



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:57 AM UTC

PDB ID : 3WIA / pdb_00003wia
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

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

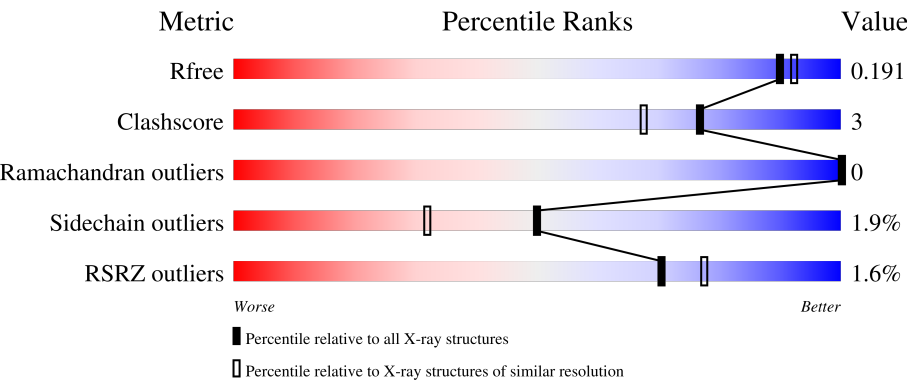
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	287	
1	B	287	
1	C	287	
1	D	287	
1	E	287	

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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	 4% 89% 6% • 5%
1	I	287	 % 87% 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	G	404	-	-	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			

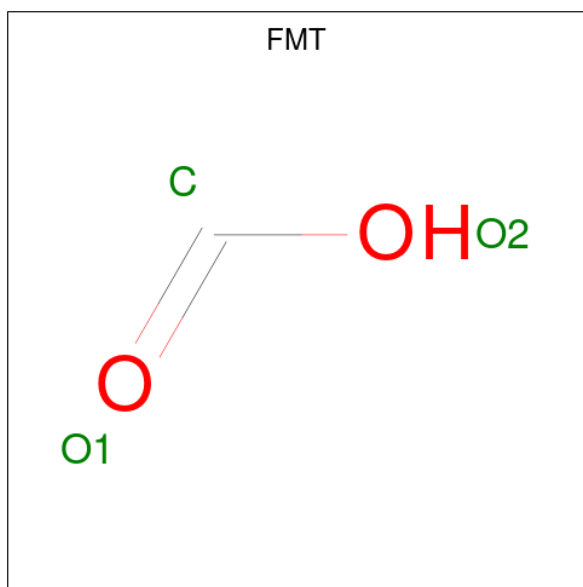
There are 9 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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 (CCD ID: FMT) (formula: CH₂O₂).



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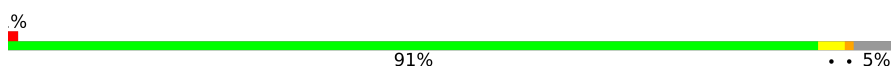
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	225	Total 225	O 225	0	0
4	F	222	Total 222	O 222	0	0
4	G	223	Total 223	O 223	0	0
4	H	211	Total 211	O 211	0	0
4	I	221	Total 221	O 221	0	0

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: 

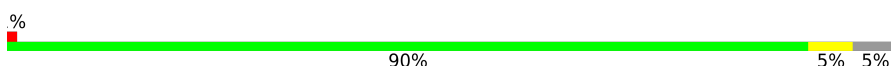


- Molecule 1: Nitrite reductase

Chain B: 

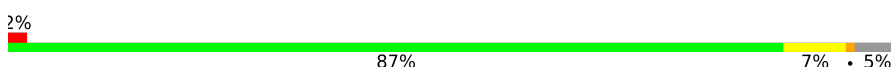


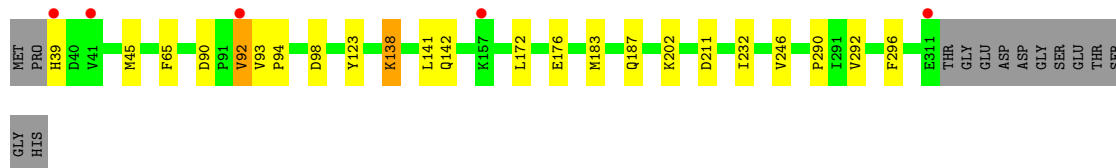
- Molecule 1: Nitrite reductase

Chain C: 

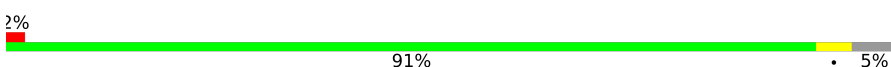


- Molecule 1: Nitrite reductase

Chain D: 

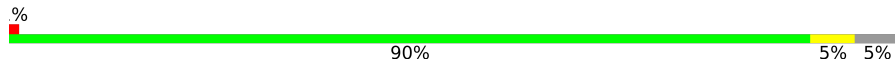


- Molecule 1: Nitrite reductase

Chain E: 



● Molecule 1: Nitrite reductase

Chain F:  %



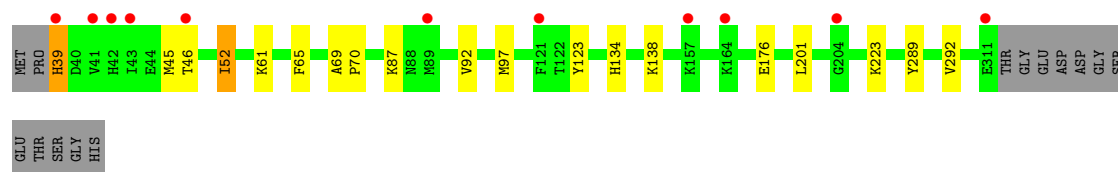
● Molecule 1: Nitrite reductase

Chain G:  %



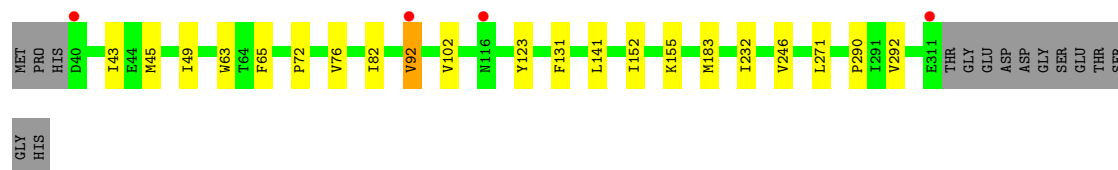
● Molecule 1: Nitrite reductase

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

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: CU, FMT

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	0.74	0/2192	0.83	1/2986 (0.0%)
1	B	0.75	0/2192	0.83	0/2986
1	C	0.74	0/2192	0.85	0/2986
1	D	0.73	0/2192	0.82	1/2986 (0.0%)
1	E	0.75	0/2192	0.83	0/2986
1	F	0.76	0/2192	0.86	1/2986 (0.0%)
1	G	0.73	0/2192	0.83	1/2986 (0.0%)
1	H	0.71	0/2192	0.85	0/2986
1	I	0.72	0/2181	0.86	3/2971 (0.1%)
All	All	0.74	0/19717	0.84	7/26859 (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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	92	VAL	N-CA-C	7.75	118.17	111.90
1	G	129	GLY	N-CA-C	5.95	117.99	110.38
1	A	129	GLY	N-CA-C	5.57	117.51	110.38
1	F	40	ASP	N-CA-C	5.51	117.71	108.96
1	I	102	VAL	N-CA-C	5.38	117.31	108.97
1	D	92	VAL	N-CA-C	5.29	116.36	111.81
1	I	92	VAL	CB-CA-C	5.04	116.14	111.30

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	8	0
1	B	2132	0	2080	14	0
1	C	2132	0	2080	10	0
1	D	2132	0	2080	15	0
1	E	2132	0	2080	14	0
1	F	2132	0	2080	11	0
1	G	2132	0	2080	14	0
1	H	2132	0	2080	13	0
1	I	2122	0	2073	14	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	A	6	0	2	0	0
3	B	6	0	2	0	0
3	C	6	0	2	2	0
3	D	9	0	3	3	0
3	E	6	0	2	0	0
3	F	3	0	1	0	0
3	G	6	0	2	2	0
3	H	6	0	2	1	0
3	I	6	0	2	2	0
4	A	251	0	0	5	0
4	B	221	0	0	1	0
4	C	232	0	0	6	1
4	D	223	0	0	1	0
4	E	225	0	0	0	0
4	F	222	0	0	1	0
4	G	223	0	0	5	0
4	H	211	0	0	1	1
4	I	221	0	0	1	0
All	All	21279	0	18731	111	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 (111) 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
1:F:45:MET:CE	1:F:65:PHE:HB3	1.71	1.19
1:I:45:MET:HE2	1:I:65:PHE:HB3	1.23	1.09
1:I:45:MET:CE	1:I:65:PHE:HB3	1.83	1.08
1:F:45:MET:HE2	1:F:65:PHE:HB3	1.43	1.01
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
1:D:92:VAL:HG23	1:D:93:VAL:HG23	1.48	0.94
1:B:45:MET:HE2	1:B:65:PHE:HB3	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:HIS:HA	4:B:501:HOH:O	1.69	0.92
1:G:246:VAL:HG22	3:G:404:FMT:H	1.52	0.91
1:E:45:MET:HE3	1:E:72:PRO:HG2	1.48	0.91
1:D:45:MET:HE3	1:D:65:PHE:HB3	1.54	0.89
1:E:45:MET:CE	1:E:72:PRO:HG2	2.03	0.88
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
1:B:45:MET:HE3	1:B:72:PRO:CG	2.13	0.79
1:B:45:MET:HE3	1:B:72:PRO:HG2	1.64	0.79
1:C:155:LYS:HD3	4:C:520:HOH:O	1.84	0.78
1:B:45:MET:CE	1:B:65:PHE:HB3	2.13	0.78
1:E:45:MET:CE	1:E:72:PRO:CG	2.64	0.75
1:E:45:MET:HE1	1:E:72:PRO:HD2	1.69	0.73
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:H:45:MET:HE3	1:H:65:PHE:HB3	1.75	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
1:F:45:MET:HE3	1:F:65:PHE:HB3	1.70	0.69
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:I:45:MET:HE2	1:I:65:PHE:CB	2.15	0.65
1:E:45:MET:HE3	1:E:72:PRO:CG	2.22	0.60
1:H:39:HIS:HB2	4:H:632:HOH:O	2.01	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:G:134:HIS:CE1	3:H:401:FMT:H	2.39	0.58
1:C:155:LYS:CD	4:C:520:HOH:O	2.49	0.57
1:E:45:MET:HE1	1:E:72:PRO:CD	2.34	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
1:A:138:LYS:NZ	4:A:749:HOH:O	2.39	0.55
1:F:45:MET:HE1	1:F:65:PHE:CB	2.36	0.54
1:B:45:MET:CE	1:B:72:PRO:HD2	2.37	0.53
1:A:89:MET:HE3	4:A:546:HOH:O	2.08	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:45:MET:HE1	1:H:97:MET:HE1	1.92	0.52
1:H:134:HIS:HE1	3:I:401:FMT:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LYS:HD2	4:C:578:HOH:O	2.08	0.52
1:I:45:MET:HE3	1:I:72:PRO:HD2	1.92	0.51
1:H:45:MET:CE	1:H:65:PHE:CD1	2.95	0.49
1:E:45:MET:HE1	1:E:72:PRO:CG	2.42	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:49:ILE:CG2	1:E:61:LYS:HG2	2.43	0.48
1:E:45:MET:CE	1:E:72:PRO:HD2	2.42	0.48
1:E:45:MET:HE1	1:E:72:PRO:HG2	1.90	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:H:45:MET:HE1	1:H:97:MET:CE	2.44	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:A:89:MET:HA	1:A:89:MET:HE2	1.96	0.46
1:F:45:MET:HE2	1:F:65:PHE:CB	2.27	0.46
1:F:203:PRO:HG2	1:I:76:VAL:HA	1.97	0.46
1:G:89:MET:HA	1:G:89:MET:HE2	1.98	0.45
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
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:B:45:MET:HE1	1:B:72:PRO:HD2	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:45:MET:HE1	1:I:65:PHE:CB	2.47	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:B:45:MET:HE3	1:B:72:PRO:CD	2.49	0.42
1:B:211:ASP:OD1	1:B:211:ASP:C	2.62	0.42
1:H:69:ALA:HA	1:H:70:PRO:C	2.43	0.42
1:E:155:LYS:HA	1:E:156:PRO:HD3	1.94	0.42
1:D:138:LYS:N	1:D:138:LYS:HE2	2.35	0.42
1:C:39:HIS:CD2	4:C:552:HOH:O	2.73	0.42
1:F:131:PHE:HB2	1:F:152:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ASP:OD1	1:D:211:ASP:C	2.63	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: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:D:141:LEU:HD23	1:D:183:MET:HE1	2.03	0.40
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:H:45:MET:HE3	1:H:65:PHE:CB	2.49	0.40
1:H:45:MET:HE3	1:H:65:PHE:CD1	2.55	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
1:I:141:LEU:HD23	1:I:183:MET:HE1	2.03	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 ⓘ

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	A	271/287 (94%)	263 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	271/287 (94%)	264 (97%)	7 (3%)	0	100	100
1	C	271/287 (94%)	264 (97%)	7 (3%)	0	100	100
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%)	232 (98%)	5 (2%)	47	27
1	B	237/248 (96%)	233 (98%)	4 (2%)	53	36
1	C	237/248 (96%)	233 (98%)	4 (2%)	53	36
1	D	237/248 (96%)	233 (98%)	4 (2%)	53	36
1	E	237/248 (96%)	234 (99%)	3 (1%)	61	46
1	F	237/248 (96%)	232 (98%)	5 (2%)	47	27
1	G	237/248 (96%)	232 (98%)	5 (2%)	47	27
1	H	237/248 (96%)	228 (96%)	9 (4%)	29	9
1	I	236/248 (95%)	234 (99%)	2 (1%)	73	63
All	All	2132/2232 (96%)	2091 (98%)	41 (2%)	50	32

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	89	MET
1	A	123	TYR
1	A	176	GLU
1	A	296	PHE
1	B	39	HIS
1	B	123	TYR
1	B	176	GLU
1	B	202	LYS
1	C	123	TYR
1	C	157	LYS
1	C	176	GLU
1	C	183	MET
1	D	123	TYR
1	D	138	LYS
1	D	176	GLU
1	D	202	LYS
1	E	92	VAL
1	E	123	TYR
1	E	176	GLU
1	F	39	HIS
1	F	44	GLU
1	F	123	TYR
1	F	183	MET
1	F	201	LEU
1	G	61	LYS
1	G	123	TYR
1	G	176	GLU
1	G	183	MET
1	G	296	PHE
1	H	39	HIS
1	H	52	ILE
1	H	61	LYS
1	H	92	VAL
1	H	123	TYR
1	H	138	LYS
1	H	176	GLU
1	H	201	LEU
1	H	223	LYS
1	I	92	VAL
1	I	123	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	295	GLN
1	B	77	ASN
1	B	233	ASN
1	B	295	GLN
1	C	233	ASN
1	C	295	GLN
1	D	77	ASN
1	D	295	GLN
1	E	264	GLN
1	E	295	GLN
1	E	300	GLN
1	F	77	ASN
1	F	260	ASN
1	F	295	GLN
1	G	77	ASN
1	G	233	ASN
1	G	295	GLN
1	H	295	GLN
1	I	295	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](#)

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	C	404	-	2,2,2	0.76	0	1,1,1	0.30	0
3	FMT	G	404	2	2,2,2	0.65	0	1,1,1	0.02	0
3	FMT	F	403	-	2,2,2	0.79	0	1,1,1	0.35	0
3	FMT	G	403	-	2,2,2	0.71	0	1,1,1	0.32	0
3	FMT	C	401	-	2,2,2	0.73	0	1,1,1	0.22	0
3	FMT	D	405	2	2,2,2	0.76	0	1,1,1	0.13	0
3	FMT	B	401	2	2,2,2	0.67	0	1,1,1	0.12	0
3	FMT	E	403	-	2,2,2	0.71	0	1,1,1	0.22	0
3	FMT	E	404	-	2,2,2	0.77	0	1,1,1	0.04	0
3	FMT	B	404	-	2,2,2	0.70	0	1,1,1	0.20	0
3	FMT	D	403	-	2,2,2	0.67	0	1,1,1	0.21	0
3	FMT	D	404	2	2,2,2	0.71	0	1,1,1	0.06	0
3	FMT	H	404	-	2,2,2	0.63	0	1,1,1	0.17	0
3	FMT	I	401	-	2,2,2	0.66	0	1,1,1	0.18	0
3	FMT	A	403	-	2,2,2	0.63	0	1,1,1	0.26	0
3	FMT	A	404	2	2,2,2	0.69	0	1,1,1	0.12	0
3	FMT	H	401	-	2,2,2	0.77	0	1,1,1	0.02	0
3	FMT	I	404	-	2,2,2	0.78	0	1,1,1	0.23	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.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	404	FMT	1	0
3	G	404	FMT	2	0
3	C	401	FMT	1	0
3	D	405	FMT	1	0
3	D	403	FMT	1	0
3	D	404	FMT	1	0
3	I	401	FMT	2	0
3	H	401	FMT	1	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, 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	273/287 (95%)	0.00	4 (1%) 72 78	17, 23, 34, 48	0
1	B	273/287 (95%)	-0.00	2 (0%) 84 88	17, 23, 32, 45	0
1	C	273/287 (95%)	-0.02	4 (1%) 72 78	17, 22, 33, 45	0
1	D	273/287 (95%)	0.03	5 (1%) 67 75	17, 23, 35, 48	0
1	E	273/287 (95%)	-0.03	5 (1%) 67 75	16, 23, 33, 43	0
1	F	273/287 (95%)	-0.04	3 (1%) 78 84	17, 22, 32, 49	0
1	G	273/287 (95%)	0.04	2 (0%) 84 88	16, 23, 34, 49	0
1	H	273/287 (95%)	0.33	11 (4%) 42 48	17, 26, 38, 54	0
1	I	272/287 (94%)	0.08	4 (1%) 72 78	17, 24, 34, 47	0
All	All	2456/2583 (95%)	0.04	40 (1%) 70 77	16, 23, 35, 54	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	39	HIS	4.5
1	C	204	GLY	4.2
1	H	39	HIS	4.0
1	G	39	HIS	3.9
1	H	89	MET	3.7
1	B	39	HIS	3.7
1	A	39	HIS	3.5
1	C	39	HIS	3.5
1	E	157	LYS	3.5
1	B	89	MET	3.4
1	H	204	GLY	3.4
1	D	39	HIS	3.3
1	E	39	HIS	3.3
1	F	311	GLU	3.0
1	I	116	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	40	ASP	2.9
1	H	41	VAL	2.7
1	A	46	THR	2.7
1	C	203	PRO	2.7
1	E	89	MET	2.6
1	I	311	GLU	2.6
1	H	42	HIS	2.5
1	C	89	MET	2.5
1	A	116	ASN	2.4
1	D	311	GLU	2.4
1	F	89	MET	2.4
1	E	311	GLU	2.3
1	D	41	VAL	2.3
1	D	92	VAL	2.3
1	H	46	THR	2.2
1	E	44	GLU	2.2
1	G	311	GLU	2.2
1	A	311	GLU	2.2
1	H	157	LYS	2.1
1	H	121	PHE	2.1
1	H	164	LYS	2.1
1	I	92	VAL	2.1
1	D	157	LYS	2.1
1	H	311	GLU	2.0
1	H	43	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	FMT	B	404	3/3	0.79	0.35	27,27,28,28	3
3	FMT	D	403	3/3	0.80	0.27	26,26,26,26	3
3	FMT	E	404	3/3	0.81	0.33	29,29,30,30	3
3	FMT	G	403	3/3	0.82	0.25	26,26,26,26	3
3	FMT	C	404	3/3	0.83	0.32	24,24,24,24	3
3	FMT	I	401	3/3	0.83	0.26	28,28,28,28	3
3	FMT	E	403	3/3	0.84	0.27	27,27,27,28	3
3	FMT	I	404	3/3	0.84	0.31	24,24,25,26	3
3	FMT	H	404	3/3	0.85	0.29	27,27,27,27	3
3	FMT	A	403	3/3	0.86	0.33	27,27,27,28	3
3	FMT	G	404	3/3	0.87	0.22	27,27,28,28	3
3	FMT	H	401	3/3	0.88	0.14	25,25,25,25	3
3	FMT	A	404	3/3	0.89	0.16	24,24,25,26	3
3	FMT	F	403	3/3	0.89	0.31	24,24,24,25	3
3	FMT	B	401	3/3	0.91	0.14	23,23,23,24	3
3	FMT	D	405	3/3	0.92	0.19	26,26,27,27	3
3	FMT	D	404	3/3	0.92	0.11	26,26,26,27	3
3	FMT	C	401	3/3	0.95	0.15	27,27,28,29	3
2	CU	H	402	1/1	0.98	0.04	28,28,28,28	0
2	CU	I	402	1/1	0.99	0.03	23,23,23,23	0
2	CU	I	403	1/1	0.99	0.02	23,23,23,23	0
2	CU	B	402	1/1	0.99	0.03	23,23,23,23	0
2	CU	C	403	1/1	0.99	0.02	22,22,22,22	0
2	CU	D	401	1/1	0.99	0.02	21,21,21,21	0
2	CU	F	401	1/1	0.99	0.02	22,22,22,22	0
2	CU	F	402	1/1	0.99	0.02	23,23,23,23	0
2	CU	G	402	1/1	0.99	0.03	23,23,23,23	0
2	CU	A	402	1/1	0.99	0.02	23,23,23,23	0
2	CU	H	403	1/1	0.99	0.03	25,25,25,25	0
2	CU	E	401	1/1	1.00	0.02	23,23,23,23	0
2	CU	E	402	1/1	1.00	0.02	22,22,22,22	0
2	CU	C	402	1/1	1.00	0.02	21,21,21,21	0
2	CU	A	401	1/1	1.00	0.02	22,22,22,22	0
2	CU	G	401	1/1	1.00	0.01	21,21,21,21	0
2	CU	B	403	1/1	1.00	0.02	22,22,22,22	0
2	CU	D	402	1/1	1.00	0.02	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.