



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 11:43 PM EDT

PDB ID : 3WIA  
Title : Crystal structure of the N-terminal 1-37 residues deleted mutant of Geobacillus copper nitrite reductase  
Authors : Fukuda, Y.; Nojiri, M.  
Deposited on : 2013-09-09  
Resolution : 1.77 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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:

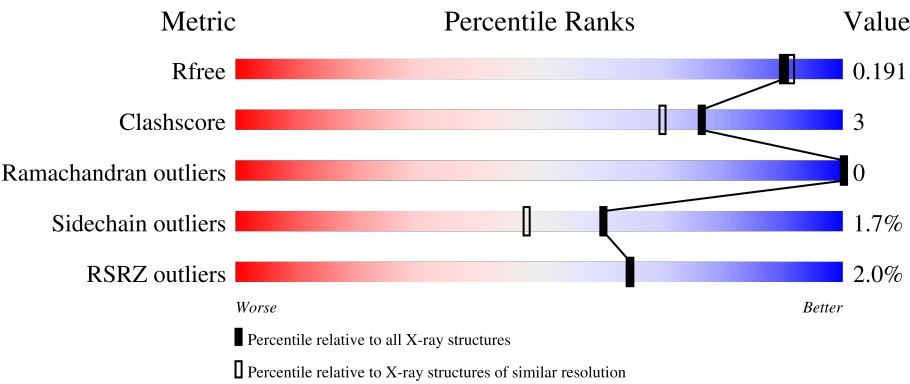
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

# 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 1.77 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	287	<div><div>0%</div><div>92%</div><div>5%</div></div>
1	B	287	<div><div>2%</div><div>90%</div><div>5%</div><div>5%</div></div>
1	C	287	<div><div>2%</div><div>91%</div><div>5%</div><div>5%</div></div>
1	D	287	<div><div>2%</div><div>88%</div><div>7%</div><div>5%</div></div>
1	E	287	<div><div>2%</div><div>91%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	287	 90% 5% 5%
1	G	287	 89% 6% 5%
1	H	287	 90% 5% 5%
1	I	287	 88% 7% 5%

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
3	FMT	A	404	-	-	X	-
3	FMT	C	401	-	-	X	-
3	FMT	D	404	-	-	X	-
3	FMT	D	405	-	-	X	-
3	FMT	E	404	-	-	X	-
3	FMT	G	404	-	-	X	-
3	FMT	H	401	-	-	X	-
3	FMT	I	401	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21279 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 Nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2132	1364	359	398	11			
1	B	273	Total	C	N	O	S	0	0	0
			2132	1364	359	398	11			
1	C	273	Total	C	N	O	S	0	0	0
			2132	1364	359	398	11			
1	D	273	Total	C	N	O	S	0	0	0
			2132	1364	359	398	11			
1	E	273	Total	C	N	O	S	0	0	0
			2132	1364	359	398	11			
1	F	273	Total	C	N	O	S	0	0	0
			2132	1364	359	398	11			
1	G	273	Total	C	N	O	S	0	0	0
			2132	1364	359	398	11			
1	H	273	Total	C	N	O	S	0	0	0
			2132	1364	359	398	11			
1	I	272	Total	C	N	O	S	0	0	0
			2122	1358	356	397	11			

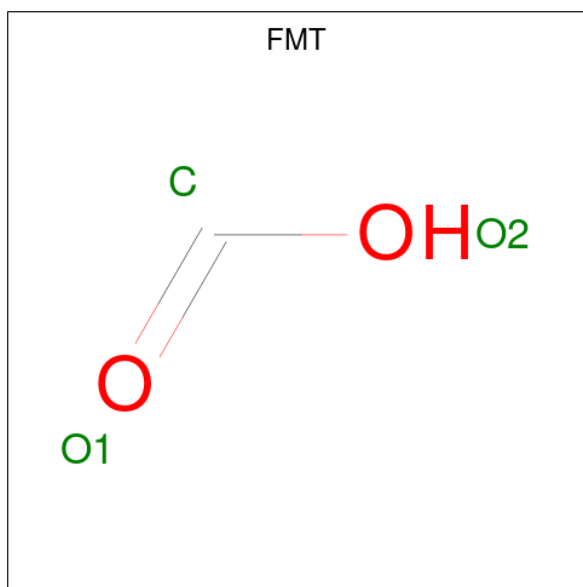
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	expression tag	UNP Q5L1X8
B	37	MET	-	expression tag	UNP Q5L1X8
C	37	MET	-	expression tag	UNP Q5L1X8
D	37	MET	-	expression tag	UNP Q5L1X8
E	37	MET	-	expression tag	UNP Q5L1X8
F	37	MET	-	expression tag	UNP Q5L1X8
G	37	MET	-	expression tag	UNP Q5L1X8
H	37	MET	-	expression tag	UNP Q5L1X8
I	37	MET	-	expression tag	UNP Q5L1X8

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0
2	E	2	Total Cu 2 2	0	0
2	F	2	Total Cu 2 2	0	0
2	G	2	Total Cu 2 2	0	0
2	H	2	Total Cu 2 2	0	0
2	I	2	Total Cu 2 2	0	0

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	E	1	Total C O 3 1 2	0	0
3	E	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	I	1	Total C O 3 1 2	0	0
3	I	1	Total C O 3 1 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	251	Total O 251 251	0	0
4	B	221	Total O 221 221	0	0
4	C	232	Total O 232 232	0	0
4	D	223	Total O 223 223	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	225	Total 225	O 225	0	0
4	F	222	Total 222	O 222	0	0
4	G	223	Total 223	O 223	0	0
4	H	211	Total 211	O 211	0	0
4	I	221	Total 221	O 221	0	0

### 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.

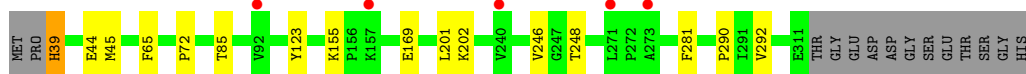
- Molecule 1: Nitrite reductase

Chain A: 



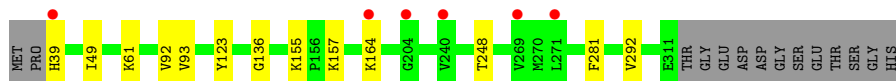
- Molecule 1: Nitrite reductase

Chain B: 




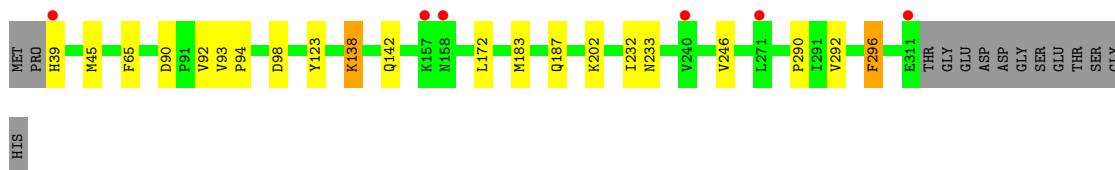
- Molecule 1: Nitrite reductase

Chain C: 



- Molecule 1: Nitrite reductase

Chain D: 



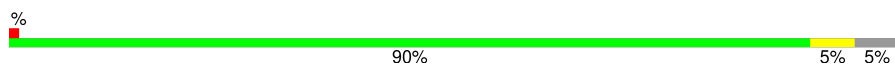
- Molecule 1: Nitrite reductase

Chain E: 






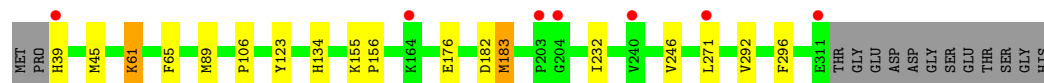
## ● Molecule 1: Nitrite reductase

Chain F: 

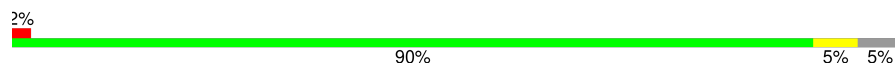


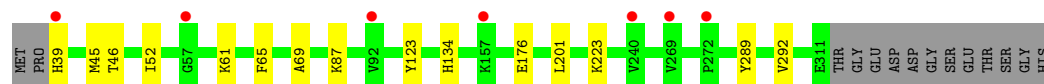
## ● Molecule 1: Nitrite reductase

Chain G: 




## ● Molecule 1: Nitrite reductase

Chain H: 



## ● Molecule 1: Nitrite reductase

Chain I: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.32Å 164.99Å 126.56Å 90.00° 102.27° 90.00°	Depositor
Resolution (Å)	42.70 – 1.77 42.70 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.4 (42.70-1.77) 98.4 (42.70-1.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.171 , 0.192 0.171 , 0.191	Depositor DCC
$R_{free}$ test set	17225 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	21279	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.65	0/2192	0.69	0/2986
1	B	0.65	0/2192	0.68	0/2986
1	C	0.63	0/2192	0.69	0/2986
1	D	0.62	0/2192	0.69	0/2986
1	E	0.66	0/2192	0.67	0/2986
1	F	0.67	0/2192	0.71	0/2986
1	G	0.64	0/2192	0.68	1/2986 (0.0%)
1	H	0.61	0/2192	0.67	0/2986
1	I	0.61	0/2181	0.68	0/2971
All	All	0.64	0/19717	0.68	1/26859 (0.0%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	0	9

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	182	ASP	CB-CG-OD1	5.29	123.06	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	VAL	Peptide
1	B	292	VAL	Peptide
1	C	292	VAL	Peptide
1	D	292	VAL	Peptide
1	E	292	VAL	Peptide
1	F	292	VAL	Peptide
1	G	292	VAL	Peptide
1	H	292	VAL	Peptide
1	I	292	VAL	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2132	0	2080	6	0
1	B	2132	0	2080	14	0
1	C	2132	0	2080	10	0
1	D	2132	0	2080	13	0
1	E	2132	0	2080	14	0
1	F	2132	0	2080	12	0
1	G	2132	0	2080	13	0
1	H	2132	0	2080	9	0
1	I	2122	0	2073	11	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6	0	2	2	0
3	B	6	0	2	0	0
3	C	6	0	2	4	0
3	D	9	0	3	5	0
3	E	6	0	2	2	0
3	F	3	0	1	0	0
3	G	6	0	2	4	0
3	H	6	0	2	3	0
3	I	6	0	2	4	0
4	A	251	0	0	6	0
4	B	221	0	0	2	0
4	C	232	0	0	8	1
4	D	223	0	0	3	0
4	E	225	0	0	2	0
4	F	222	0	0	1	0
4	G	223	0	0	9	0
4	H	211	0	0	1	1
4	I	221	0	0	3	0
All	All	21279	0	18731	114	1

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

All (114) 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:G:89:MET:HG3	4:G:659:HOH:O	1.33	1.28
3:D:404:FMT:H	4:D:663:HOH:O	1.12	1.22
3:A:404:FMT:H	4:A:690:HOH:O	1.36	1.20
1:F:45:MET:CE	1:F:65:PHE:HB3	1.71	1.19
1:I:45:MET:HE2	1:I:65:PHE:HB3	1.21	1.15
1:B:45:MET:HE2	1:B:65:PHE:HB3	1.28	1.11
1:I:45:MET:CE	1:I:65:PHE:HB3	1.83	1.08
3:C:401:FMT:H	4:C:675:HOH:O	1.56	1.03
1:D:39:HIS:HA	4:D:501:HOH:O	1.63	0.98
1:C:92:VAL:HG23	1:C:93:VAL:HG23	1.45	0.97
3:E:404:FMT:H	4:E:666:HOH:O	1.62	0.97
1:F:45:MET:HE2	1:F:65:PHE:HB3	1.46	0.95
1:D:92:VAL:HG23	1:D:93:VAL:HG23	1.48	0.94
3:G:404:FMT:C	4:G:666:HOH:O	2.15	0.94
1:B:39:HIS:HA	4:B:501:HOH:O	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:VAL:HG22	3:G:404:FMT:H	1.52	0.91
3:I:401:FMT:O2	4:I:658:HOH:O	1.88	0.90
1:E:45:MET:CE	1:E:72:PRO:HG2	2.03	0.89
1:A:89:MET:HG3	4:A:741:HOH:O	1.75	0.86
1:F:45:MET:CE	1:F:65:PHE:CB	2.54	0.86
3:C:401:FMT:C	4:C:675:HOH:O	2.19	0.86
3:A:404:FMT:C	4:A:690:HOH:O	2.07	0.85
1:D:45:MET:HE3	1:D:65:PHE:HB3	1.59	0.84
3:E:404:FMT:C	4:E:666:HOH:O	2.23	0.82
1:I:45:MET:HE2	1:I:65:PHE:CB	2.09	0.79
1:C:155:LYS:HD3	4:C:520:HOH:O	1.84	0.78
1:F:45:MET:HE3	1:F:65:PHE:HB3	1.65	0.78
1:E:45:MET:HE3	1:E:72:PRO:HG2	1.64	0.77
4:G:665:HOH:O	3:H:401:FMT:C	2.31	0.77
1:E:45:MET:CE	1:E:72:PRO:CG	2.64	0.75
4:G:665:HOH:O	3:H:401:FMT:H	1.86	0.74
1:G:39:HIS:HA	4:G:501:HOH:O	1.88	0.73
1:G:246:VAL:CG2	3:G:404:FMT:H	2.18	0.73
1:B:45:MET:CE	1:B:65:PHE:HB3	2.13	0.71
1:E:45:MET:HE1	1:E:72:PRO:HG2	1.72	0.69
1:D:45:MET:CE	1:D:65:PHE:HB3	2.22	0.69
1:I:45:MET:CE	1:I:65:PHE:CB	2.65	0.69
3:G:404:FMT:H	4:G:666:HOH:O	1.88	0.67
1:A:44:GLU:HG2	1:A:85:THR:HB	1.77	0.67
1:A:116:ASN:ND2	4:A:654:HOH:O	2.27	0.67
1:E:45:MET:HE1	1:E:72:PRO:HD2	1.78	0.65
1:B:45:MET:HE3	1:B:72:PRO:CG	2.27	0.64
3:I:401:FMT:C	4:I:658:HOH:O	2.39	0.62
1:H:39:HIS:HB2	4:H:632:HOH:O	2.01	0.60
1:F:45:MET:HE2	1:F:65:PHE:CB	2.26	0.60
3:C:401:FMT:O1	4:C:672:HOH:O	2.17	0.59
1:D:90:ASP:OD1	1:D:92:VAL:HG22	2.03	0.58
3:D:404:FMT:C	1:E:246:VAL:HG22	2.34	0.58
1:E:45:MET:HE3	1:E:72:PRO:CG	2.31	0.58
1:G:134:HIS:CE1	3:H:401:FMT:H	2.39	0.58
1:B:45:MET:HE3	1:B:72:PRO:HG2	1.85	0.58
1:C:155:LYS:CD	4:C:520:HOH:O	2.49	0.57
1:B:45:MET:HE1	1:B:72:PRO:HD2	1.87	0.57
1:E:45:MET:HE1	1:E:72:PRO:CG	2.32	0.57
1:A:89:MET:CG	4:A:741:HOH:O	2.44	0.56
1:F:56:LYS:HE2	1:F:217:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:MET:HE1	1:E:72:PRO:CD	2.36	0.56
1:A:138:LYS:NZ	4:A:749:HOH:O	2.39	0.55
1:B:45:MET:CE	1:B:72:PRO:HD2	2.37	0.53
1:G:39:HIS:CD2	4:G:668:HOH:O	2.61	0.53
1:C:61:LYS:HB2	1:C:61:LYS:NZ	2.25	0.52
1:C:164:LYS:HG3	4:C:521:HOH:O	2.09	0.52
1:H:134:HIS:HE1	3:I:401:FMT:H	1.75	0.52
1:C:61:LYS:HD2	4:C:578:HOH:O	2.08	0.52
1:H:45:MET:HE3	1:H:65:PHE:HB3	1.93	0.51
1:H:45:MET:CE	1:H:65:PHE:CD1	2.95	0.49
1:D:296:PHE:CZ	3:D:405:FMT:H	2.48	0.49
1:D:246:VAL:HB	1:D:290:PRO:HD2	1.94	0.49
1:E:45:MET:CE	1:E:72:PRO:HD2	2.42	0.48
1:F:45:MET:HE1	1:F:65:PHE:CB	2.39	0.48
1:E:49:ILE:CG2	1:E:61:LYS:HG2	2.43	0.48
1:G:183:MET:HG3	4:G:555:HOH:O	2.13	0.47
1:H:134:HIS:CE1	3:I:401:FMT:H	2.49	0.47
1:B:246:VAL:HB	1:B:290:PRO:HD2	1.97	0.47
1:F:202:LYS:HG3	4:F:552:HOH:O	2.14	0.47
1:I:246:VAL:HB	1:I:290:PRO:HD2	1.96	0.47
1:F:203:PRO:HG2	1:I:76:VAL:HA	1.97	0.46
1:B:155:LYS:NZ	4:B:697:HOH:O	2.45	0.46
1:H:46:THR:HG22	1:H:87:LYS:HB3	1.98	0.45
1:D:187:GLN:HG2	1:E:300:GLN:HG2	1.98	0.45
3:D:405:FMT:O2	4:D:664:HOH:O	2.21	0.45
1:C:248:THR:HG21	1:C:281:PHE:CD1	2.51	0.44
1:D:93:VAL:HG12	1:D:94:PRO:O	2.17	0.44
1:B:44:GLU:HG3	1:B:85:THR:HB	1.99	0.44
1:E:45:MET:CE	1:E:72:PRO:CD	2.95	0.44
1:B:169:GLU:HG3	1:B:201:LEU:HD13	2.00	0.44
1:D:142:GLN:HB2	1:D:183:MET:SD	2.57	0.44
1:G:45:MET:CE	1:G:65:PHE:HB3	2.49	0.43
1:I:232:ILE:HD12	1:I:271:LEU:HD11	2.00	0.43
1:I:49:ILE:HD12	1:I:63:TRP:CD1	2.54	0.43
1:G:232:ILE:HD12	1:G:271:LEU:HD11	2.01	0.43
1:I:43:ILE:HD12	1:I:82:ILE:HG23	2.00	0.42
1:E:155:LYS:HA	1:E:156:PRO:HD3	1.94	0.42
1:H:45:MET:HE1	1:H:65:PHE:CG	2.55	0.42
1:D:138:LYS:N	1:D:138:LYS:HE2	2.35	0.42
1:F:45:MET:HE2	1:F:65:PHE:CG	2.54	0.42
1:C:39:HIS:CD2	4:C:552:HOH:O	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:PHE:HB2	1:F:152:ILE:HG23	2.01	0.42
1:H:52:ILE:HD12	1:H:69:ALA:HB3	2.01	0.41
1:C:49:ILE:CG2	1:C:61:LYS:HG2	2.50	0.41
1:A:228:ILE:O	1:A:280:GLU:HA	2.21	0.41
1:F:45:MET:CE	1:F:65:PHE:CG	3.04	0.41
1:I:155:LYS:NZ	4:I:648:HOH:O	2.53	0.41
1:B:45:MET:CE	1:B:72:PRO:HG2	2.51	0.41
1:D:172:LEU:O	1:D:232:ILE:HA	2.21	0.41
1:G:61:LYS:HB2	1:G:61:LYS:HE2	1.62	0.41
1:G:61:LYS:HD2	4:G:656:HOH:O	2.21	0.40
1:G:155:LYS:HA	1:G:156:PRO:HD3	1.95	0.40
1:B:248:THR:HG21	1:B:281:PHE:CD1	2.56	0.40
1:G:106:PRO:HG2	1:H:289:TYR:HA	2.02	0.40
1:I:131:PHE:HB2	1:I:152:ILE:HG23	2.03	0.40
1:D:98:ASP:OD1	3:D:403:FMT:O1	2.40	0.40
1:C:136:GLY:HA3	3:C:404:FMT:H	2.02	0.40
1:B:169:GLU:HG3	1:B:201:LEU:CD1	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:524:HOH:O	4:H:707:HOH:O[1_554]	2.19	0.01

## 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	271/287 (94%)	263 (97%)	8 (3%)	0	100	100
1	B	271/287 (94%)	264 (97%)	7 (3%)	0	100	100
1	C	271/287 (94%)	264 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	271/287 (94%)	265 (98%)	6 (2%)	0	100	100
1	E	271/287 (94%)	265 (98%)	6 (2%)	0	100	100
1	F	271/287 (94%)	266 (98%)	5 (2%)	0	100	100
1	G	271/287 (94%)	266 (98%)	5 (2%)	0	100	100
1	H	271/287 (94%)	263 (97%)	8 (3%)	0	100	100
1	I	270/287 (94%)	265 (98%)	5 (2%)	0	100	100
All	All	2438/2583 (94%)	2381 (98%)	57 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/248 (96%)	234 (99%)	3 (1%)	69	59
1	B	237/248 (96%)	234 (99%)	3 (1%)	69	59
1	C	237/248 (96%)	235 (99%)	2 (1%)	81	76
1	D	237/248 (96%)	232 (98%)	5 (2%)	53	38
1	E	237/248 (96%)	234 (99%)	3 (1%)	69	59
1	F	237/248 (96%)	231 (98%)	6 (2%)	47	31
1	G	237/248 (96%)	232 (98%)	5 (2%)	53	38
1	H	237/248 (96%)	232 (98%)	5 (2%)	53	38
1	I	236/248 (95%)	231 (98%)	5 (2%)	53	38
All	All	2132/2232 (96%)	2095 (98%)	37 (2%)	60	48

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	123	TYR

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Mol	Chain	Res	Type
1	A	296	PHE
1	B	39	HIS
1	B	123	TYR
1	B	202	LYS
1	C	123	TYR
1	C	157	LYS
1	D	123	TYR
1	D	138	LYS
1	D	202	LYS
1	D	233	ASN
1	D	296	PHE
1	E	92	VAL
1	E	123	TYR
1	E	296	PHE
1	F	39	HIS
1	F	123	TYR
1	F	183	MET
1	F	191	PRO
1	F	201	LEU
1	F	296	PHE
1	G	61	LYS
1	G	123	TYR
1	G	176	GLU
1	G	183	MET
1	G	296	PHE
1	H	61	LYS
1	H	123	TYR
1	H	176	GLU
1	H	201	LEU
1	H	223	LYS
1	I	40	ASP
1	I	92	VAL
1	I	123	TYR
1	I	233	ASN
1	I	296	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

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](#)

Of 36 ligands modelled in this entry, 18 are monoatomic - leaving 18 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	FMT	E	404	-	2,2,2	0.77	0	1,1,1	0.04	0
3	FMT	F	403	-	2,2,2	0.79	0	1,1,1	0.35	0
3	FMT	I	401	-	2,2,2	0.66	0	1,1,1	0.18	0
3	FMT	C	404	-	2,2,2	0.76	0	1,1,1	0.30	0
3	FMT	D	403	-	2,2,2	0.67	0	1,1,1	0.21	0
3	FMT	B	404	-	2,2,2	0.70	0	1,1,1	0.20	0
3	FMT	A	404	2	2,2,2	0.69	0	1,1,1	0.12	0
3	FMT	G	403	-	2,2,2	0.71	0	1,1,1	0.32	0
3	FMT	G	404	2	2,2,2	0.65	0	1,1,1	0.02	0
3	FMT	B	401	2	2,2,2	0.67	0	1,1,1	0.12	0
3	FMT	I	404	-	2,2,2	0.78	0	1,1,1	0.23	0
3	FMT	D	404	2	2,2,2	0.71	0	1,1,1	0.06	0
3	FMT	E	403	-	2,2,2	0.71	0	1,1,1	0.22	0
3	FMT	H	401	-	2,2,2	0.77	0	1,1,1	0.02	0
3	FMT	D	405	2	2,2,2	0.76	0	1,1,1	0.13	0
3	FMT	H	404	-	2,2,2	0.63	0	1,1,1	0.17	0
3	FMT	A	403	-	2,2,2	0.63	0	1,1,1	0.26	0
3	FMT	C	401	-	2,2,2	0.73	0	1,1,1	0.22	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 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	404	FMT	2	0
3	I	401	FMT	4	0
3	C	404	FMT	1	0
3	D	403	FMT	1	0
3	A	404	FMT	2	0
3	G	404	FMT	4	0
3	D	404	FMT	2	0
3	H	401	FMT	3	0
3	D	405	FMT	2	0
3	C	401	FMT	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	273/287 (95%)	-0.29	4 (1%) 73 73	17, 23, 34, 48	0
1	B	273/287 (95%)	-0.18	5 (1%) 68 68	17, 23, 32, 45	0
1	C	273/287 (95%)	-0.26	6 (2%) 62 61	17, 22, 33, 45	0
1	D	273/287 (95%)	-0.23	6 (2%) 62 61	17, 23, 35, 48	0
1	E	273/287 (95%)	-0.30	5 (1%) 68 68	16, 23, 33, 43	0
1	F	273/287 (95%)	-0.29	4 (1%) 73 73	17, 22, 32, 49	0
1	G	273/287 (95%)	-0.28	7 (2%) 56 55	16, 23, 34, 49	0
1	H	273/287 (95%)	-0.07	7 (2%) 56 55	17, 26, 38, 54	0
1	I	272/287 (94%)	-0.12	6 (2%) 62 61	17, 24, 34, 47	0
All	All	2456/2583 (95%)	-0.22	50 (2%) 65 65	16, 23, 35, 54	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	39	HIS	4.6
1	D	39	HIS	3.9
1	A	39	HIS	3.6
1	C	39	HIS	3.2
1	I	271	LEU	3.1
1	G	203	PRO	2.9
1	F	39	HIS	2.8
1	C	271	LEU	2.8
1	I	311	GLU	2.7
1	D	158	ASN	2.7
1	C	164	LYS	2.7
1	E	157	LYS	2.7
1	F	271	LEU	2.6
1	F	311	GLU	2.6
1	D	240	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	240	VAL	2.5
1	E	39	HIS	2.5
1	H	92	VAL	2.5
1	B	92	VAL	2.4
1	I	240	VAL	2.4
1	D	157	LYS	2.4
1	C	240	VAL	2.3
1	B	240	VAL	2.3
1	I	164	LYS	2.3
1	D	271	LEU	2.3
1	G	164	LYS	2.3
1	A	240	VAL	2.2
1	C	204	GLY	2.2
1	F	240	VAL	2.2
1	B	271	LEU	2.2
1	H	39	HIS	2.2
1	G	240	VAL	2.2
1	H	157	LYS	2.2
1	G	271	LEU	2.1
1	E	311	GLU	2.1
1	H	272	PRO	2.1
1	H	57	GLY	2.1
1	A	203	PRO	2.1
1	B	157	LYS	2.1
1	E	92	VAL	2.1
1	A	158	ASN	2.1
1	H	269	VAL	2.1
1	I	224	VAL	2.1
1	G	311	GLU	2.0
1	C	269	VAL	2.0
1	B	273	ALA	2.0
1	D	311	GLU	2.0
1	E	240	VAL	2.0
1	I	243	PHE	2.0
1	G	204	GLY	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 [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( $\text{\AA}^2$ )	Q<0.9
3	FMT	H	401	3/3	0.72	0.36	25,25,25,25	3
3	FMT	E	404	3/3	0.78	0.31	29,29,30,30	3
3	FMT	E	403	3/3	0.83	0.25	27,27,27,28	3
3	FMT	D	403	3/3	0.87	0.36	26,26,26,26	3
3	FMT	G	403	3/3	0.87	0.29	26,26,26,26	3
3	FMT	A	404	3/3	0.87	0.34	24,24,25,26	3
3	FMT	G	404	3/3	0.88	0.35	27,27,28,28	3
3	FMT	B	404	3/3	0.88	0.33	27,27,28,28	3
3	FMT	I	404	3/3	0.88	0.32	24,24,25,26	3
3	FMT	D	404	3/3	0.89	0.21	26,26,26,27	3
3	FMT	B	401	3/3	0.91	0.37	23,23,23,24	3
3	FMT	I	401	3/3	0.91	0.38	28,28,28,28	3
3	FMT	C	404	3/3	0.91	0.31	24,24,24,24	3
3	FMT	F	403	3/3	0.92	0.34	24,24,24,25	3
3	FMT	D	405	3/3	0.93	0.42	26,26,27,27	3
3	FMT	H	404	3/3	0.93	0.30	27,27,27,27	3
3	FMT	A	403	3/3	0.94	0.46	27,27,27,28	3
3	FMT	C	401	3/3	0.96	0.29	27,27,28,29	3
2	CU	H	402	1/1	0.99	0.05	28,28,28,28	0
2	CU	H	403	1/1	0.99	0.06	25,25,25,25	0
2	CU	I	402	1/1	0.99	0.07	23,23,23,23	0
2	CU	I	403	1/1	0.99	0.06	23,23,23,23	0
2	CU	A	402	1/1	0.99	0.07	23,23,23,23	0
2	CU	B	402	1/1	0.99	0.04	23,23,23,23	0
2	CU	C	402	1/1	0.99	0.07	21,21,21,21	0
2	CU	C	403	1/1	0.99	0.06	22,22,22,22	0
2	CU	F	401	1/1	0.99	0.06	22,22,22,22	0
2	CU	G	401	1/1	0.99	0.05	21,21,21,21	0
2	CU	G	402	1/1	0.99	0.05	23,23,23,23	0
2	CU	E	401	1/1	1.00	0.03	23,23,23,23	0
2	CU	E	402	1/1	1.00	0.08	22,22,22,22	0
2	CU	A	401	1/1	1.00	0.05	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CU	F	402	1/1	1.00	0.06	23,23,23,23	0
2	CU	B	403	1/1	1.00	0.05	22,22,22,22	0
2	CU	D	401	1/1	1.00	0.06	21,21,21,21	0
2	CU	D	402	1/1	1.00	0.05	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.