Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:48 PM GMT

PDB ID	:	1CFZ
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

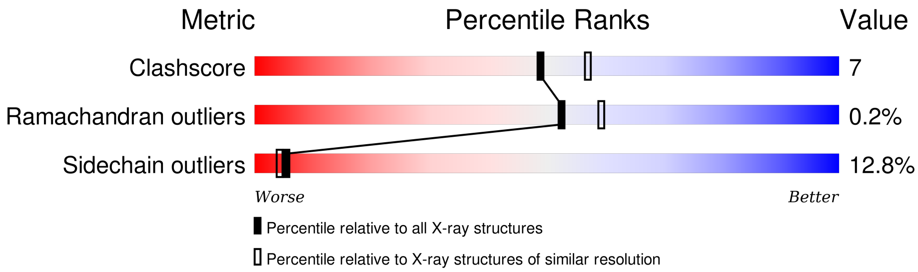
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	162	78% 19% •
1	B	162	75% 22% •
1	C	162	72% 25% •
1	D	162	76% 19% 5% •
1	E	162	69% 29% •
1	F	162	69% 27% •

2 Entry composition (i)

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 1225	C 780	N 204	O 235	S 6	0	0	0
1	B	162	Total 1225	C 780	N 204	O 235	S 6	0	0	0
1	C	162	Total 1225	C 780	N 204	O 235	S 6	0	0	0
1	D	162	Total 1225	C 780	N 204	O 235	S 6	0	0	0
1	E	162	Total 1225	C 780	N 204	O 235	S 6	0	0	0
1	F	162	Total 1225	C 780	N 204	O 235	S 6	0	0	0

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 3 is water.

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

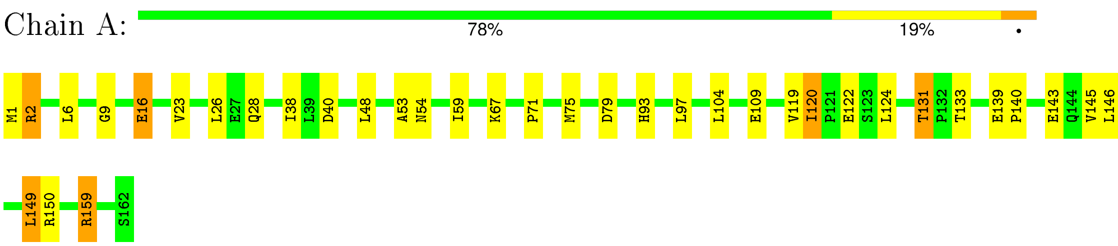
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

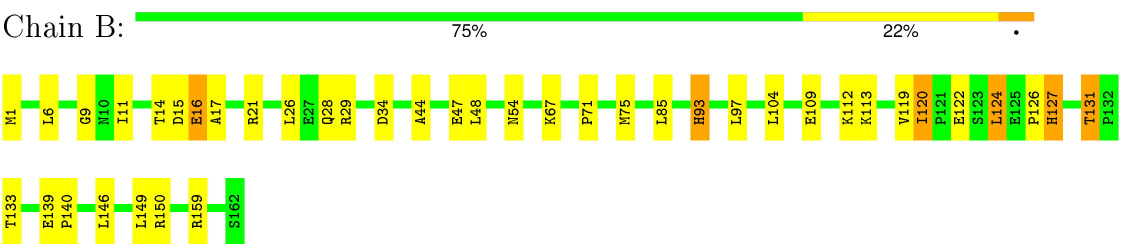
- Molecule 1: HYDROGENASE 2 MATURATION PROTEASE

Chain A:



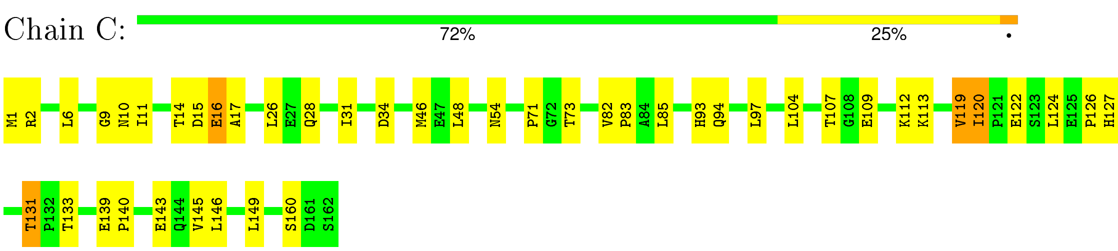
- Molecule 1: HYDROGENASE 2 MATURATION PROTEASE

Chain B:



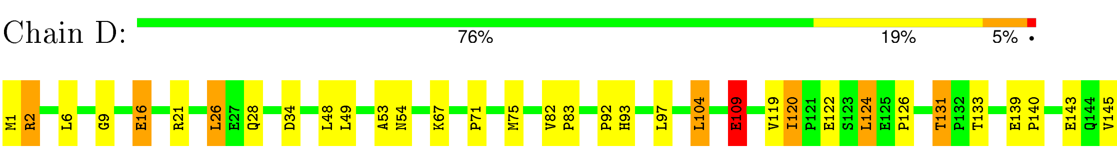
- Molecule 1: HYDROGENASE 2 MATURATION PROTEASE

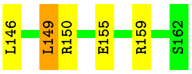
Chain C:



- Molecule 1: HYDROGENASE 2 MATURATION PROTEASE

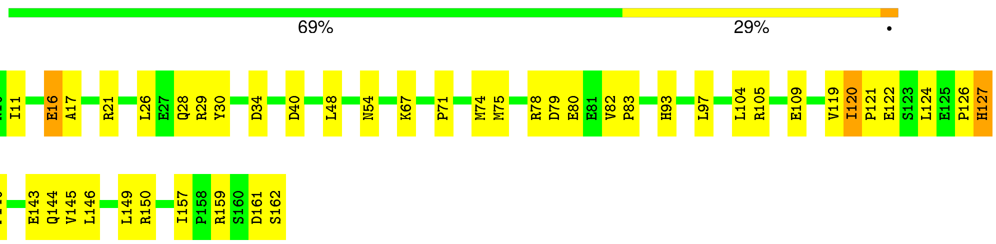
Chain D:





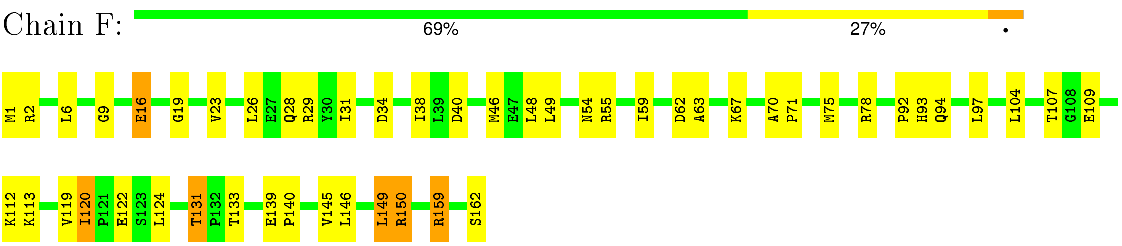
• Molecule 1: HYDROGENASE 2 MATURATION PROTEASE

Chain E:



• Molecule 1: HYDROGENASE 2 MATURATION PROTEASE

Chain F:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 (i)

5.1 Standard geometry (i)

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	0.58	0/1242	1.33	5/1686 (0.3%)
1	B	0.59	0/1242	1.41	7/1686 (0.4%)
1	C	0.59	0/1242	1.41	8/1686 (0.5%)
1	D	0.61	0/1242	1.39	11/1686 (0.7%)
1	E	0.58	0/1242	1.40	13/1686 (0.8%)
1	F	0.59	0/1242	1.39	10/1686 (0.6%)
All	All	0.59	0/7452	1.39	54/10116 (0.5%)

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

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	16	GLU	OE1-CD-OE2	-16.22	103.84	123.30
1	C	94	GLN	OE1-CD-NE2	-16.15	84.75	121.90
1	C	16	GLU	OE1-CD-OE2	-13.20	107.46	123.30
1	F	16	GLU	OE1-CD-OE2	-12.35	108.48	123.30
1	D	2	ARG	NE-CZ-NH2	-12.22	114.19	120.30
1	C	94	GLN	CG-CD-OE1	11.72	145.03	121.60
1	E	150	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	B	16	GLU	CG-CD-OE2	9.34	136.98	118.30
1	E	16	GLU	OE1-CD-OE2	-9.23	112.23	123.30
1	C	2	ARG	NE-CZ-NH2	-8.92	115.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	2	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	D	150	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	B	29	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	D	2	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	E	21	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	E	159	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	D	16	GLU	OE1-CD-OE2	-7.67	114.10	123.30
1	A	16	GLU	OE1-CD-OE2	-7.57	114.22	123.30
1	F	16	GLU	CG-CD-OE2	7.23	132.77	118.30
1	F	29	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	C	16	GLU	CG-CD-OE2	7.08	132.46	118.30
1	F	150	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	E	78	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	E	79	ASP	CB-CG-OD1	6.79	124.41	118.30
1	E	16	GLU	CG-CD-OE2	6.65	131.61	118.30
1	B	159	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	A	2	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	F	159	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	E	150	ARG	CA-CB-CG	6.27	127.19	113.40
1	A	79	ASP	CB-CG-OD1	6.17	123.86	118.30
1	E	2	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	F	159	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	A	159	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	F	2	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	F	78	ARG	NE-CZ-NH2	5.77	123.18	120.30
1	D	109	GLU	CA-CB-CG	-5.75	100.76	113.40
1	B	159	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	F	55	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	D	150	ARG	CA-CB-CG	5.67	125.88	113.40
1	D	155	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	D	124	LEU	CA-CB-CG	5.64	128.26	115.30
1	B	150	ARG	CD-NE-CZ	5.57	131.40	123.60
1	C	94	GLN	CG-CD-NE2	5.56	130.05	116.70
1	E	29	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	124	LEU	CA-CB-CG	5.47	127.88	115.30
1	E	159	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	A	40	ASP	CB-CG-OD2	5.44	123.19	118.30
1	D	26	LEU	CA-CB-CG	5.31	127.51	115.30
1	C	2	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	F	94	GLN	OE1-CD-NE2	-5.03	110.33	121.90
1	E	30	TYR	O-C-N	5.03	130.74	122.70
1	C	119	VAL	CA-CB-CG1	5.02	118.44	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	159	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	D	149	LEU	CA-CB-CG	5.01	126.81	115.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1225	0	1275	18	0
1	B	1225	0	1275	14	1
1	C	1225	0	1275	28	0
1	D	1225	0	1275	17	2
1	E	1225	0	1275	23	0
1	F	1225	0	1275	22	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	1	0
All	All	7630	0	7650	108	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 7.

All (108) 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
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: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: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:D:54:ASN:CG	1:D:109:GLU:HG2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:139:GLU:HB3	1:F:140:PRO:CD	2.43	0.47
1:E:11:ILE:HD13	1:E:17:ALA:HB1	1.95	0.47
1:A:9:GLY:HA2	1:A:16:GLU:OE1	2.14	0.47
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:A:54:ASN:CG	1:A:109:GLU:HG2	2.36	0.46
1:E:40:ASP:C	1:E:40:ASP:OD2	2.54	0.46
1:B:112:LYS:HE2	1:B:113:LYS:HB2	1.98	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:A:67:LYS:HD3	1:A:75:MET:HE1	1.98	0.45
1:E:139:GLU:O	1:E:143:GLU:HG3	2.15	0.45
1:D:9:GLY:HA2	1:D:16:GLU:OE1	2.17	0.45
1:C:11:ILE:HG12	3:C:181:HOH:O	2.16	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:D:67:LYS:HD3	1:D:75:MET:HE1	2.00	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: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:D:21:ARG:HD3	3:D:194:HOH:O	2.19	0.42
1:C:107:THR:CG2	1:F:107:THR:HA	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ALA:HB1	1:B:47:GLU:HG2	2.02	0.42
1:D:67:LYS:HD3	1:D:75:MET:SD	2.60	0.41
1:C:85:LEU:HG	1:C:85:LEU:O	2.19	0.41
1:F:54:ASN:CG	1:F:109:GLU:HG2	2.41	0.41
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:B:85:LEU:HG	1:B:85:LEU:O	2.20	0.41
1:F:23:VAL:HG13	1:F:38:ILE:CG2	2.50	0.41
1:C:14:THR:HG22	1:C:15:ASP:N	2.35	0.41
1:F:31:ILE:HG13	1:F:159:ARG:HG2	2.02	0.41
1:C:54:ASN:CG	1:C:109:GLU:HG2	2.40	0.41
1:C:126:PRO:O	1:C:127:HIS:HB2	2.21	0.41
1:F:70:ALA:HA	1:F:71:PRO:HD3	1.98	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:A:2:ARG:NH2	1:A:53:ALA:O	2.54	0.41
1:F:139:GLU:CB	1:F:140:PRO:HD3	2.48	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:B:67:LYS:HD3	1:B:75:MET:HE1	2.02	0.41
1:E:120:ILE:HD12	1:E:121:PRO:HD2	2.02	0.40
1:B:14:THR:HG22	1:B:15:ASP:N	2.36	0.40
1:E:126:PRO:O	1:E:127:HIS:HB2	2.21	0.40
1:F:40:ASP:C	1:F:40:ASP:OD2	2.59	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 (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	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
1	B	160/162 (99%)	153 (96%)	6 (4%)	1 (1%)	30	29
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%)	30	29
1	F	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
All	All	960/972 (99%)	914 (95%)	44 (5%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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%)	118 (88%)	16 (12%)	6	5
1	B	134/134 (100%)	117 (87%)	17 (13%)	5	4
1	C	134/134 (100%)	117 (87%)	17 (13%)	5	4
1	D	134/134 (100%)	116 (87%)	18 (13%)	5	4
1	E	134/134 (100%)	116 (87%)	18 (13%)	5	4
1	F	134/134 (100%)	117 (87%)	17 (13%)	5	4
All	All	804/804 (100%)	701 (87%)	103 (13%)	5	4

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	LEU
1	A	26	LEU
1	A	28	GLN
1	A	48	LEU
1	A	93	HIS
1	A	97	LEU
1	A	104	LEU
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	B	1	MET
1	B	6	LEU
1	B	21	ARG
1	B	26	LEU
1	B	28	GLN
1	B	34	ASP
1	B	48	LEU
1	B	93	HIS
1	B	97	LEU
1	B	104	LEU
1	B	119	VAL
1	B	120	ILE
1	B	124	LEU
1	B	131	THR
1	B	133	THR
1	B	146	LEU
1	B	149	LEU
1	C	1	MET
1	C	6	LEU
1	C	26	LEU
1	C	28	GLN
1	C	34	ASP
1	C	48	LEU
1	C	93	HIS
1	C	97	LEU
1	C	104	LEU
1	C	119	VAL

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Mol	Chain	Res	Type
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	D	1	MET
1	D	6	LEU
1	D	26	LEU
1	D	28	GLN
1	D	34	ASP
1	D	48	LEU
1	D	93	HIS
1	D	97	LEU
1	D	104	LEU
1	D	109	GLU
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	E	1	MET
1	E	6	LEU
1	E	26	LEU
1	E	28	GLN
1	E	34	ASP
1	E	48	LEU
1	E	93	HIS
1	E	97	LEU
1	E	104	LEU
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

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Mol	Chain	Res	Type
1	E	162	SER
1	F	1	MET
1	F	6	LEU
1	F	26	LEU
1	F	28	GLN
1	F	34	ASP
1	F	48	LEU
1	F	93	HIS
1	F	97	LEU
1	F	104	LEU
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

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

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 carbohydrates 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.