Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 03:50 PM JST

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PDB ID	:	5JZM
Title	:	Structure of wild type Amidase from Vibrio cholerae 0395 at low temparature at 1.8 Angstroms resolution.
Authors	:	Chowdhury, S.R.; Sen, U.
Deposited on	:	2016-05-17
Resolution	:	1.87 Å(reported)

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 1.87 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.
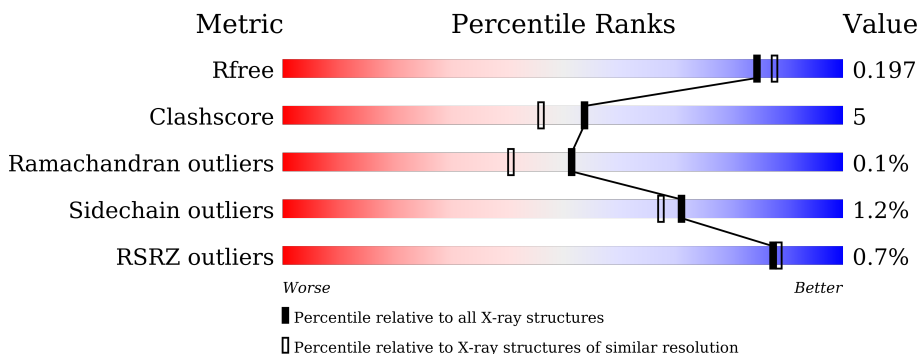
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	288	90% ... 7% ..
1	B	288	88% ... 10% .
1	C	288	88% ... 9% .
1	D	288	87% ... 10% ..
1	E	288	86% ... 11% ..
1	F	288	89% ... 8% .

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14669 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 Intracellular protease/amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	B	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	C	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	D	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	E	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			
1	F	281	Total	C	N	O	S	0	0	0
			2163	1390	352	411	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A0H3AFW5
A	0	SER	-	expression tag	UNP A0A0H3AFW5
B	-1	GLY	-	expression tag	UNP A0A0H3AFW5
B	0	SER	-	expression tag	UNP A0A0H3AFW5
C	-1	GLY	-	expression tag	UNP A0A0H3AFW5
C	0	SER	-	expression tag	UNP A0A0H3AFW5
D	-1	GLY	-	expression tag	UNP A0A0H3AFW5
D	0	SER	-	expression tag	UNP A0A0H3AFW5
E	-1	GLY	-	expression tag	UNP A0A0H3AFW5
E	0	SER	-	expression tag	UNP A0A0H3AFW5
F	-1	GLY	-	expression tag	UNP A0A0H3AFW5
F	0	SER	-	expression tag	UNP A0A0H3AFW5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	317	Total 317	O 317	0	0
2	B	317	Total 317	O 317	0	0
2	C	292	Total 292	O 292	0	0
2	D	297	Total 297	O 297	0	0
2	E	253	Total 253	O 253	0	0
2	F	215	Total 215	O 215	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 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: Intracellular protease/amidase
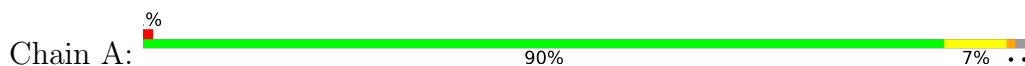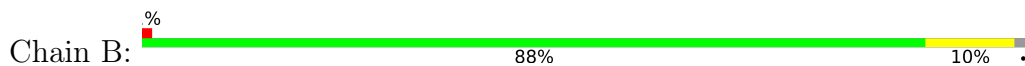
Chain A:

- Molecule 1: Intracellular protease/amidase

Chain B:

- Molecule 1: Intracellular protease/amidase

Chain C:

- Molecule 1: Intracellular protease/amidase

Chain D:

- Molecule 1: Intracellular protease/amidase

Chain E:

GLY SER MET THR THR VAL M5 H9 P10 T11 D36 A40 H41 Y42 I53 H76 H86 M111 P112 R113 Y122 Q126 R130 Q131 P132 E145 D146 L164 P165 D166 S167 Q168 F183 S186 L202 T219 P220 K258 T261 S264 P265

N269 V283 E284 Q285 LYS

• Molecule 1: Intracellular protease/amidase

%

Chain F:	89%	8%	•

GLY SER MET THR THR VAL M5 N6 D7 K8 H9 D17 Y42 P43 T44 H86 R113 E114 D115 Q116 D137 L143 L164 P165 Q168 S186 T219 P220 Q252 Q255 K258 T261 S264 P265 N269 E282 Q285 LYS
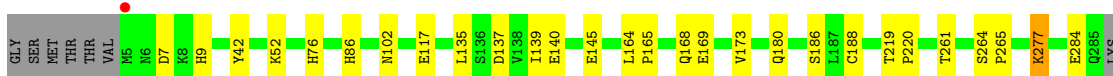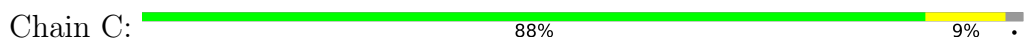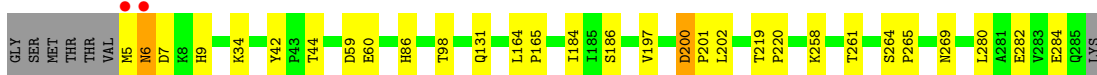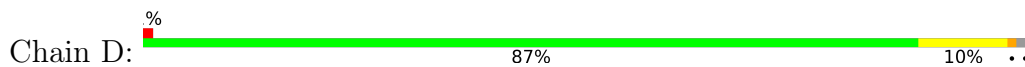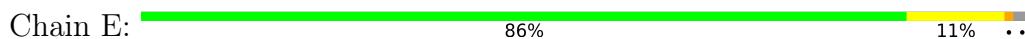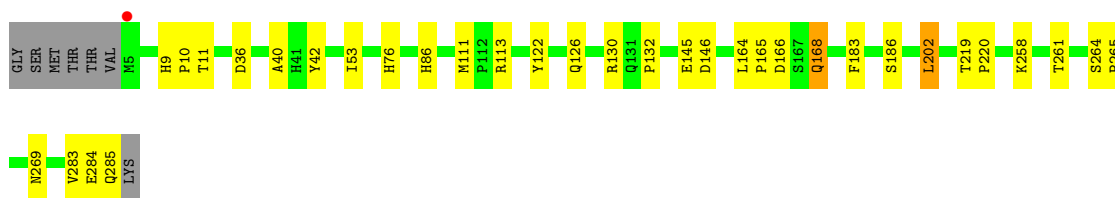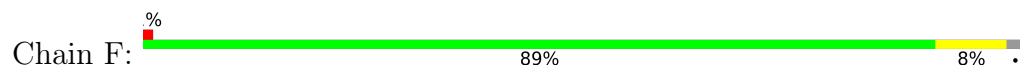
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.92Å　　79.72Å　　133.58Å 90.00°　　95.04°　　90.00°	Depositor
Resolution (Å)	36.31　–　1.87 43.36　–　1.87	Depositor EDS
% Data completeness (in resolution range)	93.0 (36.31-1.87) 88.5 (43.36-1.87)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.158　,　0.196 0.160　,　0.197	Depositor DCC
R_{free} test set	2000 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.2	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14669	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

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	0/2225	0.67	0/3023
1	B	0.58	0/2225	0.65	1/3023 (0.0%)
1	C	0.56	0/2225	0.63	0/3023
1	D	0.59	0/2225	0.67	2/3023 (0.1%)
1	E	0.69	2/2225 (0.1%)	0.69	3/3023 (0.1%)
1	F	0.48	0/2225	0.57	0/3023
All	All	0.59	2/13350 (0.0%)	0.65	6/18138 (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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	132	PRO	N-CD	5.57	1.55	1.47
1	E	10	PRO	N-CD	5.24	1.55	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	285	GLN	N-CA-C	-6.80	92.64	111.00
1	D	200	ASP	C-N-CD	5.68	140.33	128.40
1	D	200	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	200	ASP	CB-CG-OD1	5.58	123.32	118.30
1	E	111	MET	C-N-CD	5.45	139.85	128.40
1	E	9	HIS	C-N-CD	5.30	139.54	128.40

There are no chirality outliers.

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All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	284	GLU	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	2163	0	2072	20	0
1	B	2163	0	2072	17	0
1	C	2163	0	2072	24	0
1	D	2163	0	2072	27	0
1	E	2163	0	2072	30	0
1	F	2163	0	2072	20	0
2	A	317	0	0	3	0
2	B	317	0	0	3	2
2	C	292	0	0	10	1
2	D	297	0	0	12	2
2	E	253	0	0	9	1
2	F	215	0	0	9	0
All	All	14669	0	12432	134	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 5.

All (134) 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:283:VAL:C	1:A:284:GLU:OE2	1.78	1.20
1:A:283:VAL:O	1:A:284:GLU:OE2	1.62	1.16
1:C:137:ASP:HB3	2:C:501:HOH:O	1.49	1.11
1:D:6:ASN:HA	2:D:302:HOH:O	1.65	0.96
1:E:283:VAL:HG23	1:E:284:GLU:HG3	1.56	0.88
1:F:252:GLN:HG2	2:F:307:HOH:O	1.75	0.87
1:A:282:GLU:O	1:A:284:GLU:N	2.08	0.87
1:E:284:GLU:O	2:E:301:HOH:O	1.93	0.87
1:F:116:GLN:OE1	2:F:301:HOH:O	1.93	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:ASP:OD1	2:D:301:HOH:O	1.94	0.85
1:D:34:LYS:CE	2:D:435:HOH:O	2.25	0.83
1:E:166:ASP:OD1	2:E:302:HOH:O	1.96	0.82
1:D:34:LYS:HE2	2:D:435:HOH:O	1.81	0.81
1:F:252:GLN:OE1	2:F:302:HOH:O	1.99	0.79
1:E:11:THR:OG1	2:E:303:HOH:O	2.00	0.78
1:F:252:GLN:CG	2:F:307:HOH:O	2.30	0.77
1:B:140:GLU:HG3	2:B:318:HOH:O	1.85	0.76
1:F:258:LYS:NZ	1:F:282:GLU:OE2	2.19	0.75
1:E:146:ASP:OD1	2:E:304:HOH:O	2.03	0.74
1:A:116:GLN:OE1	2:A:301:HOH:O	2.06	0.73
1:B:5:MET:CB	1:B:9:HIS:CE1	2.73	0.72
1:E:36:ASP:HB2	2:E:339:HOH:O	1.88	0.71
1:D:280:LEU:O	1:D:284:GLU:HG2	1.91	0.71
1:C:169:GLU:OE1	2:C:301:HOH:O	2.07	0.71
1:A:283:VAL:O	1:A:284:GLU:CD	2.29	0.69
1:B:5:MET:CB	1:B:9:HIS:HE1	2.06	0.69
1:D:5:MET:O	2:D:302:HOH:O	2.09	0.68
1:C:52:LYS:HD2	2:C:366:HOH:O	1.94	0.68
1:C:137:ASP:CB	2:C:501:HOH:O	2.24	0.68
1:E:283:VAL:HG23	1:E:284:GLU:CG	2.22	0.68
1:D:7:ASP:OD1	1:D:9:HIS:HD2	1.77	0.67
1:D:6:ASN:ND2	2:D:302:HOH:O	2.27	0.66
1:C:188:CYS:SG	2:C:313:HOH:O	2.33	0.65
1:B:140:GLU:OE1	2:B:301:HOH:O	2.14	0.65
1:C:42:TYR:OH	1:C:86:HIS:HD2	1.79	0.65
1:C:139:ILE:HD11	1:C:173:VAL:HG23	1.79	0.64
1:C:139:ILE:HD11	1:C:173:VAL:CG2	2.28	0.64
1:D:6:ASN:CG	2:D:302:HOH:O	2.36	0.63
1:B:258:LYS:NZ	1:B:282:GLU:OE2	2.32	0.62
1:E:130:ARG:HD2	2:E:315:HOH:O	2.00	0.62
1:A:202:LEU:HD21	1:A:203:PHE:CE2	2.37	0.59
2:C:328:HOH:O	1:E:168:GLN:HG2	2.02	0.58
1:E:283:VAL:CG2	1:E:284:GLU:HG3	2.30	0.58
1:F:86:HIS:HE1	1:F:269:ASN:OD1	1.87	0.57
1:A:171:LYS:HG3	1:A:197:VAL:HA	1.86	0.57
1:D:7:ASP:OD1	1:D:9:HIS:CD2	2.56	0.57
1:F:255:GLN:HG2	2:F:376:HOH:O	2.05	0.56
1:F:264:SER:HB2	1:F:265:PRO:CD	2.36	0.56
1:A:273:GLN:O	1:A:277:LYS:HG2	2.05	0.56
1:D:197:VAL:HG11	1:D:202:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:SER:HB2	1:D:265:PRO:CD	2.37	0.54
1:C:180:GLN:OE1	1:E:168:GLN:NE2	2.26	0.54
1:E:42:TYR:OH	1:E:86:HIS:HD2	1.90	0.54
1:A:284:GLU:OE2	1:A:284:GLU:N	2.39	0.54
1:A:42:TYR:OH	1:A:86:HIS:HD2	1.91	0.54
1:E:86:HIS:HE1	1:E:269:ASN:OD1	1.91	0.54
1:C:168:GLN:HG3	2:C:485:HOH:O	2.08	0.53
1:F:114:GLU:O	1:F:114:GLU:HG3	2.08	0.53
1:C:264:SER:HB2	1:C:265:PRO:CD	2.39	0.53
1:F:264:SER:HB2	1:F:265:PRO:HD2	1.91	0.53
1:D:42:TYR:OH	1:D:86:HIS:HD2	1.92	0.52
1:B:136:SER:HB3	1:B:169:GLU:OE2	2.08	0.52
1:B:86:HIS:HE1	1:B:269:ASN:OD1	1.93	0.52
1:F:219:THR:N	1:F:220:PRO:CD	2.73	0.52
1:C:145:GLU:OE1	2:C:303:HOH:O	2.19	0.52
1:D:86:HIS:HE1	1:D:269:ASN:OD1	1.92	0.52
1:F:137:ASP:OD2	2:F:305:HOH:O	2.18	0.51
1:F:168:GLN:OE1	2:F:306:HOH:O	2.20	0.50
1:F:252:GLN:CD	2:F:307:HOH:O	2.49	0.50
1:D:264:SER:HB2	1:D:265:PRO:HD2	1.94	0.50
1:B:42:TYR:OH	1:B:86:HIS:HD2	1.94	0.50
1:E:122:TYR:CE2	1:E:126:GLN:HG3	2.47	0.49
1:C:264:SER:HB2	1:C:265:PRO:HD2	1.95	0.49
1:E:202:LEU:HD23	1:E:202:LEU:N	2.26	0.49
1:D:131:GLN:HG2	2:D:415:HOH:O	2.13	0.48
1:D:202:LEU:HD23	1:D:202:LEU:N	2.29	0.48
1:E:264:SER:HB2	1:E:265:PRO:HD2	1.96	0.48
1:D:6:ASN:CA	2:D:302:HOH:O	2.42	0.48
1:B:186:SER:O	1:B:261:THR:HA	2.14	0.48
1:E:202:LEU:H	1:E:202:LEU:CD2	2.27	0.47
1:E:76:HIS:HE1	2:E:422:HOH:O	1.98	0.47
1:E:164:LEU:HB2	1:E:165:PRO:HD3	1.96	0.46
1:A:86:HIS:HE1	1:A:269:ASN:OD1	1.99	0.46
1:D:258:LYS:NZ	1:D:282:GLU:OE2	2.45	0.46
1:E:113:ARG:NE	2:E:310:HOH:O	2.45	0.46
1:B:52:LYS:HG2	1:B:93:SER:HB3	1.97	0.46
1:B:280:LEU:O	1:B:284:GLU:HG3	2.16	0.46
1:D:219:THR:N	1:D:220:PRO:CD	2.79	0.46
2:A:431:HOH:O	1:B:130:ARG:HD3	2.15	0.46
1:C:140:GLU:HB3	1:F:143:LEU:HB2	1.98	0.45
1:C:186:SER:O	1:C:261:THR:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ILE:HD12	1:E:53:ILE:N	2.31	0.45
1:F:186:SER:O	1:F:261:THR:HA	2.16	0.45
1:E:183:PHE:CE1	1:E:258:LYS:HD3	2.51	0.45
1:E:202:LEU:N	1:E:202:LEU:CD2	2.79	0.45
1:D:186:SER:O	1:D:261:THR:HA	2.17	0.44
1:C:277:LYS:HB3	1:C:277:LYS:NZ	2.32	0.44
1:F:252:GLN:CD	2:F:302:HOH:O	2.48	0.44
1:C:102:ASN:HB3	1:D:60:GLU:OE1	2.17	0.44
1:A:102:ASN:HB3	1:A:103:PRO:HD2	1.99	0.44
1:E:130:ARG:NH2	2:E:315:HOH:O	2.51	0.43
1:F:164:LEU:HB2	1:F:165:PRO:HD3	2.00	0.43
1:E:40:ALA:HA	1:E:86:HIS:CD2	2.53	0.43
1:A:202:LEU:HD21	1:A:203:PHE:CD2	2.53	0.43
1:C:42:TYR:OH	1:C:86:HIS:CD2	2.67	0.43
1:C:137:ASP:CG	2:C:501:HOH:O	2.52	0.43
1:C:76:HIS:HE1	2:C:450:HOH:O	2.02	0.43
1:E:219:THR:OG1	1:E:220:PRO:HD3	2.19	0.43
1:B:219:THR:N	1:B:220:PRO:CD	2.82	0.43
1:A:102:ASN:HB3	1:B:60:GLU:OE1	2.18	0.43
1:B:252:GLN:OE1	2:B:302:HOH:O	2.22	0.42
1:D:59:ASP:HB3	1:D:98:THR:HB	2.02	0.42
1:F:42:TYR:OH	1:F:86:HIS:HD2	2.02	0.42
1:C:7:ASP:OD1	1:C:9:HIS:CD2	2.72	0.42
1:C:219:THR:N	1:C:220:PRO:CD	2.83	0.42
1:D:9:HIS:CD2	2:D:311:HOH:O	2.72	0.42
1:E:264:SER:HB2	1:E:265:PRO:CD	2.48	0.42
1:A:264:SER:HB2	1:A:265:PRO:CD	2.50	0.41
1:A:164:LEU:HB2	1:A:165:PRO:HD3	2.01	0.41
1:A:164:LEU:N	1:A:165:PRO:CD	2.82	0.41
1:B:59:ASP:HB3	1:B:98:THR:HB	2.02	0.41
1:D:184:ILE:HD12	2:D:563:HOH:O	2.19	0.41
1:D:164:LEU:HB2	1:D:165:PRO:HD3	2.03	0.41
1:D:201:PRO:HD2	2:D:301:HOH:O	2.20	0.41
1:A:197:VAL:HG11	1:A:202:LEU:CD2	2.50	0.41
1:C:135:LEU:O	1:C:139:ILE:HG12	2.19	0.41
1:E:219:THR:N	1:E:220:PRO:CD	2.84	0.41
1:F:7:ASP:OD2	1:F:9:HIS:ND1	2.54	0.41
1:A:125:TYR:OH	2:A:302:HOH:O	2.13	0.41
1:C:164:LEU:N	1:C:165:PRO:CD	2.84	0.41
1:E:186:SER:O	1:E:261:THR:HA	2.21	0.41
1:A:186:SER:O	1:A:261:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:TYR:OH	1:E:86:HIS:CD2	2.72	0.41
1:B:197:VAL:HG11	1:B:202:LEU:HD21	2.03	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)
2:B:543:HOH:O	2:D:481:HOH:O[2_555]	1.87	0.33
2:B:397:HOH:O	2:D:587:HOH:O[2_555]	1.95	0.25
2:C:508:HOH:O	2:E:320:HOH:O[2_546]	2.11	0.09

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	279/288 (97%)	268 (96%)	10 (4%)	1 (0%)	34	22
1	B	279/288 (97%)	269 (96%)	10 (4%)	0	100	100
1	C	279/288 (97%)	268 (96%)	11 (4%)	0	100	100
1	D	279/288 (97%)	270 (97%)	9 (3%)	0	100	100
1	E	279/288 (97%)	269 (96%)	10 (4%)	0	100	100
1	F	279/288 (97%)	269 (96%)	10 (4%)	0	100	100
All	All	1674/1728 (97%)	1613 (96%)	60 (4%)	1 (0%)	51	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	VAL

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	226/234 (97%)	224 (99%)	2 (1%)	78	76
1	B	226/234 (97%)	222 (98%)	4 (2%)	59	52
1	C	226/234 (97%)	224 (99%)	2 (1%)	78	76
1	D	226/234 (97%)	224 (99%)	2 (1%)	78	76
1	E	226/234 (97%)	223 (99%)	3 (1%)	69	64
1	F	226/234 (97%)	223 (99%)	3 (1%)	69	64
All	All	1356/1404 (97%)	1340 (99%)	16 (1%)	71	67

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	LEU
1	A	277	LYS
1	B	93	SER
1	B	146	ASP
1	B	168	GLN
1	B	236	GLN
1	C	117	GLU
1	C	277	LYS
1	D	6	ASN
1	D	44	THR
1	E	145	GLU
1	E	168	GLN
1	E	202	LEU
1	F	7	ASP
1	F	17	ASP
1	F	113	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS

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Mol	Chain	Res	Type
1	A	86	HIS
1	A	116	GLN
1	B	9	HIS
1	B	41	HIS
1	B	76	HIS
1	B	86	HIS
1	B	168	GLN
1	B	252	GLN
1	C	9	HIS
1	C	76	HIS
1	C	86	HIS
1	C	168	GLN
1	D	9	HIS
1	D	76	HIS
1	D	86	HIS
1	E	76	HIS
1	E	86	HIS
1	F	86	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	281/288 (97%)	-0.48	2 (0%)	87	88	11, 16, 29, 81	0
1	B	281/288 (97%)	-0.49	2 (0%)	87	88	10, 15, 30, 66	0
1	C	281/288 (97%)	-0.51	1 (0%)	92	93	12, 17, 32, 53	0
1	D	281/288 (97%)	-0.49	2 (0%)	87	88	10, 16, 30, 70	0
1	E	281/288 (97%)	-0.33	1 (0%)	92	93	13, 22, 38, 77	0
1	F	281/288 (97%)	-0.15	4 (1%)	75	77	14, 23, 47, 64	0
All	All	1686/1728 (97%)	-0.41	12 (0%)	87	88	10, 18, 37, 81	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	GLN	5.5
1	E	5	MET	4.3
1	D	6	ASN	3.9
1	D	5	MET	3.1
1	F	9	HIS	3.0
1	C	5	MET	3.0
1	B	5	MET	2.8
1	B	285	GLN	2.5
1	A	283	VAL	2.5
1	F	44	THR	2.4
1	F	285	GLN	2.4
1	F	6	ASN	2.1

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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.