



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 06:02 PM EST

PDB ID : 3MFN
Title : Dfer_2879 protein of unknown function from Dyadobacter fermentans
Authors : Osipiuk, J.; Xu, X.; Cui, H.; Chin, S.; Eisen, J.; Wu, D.; Kerfeld, C.; Savchenko, A.; Edwards, A.M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2010-04-02
Resolution : 2.02 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

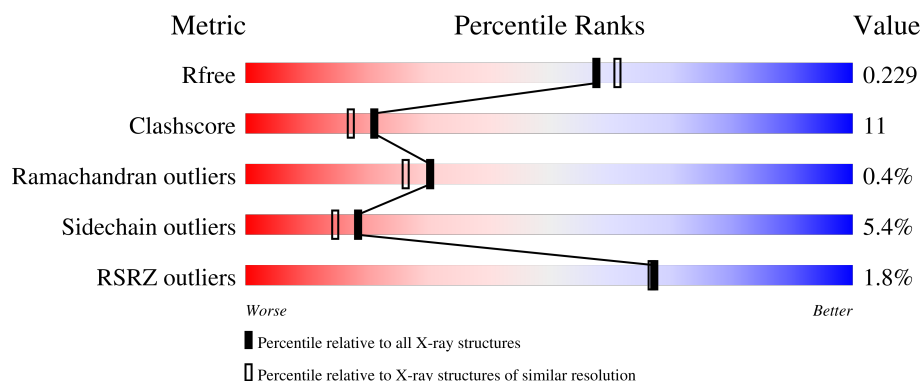
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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}	164625	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (2.04-2.00)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	157	 66% 11% • 20%
1	B	157	 70% 9% • 20%
1	C	157	 62% 16% • 20%
1	D	157	 64% 10% • 24%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4346 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	Se	0	12	0
			1085	699	190	194	2			
1	B	126	Total	C	N	O	Se	0	8	0
			1068	687	186	193	2			
1	C	125	Total	C	N	O	Se	0	4	0
			1038	668	176	191	3			
1	D	120	Total	C	N	O	Se	0	6	0
			1005	650	167	184	4			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	expression tag	UNP C6W4J3
A	-20	GLY	-	expression tag	UNP C6W4J3
A	-19	SER	-	expression tag	UNP C6W4J3
A	-18	SER	-	expression tag	UNP C6W4J3
A	-17	HIS	-	expression tag	UNP C6W4J3
A	-16	HIS	-	expression tag	UNP C6W4J3
A	-15	HIS	-	expression tag	UNP C6W4J3
A	-14	HIS	-	expression tag	UNP C6W4J3
A	-13	HIS	-	expression tag	UNP C6W4J3
A	-12	HIS	-	expression tag	UNP C6W4J3
A	-11	SER	-	expression tag	UNP C6W4J3
A	-10	SER	-	expression tag	UNP C6W4J3
A	-9	GLY	-	expression tag	UNP C6W4J3
A	-8	ARG	-	expression tag	UNP C6W4J3
A	-7	GLU	-	expression tag	UNP C6W4J3
A	-6	ASN	-	expression tag	UNP C6W4J3
A	-5	LEU	-	expression tag	UNP C6W4J3
A	-4	TYR	-	expression tag	UNP C6W4J3
A	-3	PHE	-	expression tag	UNP C6W4J3
A	-2	GLN	-	expression tag	UNP C6W4J3
A	-1	GLY	-	expression tag	UNP C6W4J3

Continued on next page...

Continued from previous page...

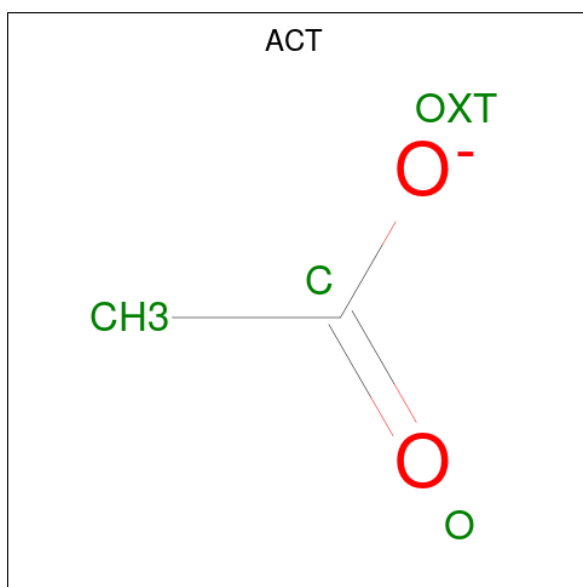
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP C6W4J3
A	134	GLY	-	expression tag	UNP C6W4J3
A	135	SER	-	expression tag	UNP C6W4J3
B	-21	MSE	-	expression tag	UNP C6W4J3
B	-20	GLY	-	expression tag	UNP C6W4J3
B	-19	SER	-	expression tag	UNP C6W4J3
B	-18	SER	-	expression tag	UNP C6W4J3
B	-17	HIS	-	expression tag	UNP C6W4J3
B	-16	HIS	-	expression tag	UNP C6W4J3
B	-15	HIS	-	expression tag	UNP C6W4J3
B	-14	HIS	-	expression tag	UNP C6W4J3
B	-13	HIS	-	expression tag	UNP C6W4J3
B	-12	HIS	-	expression tag	UNP C6W4J3
B	-11	SER	-	expression tag	UNP C6W4J3
B	-10	SER	-	expression tag	UNP C6W4J3
B	-9	GLY	-	expression tag	UNP C6W4J3
B	-8	ARG	-	expression tag	UNP C6W4J3
B	-7	GLU	-	expression tag	UNP C6W4J3
B	-6	ASN	-	expression tag	UNP C6W4J3
B	-5	LEU	-	expression tag	UNP C6W4J3
B	-4	TYR	-	expression tag	UNP C6W4J3
B	-3	PHE	-	expression tag	UNP C6W4J3
B	-2	GLN	-	expression tag	UNP C6W4J3
B	-1	GLY	-	expression tag	UNP C6W4J3
B	0	HIS	-	expression tag	UNP C6W4J3
B	134	GLY	-	expression tag	UNP C6W4J3
B	135	SER	-	expression tag	UNP C6W4J3
C	-21	MSE	-	expression tag	UNP C6W4J3
C	-20	GLY	-	expression tag	UNP C6W4J3
C	-19	SER	-	expression tag	UNP C6W4J3
C	-18	SER	-	expression tag	UNP C6W4J3
C	-17	HIS	-	expression tag	UNP C6W4J3
C	-16	HIS	-	expression tag	UNP C6W4J3
C	-15	HIS	-	expression tag	UNP C6W4J3
C	-14	HIS	-	expression tag	UNP C6W4J3
C	-13	HIS	-	expression tag	UNP C6W4J3
C	-12	HIS	-	expression tag	UNP C6W4J3
C	-11	SER	-	expression tag	UNP C6W4J3
C	-10	SER	-	expression tag	UNP C6W4J3
C	-9	GLY	-	expression tag	UNP C6W4J3
C	-8	ARG	-	expression tag	UNP C6W4J3
C	-7	GLU	-	expression tag	UNP C6W4J3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ASN	-	expression tag	UNP C6W4J3
C	-5	LEU	-	expression tag	UNP C6W4J3
C	-4	TYR	-	expression tag	UNP C6W4J3
C	-3	PHE	-	expression tag	UNP C6W4J3
C	-2	GLN	-	expression tag	UNP C6W4J3
C	-1	GLY	-	expression tag	UNP C6W4J3
C	0	HIS	-	expression tag	UNP C6W4J3
C	134	GLY	-	expression tag	UNP C6W4J3
C	135	SER	-	expression tag	UNP C6W4J3
D	-21	MSE	-	expression tag	UNP C6W4J3
D	-20	GLY	-	expression tag	UNP C6W4J3
D	-19	SER	-	expression tag	UNP C6W4J3
D	-18	SER	-	expression tag	UNP C6W4J3
D	-17	HIS	-	expression tag	UNP C6W4J3
D	-16	HIS	-	expression tag	UNP C6W4J3
D	-15	HIS	-	expression tag	UNP C6W4J3
D	-14	HIS	-	expression tag	UNP C6W4J3
D	-13	HIS	-	expression tag	UNP C6W4J3
D	-12	HIS	-	expression tag	UNP C6W4J3
D	-11	SER	-	expression tag	UNP C6W4J3
D	-10	SER	-	expression tag	UNP C6W4J3
D	-9	GLY	-	expression tag	UNP C6W4J3
D	-8	ARG	-	expression tag	UNP C6W4J3
D	-7	GLU	-	expression tag	UNP C6W4J3
D	-6	ASN	-	expression tag	UNP C6W4J3
D	-5	LEU	-	expression tag	UNP C6W4J3
D	-4	TYR	-	expression tag	UNP C6W4J3
D	-3	PHE	-	expression tag	UNP C6W4J3
D	-2	GLN	-	expression tag	UNP C6W4J3
D	-1	GLY	-	expression tag	UNP C6W4J3
D	0	HIS	-	expression tag	UNP C6W4J3
D	134	GLY	-	expression tag	UNP C6W4J3
D	135	SER	-	expression tag	UNP C6W4J3

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

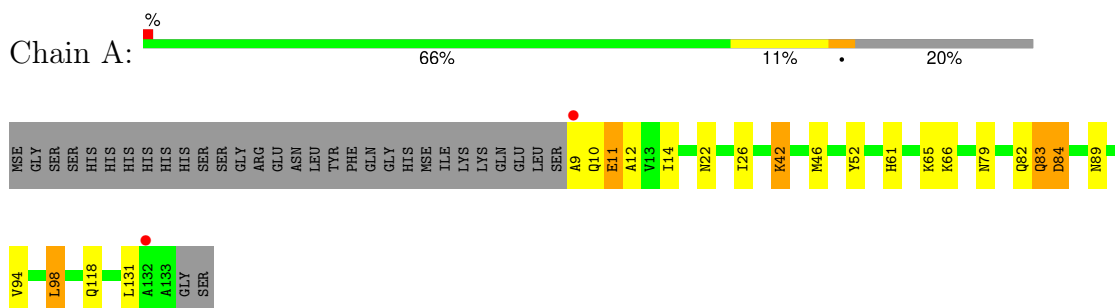
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total	O	0	1
			50	50		
3	B	42	Total	O	0	0
			42	42		
3	C	41	Total	O	0	0
			41	41		
3	D	13	Total	O	0	0
			13	13		

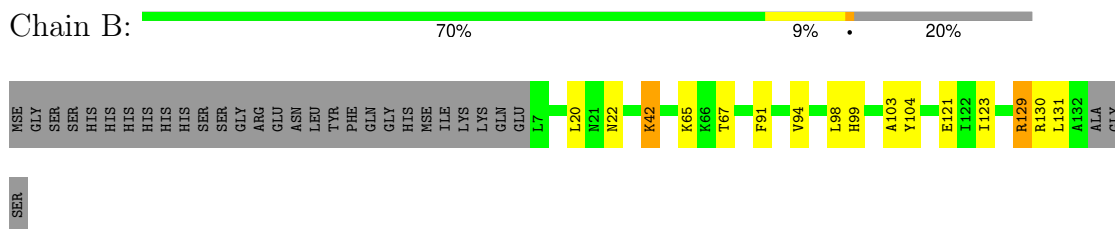
3 Residue-property plots [i](#)

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. 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. 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.

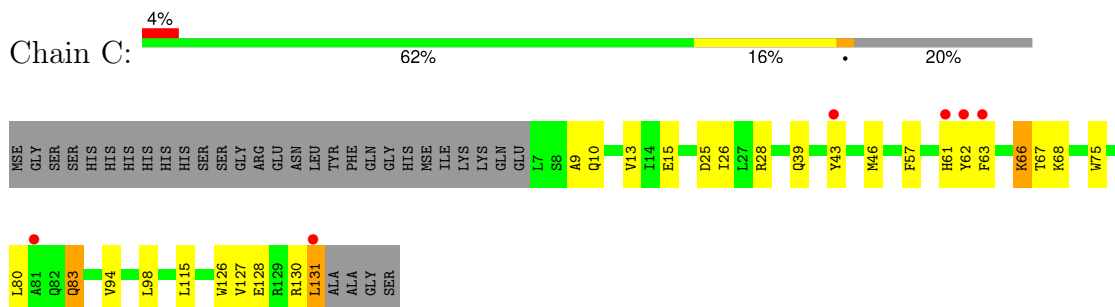
- Molecule 1: Uncharacterized protein



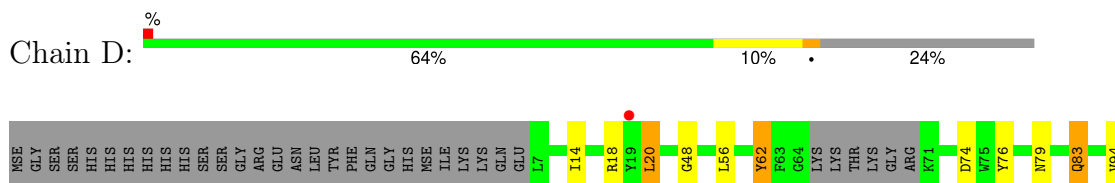
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



L98	M102	F117	E121	I124	D125	W126	L131	A132	ALA	GLY	SER
-----	------	------	------	------	------	------	------	------	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.78Å 83.65Å 93.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.30 – 2.02 35.30 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.30-2.02) 99.2 (35.30-2.02)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.188 , 0.227 0.185 , 0.229	Depositor DCC
R_{free} test set	1802 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4346	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT

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	0.99	0/1139	0.86	0/1521
1	B	0.84	0/1110	0.75	0/1484
1	C	0.86	0/1065	0.77	0/1425
1	D	0.73	0/1041	0.72	0/1395
All	All	0.86	0/4355	0.78	0/5825

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	1085	0	1112	33	0
1	B	1068	0	1083	22	0
1	C	1038	0	1038	24	0
1	D	1005	0	998	25	0
2	A	4	0	3	5	0
3	A	50	0	0	0	0
3	B	42	0	0	2	0
3	C	41	0	0	0	0
3	D	13	0	0	0	0
All	All	4346	0	4234	91	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 11.

All (91) 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:A:42[B]:LYS:NZ	1:B:22[B]:ASN:HB2	1.52	1.25
1:A:42[B]:LYS:NZ	1:B:22[B]:ASN:CB	2.06	1.19
2:A:301:ACT:CH3	1:B:104:TYR:OH	1.99	1.09
1:A:10[B]:GLN:HG3	1:A:131:LEU:HD13	1.34	1.07
1:D:98:LEU:HA	1:D:102[A]:MSE:HE2	1.38	1.03
2:A:301:ACT:H3	1:B:104:TYR:OH	1.57	1.02
1:A:10[B]:GLN:CG	1:A:131:LEU:HD13	1.92	1.00
1:A:22[B]:ASN:HB2	1:B:42[B]:LYS:NZ	1.80	0.97
1:A:42[B]:LYS:NZ	1:B:22[B]:ASN:CG	2.25	0.90
1:A:22[B]:ASN:CB	1:B:42[B]:LYS:NZ	2.36	0.88
1:B:22[B]:ASN:ND2	3:B:161:HOH:O	2.08	0.86
1:A:10[B]:GLN:OE1	1:A:12:ALA:HB3	1.80	0.81
1:D:98:LEU:HG	1:D:102[A]:MSE:HE1	1.61	0.81
2:A:301:ACT:H1	1:B:104:TYR:OH	1.83	0.77
1:A:52:TYR:OH	2:A:301:ACT:O	2.03	0.76
1:C:43:TYR:CD1	1:C:46[A]:MSE:CE	2.69	0.75
1:C:94:VAL:HG13	1:C:98:LEU:HD22	1.67	0.75
1:C:43:TYR:HD1	1:C:46[A]:MSE:CE	1.99	0.74
1:A:42[B]:LYS:NZ	1:B:22[B]:ASN:OD1	2.22	0.72
1:D:98:LEU:HG	1:D:102[A]:MSE:CE	2.20	0.72
1:A:9:ALA:HB3	1:A:11:GLU:OE1	1.90	0.71
1:A:94:VAL:HG13	1:A:98:LEU:HD22	1.75	0.69
1:D:48:GLY:HA2	1:D:102[A]:MSE:HE3	1.72	0.68
1:D:98:LEU:HA	1:D:102[A]:MSE:CE	2.18	0.68
1:A:10[B]:GLN:HG3	1:A:131:LEU:CD1	2.20	0.68
1:C:43:TYR:CD1	1:C:46[A]:MSE:HE2	2.29	0.67
1:A:42[B]:LYS:HE3	1:B:22[B]:ASN:OD1	1.94	0.66
1:A:22[B]:ASN:HD21	1:A:26:ILE:HD11	1.62	0.64
1:A:79:ASN:O	1:A:82[A]:GLN:HG2	1.96	0.63
1:A:22[A]:ASN:OD1	1:B:42[A]:LYS:HD2	1.97	0.63
1:D:98:LEU:CA	1:D:102[A]:MSE:HE2	2.24	0.63
1:D:48:GLY:CA	1:D:102[A]:MSE:HE3	2.29	0.62
1:D:56:LEU:HD22	1:D:76:TYR:CZ	2.34	0.62
1:C:9:ALA:HB1	1:C:131:LEU:HD21	1.80	0.62
1:A:42[B]:LYS:CE	1:B:22[B]:ASN:OD1	2.47	0.61
1:C:13:VAL:HG11	1:C:128:GLU:HB2	1.83	0.61
1:C:43:TYR:CE1	1:C:46[A]:MSE:HE1	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:LEU:HD22	1:D:124:ILE:CD1	2.32	0.60
1:D:131:LEU:O	1:D:132:ALA:HB2	2.01	0.60
1:D:83:GLN:HG2	1:D:126:TRP:CH2	2.37	0.59
1:D:131:LEU:O	1:D:132:ALA:CB	2.52	0.57
1:D:62:TYR:O	1:D:62:TYR:HD2	1.89	0.56
1:C:9:ALA:HB1	1:C:131:LEU:CD2	2.35	0.56
1:D:83:GLN:HG2	1:D:126:TRP:HH2	1.70	0.54
1:C:43:TYR:HD1	1:C:46[A]:MSE:HE2	1.67	0.54
1:B:129:ARG:HD2	3:B:145:HOH:O	2.07	0.54
1:D:62:TYR:HD2	1:D:62:TYR:C	2.11	0.54
1:C:63:PHE:HZ	1:C:80:LEU:HD23	1.75	0.51
1:C:83:GLN:HG2	1:C:126:TRP:CZ2	2.45	0.51
1:B:94:VAL:HG13	1:B:98:LEU:HD22	1.92	0.51
1:C:62:TYR:HB2	1:C:127:VAL:HG13	1.93	0.51
1:A:22[B]:ASN:HD21	1:A:26:ILE:CD1	2.24	0.51
1:C:43:TYR:HE1	1:C:46[A]:MSE:HE1	1.75	0.51
1:A:46:MSE:HE1	1:B:22[B]:ASN:OD1	2.10	0.51
1:D:62:TYR:C	1:D:62:TYR:CD2	2.82	0.51
1:D:20:LEU:HD22	1:D:124:ILE:HD12	1.92	0.51
1:D:20:LEU:CD2	1:D:124:ILE:HD12	2.41	0.50
1:C:66:LYS:HD2	1:C:75:TRP:CD1	2.47	0.49
1:B:91:PHE:HA	1:B:123:ILE:HD11	1.94	0.48
1:C:43:TYR:CE1	1:C:46[A]:MSE:CE	2.96	0.48
1:A:89:ASN:ND2	1:C:39:GLN:HE22	2.10	0.48
1:A:22[B]:ASN:HB3	1:B:42[B]:LYS:NZ	2.27	0.48
1:A:83:GLN:O	1:A:84:ASP:HB2	2.14	0.47
1:C:83:GLN:HG3	1:C:130:ARG:NH2	2.31	0.46
1:A:118[B]:GLN:HE21	1:A:118[B]:GLN:HA	1.81	0.46
1:C:15:GLU:HB3	1:C:57[B]:PHE:HE2	1.82	0.45
1:C:25:ASP:OD1	1:C:28:ARG:NH1	2.39	0.45
1:A:14:ILE:HD12	1:A:14:ILE:N	2.32	0.45
1:C:26:ILE:HD13	1:C:46[A]:MSE:HG2	1.99	0.45
1:A:9:ALA:O	1:A:61[A]:HIS:CE1	2.69	0.45
1:D:20:LEU:HD23	1:D:121[B]:GLU:OE2	2.16	0.45
1:C:57[B]:PHE:CE1	1:C:61:HIS:NE2	2.85	0.45
1:D:79[B]:ASN:HD22	1:D:79[B]:ASN:HA	1.63	0.44
1:C:15:GLU:HB3	1:C:57[B]:PHE:CE2	2.53	0.44
1:C:43:TYR:CD1	1:C:46[A]:MSE:HE1	2.51	0.43
1:D:48:GLY:HA2	1:D:102[A]:MSE:CE	2.44	0.43
1:D:94:VAL:HG13	1:D:98:LEU:HD22	2.00	0.43
1:B:20:LEU:HD21	1:B:121[A]:GLU:HG2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10[B]:GLN:CD	1:A:131:LEU:HD13	2.38	0.42
1:A:22[B]:ASN:ND2	1:A:26:ILE:CD1	2.83	0.41
2:A:301:ACT:H1	1:B:104:TYR:CZ	2.55	0.41
1:D:98:LEU:CG	1:D:102[A]:MSE:CE	2.95	0.41
1:A:65:LYS:HE3	1:D:74:ASP:OD2	2.21	0.41
1:B:42[A]:LYS:HE2	1:B:42[A]:LYS:HB3	1.89	0.41
1:B:99:HIS:O	1:B:103:ALA:HB3	2.21	0.40
1:C:83:GLN:HG2	1:C:126:TRP:CH2	2.56	0.40
1:D:117:PHE:O	1:D:121[A]:GLU:HG3	2.22	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	135/157 (86%)	132 (98%)	2 (2%)	1 (1%)	19	14
1	B	132/157 (84%)	127 (96%)	4 (3%)	1 (1%)	16	11
1	C	127/157 (81%)	118 (93%)	9 (7%)	0	100	100
1	D	122/157 (78%)	119 (98%)	3 (2%)	0	100	100
All	All	516/628 (82%)	496 (96%)	18 (4%)	2 (0%)	30	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ASP
1	B	131	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	114/126 (90%)	108 (95%)	6 (5%)	19	15
1	B	112/126 (89%)	105 (94%)	7 (6%)	15	11
1	C	108/126 (86%)	101 (94%)	7 (6%)	14	10
1	D	105/126 (83%)	100 (95%)	5 (5%)	21	18
All	All	439/504 (87%)	414 (94%)	25 (6%)	18	13

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	42[A]	LYS
1	A	42[B]	LYS
1	A	66	LYS
1	A	83	GLN
1	A	98	LEU
1	B	42[A]	LYS
1	B	42[B]	LYS
1	B	65[A]	LYS
1	B	65[B]	LYS
1	B	67	THR
1	B	129	ARG
1	B	130	ARG
1	C	10	GLN
1	C	66	LYS
1	C	67	THR
1	C	68	LYS
1	C	83	GLN
1	C	115	LEU
1	C	131	LEU
1	D	14	ILE
1	D	18	ARG
1	D	20	LEU
1	D	62	TYR
1	D	83	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	83	GLN
1	A	89	ASN
1	C	22	ASN
1	D	118	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	ACT	A	301	-	3,3,3	0.95	0	3,3,3	2.14	2 (66%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	301	ACT	OXT-C-CH3	2.76	126.62	115.05
2	A	301	ACT	OXT-C-O	-2.40	113.11	122.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ACT	5	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](#)

Warning: The R factor obtained from EDS is 0.2535, which does not match the depositor's R factor of 0.188. Please interpret the results in this section carefully.

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	123/157 (78%)	-0.22	2 (1%) 70 70	12, 22, 40, 47	12 (9%)
1	B	124/157 (78%)	0.01	0 100 100	12, 24, 37, 42	8 (6%)
1	C	123/157 (78%)	0.47	6 (4%) 36 35	10, 22, 42, 54	3 (2%)
1	D	118/157 (75%)	0.22	1 (0%) 82 82	11, 22, 36, 39	4 (3%)
All	All	488/628 (77%)	0.12	9 (1%) 67 67	10, 22, 39, 54	27 (5%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	62	TYR	4.5
1	C	131	LEU	3.5
1	C	63	PHE	3.2
1	A	132	ALA	3.1
1	D	19	TYR	2.4
1	C	43	TYR	2.3
1	A	9	ALA	2.3
1	C	81	ALA	2.2
1	C	61	HIS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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, 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(\AA^2)	Q<0.9
2	ACT	A	301	4/4	0.90	0.16	42,43,44,45	4

6.5 Other polymers [i](#)

There are no such residues in this entry.