



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:26 PM UTC

PDB ID : 8FUH / pdb_00008fuh
Title : Rubrerythrin from *B. pseudomallei*: apo form
Authors : Monteiro, D.C.F.; Snell, M.E.; Budziszewski, G.R.; Bowman, S.E.J.
Deposited on : 2023-01-17
Resolution : 1.85 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

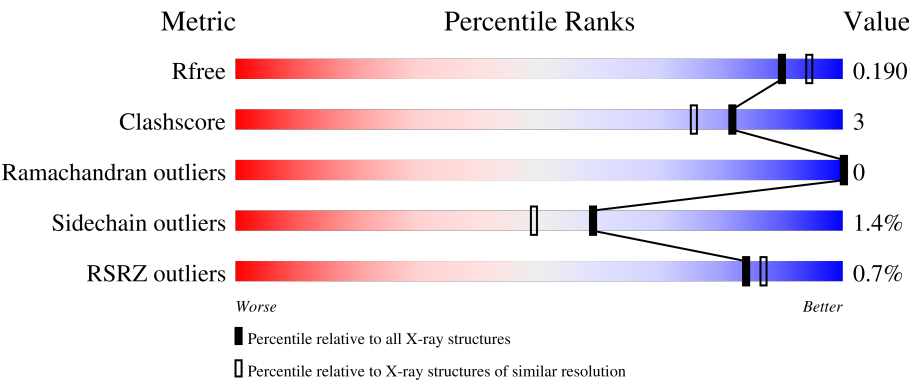
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	5	169	% 77% 5% 18%
1	A	169	% 78% • 18%
1	B	169	% 74% 8% 18%
1	M	169	% 77% 5% 18%
1	S	169	% 76% 6% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Y	169	% 77% 5% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13649 atoms, of which 6151 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 Rubrerythrin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	139	Total	C	H	N	O	S	70	1	0
			2098	671	1015	189	221	2			
1	B	139	Total	C	H	N	O	S	70	2	0
			2120	678	1028	190	222	2			
1	M	139	Total	C	H	N	O	S	72	2	0
			2121	677	1029	192	221	2			
1	S	139	Total	C	H	N	O	S	70	1	0
			2101	672	1017	189	221	2			
1	Y	139	Total	C	H	N	O	S	72	2	0
			2118	676	1027	192	221	2			
1	5	139	Total	C	H	N	O	S	70	1	0
			2098	671	1015	189	221	2			

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	initiating methionine	UNP Q3JK21
A	-27	GLY	-	expression tag	UNP Q3JK21
A	-26	SER	-	expression tag	UNP Q3JK21
A	-25	SER	-	expression tag	UNP Q3JK21
A	-24	HIS	-	expression tag	UNP Q3JK21
A	-23	HIS	-	expression tag	UNP Q3JK21
A	-22	HIS	-	expression tag	UNP Q3JK21
A	-21	HIS	-	expression tag	UNP Q3JK21
A	-20	HIS	-	expression tag	UNP Q3JK21
A	-19	HIS	-	expression tag	UNP Q3JK21
A	-18	SER	-	expression tag	UNP Q3JK21
A	-17	SER	-	expression tag	UNP Q3JK21
A	-16	GLY	-	expression tag	UNP Q3JK21
A	-15	LEU	-	expression tag	UNP Q3JK21
A	-14	VAL	-	expression tag	UNP Q3JK21
A	-13	PRO	-	expression tag	UNP Q3JK21
A	-12	ARG	-	expression tag	UNP Q3JK21

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	GLY	-	expression tag	UNP Q3JK21
A	-10	SER	-	expression tag	UNP Q3JK21
A	-9	HIS	-	expression tag	UNP Q3JK21
A	-8	MET	-	expression tag	UNP Q3JK21
A	-7	GLU	-	expression tag	UNP Q3JK21
A	-6	ASN	-	expression tag	UNP Q3JK21
A	-5	LEU	-	expression tag	UNP Q3JK21
A	-4	TYR	-	expression tag	UNP Q3JK21
A	-3	PHE	-	expression tag	UNP Q3JK21
A	-2	GLN	-	expression tag	UNP Q3JK21
A	-1	GLY	-	expression tag	UNP Q3JK21
A	0	SER	-	expression tag	UNP Q3JK21
B	-28	MET	-	initiating methionine	UNP Q3JK21
B	-27	GLY	-	expression tag	UNP Q3JK21
B	-26	SER	-	expression tag	UNP Q3JK21
B	-25	SER	-	expression tag	UNP Q3JK21
B	-24	HIS	-	expression tag	UNP Q3JK21
B	-23	HIS	-	expression tag	UNP Q3JK21
B	-22	HIS	-	expression tag	UNP Q3JK21
B	-21	HIS	-	expression tag	UNP Q3JK21
B	-20	HIS	-	expression tag	UNP Q3JK21
B	-19	HIS	-	expression tag	UNP Q3JK21
B	-18	SER	-	expression tag	UNP Q3JK21
B	-17	SER	-	expression tag	UNP Q3JK21
B	-16	GLY	-	expression tag	UNP Q3JK21
B	-15	LEU	-	expression tag	UNP Q3JK21
B	-14	VAL	-	expression tag	UNP Q3JK21
B	-13	PRO	-	expression tag	UNP Q3JK21
B	-12	ARG	-	expression tag	UNP Q3JK21
B	-11	GLY	-	expression tag	UNP Q3JK21
B	-10	SER	-	expression tag	UNP Q3JK21
B	-9	HIS	-	expression tag	UNP Q3JK21
B	-8	MET	-	expression tag	UNP Q3JK21
B	-7	GLU	-	expression tag	UNP Q3JK21
B	-6	ASN	-	expression tag	UNP Q3JK21
B	-5	LEU	-	expression tag	UNP Q3JK21
B	-4	TYR	-	expression tag	UNP Q3JK21
B	-3	PHE	-	expression tag	UNP Q3JK21
B	-2	GLN	-	expression tag	UNP Q3JK21
B	-1	GLY	-	expression tag	UNP Q3JK21
B	0	SER	-	expression tag	UNP Q3JK21
M	-28	MET	-	initiating methionine	UNP Q3JK21

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	-27	GLY	-	expression tag	UNP Q3JK21
M	-26	SER	-	expression tag	UNP Q3JK21
M	-25	SER	-	expression tag	UNP Q3JK21
M	-24	HIS	-	expression tag	UNP Q3JK21
M	-23	HIS	-	expression tag	UNP Q3JK21
M	-22	HIS	-	expression tag	UNP Q3JK21
M	-21	HIS	-	expression tag	UNP Q3JK21
M	-20	HIS	-	expression tag	UNP Q3JK21
M	-19	HIS	-	expression tag	UNP Q3JK21
M	-18	SER	-	expression tag	UNP Q3JK21
M	-17	SER	-	expression tag	UNP Q3JK21
M	-16	GLY	-	expression tag	UNP Q3JK21
M	-15	LEU	-	expression tag	UNP Q3JK21
M	-14	VAL	-	expression tag	UNP Q3JK21
M	-13	PRO	-	expression tag	UNP Q3JK21
M	-12	ARG	-	expression tag	UNP Q3JK21
M	-11	GLY	-	expression tag	UNP Q3JK21
M	-10	SER	-	expression tag	UNP Q3JK21
M	-9	HIS	-	expression tag	UNP Q3JK21
M	-8	MET	-	expression tag	UNP Q3JK21
M	-7	GLU	-	expression tag	UNP Q3JK21
M	-6	ASN	-	expression tag	UNP Q3JK21
M	-5	LEU	-	expression tag	UNP Q3JK21
M	-4	TYR	-	expression tag	UNP Q3JK21
M	-3	PHE	-	expression tag	UNP Q3JK21
M	-2	GLN	-	expression tag	UNP Q3JK21
M	-1	GLY	-	expression tag	UNP Q3JK21
M	0	SER	-	expression tag	UNP Q3JK21
S	-28	MET	-	initiating methionine	UNP Q3JK21
S	-27	GLY	-	expression tag	UNP Q3JK21
S	-26	SER	-	expression tag	UNP Q3JK21
S	-25	SER	-	expression tag	UNP Q3JK21
S	-24	HIS	-	expression tag	UNP Q3JK21
S	-23	HIS	-	expression tag	UNP Q3JK21
S	-22	HIS	-	expression tag	UNP Q3JK21
S	-21	HIS	-	expression tag	UNP Q3JK21
S	-20	HIS	-	expression tag	UNP Q3JK21
S	-19	HIS	-	expression tag	UNP Q3JK21
S	-18	SER	-	expression tag	UNP Q3JK21
S	-17	SER	-	expression tag	UNP Q3JK21
S	-16	GLY	-	expression tag	UNP Q3JK21
S	-15	LEU	-	expression tag	UNP Q3JK21

Continued on next page...

Continued from previous page...

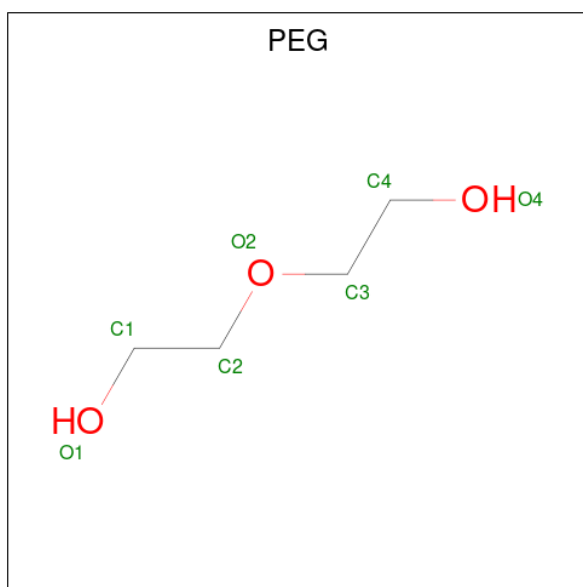
Chain	Residue	Modelled	Actual	Comment	Reference
S	-14	VAL	-	expression tag	UNP Q3JK21
S	-13	PRO	-	expression tag	UNP Q3JK21
S	-12	ARG	-	expression tag	UNP Q3JK21
S	-11	GLY	-	expression tag	UNP Q3JK21
S	-10	SER	-	expression tag	UNP Q3JK21
S	-9	HIS	-	expression tag	UNP Q3JK21
S	-8	MET	-	expression tag	UNP Q3JK21
S	-7	GLU	-	expression tag	UNP Q3JK21
S	-6	ASN	-	expression tag	UNP Q3JK21
S	-5	LEU	-	expression tag	UNP Q3JK21
S	-4	TYR	-	expression tag	UNP Q3JK21
S	-3	PHE	-	expression tag	UNP Q3JK21
S	-2	GLN	-	expression tag	UNP Q3JK21
S	-1	GLY	-	expression tag	UNP Q3JK21
S	0	SER	-	expression tag	UNP Q3JK21
Y	-28	MET	-	initiating methionine	UNP Q3JK21
Y	-27	GLY	-	expression tag	UNP Q3JK21
Y	-26	SER	-	expression tag	UNP Q3JK21
Y	-25	SER	-	expression tag	UNP Q3JK21
Y	-24	HIS	-	expression tag	UNP Q3JK21
Y	-23	HIS	-	expression tag	UNP Q3JK21
Y	-22	HIS	-	expression tag	UNP Q3JK21
Y	-21	HIS	-	expression tag	UNP Q3JK21
Y	-20	HIS	-	expression tag	UNP Q3JK21
Y	-19	HIS	-	expression tag	UNP Q3JK21
Y	-18	SER	-	expression tag	UNP Q3JK21
Y	-17	SER	-	expression tag	UNP Q3JK21
Y	-16	GLY	-	expression tag	UNP Q3JK21
Y	-15	LEU	-	expression tag	UNP Q3JK21
Y	-14	VAL	-	expression tag	UNP Q3JK21
Y	-13	PRO	-	expression tag	UNP Q3JK21
Y	-12	ARG	-	expression tag	UNP Q3JK21
Y	-11	GLY	-	expression tag	UNP Q3JK21
Y	-10	SER	-	expression tag	UNP Q3JK21
Y	-9	HIS	-	expression tag	UNP Q3JK21
Y	-8	MET	-	expression tag	UNP Q3JK21
Y	-7	GLU	-	expression tag	UNP Q3JK21
Y	-6	ASN	-	expression tag	UNP Q3JK21
Y	-5	LEU	-	expression tag	UNP Q3JK21
Y	-4	TYR	-	expression tag	UNP Q3JK21
Y	-3	PHE	-	expression tag	UNP Q3JK21
Y	-2	GLN	-	expression tag	UNP Q3JK21

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-1	GLY	-	expression tag	UNP Q3JK21
Y	0	SER	-	expression tag	UNP Q3JK21
5	-28	MET	-	initiating methionine	UNP Q3JK21
5	-27	GLY	-	expression tag	UNP Q3JK21
5	-26	SER	-	expression tag	UNP Q3JK21
5	-25	SER	-	expression tag	UNP Q3JK21
5	-24	HIS	-	expression tag	UNP Q3JK21
5	-23	HIS	-	expression tag	UNP Q3JK21
5	-22	HIS	-	expression tag	UNP Q3JK21
5	-21	HIS	-	expression tag	UNP Q3JK21
5	-20	HIS	-	expression tag	UNP Q3JK21
5	-19	HIS	-	expression tag	UNP Q3JK21
5	-18	SER	-	expression tag	UNP Q3JK21
5	-17	SER	-	expression tag	UNP Q3JK21
5	-16	GLY	-	expression tag	UNP Q3JK21
5	-15	LEU	-	expression tag	UNP Q3JK21
5	-14	VAL	-	expression tag	UNP Q3JK21
5	-13	PRO	-	expression tag	UNP Q3JK21
5	-12	ARG	-	expression tag	UNP Q3JK21
5	-11	GLY	-	expression tag	UNP Q3JK21
5	-10	SER	-	expression tag	UNP Q3JK21
5	-9	HIS	-	expression tag	UNP Q3JK21
5	-8	MET	-	expression tag	UNP Q3JK21
5	-7	GLU	-	expression tag	UNP Q3JK21
5	-6	ASN	-	expression tag	UNP Q3JK21
5	-5	LEU	-	expression tag	UNP Q3JK21
5	-4	TYR	-	expression tag	UNP Q3JK21
5	-3	PHE	-	expression tag	UNP Q3JK21
5	-2	GLN	-	expression tag	UNP Q3JK21
5	-1	GLY	-	expression tag	UNP Q3JK21
5	0	SER	-	expression tag	UNP Q3JK21

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

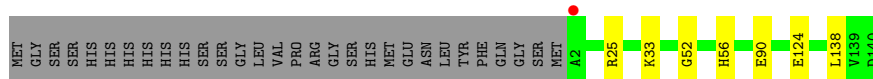


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	1	0
			17	4	10	3		
2	S	1	Total	C	H	O	1	0
			17	4	10	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total	O	0	4
			157	157		
3	B	168	Total	O	0	6
			174	174		
3	M	169	Total	O	0	5
			174	174		
3	S	144	Total	O	0	3
			147	147		
3	Y	153	Total	O	0	1
			154	154		
3	5	149	Total	O	0	4
			153	153		

- Molecule 1: Rubrerythrin



Label	Value
NET	100
GLY	99
SER	98
SER	97
HIS	96
HIS	95
HIS	94
HIS	93
HIS	92
HIS	91
SER	90
SER	89
GLY	88
LEU	87
VAL	86
PRO	85
ARG	84
GLY	83
SER	82
HIS	81
MET	80
GLU	79
ASN	78
LEU	77
TYR	76
PHE	75
GLN	74
GLY	73
SER	72
MET	71
A2	70
Q3	69
K8	68
K14	67
F17	66
R25	65
D35	64
I42	63
H58	62
L61	61
E62	60
E90	59
R106	58
L120	57
E124	56
E130	55

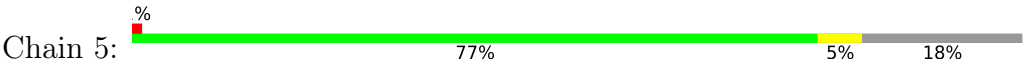
Residue	Score	Color
Met	1.00	Red
Gly	0.99	Yellow
Ser	0.98	Yellow
Ser	0.97	Yellow
His	0.96	Yellow
His	0.95	Yellow
His	0.94	Yellow
His	0.93	Yellow
His	0.92	Yellow
His	0.91	Yellow
Ser	0.90	Yellow
Ser	0.89	Yellow
Gly	0.88	Yellow
Leu	0.87	Yellow
Val	0.86	Yellow
Pro	0.85	Yellow
Arg	0.84	Yellow
Gly	0.83	Yellow
Ser	0.82	Yellow
His	0.81	Yellow
Met	0.80	Yellow
Glu	0.79	Yellow
Asn	0.78	Yellow
Leu	0.77	Yellow
Tyr	0.76	Yellow
Phe	0.75	Yellow
Gln	0.74	Yellow
Gly	0.73	Yellow
Ser	0.72	Yellow
Met	0.71	Yellow
Met	0.70	Yellow
Asp	0.69	Yellow
Asp	0.68	Yellow
Asp	0.67	Yellow
Asp	0.66	Yellow
Asp	0.65	Yellow
Asp	0.64	Yellow
Asp	0.63	Yellow
Asp	0.62	Yellow
Asp	0.61	Yellow
Asp	0.60	Yellow
Asp	0.59	Yellow
Asp	0.58	Yellow
Asp	0.57	Yellow
Asp	0.56	Yellow
Asp	0.55	Yellow
Asp	0.54	Yellow
Asp	0.53	Yellow
Asp	0.52	Yellow
Asp	0.51	Yellow
Asp	0.50	Yellow
Asp	0.49	Yellow
Asp	0.48	Yellow
Asp	0.47	Yellow
Asp	0.46	Yellow
Asp	0.45	Yellow
Asp	0.44	Yellow
Asp	0.43	Yellow
Asp	0.42	Yellow
Asp	0.41	Yellow
Asp	0.40	Yellow
Asp	0.39	Yellow
Asp	0.38	Yellow
Asp	0.37	Yellow
Asp	0.36	Yellow
Asp	0.35	Yellow
Asp	0.34	Yellow
Asp	0.33	Yellow
Asp	0.32	Yellow
Asp	0.31	Yellow
Asp	0.30	Yellow
Asp	0.29	Yellow
Asp	0.28	Yellow
Asp	0.27	Yellow
Asp	0.26	Yellow
Asp	0.25	Yellow
Asp	0.24	Yellow
Asp	0.23	Yellow
Asp	0.22	Yellow
Asp	0.21	Yellow
Asp	0.20	Yellow
Asp	0.19	Yellow
Asp	0.18	Yellow
Asp	0.17	Yellow
Asp	0.16	Yellow
Asp	0.15	Yellow
Asp	0.14	Yellow
Asp	0.13	Yellow
Asp	0.12	Yellow
Asp	0.11	Yellow
Asp	0.10	Yellow
Asp	0.09	Yellow
Asp	0.08	Yellow
Asp	0.07	Yellow
Asp	0.06	Yellow
Asp	0.05	Yellow
Asp	0.04	Yellow
Asp	0.03	Yellow
Asp	0.02	Yellow
Asp	0.01	Yellow
Asp	0.00	Yellow

Residue	Score
Met	1.00
Gly	0.99
Ser	0.98
His	0.97
His	0.96
His	0.95
His	0.94
His	0.93
His	0.92
Ser	0.91
Ser	0.90
Gly	0.89
Leu	0.88
Val	0.87
Pro	0.86
Arg	0.85
Gly	0.84
Ser	0.83
His	0.82
Met	0.81
Glu	0.80
Asn	0.79
Leu	0.78
Tyr	0.77
Phe	0.76
Gln	0.75
Gly	0.74
Ser	0.73
Met	0.72
A2	0.71
E11	0.70
R25	0.69
Y29	0.68
D35	0.67
R47	0.66
L61	0.65
L83	0.64
E90	0.63
D96	0.62
E124	0.61
S146	0.60

Residue	B-factor (Å²)
MET	60
GLY	70
SER	80
HIS	90
HIS	100
HIS	110
HIS	120
HIS	130
SER	140
SER	150
GLY	160
LEU	170
VAL	180
PRO	190
ARG	200
GLY	210
SER	220
HIS	230
MET	240
GLU	250
ASN	260
LEU	270
TYR	280
PHE	290
GLN	300
GLY	310
SER	320
MET	330
A2	340
R25	350
D35	360
G52	370
G59	380
H60	390
L61	400
E90	410
L120	420
E124	430
G125	440



WORLD WIDE
PDB
PROTEIN DATA BANK



MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MET	GLU	ASN	LEU	TYR	PHE	GLN	GLY	SER	MET	A2	R25	G52	E90	T91	Y94	T95	D96	W116	E124	R125	D140
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	202.37Å 202.37Å 70.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.75 – 1.85 28.75 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (28.75-1.85) 90.0 (28.75-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.68 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.150 , 0.188 0.151 , 0.190	Depositor DCC
R_{free} test set	5014 reflections (5.48%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13649	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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

5.1 Standard geometry

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

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	5	0.62	0/1108	0.98	0/1494
1	A	0.65	0/1108	1.02	0/1494
1	B	0.65	0/1117	1.03	0/1506
1	M	0.67	0/1120	0.97	0/1509
1	S	0.60	0/1109	1.02	0/1495
1	Y	0.62	0/1119	0.95	0/1508
All	All	0.63	0/6681	0.99	0/9006

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	M	0	1
1	S	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	47	ARG	Sidechain
1	S	47	ARG	Sidechain

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	5	1083	1015	1010	7	0
1	A	1083	1015	1010	5	0
1	B	1092	1028	1022	8	0
1	M	1092	1029	1025	7	0
1	S	1084	1017	1012	7	0
1	Y	1091	1027	1023	7	0
2	A	7	10	10	0	0
2	S	7	10	10	0	0
3	5	153	0	0	1	0
3	A	157	0	0	0	0
3	B	174	0	0	3	0
3	M	174	0	0	1	0
3	S	147	0	0	1	0
3	Y	154	0	0	0	0
All	All	7498	6151	6122	32	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 3.

All (32) 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:33:LYS:NZ	3:B:314[B]:HOH:O	2.36	0.59
1:B:90:GLU:OE1	1:B:124:GLU:OE1	2.24	0.55
1:A:56:HIS:CD2	1:B:120:LEU:HD22	2.42	0.55
1:M:42:ILE:HD12	1:S:83:LEU:HD11	1.89	0.54
1:B:14:LYS:NZ	3:B:201:HOH:O	2.38	0.53
1:B:106:ARG:HD2	3:B:278:HOH:O	2.10	0.51
1:M:3:GLN:N	1:M:3:GLN:OE1	2.45	0.49
1:A:52:GLY:HA2	1:Y:35:ASP:HB3	1.94	0.49
1:5:125:ARG:NH1	3:5:201:HOH:O	2.43	0.48
1:M:11[B]:GLU:HG2	3:M:318:HOH:O	2.13	0.48
1:S:11[A]:GLU:HG2	3:S:412:HOH:O	2.14	0.48
1:S:90:GLU:OE1	1:S:124:GLU:OE1	2.32	0.47
1:5:90:GLU:OE1	1:5:124:GLU:OE1	2.31	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:PHE:CE1	1:B:61:LEU:HG	2.50	0.46
1:B:35:ASP:HB3	1:5:52:GLY:HA2	1.97	0.46
1:Y:59:GLY:HA3	1:5:116:TRP:CZ2	2.51	0.46
1:B:58:HIS:O	1:B:62[A]:GLU:HG3	2.17	0.44
1:Y:120:LEU:O	1:Y:124:GLU:HG2	2.18	0.44
1:Y:60:HIS:HD1	1:5:116:TRP:HE1	1.66	0.44
1:5:91:THR:HA	1:5:94:TYR:CE2	2.53	0.44
1:S:96:ASP:OD1	1:S:96:ASP:C	2.62	0.42
1:M:3:GLN:H	1:M:3:GLN:CD	2.28	0.42
1:Y:90:GLU:OE1	1:Y:124:GLU:OE1	2.37	0.42
1:A:90:GLU:OE1	1:A:124:GLU:OE1	2.38	0.41
1:M:94:TYR:CD2	1:M:125:ARG:HA	2.56	0.41
1:S:61:LEU:HD23	1:S:61:LEU:HA	1.89	0.41
1:S:35:ASP:HB3	1:Y:52:GLY:HA2	2.03	0.41
1:A:138:LEU:HD13	1:B:42[B]:ILE:CD1	2.51	0.41
1:Y:61:LEU:HD23	1:Y:61:LEU:HA	1.93	0.41
1:M:61:LEU:HD23	1:S:29:TYR:CG	2.57	0.40
1:M:91:THR:HA	1:M:94:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

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	5	138/169 (82%)	136 (99%)	2 (1%)	0	100	100
1	A	138/169 (82%)	133 (96%)	5 (4%)	0	100	100
1	B	139/169 (82%)	136 (98%)	3 (2%)	0	100	100
1	M	139/169 (82%)	135 (97%)	4 (3%)	0	100	100
1	S	138/169 (82%)	134 (97%)	4 (3%)	0	100	100
1	Y	139/169 (82%)	134 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	831/1014 (82%)	808 (97%)	23 (3%)	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	5	106/131 (81%)	105 (99%)	1 (1%)	70	64
1	A	106/131 (81%)	105 (99%)	1 (1%)	70	64
1	B	107/131 (82%)	104 (97%)	3 (3%)	38	23
1	M	107/131 (82%)	106 (99%)	1 (1%)	70	64
1	S	106/131 (81%)	105 (99%)	1 (1%)	70	64
1	Y	107/131 (82%)	105 (98%)	2 (2%)	50	38
All	All	639/786 (81%)	630 (99%)	9 (1%)	59	49

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	B	3	GLN
1	B	8	LYS
1	B	25	ARG
1	M	25	ARG
1	S	25	ARG
1	Y	25	ARG
1	Y	61	LEU
1	5	25	ARG

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	39	GLN
1	B	39	GLN
1	M	39	GLN
1	S	39	GLN
1	5	39	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](#)

2 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	PEG	A	201	-	6,6,6	0.35	0	5,5,5	0.18	0
2	PEG	S	201	-	6,6,6	0.42	0	5,5,5	0.27	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
2	PEG	A	201	-	-	2/4/4/4	-
2	PEG	S	201	-	-	2/4/4/4	-

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
2	A	201	PEG	O1-C1-C2-O2
2	S	201	PEG	O2-C3-C4-O4
2	S	201	PEG	C4-C3-O2-C2
2	A	201	PEG	O2-C3-C4-O4

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 [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, 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	5	139/169 (82%)	-0.40	1 (0%) 84 87	17, 27, 52, 76	1 (0%)
1	A	139/169 (82%)	-0.66	1 (0%) 84 87	15, 22, 40, 63	1 (0%)
1	B	139/169 (82%)	-0.71	1 (0%) 84 87	10, 21, 41, 68	2 (1%)
1	M	139/169 (82%)	-0.64	1 (0%) 84 87	14, 22, 44, 86	2 (1%)
1	S	139/169 (82%)	-0.48	1 (0%) 84 87	15, 26, 46, 73	1 (0%)
1	Y	139/169 (82%)	-0.57	1 (0%) 84 87	13, 24, 47, 87	2 (1%)
All	All	834/1014 (82%)	-0.58	6 (0%) 84 87	10, 24, 46, 87	9 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	5	2	ALA	5.6
1	M	2	ALA	3.9
1	S	2	ALA	3.7
1	A	2	ALA	2.7
1	B	2	ALA	2.7
1	Y	2	ALA	2.5

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 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($\text{\AA}^2$)	Q<0.9
2	PEG	A	201	7/7	0.76	0.19	45,61,72,82	1
2	PEG	S	201	7/7	0.79	0.17	56,67,70,70	1

6.5 Other polymers [i](#)

There are no such residues in this entry.