



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:30 pm GMT

PDB ID : 3WJ2  
Title : Crystal structure of ESTFA (FE-lacking apo form)  
Authors : Ohara, K.; Unno, H.; Oshima, Y.; Furukawa, K.; Fujino, N.; Hirooka, K.; Hemmi, H.; Takahashi, S.; Nishino, T.; Kusunoki, M.; Nakayama, T.  
Deposited on : 2013-10-03  
Resolution : 1.61 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949



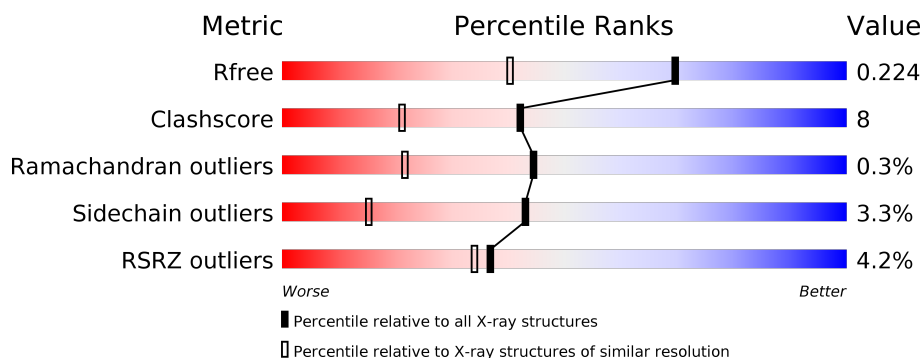
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.61 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))
$R_{free}$	100719	3539 (1.64-1.60)
Clashscore	112137	3855 (1.64-1.60)
Ramachandran outliers	110173	3764 (1.64-1.60)
Sidechain outliers	110143	3763 (1.64-1.60)
RSRZ outliers	101464	3562 (1.64-1.60)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	308	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>
1	B	308	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
1	C	308	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	D	308	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>



## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10427 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 Carboxylesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2355	1502	394	446	13			
1	B	300	Total	C	N	O	S	0	0	0
			2363	1506	396	448	13			
1	C	300	Total	C	N	O	S	0	0	0
			2363	1506	396	448	13			
1	D	300	Total	C	N	O	S	0	0	0
			2363	1506	396	448	13			

- Molecule 2 is water.

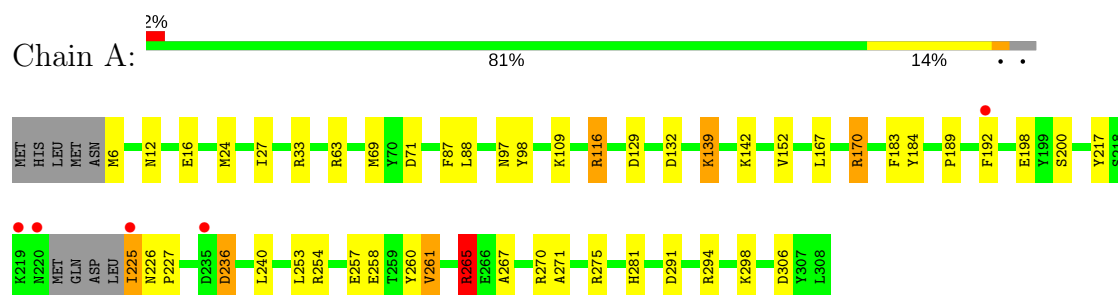
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	286	Total	O	0	0
			286	286		
2	B	284	Total	O	0	0
			284	284		
2	C	219	Total	O	0	0
			219	219		
2	D	194	Total	O	0	0
			194	194		



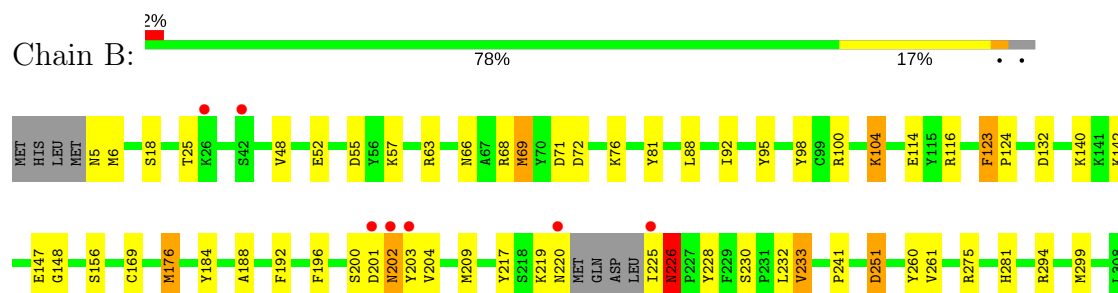
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

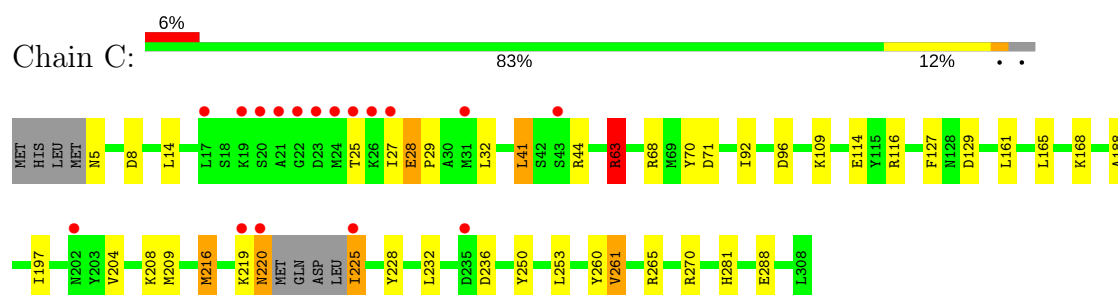
#### • Molecule 1: Carboxylesterase



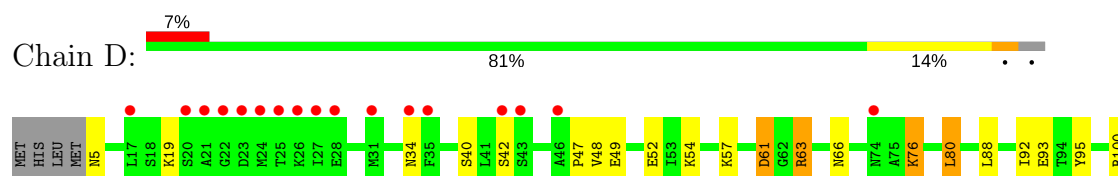
#### • Molecule 1: Carboxylesterase



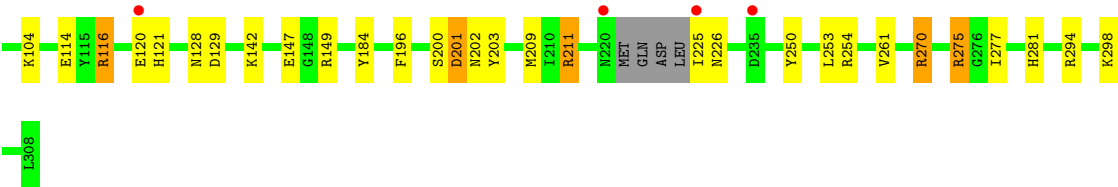
#### • Molecule 1: Carboxylesterase



#### • Molecule 1: Carboxylesterase









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.80Å 137.36Å 76.88Å 90.00° 91.47° 90.00°	Depositor
Resolution (Å)	46.37 – 1.61 46.36 – 1.61	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.37-1.61) 98.9 (46.36-1.61)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.86 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.188 , 0.225 0.186 , 0.224	Depositor DCC
$R_{free}$ test set	8367 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10427	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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	1.41	10/2406 (0.4%)	1.53	26/3245 (0.8%)
1	B	1.46	8/2414 (0.3%)	1.39	23/3256 (0.7%)
1	C	1.32	8/2414 (0.3%)	1.23	12/3256 (0.4%)
1	D	1.29	2/2414 (0.1%)	1.24	11/3256 (0.3%)
All	All	1.37	28/9648 (0.3%)	1.35	72/13013 (0.6%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	261	VAL	CB-CG1	-8.36	1.35	1.52
1	B	176	MET	CB-CG	8.11	1.77	1.51
1	A	261	VAL	CB-CG1	-7.81	1.36	1.52
1	A	261	VAL	CB-CG2	-7.60	1.36	1.52
1	B	261	VAL	CB-CG2	-7.54	1.37	1.52
1	C	228	TYR	CE1-CZ	6.96	1.47	1.38
1	A	257	GLU	CD-OE2	6.56	1.32	1.25
1	B	95	TYR	CD1-CE1	6.28	1.48	1.39
1	B	123	PHE	CE1-CZ	6.23	1.49	1.37
1	C	70	TYR	CE1-CZ	6.20	1.46	1.38
1	C	288	GLU	CD-OE2	-6.18	1.18	1.25
1	B	217	TYR	CD1-CE1	5.75	1.48	1.39
1	A	265	ARG	CZ-NH1	-5.73	1.25	1.33
1	A	217	TYR	CG-CD2	5.50	1.46	1.39
1	A	87	PHE	CD1-CE1	5.48	1.50	1.39
1	B	226	ASN	N-CA	-5.43	1.35	1.46
1	D	261	VAL	CA-CB	5.43	1.66	1.54
1	D	203	TYR	CD1-CE1	5.40	1.47	1.39
1	A	217	TYR	CD1-CE1	5.39	1.47	1.39
1	A	267	ALA	CA-CB	5.35	1.63	1.52
1	B	233	VAL	CB-CG2	-5.30	1.41	1.52
1	C	168	LYS	CD-CE	5.28	1.64	1.51
1	C	70	TYR	CG-CD2	5.25	1.46	1.39
1	A	152	VAL	CB-CG1	5.12	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	260	TYR	CD2-CE2	5.10	1.47	1.39
1	C	250	TYR	CD1-CE1	5.10	1.47	1.39
1	B	217	TYR	CE2-CZ	-5.03	1.32	1.38
1	A	33	ARG	CZ-NH1	5.02	1.39	1.33

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ARG	NE-CZ-NH1	-25.54	107.53	120.30
1	A	116	ARG	NE-CZ-NH2	-20.14	110.23	120.30
1	A	116	ARG	NE-CZ-NH1	19.97	130.28	120.30
1	A	265	ARG	NE-CZ-NH2	13.56	127.08	120.30
1	B	299	MET	CG-SD-CE	-13.34	78.86	100.20
1	B	116	ARG	NE-CZ-NH1	-10.43	115.09	120.30
1	A	170	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	A	116	ARG	CD-NE-CZ	10.06	137.69	123.60
1	D	275	ARG	NE-CZ-NH1	-9.86	115.37	120.30
1	A	170	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	B	98	TYR	CB-CG-CD2	-9.46	115.32	121.00
1	B	275	ARG	NE-CZ-NH2	-8.91	115.85	120.30
1	A	294	ARG	NE-CZ-NH1	8.89	124.74	120.30
1	C	68	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	B	251	ASP	CB-CG-OD1	8.28	125.76	118.30
1	D	116	ARG	NE-CZ-NH1	-8.23	116.19	120.30
1	B	176	MET	CB-CG-SD	-7.91	88.68	112.40
1	B	251	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	C	216	MET	CG-SD-CE	-7.75	87.81	100.20
1	A	265	ARG	CD-NE-CZ	-7.50	113.09	123.60
1	B	176	MET	CG-SD-CE	-7.34	88.45	100.20
1	A	98	TYR	CB-CG-CD2	-7.26	116.65	121.00
1	C	96	ASP	CB-CG-OD1	6.82	124.43	118.30
1	D	80	LEU	CB-CG-CD1	6.71	122.41	111.00
1	B	98	TYR	CD1-CE1-CZ	-6.59	113.87	119.80
1	D	270	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	C	63	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	C	220	ASN	N-CA-C	6.49	128.53	111.00
1	B	88	LEU	CB-CG-CD2	-6.49	99.97	111.00
1	C	8	ASP	CB-CG-OD2	6.36	124.03	118.30
1	C	219	LYS	C-N-CA	6.33	137.52	121.70
1	C	270	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A	132	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	270	ARG	NE-CZ-NH1	6.25	123.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	254	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	B	260	TYR	CB-CG-CD1	-6.16	117.30	121.00
1	A	116	ARG	CG-CD-NE	-6.11	98.98	111.80
1	B	69	MET	CG-SD-CE	6.11	109.97	100.20
1	D	254	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	265	ARG	CB-CG-CD	5.94	127.05	111.60
1	A	184	TYR	CD1-CE1-CZ	-5.94	114.45	119.80
1	B	55	ASP	CB-CG-OD1	-5.73	113.14	118.30
1	C	236	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	132	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	183	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	B	294	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	6	MET	CG-SD-CE	5.64	109.22	100.20
1	B	184	TYR	CG-CD1-CE1	-5.63	116.79	121.30
1	D	116	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	A	294	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	258	GLU	OE1-CD-OE2	-5.48	116.72	123.30
1	B	184	TYR	CZ-CE2-CD2	-5.45	114.90	119.80
1	B	100	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	183	PHE	CG-CD2-CE2	-5.42	114.83	120.80
1	C	68	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	D	254	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	298	LYS	CD-CE-NZ	-5.34	99.42	111.70
1	B	81	TYR	CB-CG-CD1	-5.31	117.82	121.00
1	B	68	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	265	ARG	NH1-CZ-NH2	5.29	125.22	119.40
1	D	270	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	88	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	D	184	TYR	CZ-CE2-CD2	-5.18	115.14	119.80
1	A	260	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	C	261	VAL	CB-CA-C	5.09	121.06	111.40
1	B	95	TYR	CG-CD2-CE2	-5.07	117.25	121.30
1	C	265	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	98	TYR	CD1-CE1-CZ	-5.03	115.28	119.80
1	D	95	TYR	CZ-CE2-CD2	5.03	124.32	119.80
1	D	250	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	A	306	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.



## 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	2355	0	2318	36	0
1	B	2363	0	2324	50	0
1	C	2363	0	2324	24	0
1	D	2363	0	2324	44	0
2	A	286	0	0	14	0
2	B	284	0	0	14	0
2	C	219	0	0	2	0
2	D	194	0	0	16	0
All	All	10427	0	9290	148	0

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 (148) 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:B:176:MET:CB	1:B:176:MET:CG	1.77	1.59
1:B:69:MET:HG3	2:B:449:HOH:O	1.09	1.24
1:A:116:ARG:HD3	1:A:129:ASP:OD2	1.41	1.21
1:A:116:ARG:CD	1:A:129:ASP:OD2	1.92	1.17
1:B:219:LYS:HE2	2:B:512:HOH:O	1.52	1.09
1:A:225:ILE:O	1:A:225:ILE:HD13	1.54	1.08
1:C:116:ARG:NH1	1:C:129:ASP:OD1	1.87	1.07
1:D:48:VAL:CG1	1:D:104:LYS:HD2	1.88	1.01
1:D:63:ARG:HG3	1:D:116:ARG:NH1	1.77	0.99
1:B:176:MET:CB	1:B:176:MET:SD	2.50	0.98
1:A:170:ARG:NH2	1:A:236:ASP:O	1.97	0.96
1:B:69:MET:CG	2:B:449:HOH:O	1.80	0.96
1:B:201:ASP:O	1:B:203:TYR:N	2.01	0.93
1:B:5:ASN:N	2:B:661:HOH:O	1.99	0.93
1:D:128:ASN:ND2	2:D:577:HOH:O	2.02	0.91
1:A:116:ARG:HD2	1:A:129:ASP:OD2	1.72	0.89
1:B:220:ASN:C	2:B:451:HOH:O	2.11	0.88
1:D:48:VAL:HG11	1:D:104:LYS:HD2	1.56	0.88
1:A:225:ILE:O	1:A:225:ILE:CD1	2.21	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ASN:N	2:D:448:HOH:O	2.07	0.87
1:D:48:VAL:HG13	1:D:104:LYS:HD2	1.55	0.85
1:D:34:ASN:HB2	2:D:456:HOH:O	1.76	0.85
1:A:291:ASP:OD2	1:D:270:ARG:HD2	1.77	0.83
1:B:72:ASP:OD2	1:B:104:LYS:HE3	1.76	0.83
1:B:204:VAL:HB	2:B:634:HOH:O	1.77	0.83
1:A:265:ARG:HD2	1:A:271:ALA:HB3	1.61	0.83
1:D:120:GLU:HG3	2:D:455:HOH:O	1.79	0.82
1:D:142:LYS:NZ	2:D:573:HOH:O	2.15	0.79
1:C:14:LEU:HD22	1:C:204:VAL:HG21	1.64	0.79
1:B:176:MET:HE1	1:B:241:PRO:HG3	1.68	0.76
1:C:116:ARG:NH1	1:C:129:ASP:CG	2.38	0.76
1:B:176:MET:HB3	1:B:176:MET:SD	2.26	0.75
1:D:34:ASN:HB2	2:D:570:HOH:O	1.86	0.74
1:A:265:ARG:NH1	2:A:448:HOH:O	2.01	0.74
1:C:63:ARG:HG3	1:C:116:ARG:NH1	2.03	0.73
1:B:201:ASP:C	1:B:203:TYR:H	1.92	0.72
1:D:116:ARG:HD2	1:D:121:HIS:CE1	2.24	0.72
1:A:265:ARG:NH2	2:A:448:HOH:O	2.24	0.71
1:A:225:ILE:O	1:A:225:ILE:CG1	2.39	0.70
1:D:63:ARG:HG3	1:D:116:ARG:HH12	1.51	0.70
1:A:227:PRO:HD3	2:A:578:HOH:O	1.91	0.69
1:B:5:ASN:N	2:B:561:HOH:O	2.25	0.69
1:B:76:LYS:HG3	1:B:147:GLU:HB2	1.75	0.69
1:A:265:ARG:CZ	2:A:448:HOH:O	2.38	0.68
1:B:57:LYS:NZ	1:B:66:ASN:HD21	1.90	0.68
1:C:14:LEU:CD2	1:C:204:VAL:HG21	2.24	0.68
1:B:226:ASN:HD22	1:B:228:TYR:H	1.42	0.67
1:A:225:ILE:HA	2:A:515:HOH:O	1.94	0.67
1:A:24:MET:HB3	1:A:27:ILE:HD12	1.75	0.67
1:C:71:ASP:OD1	1:C:109:LYS:NZ	2.27	0.66
1:A:198:GLU:O	1:C:5:ASN:N	2.29	0.65
2:A:565:HOH:O	1:B:233:VAL:HG12	1.96	0.64
1:D:209:MET:HG3	2:D:445:HOH:O	1.97	0.64
1:C:63:ARG:HE	1:C:116:ARG:HH12	1.46	0.64
1:C:225:ILE:O	1:C:225:ILE:HG22	1.99	0.63
1:B:176:MET:CE	1:B:176:MET:HB3	2.29	0.62
1:B:176:MET:CB	1:B:176:MET:CE	2.77	0.62
1:C:116:ARG:NH1	1:C:129:ASP:OD2	2.33	0.61
1:B:196:PHE:O	1:B:200:SER:HB3	2.01	0.61
1:B:176:MET:HE1	1:B:241:PRO:CG	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:GLU:HG3	1:B:71:ASP:HB3	1.81	0.61
1:D:225:ILE:N	2:D:419:HOH:O	2.33	0.60
1:A:71:ASP:OD2	1:A:109:LYS:NZ	2.34	0.60
1:A:226:ASN:HA	2:A:578:HOH:O	2.01	0.60
1:D:19:LYS:HD3	1:D:202:ASN:HD22	1.64	0.60
1:D:225:ILE:HA	2:D:419:HOH:O	2.01	0.59
1:D:270:ARG:HD3	2:D:545:HOH:O	2.01	0.59
1:B:48:VAL:CG1	1:B:104:LYS:HD2	2.34	0.58
1:B:200:SER:OG	2:B:545:HOH:O	2.14	0.57
1:D:63:ARG:HE	1:D:116:ARG:HH12	1.51	0.57
1:A:167:LEU:HD23	1:A:240:LEU:HD21	1.86	0.57
1:A:253:LEU:HD12	1:A:281:HIS:CE1	2.39	0.57
1:C:253:LEU:HD12	1:C:281:HIS:CE1	2.40	0.57
1:D:57:LYS:NZ	1:D:66:ASN:HD21	2.02	0.57
1:B:220:ASN:ND2	2:B:655:HOH:O	2.25	0.57
1:D:49:GLU:O	1:D:104:LYS:HE2	2.05	0.56
1:B:140:LYS:HD3	2:B:572:HOH:O	2.05	0.56
1:B:76:LYS:HG2	1:B:148:GLY:N	2.21	0.55
1:D:48:VAL:HG13	1:D:104:LYS:CD	2.33	0.55
1:D:48:VAL:CG1	1:D:104:LYS:CD	2.75	0.55
1:A:170:ARG:HG2	2:A:609:HOH:O	2.06	0.55
1:B:201:ASP:OD1	1:B:201:ASP:C	2.46	0.54
1:B:230:SER:O	1:B:233:VAL:HG22	2.07	0.54
1:D:76:LYS:HE2	2:D:550:HOH:O	2.08	0.54
1:D:120:GLU:CG	2:D:455:HOH:O	2.46	0.53
1:C:188:ALA:HB2	1:C:232:LEU:HD12	1.90	0.53
1:B:57:LYS:HZ3	1:B:66:ASN:HD21	1.56	0.52
1:B:76:LYS:HA	2:B:640:HOH:O	2.09	0.52
1:A:142:LYS:HG2	2:A:659:HOH:O	2.09	0.52
1:B:25:THR:HG22	1:B:209:MET:SD	2.50	0.51
1:B:202:ASN:O	2:B:663:HOH:O	2.19	0.51
1:A:116:ARG:CD	1:A:129:ASP:CG	2.75	0.51
1:D:92:ILE:HG13	1:D:114:GLU:HG3	1.92	0.51
1:B:188:ALA:HB2	1:B:232:LEU:HD12	1.92	0.51
1:D:63:ARG:HG3	1:D:116:ARG:HH11	1.72	0.50
1:A:116:ARG:HD2	1:A:129:ASP:CG	2.29	0.50
1:C:225:ILE:HD12	1:C:225:ILE:N	2.26	0.50
1:D:57:LYS:HZ3	1:D:66:ASN:HD21	1.58	0.50
1:D:196:PHE:O	1:D:200:SER:HB3	2.12	0.50
1:B:57:LYS:HZ2	1:B:66:ASN:HD21	1.61	0.49
1:B:251:ASP:OD2	1:B:281:HIS:HD2	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:GLU:HG3	1:C:29:PRO:N	2.27	0.48
1:D:93:GLU:HG2	2:D:513:HOH:O	2.12	0.48
1:C:253:LEU:HD12	1:C:281:HIS:HE1	1.79	0.48
1:C:209:MET:HG3	2:C:510:HOH:O	2.14	0.47
1:D:76:LYS:HG2	1:D:147:GLU:HB2	1.94	0.47
1:A:227:PRO:CD	2:A:578:HOH:O	2.55	0.47
1:B:156:SER:OG	1:B:281:HIS:HE1	1.97	0.47
1:A:6:MET:N	2:A:664:HOH:O	2.48	0.47
1:A:189:PRO:HG3	2:A:515:HOH:O	2.14	0.46
1:D:5:ASN:CA	2:D:448:HOH:O	2.59	0.46
1:A:139:LYS:HE2	1:A:139:LYS:HB2	1.49	0.46
1:C:5:ASN:C	1:C:5:ASN:OD1	2.53	0.46
1:C:225:ILE:HA	2:C:596:HOH:O	2.16	0.45
1:D:211:ARG:HD2	1:D:211:ARG:HA	1.69	0.45
1:B:123:PHE:CD1	1:B:124:PRO:HA	2.52	0.45
1:B:226:ASN:ND2	1:B:228:TYR:H	2.13	0.45
1:D:201:ASP:HB2	2:D:481:HOH:O	2.17	0.45
1:A:12:ASN:O	1:A:16:GLU:HG2	2.17	0.45
1:B:18:SER:OG	1:B:203:TYR:O	2.35	0.45
1:A:275:ARG:HB3	1:D:275:ARG:HB3	1.99	0.44
1:C:25:THR:HG21	1:C:208:LYS:HG2	1.99	0.44
1:A:69:MET:HE3	2:A:480:HOH:O	2.17	0.44
1:D:116:ARG:NH1	1:D:129:ASP:OD1	2.50	0.44
1:B:69:MET:SD	1:B:71:ASP:HB2	2.58	0.44
1:D:47:PRO:HB3	1:D:100:ARG:CD	2.47	0.44
1:A:192:PHE:CZ	1:B:192:PHE:CZ	3.06	0.42
1:B:176:MET:HE1	1:B:176:MET:HB3	1.99	0.42
1:C:127:PHE:HA	1:C:161:LEU:HD22	2.01	0.42
1:D:63:ARG:NE	1:D:116:ARG:HH12	2.17	0.42
1:D:63:ARG:CG	1:D:116:ARG:NH1	2.66	0.42
1:A:265:ARG:HD3	1:A:265:ARG:HH11	1.19	0.42
1:B:92:ILE:HG13	1:B:114:GLU:HG3	2.01	0.42
1:B:201:ASP:C	1:B:203:TYR:N	2.59	0.42
1:B:209:MET:HG3	2:B:406:HOH:O	2.19	0.41
1:D:116:ARG:HD2	1:D:121:HIS:ND1	2.34	0.41
1:C:41:LEU:O	1:C:44:ARG:HB2	2.20	0.41
1:A:225:ILE:N	2:A:658:HOH:O	2.54	0.41
1:B:196:PHE:O	1:B:200:SER:CB	2.69	0.41
1:C:92:ILE:HG13	1:C:114:GLU:HG3	2.03	0.41
1:C:32:LEU:HD21	1:C:209:MET:HE1	2.03	0.41
1:B:169:CYS:HB3	1:B:176:MET:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LEU:HD12	1:D:281:HIS:CE1	2.55	0.41
1:A:6:MET:HG3	1:C:197:ILE:HG13	2.03	0.40
1:A:261:VAL:HG21	1:D:277:ILE:HG21	2.03	0.40
1:D:294:ARG:O	1:D:298:LYS:HG3	2.21	0.40
1:B:5:ASN:C	2:B:661:HOH:O	2.59	0.40
1:D:209:MET:CG	2:D:445:HOH:O	2.65	0.40

There are no symmetry-related clashes.

## 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	295/308 (96%)	286 (97%)	9 (3%)	0	100	100
1	B	296/308 (96%)	287 (97%)	8 (3%)	1 (0%)	44	22
1	C	296/308 (96%)	283 (96%)	13 (4%)	0	100	100
1	D	296/308 (96%)	275 (93%)	19 (6%)	2 (1%)	25	7
All	All	1183/1232 (96%)	1131 (96%)	49 (4%)	3 (0%)	44	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	202	ASN
1	D	42	SER
1	D	61	ASP

### 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	251/260 (96%)	244 (97%)	7 (3%)	49	20
1	B	252/260 (97%)	247 (98%)	5 (2%)	60	33
1	C	252/260 (97%)	243 (96%)	9 (4%)	40	13
1	D	252/260 (97%)	240 (95%)	12 (5%)	30	7
All	All	1007/1040 (97%)	974 (97%)	33 (3%)	43	15

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	97	ASN
1	A	139	LYS
1	A	200	SER
1	A	225	ILE
1	A	236	ASP
1	A	265	ARG
1	B	63	ARG
1	B	104	LYS
1	B	142	LYS
1	B	225	ILE
1	B	226	ASN
1	C	27	ILE
1	C	28	GLU
1	C	41	LEU
1	C	63	ARG
1	C	165	LEU
1	C	216	MET
1	C	220	ASN
1	C	225	ILE
1	C	261	VAL
1	D	40	SER
1	D	52	GLU
1	D	54	LYS
1	D	61	ASP
1	D	63	ARG
1	D	76	LYS
1	D	80	LEU
1	D	88	LEU
1	D	149	ARG

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Mol	Chain	Res	Type
1	D	201	ASP
1	D	211	ARG
1	D	226	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	295	ASN
1	B	66	ASN
1	B	226	ASN
1	B	281	HIS
1	B	295	ASN
1	C	34	ASN
1	C	226	ASN
1	C	295	ASN
1	D	34	ASN
1	D	66	ASN
1	D	128	ASN
1	D	202	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	299/308 (97%)	-0.09	5 (1%) 70 70	9, 20, 35, 48	0
1	B	300/308 (97%)	-0.09	7 (2%) 61 60	8, 17, 34, 43	0
1	C	300/308 (97%)	0.23	17 (5%) 24 22	10, 21, 46, 67	0
1	D	300/308 (97%)	0.49	21 (7%) 17 15	11, 25, 52, 78	0
All	All	1199/1232 (97%)	0.14	50 (4%) 37 34	8, 21, 42, 78	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	ILE	7.0
1	C	225	ILE	6.0
1	D	27	ILE	5.9
1	D	24	MET	5.4
1	D	31	MET	5.1
1	D	26	LYS	4.5
1	D	23	ASP	4.5
1	A	220	ASN	4.4
1	D	220	ASN	4.3
1	D	20	SER	4.2
1	C	27	ILE	4.1
1	D	21	ALA	4.1
1	D	17	LEU	4.1
1	C	26	LYS	4.1
1	B	203	TYR	4.0
1	C	20	SER	4.0
1	D	25	THR	3.9
1	C	24	MET	3.8
1	D	35	PHE	3.7
1	A	225	ILE	3.7
1	D	34	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	219	LYS	3.5
1	D	46	ALA	3.5
1	D	225	ILE	3.4
1	C	21	ALA	3.3
1	C	23	ASP	3.3
1	C	25	THR	3.1
1	D	43	SER	3.0
1	C	202	ASN	3.0
1	D	28	GLU	3.0
1	C	235	ASP	2.9
1	B	26	LYS	2.9
1	D	235	ASP	2.9
1	D	42	SER	2.8
1	A	219	LYS	2.7
1	B	202	ASN	2.6
1	C	43	SER	2.6
1	A	192	PHE	2.5
1	A	235	ASP	2.5
1	D	22	GLY	2.5
1	B	220	ASN	2.5
1	C	22	GLY	2.3
1	B	42	SER	2.3
1	C	17	LEU	2.3
1	C	220	ASN	2.3
1	C	19	LYS	2.3
1	D	74	ASN	2.2
1	C	31	MET	2.1
1	B	201	ASP	2.1
1	D	120	GLU	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 carbohydrates 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.