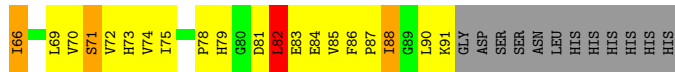
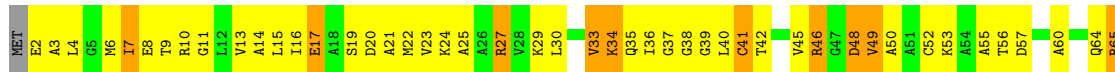




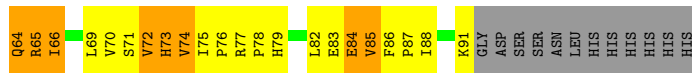
• Molecule 1: Ethanolamine utilization protein eutM



• Molecule 1: Ethanolamine utilization protein eutM



• Molecule 1: Ethanolamine utilization protein eutM



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.95Å 149.07Å 70.09Å 90.00° 120.01° 90.00°	Depositor
Resolution (Å)	46.98 – 2.70 47.01 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.98-2.70) 77.5 (47.01-2.70)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.248 , 0.336 0.258 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtrriage
Anisotropy	1.288	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 0.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.458 for l,k,-h-l 0.458 for -h-l,k,h 0.459 for h,-k,-h-l 0.458 for l,-k,h 0.468 for -h-l,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7914	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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 43.03 % 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 1.8706e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PO4

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	0.55	0/716	0.70	0/966
1	B	0.54	0/694	0.72	0/936
1	C	0.54	0/647	0.76	0/872
1	D	0.58	1/647 (0.2%)	0.71	0/872
1	E	0.58	0/643	0.75	0/867
1	F	0.52	0/643	0.71	0/867
1	G	0.54	0/705	0.69	0/951
1	H	0.54	0/643	0.81	1/867 (0.1%)
1	I	0.55	0/643	0.89	2/867 (0.2%)
1	J	0.57	0/643	0.75	0/867
1	K	0.53	0/643	0.74	0/867
1	L	0.53	0/643	0.69	0/867
All	All	0.55	1/7910 (0.0%)	0.74	3/10666 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	68	GLU	CG-CD	5.83	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	37	GLY	N-CA-C	-13.26	79.95	113.10
1	H	37	GLY	N-CA-C	-11.37	84.67	113.10
1	I	38	GLY	N-CA-C	-5.89	98.38	113.10

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	708	0	730	125	0
1	B	688	0	716	133	0
1	C	642	0	678	112	0
1	D	642	0	678	126	0
1	E	638	0	675	118	0
1	F	638	0	675	132	0
1	G	698	0	723	143	0
1	H	638	0	675	93	0
1	I	638	0	675	115	1
1	J	638	0	675	97	0
1	K	638	0	675	115	1
1	L	638	0	675	109	0
2	A	5	0	0	0	0
2	B	5	0	0	2	0
2	C	10	0	0	4	0
2	D	5	0	0	1	0
2	E	5	0	0	1	0
2	F	5	0	0	5	0
2	G	5	0	0	2	0
2	H	5	0	0	0	0
2	I	10	0	0	1	0
2	J	5	0	0	5	0
2	K	5	0	0	2	0
2	L	5	0	0	0	0
All	All	7914	0	8250	1190	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 74.

The worst 5 of 1190 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:GLN:HE22	1:D:34:LYS:NZ	1.03	1.42
1:A:7:ILE:CD1	1:A:8:GLU:N	1.88	1.35
1:C:35:GLN:NE2	1:D:34:LYS:HZ1	1.20	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2:GLU:HG3	2:J:209:PO4:O4	1.23	1.30
1:C:35:GLN:NE2	1:D:34:LYS:NZ	1.73	1.29

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)
1:I:48:ASP:OD1	1:K:27:ARG:NH2[1_454]	1.87	0.33

## 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	97/103 (94%)	82 (84%)	10 (10%)	5 (5%)	2 3
1	B	95/103 (92%)	82 (86%)	10 (10%)	3 (3%)	4 9
1	C	89/103 (86%)	71 (80%)	14 (16%)	4 (4%)	2 5
1	D	89/103 (86%)	75 (84%)	9 (10%)	5 (6%)	2 3
1	E	88/103 (85%)	71 (81%)	11 (12%)	6 (7%)	1 1
1	F	88/103 (85%)	72 (82%)	10 (11%)	6 (7%)	1 1
1	G	96/103 (93%)	83 (86%)	9 (9%)	4 (4%)	3 5
1	H	88/103 (85%)	75 (85%)	10 (11%)	3 (3%)	3 8
1	I	88/103 (85%)	72 (82%)	11 (12%)	5 (6%)	1 2
1	J	88/103 (85%)	78 (89%)	8 (9%)	2 (2%)	6 16
1	K	88/103 (85%)	69 (78%)	15 (17%)	4 (4%)	2 5
1	L	88/103 (85%)	72 (82%)	12 (14%)	4 (4%)	2 5
All	All	1082/1236 (88%)	902 (83%)	129 (12%)	51 (5%)	2 4

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	87	PRO
1	H	49	VAL
1	I	49	VAL
1	I	61	ALA
1	J	49	VAL

### 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	71/75 (95%)	59 (83%)	12 (17%)	2	5
1	B	69/75 (92%)	58 (84%)	11 (16%)	2	6
1	C	63/75 (84%)	51 (81%)	12 (19%)	1	4
1	D	63/75 (84%)	45 (71%)	18 (29%)	0	1
1	E	63/75 (84%)	51 (81%)	12 (19%)	1	4
1	F	63/75 (84%)	51 (81%)	12 (19%)	1	4
1	G	70/75 (93%)	52 (74%)	18 (26%)	0	1
1	H	63/75 (84%)	51 (81%)	12 (19%)	1	4
1	I	63/75 (84%)	51 (81%)	12 (19%)	1	4
1	J	63/75 (84%)	48 (76%)	15 (24%)	0	2
1	K	63/75 (84%)	51 (81%)	12 (19%)	1	4
1	L	63/75 (84%)	52 (82%)	11 (18%)	2	4
All	All	777/900 (86%)	620 (80%)	157 (20%)	1	3

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2	GLU
1	E	82	LEU
1	D	16	ILE
1	D	77	ARG
1	F	44	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	98	HIS
1	C	35	GLN
1	F	35	GLN
1	J	35	GLN
1	J	64	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

14 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	$\# Z  > 2$
2	PO4	I	156	-	4,4,4	0.88	0	6,6,6	0.48	0
2	PO4	C	205	-	4,4,4	0.84	0	6,6,6	0.42	0
2	PO4	F	202	-	4,4,4	0.87	0	6,6,6	0.50	0
2	PO4	L	211	-	4,4,4	0.86	0	6,6,6	0.55	0
2	PO4	D	200	-	4,4,4	0.93	0	6,6,6	0.49	0
2	PO4	J	209	-	4,4,4	0.78	0	6,6,6	0.76	0
2	PO4	B	204	-	4,4,4	0.86	0	6,6,6	0.48	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	G	206	-	4,4,4	0.84	0	6,6,6	0.61	0
2	PO4	C	155	-	4,4,4	0.88	0	6,6,6	0.45	0
2	PO4	I	208	-	4,4,4	0.90	0	6,6,6	0.43	0
2	PO4	E	201	-	4,4,4	0.93	0	6,6,6	0.42	0
2	PO4	H	207	-	4,4,4	0.93	0	6,6,6	0.51	0
2	PO4	K	210	-	4,4,4	0.87	0	6,6,6	0.58	0
2	PO4	A	203	-	4,4,4	0.76	0	6,6,6	0.61	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.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	205	PO4	2	0
2	F	202	PO4	5	0
2	D	200	PO4	1	0
2	J	209	PO4	5	0
2	B	204	PO4	2	0
2	G	206	PO4	2	0
2	C	155	PO4	2	0
2	I	208	PO4	1	0
2	E	201	PO4	1	0
2	K	210	PO4	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	99/103 (96%)	-0.31	9 (9%) 9 7	22, 34, 45, 49	9 (9%)
1	B	97/103 (94%)	-0.28	7 (7%) 15 13	24, 32, 49, 52	7 (7%)
1	C	91/103 (88%)	-0.59	1 (1%) 80 82	24, 33, 43, 49	1 (1%)
1	D	91/103 (88%)	-0.55	1 (1%) 80 82	25, 32, 42, 50	1 (1%)
1	E	90/103 (87%)	-0.64	0 100 100	22, 31, 39, 42	0
1	F	90/103 (87%)	-0.62	0 100 100	22, 32, 43, 55	0
1	G	98/103 (95%)	-0.23	8 (8%) 11 9	25, 35, 51, 55	8 (8%)
1	H	90/103 (87%)	-0.59	0 100 100	25, 32, 41, 45	0
1	I	90/103 (87%)	-0.65	0 100 100	25, 34, 45, 50	0
1	J	90/103 (87%)	-0.58	0 100 100	20, 31, 40, 45	0
1	K	90/103 (87%)	-0.58	0 100 100	24, 33, 42, 49	0
1	L	90/103 (87%)	-0.55	0 100 100	22, 33, 42, 51	0
All	All	1106/1236 (89%)	-0.51	26 (2%) 59 60	20, 33, 45, 55	26 (2%)

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	94	SER	7.3
1	G	95	SER	6.5
1	B	93	ASP	5.8
1	G	98	HIS	5.2
1	A	100	HIS	5.2

### 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
2	PO4	I	156	5/5	0.54	1.08	226,226,226,226	0
2	PO4	L	211	5/5	0.78	0.23	119,119,119,120	0
2	PO4	I	208	5/5	0.85	0.18	134,134,134,135	0
2	PO4	C	155	5/5	0.86	0.39	114,115,115,115	0
2	PO4	C	205	5/5	0.86	0.14	112,113,113,113	0
2	PO4	F	202	5/5	0.86	0.18	127,127,127,127	0
2	PO4	A	203	5/5	0.88	0.17	87,88,88,89	0
2	PO4	H	207	5/5	0.92	0.13	92,92,92,92	0
2	PO4	G	206	5/5	0.93	0.17	63,63,63,64	0
2	PO4	E	201	5/5	0.94	0.16	88,88,88,89	0
2	PO4	J	209	5/5	0.94	0.12	86,87,87,87	0
2	PO4	K	210	5/5	0.95	0.14	70,71,71,71	0
2	PO4	B	204	5/5	0.96	0.09	92,92,93,93	0
2	PO4	D	200	5/5	0.97	0.09	79,79,80,80	0

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

There are no such residues in this entry.