



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:27 AM UTC

PDB ID : 1CFZ / pdb_00001cfz
Title : HYDROGENASE MATURATING ENDOPEPTIDASE HYBD FROM E. COLI
Authors : Fritsche, E.; Paschos, A.; Beisel, H.-G.; Boeck, A.; Huber, R.
Deposited on : 1999-03-23
Resolution : 2.20 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

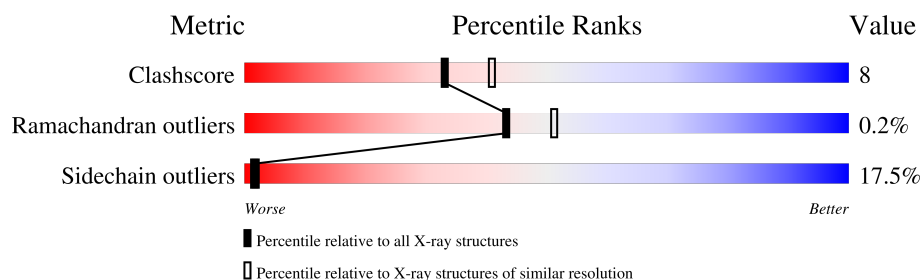
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	162	70% 25% • •
1	B	162	67% 24% 9%
1	C	162	67% 27% 6%
1	D	162	70% 23% 5% •
1	E	162	66% 28% 6%
1	F	162	63% 31% 5% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7630 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 HYDROGENASE 2 MATURATION PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1225	780	204	235	6			
1	B	162	Total	C	N	O	S	0	0	0
			1225	780	204	235	6			
1	C	162	Total	C	N	O	S	0	0	0
			1225	780	204	235	6			
1	D	162	Total	C	N	O	S	0	0	0
			1225	780	204	235	6			
1	E	162	Total	C	N	O	S	0	0	0
			1225	780	204	235	6			
1	F	162	Total	C	N	O	S	0	0	0
			1225	780	204	235	6			

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cd	0	0
			1	1		
2	B	1	Total	Cd	0	0
			1	1		
2	C	1	Total	Cd	0	0
			1	1		
2	D	1	Total	Cd	0	0
			1	1		
2	E	1	Total	Cd	0	0
			1	1		
2	F	1	Total	Cd	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total 47	O 47	0	0
3	B	68	Total 68	O 68	0	0
3	C	46	Total 46	O 46	0	0
3	D	38	Total 38	O 38	0	0
3	E	40	Total 40	O 40	0	0
3	F	35	Total 35	O 35	0	0

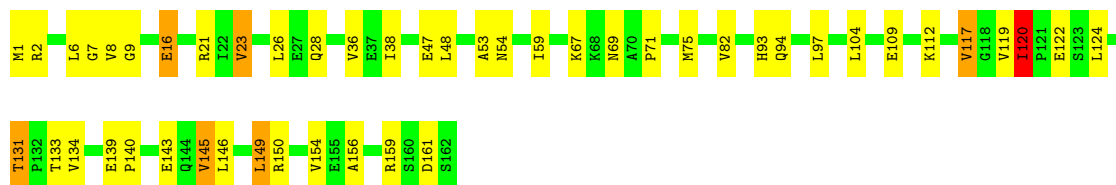
3 Residue-property plots

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.

Note EDS was not executed.

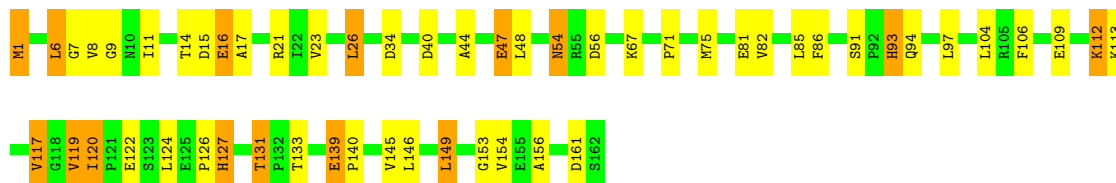
• Molecule 1: HYDROGENASE 2 MATURATION PROTEASE

Chain A: 



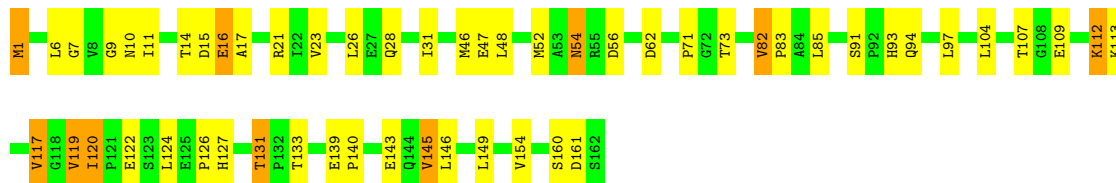
• Molecule 1: HYDROGENASE 2 MATURATION PROTEASE

Chain B: 



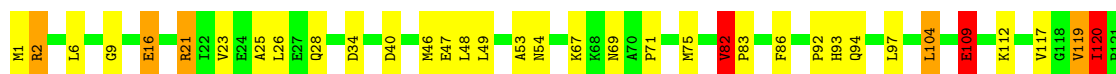
• Molecule 1: HYDROGENASE 2 MATURATION PROTEASE

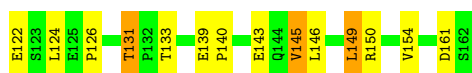
Chain C: 



• Molecule 1: HYDROGENASE 2 MATURATION PROTEASE

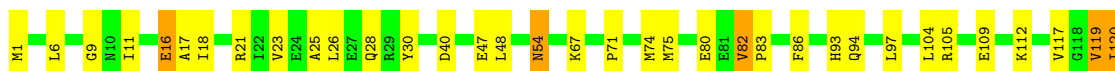
Chain D: 





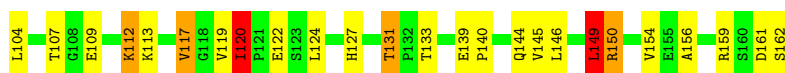
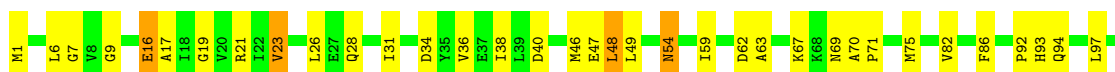
- Molecule 1: HYDROGENASE 2 MATURATION PROTEASE

Chain E:
66% 28% 6%



- Molecule 1: HYDROGENASE 2 MATURATION PROTEASE

Chain F:
63% 31% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	128.00Å 128.00Å 139.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.20	Depositor
% Data completeness (in resolution range)	95.0 (15.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	10.30	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7630	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.81	1/1242 (0.1%)	1.75	16/1686 (0.9%)
1	B	0.80	2/1242 (0.2%)	1.75	24/1686 (1.4%)
1	C	0.79	1/1242 (0.1%)	1.93	14/1686 (0.8%)
1	D	0.82	0/1242	1.77	21/1686 (1.2%)
1	E	0.76	0/1242	1.70	19/1686 (1.1%)
1	F	0.80	1/1242 (0.1%)	1.78	22/1686 (1.3%)
All	All	0.79	5/7452 (0.1%)	1.78	116/10116 (1.1%)

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	F	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	7	GLY	CA-C	6.25	1.56	1.52
1	A	7	GLY	CA-C	6.22	1.56	1.52
1	C	7	GLY	CA-C	6.04	1.56	1.52
1	B	7	GLY	CA-C	5.62	1.56	1.51
1	B	6	LEU	C-N	-5.49	1.30	1.33

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	GLN	OE1-CD-NE2	-37.85	84.75	122.60
1	D	120	ILE	CA-C-O	12.38	126.46	119.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	94	GLN	OE1-CD-NE2	-12.27	110.33	122.60
1	C	94	GLN	CG-CD-OE1	12.12	145.03	120.80
1	D	94	GLN	OE1-CD-NE2	-12.09	110.51	122.60
1	E	94	GLN	OE1-CD-NE2	-11.63	110.97	122.60
1	A	120	ILE	CA-C-O	10.04	127.70	119.47
1	A	120	ILE	CB-CA-C	9.36	119.65	110.94
1	C	94	GLN	CG-CD-NE2	9.10	130.05	116.40
1	E	161	ASP	CA-CB-CG	8.72	121.32	112.60
1	A	94	GLN	OE1-CD-NE2	-8.42	114.18	122.60
1	B	117	VAL	N-CA-CB	8.36	122.20	111.67
1	F	120	ILE	CB-CA-C	8.18	118.55	110.94
1	B	16	GLU	CB-CG-CD	8.14	126.44	112.60
1	B	16	GLU	CG-CD-OE2	8.08	136.98	118.40
1	B	94	GLN	OE1-CD-NE2	-7.99	114.61	122.60
1	D	94	GLN	CG-CD-NE2	7.96	128.34	116.40
1	B	16	GLU	OE1-CD-OE2	-7.94	103.84	122.90
1	D	161	ASP	CA-CB-CG	7.91	120.51	112.60
1	D	120	ILE	CB-CA-C	7.87	119.13	110.71
1	F	161	ASP	CA-CB-CG	7.82	120.42	112.60
1	F	120	ILE	CA-C-O	7.47	125.59	119.47
1	D	119	VAL	CA-C-N	-7.27	117.36	122.59
1	D	119	VAL	C-N-CA	-7.27	117.36	122.59
1	B	91	SER	CA-C-O	7.01	128.08	120.08
1	C	16	GLU	CB-CG-CD	6.74	124.05	112.60
1	F	150	ARG	O-C-N	-6.72	114.99	122.12
1	D	109	GLU	CA-CB-CG	-6.67	100.76	114.10
1	D	86	PHE	CA-CB-CG	6.64	120.44	113.80
1	E	150	ARG	CA-CB-CG	6.55	127.19	114.10
1	B	139	GLU	CA-C-O	6.52	125.12	118.73
1	C	16	GLU	OE1-CD-OE2	-6.43	107.46	122.90
1	B	86	PHE	CA-CB-CG	6.38	120.18	113.80
1	B	26	LEU	CA-C-O	6.33	127.47	120.82
1	A	156	ALA	CA-C-N	-6.33	116.47	123.43
1	A	156	ALA	C-N-CA	-6.33	116.47	123.43
1	F	94	GLN	CG-CD-NE2	6.33	125.89	116.40
1	A	16	GLU	CB-CG-CD	6.30	123.30	112.60
1	F	16	GLU	CG-CD-OE2	6.25	132.77	118.40
1	B	161	ASP	CA-CB-CG	6.16	118.76	112.60
1	F	17	ALA	CA-C-N	6.15	128.53	120.60
1	F	17	ALA	C-N-CA	6.15	128.53	120.60
1	C	16	GLU	CG-CD-OE2	6.11	132.46	118.40
1	E	30	TYR	O-C-N	6.10	130.74	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	GLY	CA-C-O	-6.05	115.64	120.91
1	F	16	GLU	OE1-CD-OE2	-6.01	108.48	122.90
1	C	62	ASP	CA-CB-CG	-6.00	106.61	112.60
1	D	150	ARG	CA-CB-CG	5.89	125.88	114.10
1	A	94	GLN	CG-CD-NE2	5.86	125.19	116.40
1	F	161	ASP	CB-CA-C	-5.76	104.06	111.50
1	E	16	GLU	CG-CD-OE2	5.74	131.61	118.40
1	D	16	GLU	CB-CG-CD	5.72	122.33	112.60
1	E	119	VAL	CB-CA-C	5.67	119.22	110.50
1	B	54	ASN	CA-CB-CG	-5.65	106.95	112.60
1	E	16	GLU	CB-CG-CD	5.62	122.15	112.60
1	F	36	VAL	CA-C-O	-5.58	114.51	120.59
1	D	2	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	D	145	VAL	N-CA-CB	5.54	118.89	110.58
1	E	18	ILE	CA-C-N	5.53	126.12	119.98
1	E	18	ILE	C-N-CA	5.53	126.12	119.98
1	B	81	GLU	CA-C-O	-5.53	113.85	120.10
1	F	144	GLN	CA-C-O	-5.52	114.57	120.42
1	A	145	VAL	N-CA-CB	5.51	120.75	110.77
1	F	117	VAL	N-CA-CB	5.50	118.60	111.67
1	C	145	VAL	N-CA-CB	5.49	118.82	110.58
1	E	159	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	A	161	ASP	CB-CA-C	-5.48	103.53	111.14
1	D	149	LEU	CA-C-O	5.46	126.56	120.82
1	E	145	VAL	N-CA-CB	5.46	120.65	110.77
1	E	161	ASP	CB-CA-C	-5.44	104.53	111.22
1	B	8	VAL	CA-C-O	-5.44	115.96	121.67
1	A	69	ASN	CA-CB-CG	5.43	118.03	112.60
1	B	153	GLY	CA-C-N	-5.41	116.12	123.10
1	B	153	GLY	C-N-CA	-5.41	116.12	123.10
1	B	106	PHE	CA-CB-CG	5.40	119.20	113.80
1	C	117	VAL	N-CA-CB	5.40	118.47	111.67
1	D	82	VAL	N-CA-CB	5.39	118.75	111.21
1	A	8	VAL	CA-C-O	-5.37	116.03	121.67
1	A	161	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	161	ASP	CB-CA-C	-5.32	104.54	111.40
1	D	119	VAL	CB-CA-C	5.31	118.68	110.50
1	A	117	VAL	CB-CA-C	5.31	118.57	111.19
1	E	86	PHE	CA-CB-CG	5.30	119.10	113.80
1	D	120	ILE	CA-CB-CG2	5.30	119.50	110.50
1	C	161	ASP	CB-CA-C	-5.29	104.58	111.40
1	F	127	HIS	CA-CB-CG	5.26	119.06	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	25	ALA	CA-C-N	5.25	127.27	120.44
1	D	25	ALA	C-N-CA	5.25	127.27	120.44
1	D	69	ASN	CA-CB-CG	5.25	117.85	112.60
1	F	156	ALA	CA-C-N	-5.24	117.67	123.43
1	F	156	ALA	C-N-CA	-5.24	117.67	123.43
1	D	149	LEU	O-C-N	-5.24	116.68	122.07
1	B	119	VAL	CB-CA-C	5.22	117.96	110.33
1	E	94	GLN	CG-CD-NE2	5.22	124.22	116.40
1	E	54	ASN	CA-CB-CG	-5.21	107.39	112.60
1	A	134	VAL	CA-C-O	5.21	125.39	119.92
1	B	81	GLU	CA-C-N	-5.21	112.50	122.13
1	B	81	GLU	C-N-CA	-5.21	112.50	122.13
1	B	156	ALA	CA-C-N	-5.17	117.75	123.43
1	B	156	ALA	C-N-CA	-5.17	117.75	123.43
1	E	153	GLY	CA-C-N	-5.15	116.46	123.10
1	E	153	GLY	C-N-CA	-5.15	116.46	123.10
1	C	119	VAL	CB-CA-C	5.12	117.80	110.33
1	C	91	SER	CA-C-O	5.11	124.42	119.62
1	F	69	ASN	CA-CB-CG	5.08	117.69	112.60
1	A	36	VAL	CA-C-O	-5.08	114.85	120.74
1	F	149	LEU	CA-C-N	5.08	127.08	120.28
1	F	149	LEU	C-N-CA	5.08	127.08	120.28
1	E	25	ALA	CA-C-N	5.06	127.01	120.44
1	E	25	ALA	C-N-CA	5.06	127.01	120.44
1	B	149	LEU	CA-C-N	5.05	127.55	120.28
1	B	149	LEU	C-N-CA	5.05	127.55	120.28
1	C	52	MET	N-CA-C	5.04	119.06	113.01
1	F	54	ASN	CA-CB-CG	-5.03	107.57	112.60
1	F	86	PHE	CA-CB-CG	5.03	118.83	113.80
1	C	54	ASN	CA-CB-CG	-5.02	107.58	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	19	GLY	Mainchain

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	1225	0	1275	18	0
1	B	1225	0	1275	17	1
1	C	1225	0	1275	29	0
1	D	1225	0	1275	19	2
1	E	1225	0	1275	24	0
1	F	1225	0	1275	24	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	47	0	0	1	0
3	B	68	0	0	0	2
3	C	46	0	0	1	0
3	D	38	0	0	1	0
3	E	40	0	0	1	0
3	F	35	0	0	2	0
All	All	7630	0	7650	117	3

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 8.

All (117) 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:150:ARG:HD2	1:E:144:GLN:HE21	1.23	0.99
1:D:54:ASN:ND2	1:D:109:GLU:HG2	1.93	0.83
1:A:54:ASN:ND2	1:A:109:GLU:HG2	1.99	0.77
1:B:54:ASN:ND2	1:B:109:GLU:HG2	2.00	0.76
1:F:54:ASN:ND2	1:F:109:GLU:HG2	2.03	0.74
1:C:54:ASN:ND2	1:C:109:GLU:HG2	2.04	0.73
1:C:126:PRO:HB3	1:E:157:ILE:CD1	2.19	0.73
1:F:150:ARG:HG3	3:F:181:HOH:O	1.88	0.72
1:E:54:ASN:ND2	1:E:109:GLU:HG2	2.06	0.71
1:F:139:GLU:HB3	1:F:140:PRO:HD3	1.74	0.69
1:D:54:ASN:HD21	1:D:109:GLU:HG2	1.58	0.68
1:C:10:ASN:ND2	1:E:161:ASP:HB3	2.10	0.67
1:B:54:ASN:HD21	1:B:109:GLU:HG2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:MET:HB3	1:F:46:MET:HG2	1.78	0.65
1:A:54:ASN:HD21	1:A:109:GLU:HG2	1.61	0.65
1:E:139:GLU:HB3	1:E:140:PRO:HD3	1.79	0.64
1:B:139:GLU:HB3	1:B:140:PRO:HD3	1.79	0.64
1:A:139:GLU:HB3	1:A:140:PRO:HD3	1.82	0.61
1:C:139:GLU:HB3	1:C:140:PRO:HD3	1.83	0.61
1:D:139:GLU:HB3	1:D:140:PRO:HD3	1.82	0.61
1:F:54:ASN:HD21	1:F:109:GLU:HG2	1.64	0.61
1:E:54:ASN:HD21	1:E:109:GLU:HG2	1.64	0.61
1:C:54:ASN:HD21	1:C:109:GLU:HG2	1.65	0.60
1:B:71:PRO:HA	1:B:120:ILE:HG13	1.84	0.60
1:C:31:ILE:HG22	1:D:126:PRO:HG3	1.83	0.60
1:D:122:GLU:HB3	1:D:131:THR:HG21	1.85	0.58
1:A:150:ARG:HD2	1:E:144:GLN:NE2	2.06	0.57
1:B:122:GLU:HB3	1:B:131:THR:HG21	1.87	0.56
1:C:160:SER:HA	1:D:92:PRO:HB2	1.87	0.56
1:D:71:PRO:HA	1:D:120:ILE:HG13	1.87	0.56
1:A:71:PRO:HA	1:A:120:ILE:HG13	1.88	0.55
1:C:71:PRO:HA	1:C:120:ILE:HG13	1.88	0.55
1:F:71:PRO:HA	1:F:120:ILE:HG13	1.87	0.55
1:D:54:ASN:CG	1:D:109:GLU:HG2	2.32	0.55
1:C:10:ASN:HD22	1:E:161:ASP:HB3	1.71	0.54
1:E:71:PRO:HA	1:E:120:ILE:HG13	1.88	0.54
1:F:122:GLU:HB3	1:F:131:THR:HG21	1.90	0.52
1:C:46:MET:HG2	1:F:49:LEU:HD22	1.92	0.51
1:E:122:GLU:HB3	1:E:131:THR:HG21	1.91	0.51
1:A:54:ASN:CG	1:A:109:GLU:HG2	2.36	0.51
1:E:40:ASP:OD2	1:E:40:ASP:C	2.54	0.51
1:A:122:GLU:HB3	1:A:131:THR:HG21	1.91	0.51
1:C:126:PRO:HB3	1:E:157:ILE:HD13	1.90	0.51
1:E:143:GLU:HG2	3:E:184:HOH:O	2.12	0.50
1:C:112:LYS:HE2	1:C:113:LYS:HB2	1.92	0.50
1:A:159:ARG:O	1:F:92:PRO:HG2	2.11	0.50
1:E:9:GLY:HA2	1:E:16:GLU:OE1	2.13	0.48
1:C:11:ILE:HD13	1:C:17:ALA:HB1	1.95	0.48
1:E:139:GLU:CB	1:E:140:PRO:HD3	2.44	0.48
1:A:67:LYS:HD2	3:A:204:HOH:O	2.13	0.47
1:C:122:GLU:HB3	1:C:131:THR:HG21	1.96	0.47
1:E:11:ILE:HD13	1:E:17:ALA:HB1	1.95	0.47
1:F:139:GLU:HB3	1:F:140:PRO:CD	2.43	0.47
1:A:9:GLY:HA2	1:A:16:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLY:HA2	1:B:16:GLU:OE1	2.15	0.47
1:F:59:ILE:CD1	1:F:149:LEU:HD13	2.45	0.47
1:E:67:LYS:HD3	1:E:75:MET:SD	2.55	0.47
1:A:150:ARG:HG2	1:E:74:MET:CE	2.45	0.47
1:E:82:VAL:N	1:E:83:PRO:CD	2.78	0.47
1:F:54:ASN:CG	1:F:109:GLU:HG2	2.41	0.46
1:B:112:LYS:HE2	1:B:113:LYS:HB2	1.98	0.46
1:C:54:ASN:CG	1:C:109:GLU:HG2	2.40	0.46
1:C:160:SER:HA	1:D:92:PRO:CB	2.46	0.46
1:A:139:GLU:CB	1:A:140:PRO:HD3	2.46	0.45
1:E:139:GLU:O	1:E:143:GLU:HG3	2.15	0.45
1:F:40:ASP:OD2	1:F:40:ASP:C	2.59	0.45
1:D:9:GLY:HA2	1:D:16:GLU:OE1	2.17	0.45
1:B:54:ASN:CG	1:B:109:GLU:HG2	2.42	0.45
1:C:11:ILE:HG12	3:C:181:HOH:O	2.16	0.44
1:D:67:LYS:HD3	1:D:75:MET:HE1	1.99	0.44
1:A:67:LYS:HD3	1:A:75:MET:HE1	1.99	0.44
1:D:139:GLU:CB	1:D:140:PRO:HD3	2.48	0.44
1:F:67:LYS:HD3	1:F:75:MET:SD	2.58	0.44
1:A:23:VAL:HG13	1:A:38:ILE:CG2	2.48	0.44
1:C:73:THR:HB	1:C:120:ILE:HG23	1.99	0.44
1:C:139:GLU:CB	1:C:140:PRO:HD3	2.46	0.43
1:C:139:GLU:O	1:C:143:GLU:HG3	2.18	0.43
1:B:139:GLU:HB3	1:B:140:PRO:CD	2.48	0.43
1:E:54:ASN:CG	1:E:109:GLU:HG2	2.43	0.43
1:B:126:PRO:O	1:B:127:HIS:HB2	2.18	0.43
1:F:62:ASP:OD2	1:F:63:ALA:N	2.51	0.43
1:F:9:GLY:HA2	1:F:16:GLU:OE1	2.19	0.42
1:F:112:LYS:HE2	1:F:113:LYS:HB2	2.01	0.42
1:A:59:ILE:CD1	1:A:149:LEU:HD13	2.49	0.42
1:C:1:MET:HE2	1:C:56:ASP:CG	2.43	0.42
1:C:107:THR:CG2	1:F:107:THR:HA	2.49	0.42
1:D:21:ARG:HD3	3:D:194:HOH:O	2.19	0.42
1:F:48:LEU:O	1:F:49:LEU:C	2.61	0.42
1:A:139:GLU:O	1:A:143:GLU:HG3	2.20	0.42
1:C:9:GLY:HA2	1:C:16:GLU:OE1	2.19	0.42
1:B:44:ALA:HB1	1:B:47:GLU:HG2	2.02	0.42
1:C:85:LEU:O	1:C:85:LEU:HG	2.19	0.41
1:D:46:MET:HE2	1:D:46:MET:HB2	1.92	0.41
1:D:67:LYS:HD3	1:D:75:MET:SD	2.60	0.41
1:B:85:LEU:O	1:B:85:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:LEU:CD1	1:D:104:LEU:HD13	2.51	0.41
1:D:82:VAL:N	1:D:83:PRO:CD	2.82	0.41
1:C:14:THR:HG22	1:C:15:ASP:N	2.35	0.41
1:F:23:VAL:HG13	1:F:38:ILE:CG2	2.50	0.41
1:F:31:ILE:HG13	1:F:159:ARG:HG2	2.02	0.41
1:C:126:PRO:O	1:C:127:HIS:HB2	2.21	0.41
1:A:2:ARG:NH2	1:A:53:ALA:O	2.54	0.41
1:B:11:ILE:HD13	1:B:17:ALA:HB1	2.02	0.41
1:E:80:GLU:OE2	1:E:105:ARG:NH2	2.50	0.41
1:F:70:ALA:HA	1:F:71:PRO:HD3	1.98	0.41
1:B:1:MET:HE2	1:B:56:ASP:CG	2.45	0.41
1:B:67:LYS:HD3	1:B:75:MET:HE1	2.03	0.41
1:C:11:ILE:HA	1:C:17:ALA:HB2	2.02	0.41
1:D:2:ARG:NH2	1:D:53:ALA:O	2.53	0.41
1:F:112:LYS:NZ	3:F:171:HOH:O	2.53	0.41
1:F:139:GLU:CB	1:F:140:PRO:HD3	2.48	0.41
1:B:40:ASP:OD2	1:B:40:ASP:C	2.64	0.41
1:B:14:THR:HG22	1:B:15:ASP:N	2.36	0.40
1:D:40:ASP:OD2	1:D:40:ASP:C	2.63	0.40
1:E:120:ILE:HD12	1:E:121:PRO:HD2	2.02	0.40
1:E:126:PRO:O	1:E:127:HIS:HB2	2.21	0.40
1:C:82:VAL:N	1:C:83:PRO:CD	2.84	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:GLU:CD	3:B:198:HOH:O[5_555]	2.13	0.07
1:B:93:HIS:N	1:F:162:SER:O[5_665]	2.14	0.06
1:D:109:GLU:OE2	3:B:214:HOH:O[4_665]	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	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
1	B	160/162 (99%)	153 (96%)	6 (4%)	1 (1%)	21	23
1	C	160/162 (99%)	152 (95%)	8 (5%)	0	100	100
1	D	160/162 (99%)	152 (95%)	8 (5%)	0	100	100
1	E	160/162 (99%)	151 (94%)	8 (5%)	1 (1%)	21	23
1	F	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
All	All	960/972 (99%)	914 (95%)	44 (5%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	127	HIS
1	E	127	HIS

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	134/134 (100%)	111 (83%)	23 (17%)	2	2
1	B	134/134 (100%)	111 (83%)	23 (17%)	2	2
1	C	134/134 (100%)	111 (83%)	23 (17%)	2	2
1	D	134/134 (100%)	109 (81%)	25 (19%)	1	1
1	E	134/134 (100%)	111 (83%)	23 (17%)	2	2
1	F	134/134 (100%)	110 (82%)	24 (18%)	2	1
All	All	804/804 (100%)	663 (82%)	141 (18%)	2	1

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	6	LEU
1	A	21	ARG
1	A	23	VAL
1	A	26	LEU
1	A	28	GLN
1	A	47	GLU
1	A	48	LEU
1	A	82	VAL
1	A	93	HIS
1	A	97	LEU
1	A	104	LEU
1	A	112	LYS
1	A	117	VAL
1	A	119	VAL
1	A	120	ILE
1	A	124	LEU
1	A	131	THR
1	A	133	THR
1	A	145	VAL
1	A	146	LEU
1	A	149	LEU
1	A	154	VAL
1	B	1	MET
1	B	6	LEU
1	B	21	ARG
1	B	23	VAL
1	B	26	LEU
1	B	34	ASP
1	B	47	GLU
1	B	48	LEU
1	B	82	VAL
1	B	93	HIS
1	B	97	LEU
1	B	104	LEU
1	B	112	LYS
1	B	117	VAL
1	B	119	VAL
1	B	120	ILE
1	B	124	LEU
1	B	131	THR
1	B	133	THR
1	B	145	VAL

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Mol	Chain	Res	Type
1	B	146	LEU
1	B	149	LEU
1	B	154	VAL
1	C	1	MET
1	C	6	LEU
1	C	21	ARG
1	C	23	VAL
1	C	26	LEU
1	C	28	GLN
1	C	47	GLU
1	C	48	LEU
1	C	82	VAL
1	C	93	HIS
1	C	97	LEU
1	C	104	LEU
1	C	112	LYS
1	C	117	VAL
1	C	119	VAL
1	C	120	ILE
1	C	124	LEU
1	C	131	THR
1	C	133	THR
1	C	145	VAL
1	C	146	LEU
1	C	149	LEU
1	C	154	VAL
1	D	1	MET
1	D	6	LEU
1	D	21	ARG
1	D	23	VAL
1	D	26	LEU
1	D	28	GLN
1	D	34	ASP
1	D	47	GLU
1	D	48	LEU
1	D	82	VAL
1	D	93	HIS
1	D	97	LEU
1	D	104	LEU
1	D	109	GLU
1	D	112	LYS
1	D	117	VAL

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Mol	Chain	Res	Type
1	D	119	VAL
1	D	120	ILE
1	D	124	LEU
1	D	131	THR
1	D	133	THR
1	D	145	VAL
1	D	146	LEU
1	D	149	LEU
1	D	154	VAL
1	E	1	MET
1	E	6	LEU
1	E	21	ARG
1	E	23	VAL
1	E	26	LEU
1	E	28	GLN
1	E	47	GLU
1	E	48	LEU
1	E	82	VAL
1	E	93	HIS
1	E	97	LEU
1	E	104	LEU
1	E	112	LYS
1	E	117	VAL
1	E	119	VAL
1	E	120	ILE
1	E	124	LEU
1	E	131	THR
1	E	133	THR
1	E	145	VAL
1	E	146	LEU
1	E	149	LEU
1	E	154	VAL
1	F	1	MET
1	F	6	LEU
1	F	21	ARG
1	F	23	VAL
1	F	26	LEU
1	F	28	GLN
1	F	34	ASP
1	F	47	GLU
1	F	48	LEU
1	F	82	VAL

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Mol	Chain	Res	Type
1	F	93	HIS
1	F	97	LEU
1	F	104	LEU
1	F	112	LYS
1	F	117	VAL
1	F	119	VAL
1	F	120	ILE
1	F	124	LEU
1	F	131	THR
1	F	133	THR
1	F	145	VAL
1	F	146	LEU
1	F	149	LEU
1	F	154	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	69	ASN
1	A	144	GLN
1	B	54	ASN
1	B	69	ASN
1	B	144	GLN
1	C	28	GLN
1	C	54	ASN
1	C	94	GLN
1	D	28	GLN
1	D	54	ASN
1	D	69	ASN
1	E	54	ASN
1	E	144	GLN
1	F	54	ASN
1	F	69	ASN
1	F	144	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.