

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7Y3Z
Title	:	Structure of a novel carboxylesterase FEH from Acinetobacter sp. DL-2
Authors	:	Huang, Y.; Liu, W.D.; Zhang, Y.J.; Duan, Y.J.; Lu, M.L.
Deposited on	:	2022-06-13
Resolution	:	2.30 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	$5042 \ (2.30-2.30)$
Clashscore	141614	$5643 \ (2.30-2.30)$
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575(2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	А	387	8%	13%	••
1	В	387	16%	22%	••
1	С	387	68%	27%	••
1	D	387	5% 83%	13%	•••



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11467 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Л	277	Total	С	Ν	0	\mathbf{S}	0	0	0
1	D	311	2865	1813	493	547	12	0		U
1	Λ	277	Total	С	Ν	0	S	0	0	0
1	A	511	2865	1813	493	547	12	0	0	0
1	1 B	277	Total	С	Ν	0	S	0	0	0
		377	2865	1813	493	547	12	0	0	
1	1 C	0 977	Total	С	Ν	0	S	0	0	0
	377	2865	1813	493	547	12	0	0	0	

• Molecule 1 is a protein called Fenoxa prop-p-ethyl hydrolase.

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	3	Total O 3 3	0	0
2	А	4	Total O 4 4	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Fenoxa prop-p-ethyl hydrolase



 \bullet Molecule 1: Fenoxa prop-p-ethyl hydrolase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	129.96Å 148.96 Å 156.08 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	74.48 - 2.30	Depositor
Resolution (A)	78.04 - 2.26	EDS
% Data completeness	98.6 (74.48-2.30)	Depositor
(in resolution range)	85.7 (78.04-2.26)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.33 (at 2.27 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
D D.	0.238 , 0.257	Depositor
Π, Π_{free}	0.238 , 0.258	DCC
R_{free} test set	1998 reflections (1.42%)	wwPDB-VP
Wilson B-factor $(Å^2)$	57.6	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 57.7	EDS
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11467	wwPDB-VP
Average B, all atoms $(Å^2)$	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bo	nd lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.25	0/2934	0.45	0/3999	
1	В	0.28	0/2934	0.50	0/3999	
1	С	0.35	1/2934~(0.0%)	0.57	2/3999~(0.1%)	
1	D	0.28	0/2934	0.45	0/3999	
All	All	0.29	1/11736~(0.0%)	0.50	2/15996~(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	А	0	2
1	В	0	2
1	С	0	2
1	D	0	2
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	С	180	ARG	CG-CD	-6.24	1.36	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	С	282	LEU	CB-CG-CD2	-7.41	98.41	111.00
1	С	218	ASP	CB-CG-OD1	5.40	123.16	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	234	ALA	Peptide
1	А	66	VAL	Peptide
1	В	124	ASP	Peptide
1	В	234	ALA	Peptide
1	С	124	ASP	Peptide
1	С	66	VAL	Peptide
1	D	234	ALA	Peptide
1	D	66	VAL	Peptide

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	А	2865	0	2784	34	0
1	В	2865	0	2784	59	1
1	С	2865	0	2784	103	0
1	D	2865	0	2784	34	0
2	А	4	0	0	0	0
2	D	3	0	0	1	0
All	All	11467	0	11136	224	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (224) 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:8:CYS:SG	1:B:16:LYS:NZ	2.36	0.98
1:C:126:PRO:O	1:C:141:ARG:NH2	1.95	0.98
1:B:362:LEU:HD13	1:B:363:GLY:H	1.28	0.98
1:B:219:ILE:O	1:B:222:LEU:N	2.00	0.93
1:C:80:MET:HG2	1:C:282:LEU:HG	1.55	0.88
1:B:378:LEU:HD23	1:B:378:LEU:O	1.75	0.86
1:C:79:LEU:HB3	1:C:287:THR:HG21	1.58	0.85
1:C:77:ALA:HA	1:C:80:MET:SD	2.18	0.82
1:A:276:LYS:HB2	1:A:281:ARG:HB2	1.64	0.80
1:A:198:LEU:HD11	1:A:202:GLU:HB2	1.61	0.80



	loub page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:130:GLU:OE1	1:C:130:GLU:N	2.16	0.76
1:D:289:ASP:OD1	1:D:328:ARG:NH2	2.18	0.73
1:D:219:ILE:HD11	1:C:222:LEU:HD11	1.70	0.73
1:B:8:CYS:SG	1:B:9:ASP:N	2.62	0.72
1:C:202:GLU:HG2	1:C:205:ARG:HE	1.55	0.71
1:C:61:ASP:O	1:C:205:ARG:NH1	2.23	0.71
1:C:125:GLN:HE22	1:C:234:ALA:HA	1.57	0.70
1:C:286:GLU:OE2	1:C:287:THR:N	2.25	0.69
1:B:362:LEU:CD1	1:B:363:GLY:H	2.04	0.69
1:C:210:ILE:HB	1:C:356:LYS:HA	1.73	0.68
1:C:275:GLY:HA2	1:C:283:LEU:HD12	1.75	0.67
1:C:125:GLN:O	1:C:127:PHE:N	2.28	0.67
1:C:171:ARG:HA	1:C:176:ARG:O	1.94	0.67
1:A:356:LYS:O	1:A:366:ARG:NH2	2.25	0.66
1:C:269:SER:HA	1:C:272:ALA:HB3	1.78	0.65
1:C:182:ILE:O	1:C:187:ALA:N	2.24	0.65
1:D:193:ASP:OD1	1:D:195:ARG:NH2	2.29	0.64
1:A:109:ARG:H	1:A:112:GLN:NE2	1.96	0.64
1:B:67:TRP:O	1:B:255:ALA:HA	1.97	0.64
1:A:252:ILE:HB	1:A:256:ASN:HB2	1.78	0.64
1:D:3:ASN:N	2:D:401:HOH:O	2.31	0.64
1:C:44:ASP:OD1	1:C:262:ARG:NE	2.29	0.64
1:C:125:GLN:HE21	1:C:125:GLN:HA	1.64	0.63
1:B:60:ARG:O	1:B:262:ARG:NH2	2.27	0.63
1:C:86:LEU:N	1:C:86:LEU:HD22	2.14	0.63
1:A:109:ARG:H	1:A:112:GLN:HE21	1.45	0.62
1:C:176:ARG:HB3	1:C:180:ARG:HG2	1.81	0.62
1:B:87:LEU:HD11	1:B:110:VAL:HG11	1.82	0.62
1:A:68:SER:HB2	1:A:334:GLY:HA2	1.83	0.60
1:C:61:ASP:HB3	1:C:205:ARG:NH1	2.17	0.60
1:B:289:ASP:OD1	1:B:328:ARG:NH2	2.34	0.60
1:C:46:TRP:HB2	1:C:58:TRP:CD1	2.36	0.60
1:A:200:LYS:HA	1:A:203:TYR:CD2	2.36	0.60
1:B:12:PHE:HB3	1:B:15:LEU:HD12	1.84	0.60
1:C:285:GLU:OE2	1:C:289:ASP:N	2.35	0.60
1:D:228:MET:HG3	1:D:302:VAL:O	2.02	0.59
1:B:219:ILE:HD12	1:B:219:ILE:H	1.66	0.59
1:A:16:LYS:HB2	1:A:45:MET:HE1	1.84	0.59
1:C:271:ILE:HD11	1:C:342:ILE:HG21	1.84	0.59
1:A:178:LEU:O	1:A:182:ILE:HG13	2.03	0.59
1:B:337:GLY:HA2	1:B:363:GLY:HA2	1.84	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:16:LYS:O	1:B:20:ALA:N	2.27	0.58
1:C:79:LEU:HD13	1:C:291:ILE:HD11	1.86	0.58
1:C:287:THR:O	1:C:290:LYS:N	2.36	0.58
1:B:252:ILE:HB	1:B:256:ASN:HB2	1.85	0.57
1:D:38:ASP:HB3	1:D:347:ARG:HH21	1.69	0.57
1:A:60:ARG:O	1:A:262:ARG:NH2	2.37	0.57
1:C:354:MET:HG2	1:C:355:ASN:O	2.04	0.57
1:D:60:ARG:O	1:D:262:ARG:NH2	2.37	0.57
1:A:215:LEU:HD12	1:A:215:LEU:H	1.69	0.57
1:B:10:GLN:N	1:B:10:GLN:OE1	2.38	0.56
1:C:276:LYS:HD3	1:C:281:ARG:HB2	1.87	0.56
1:A:200:LYS:HA	1:A:203:TYR:CE2	2.41	0.55
1:A:250:ALA:O	1:A:256:ASN:ND2	2.38	0.55
1:B:378:LEU:O	1:B:378:LEU:CD2	2.52	0.55
1:B:16:LYS:HG3	1:B:45:MET:CE	2.36	0.55
1:C:283:LEU:HD22	1:C:287:THR:OG1	2.05	0.55
1:B:16:LYS:HG3	1:B:45:MET:HE1	1.88	0.54
1:C:176:ARG:CB	1:C:180:ARG:HG2	2.36	0.54
1:C:286:GLU:OE2	1:C:287:THR:HG23	2.07	0.54
1:D:222:LEU:HD21	1:C:228:MET:SD	2.47	0.54
1:C:330:CYS:O	1:C:342:ILE:HG13	2.07	0.54
1:C:276:LYS:HG2	1:C:281:ARG:HH21	1.73	0.54
1:A:73:VAL:HG12	1:A:182:ILE:HD13	1.90	0.54
1:B:250:ALA:O	1:B:256:ASN:ND2	2.41	0.54
1:A:99:GLU:OE1	1:A:99:GLU:N	2.28	0.53
1:C:277:VAL:H	1:C:280:VAL:CG2	2.21	0.53
1:B:362:LEU:HD13	1:B:363:GLY:N	2.11	0.53
1:B:35:LEU:HD21	1:B:348:MET:HG2	1.91	0.53
1:D:160:LEU:HD13	1:D:235:PRO:HG2	1.90	0.53
1:D:250:ALA:O	1:D:256:ASN:ND2	2.42	0.52
1:C:288:ILE:HG22	1:C:328:ARG:HH22	1.74	0.52
1:D:219:ILE:HD12	1:D:222:LEU:HB2	1.92	0.52
1:C:68:SER:HB2	1:C:334:GLY:HA2	1.92	0.52
1:D:67:TRP:O	1:D:255:ALA:HA	2.10	0.52
1:C:81:LEU:HD21	1:C:181:PHE:CZ	2.44	0.52
1:C:228:MET:HG3	1:C:302:VAL:O	2.10	0.51
1:B:200:LYS:HA	1:B:203:TYR:CD1	2.46	0.51
1:C:250:ALA:O	1:C:256:ASN:ND2	2.44	0.51
1:C:169:VAL:O	1:C:173:ILE:HG13	2.10	0.51
1:B:190:LEU:HD11	1:B:282:LEU:HD11	1.93	0.51
1:A:354:MET:HG3	1:A:366:ARG:HH21	1.74	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:269:SER:O	1:C:273:CYS:N	2.41	0.51
1:C:284:SER:OG	1:C:285:GLU:N	2.44	0.50
1:B:17:GLU:O	1:B:21:ARG:HG2	2.12	0.50
1:D:222:LEU:HA	1:C:226:ASN:ND2	2.26	0.50
1:D:9:ASP:HB3	1:D:12:PHE:HD2	1.76	0.50
1:B:272:ALA:HB2	1:B:342:ILE:HG23	1.93	0.50
1:D:219:ILE:CD1	1:C:222:LEU:HD11	2.37	0.50
1:B:308:ARG:H	1:B:317:THR:HG21	1.76	0.50
1:C:80:MET:HE3	1:C:282:LEU:HD11	1.93	0.49
1:C:171:ARG:O	1:C:175:GLY:N	2.38	0.49
1:C:252:ILE:HB	1:C:256:ASN:HB2	1.94	0.49
1:C:316:PRO:HD3	1:C:329:ILE:O	2.11	0.49
1:C:259:SER:OG	1:C:260:ASN:N	2.45	0.49
1:A:193:ASP:OD1	1:A:195:ARG:NH2	2.43	0.49
1:C:176:ARG:HB3	1:C:180:ARG:CG	2.41	0.49
1:B:22:ASN:ND2	1:B:370:TYR:OH	2.44	0.49
1:C:182:ILE:HD12	1:C:182:ILE:H	1.76	0.49
1:A:63:VAL:O	1:A:206:VAL:HA	2.12	0.49
1:B:219:ILE:O	1:B:221:ALA:N	2.46	0.49
1:C:80:MET:HE2	1:C:181:PHE:HE2	1.78	0.49
1:C:191:ASP:O	1:C:266:ARG:NH2	2.46	0.48
1:B:219:ILE:HG23	1:B:223:GLY:O	2.13	0.48
1:C:338:SER:N	1:C:354:MET:HE1	2.28	0.48
1:C:342:ILE:HG22	1:C:349:THR:HG22	1.95	0.48
1:C:125:GLN:HA	1:C:125:GLN:NE2	2.27	0.48
1:B:88:ASP:OD1	1:B:90:ASP:N	2.44	0.48
1:C:344:THR:HG22	1:C:347:ARG:HH21	1.79	0.48
1:D:316:PRO:HD3	1:D:329:ILE:O	2.14	0.48
1:C:84:ARG:HB2	1:C:86:LEU:CD2	2.43	0.48
1:B:219:ILE:C	1:B:222:LEU:H	2.08	0.48
1:A:67:TRP:O	1:A:255:ALA:HA	2.13	0.47
1:D:16:LYS:HA	1:D:45:MET:HE1	1.95	0.47
1:C:35:LEU:HD21	1:C:37:ILE:HG13	1.96	0.47
1:C:124:ASP:N	1:C:145:GLN:OE1	2.33	0.47
1:C:344:THR:HA	1:C:347:ARG:HE	1.78	0.47
1:B:346:LYS:HD3	1:B:378:LEU:HD13	1.96	0.47
1:C:277:VAL:H	1:C:280:VAL:HG22	1.79	0.46
1:B:316:PRO:HD3	1:B:329:ILE:O	2.15	0.46
1:C:74:THR:HG23	1:C:178:LEU:HD21	1.97	0.46
1:B:60:ARG:HG2	1:B:262:ARG:NH2	2.30	0.46
1:C:276:LYS:CD	1:C:281:ARG:HB2	2.46	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:63:VAL:HG12	1:D:260:ASN:ND2	2.29	0.46
1:A:354:MET:HB3	1:A:354:MET:HE3	1.73	0.46
1:B:50:VAL:HG22	1:B:56:ALA:O	2.15	0.46
1:B:338:SER:N	1:B:354:MET:HE1	2.30	0.46
1:C:39:GLY:HA3	1:C:277:VAL:HG21	1.97	0.46
1:D:200:LYS:HA	1:D:203:TYR:CD1	2.50	0.46
1:A:259:SER:OG	1:A:260:ASN:N	2.49	0.46
1:B:64:THR:OG1	1:B:207:SER:O	2.27	0.46
1:B:299:VAL:HA	1:B:306:PRO:HA	1.98	0.46
1:B:328:ARG:HH11	1:B:344:THR:HG21	1.80	0.46
1:A:17:GLU:O	1:A:21:ARG:HG3	2.16	0.46
1:C:67:TRP:O	1:C:255:ALA:HA	2.15	0.46
1:C:141:ARG:HG3	1:C:144:THR:HG21	1.97	0.46
1:C:285:GLU:OE2	1:C:288:ILE:HB	2.16	0.46
1:B:76:LEU:O	1:B:80:MET:HG3	2.17	0.45
1:A:316:PRO:HD3	1:A:329:ILE:O	2.17	0.45
1:B:229:VAL:O	1:B:233:THR:HG23	2.16	0.45
1:C:264:LEU:HA	1:C:267:ILE:HG22	1.98	0.45
1:D:21:ARG:NH2	1:D:369:GLN:OE1	2.49	0.45
1:D:164:HIS:NE2	1:D:252:ILE:HG23	2.31	0.45
1:C:35:LEU:CD2	1:C:37:ILE:HG13	2.47	0.45
1:D:150:GLU:O	1:D:153:THR:HB	2.17	0.45
1:C:88:ASP:HB3	1:C:91:ALA:HB2	1.98	0.45
1:C:60:ARG:HG3	1:C:262:ARG:NH2	2.32	0.45
1:D:68:SER:HB2	1:D:334:GLY:HA2	1.99	0.45
1:D:222:LEU:O	1:C:222:LEU:HD21	2.17	0.45
1:C:286:GLU:OE2	1:C:286:GLU:C	2.56	0.44
1:C:120:VAL:O	1:C:120:VAL:HG23	2.17	0.44
1:A:168:GLU:OE1	1:A:171:ARG:NH1	2.50	0.44
1:B:93:VAL:HG12	1:B:108:ILE:O	2.18	0.44
1:B:297:TYR:OH	1:B:319:GLU:OE2	2.28	0.44
1:B:288:ILE:HG23	1:B:291:ILE:HD12	2.00	0.44
1:D:354:MET:HE3	1:D:354:MET:HB3	1.75	0.44
1:A:235:PRO:HA	1:A:236:PRO:HD3	1.87	0.44
1:A:346:LYS:HE2	1:A:378:LEU:HB3	2.00	0.44
1:B:225:ASP:HA	1:B:230:LYS:HD2	2.00	0.44
1:B:49:TRP:HB3	1:B:51:ASP:H	1.83	0.43
1:C:94:ALA:HA	1:C:97:TRP:O	2.18	0.43
1:C:342:ILE:CD1	1:C:344:THR:HG23	2.48	0.43
1:A:87:LEU:HD11	1:A:110:VAL:HG11	2.00	0.43
1:B:259:SER:OG	1:B:260:ASN:N	2.51	0.43



	i agem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:105:LYS:HB3	1:C:108:ILE:HD12	2.00	0.43
1:C:210:ILE:HD12	1:C:356:LYS:HB2	2.01	0.43
1:C:344:THR:HA	1:C:347:ARG:NE	2.34	0.43
1:D:224:MET:SD	1:D:224:MET:N	2.91	0.43
1:C:329:ILE:HG23	1:C:342:ILE:O	2.18	0.43
1:B:244:THR:HG23	1:B:247:TRP:H	1.83	0.43
1:B:289:ASP:O	1:B:293:GLU:HG3	2.18	0.43
1:D:81:LEU:HD11	1:D:170:VAL:HG13	2.00	0.43
1:C:226:ASN:OD1	1:C:228:MET:N	2.41	0.43
1:C:276:LYS:HD3	1:C:281:ARG:HE	1.84	0.43
1:C:337:GLY:HA2	1:C:363:GLY:HA2	2.01	0.43
1:B:68:SER:HB2	1:B:333:GLY:O	2.19	0.42
1:C:308:ARG:H	1:C:317:THR:HG21	1.84	0.42
1:C:127:PHE:HD1	1:C:141:ARG:NH2	2.17	0.42
1:B:21:ARG:HG2	1:B:21:ARG:H	1.71	0.42
1:B:317:THR:O	1:B:317:THR:OG1	2.32	0.42
1:D:281:ARG:NH1	1:D:283:LEU:O	2.52	0.42
1:C:272:ALA:O	1:C:347:ARG:NE	2.53	0.42
1:D:328:ARG:HD3	1:D:344:THR:HG21	2.00	0.42
1:A:106:ASP:OD2	1:C:125:GLN:HG2	2.19	0.42
1:A:171:ARG:HG3	1:A:177:THR:HA	2.02	0.42
1:C:7:VAL:CG1	1:C:44:ASP:HB3	2.49	0.42
1:C:284:SER:C	1:C:286:GLU:N	2.73	0.42
1:C:202:GLU:HG2	1:C:205:ARG:NE	2.29	0.42
1:D:93:VAL:HG12	1:D:110:VAL:HA	2.01	0.42
1:B:332:TRP:CE3	1:B:332:TRP:HA	2.54	0.42
1:C:76:LEU:O	1:C:80:MET:HG3	2.20	0.42
1:C:176:ARG:NH2	1:C:185:GLU:OE1	2.47	0.42
1:C:244:THR:HG22	1:C:246:GLY:N	2.35	0.42
1:D:267:ILE:O	1:D:270:VAL:HG22	2.19	0.41
1:B:264:LEU:HB3	1:B:340:ILE:HD13	2.00	0.41
1:C:83:ASP:OD1	1:C:283:LEU:HA	2.20	0.41
1:B:45:MET:H	1:B:45:MET:HG2	1.59	0.41
1:C:84:ARG:HB2	1:C:86:LEU:HD21	2.01	0.41
1:B:59:SER:OG	1:B:60:ARG:N	2.54	0.41
1:D:343:ASP:HB3	1:D:348:MET:HG3	2.02	0.41
1:C:263:ALA:O	1:C:267:ILE:HG22	2.20	0.41
1:B:125:GLN:O	1:B:127:PHE:N	2.54	0.41
1:C:82:VAL:HG12	1:C:87:LEU:O	2.20	0.41
1:A:229:VAL:O	1:A:233:THR:HB	2.20	0.41
1:C:50:VAL:HG13	1:C:207:SER:HA	2.03	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ASP:OD2	1:D:262:ARG:HD3	2.20	0.41
1:D:66:VAL:HG22	1:D:257:GLY:O	2.20	0.41
1:A:63:VAL:HG13	1:A:259:SER:N	2.36	0.41
1:C:334:GLY:N	1:C:338:SER:O	2.54	0.41
1:B:193:ASP:OD1	1:B:195:ARG:NH2	2.47	0.40
1:C:277:VAL:N	1:C:280:VAL:HG22	2.37	0.40
1:A:66:VAL:HG22	1:A:257:GLY:O	2.21	0.40
1:C:342:ILE:HD13	1:C:344:THR:HG23	2.04	0.40
1:A:59:SER:OG	1:A:60:ARG:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:MET:SD	$1:B:224:MET:CE[2_556]$	1.79	0.41

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	Perce	ntiles
1	А	375/387~(97%)	360~(96%)	15~(4%)	0	100	100
1	В	375/387~(97%)	355~(95%)	20~(5%)	0	100	100
1	С	375/387~(97%)	350~(93%)	23~(6%)	2(0%)	29	35
1	D	375/387~(97%)	359~(96%)	16 (4%)	0	100	100
All	All	1500/1548~(97%)	1424 (95%)	74 (5%)	2(0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	177	THR
	a r.	1	



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Mol	Chain	Res	Type
1	С	126	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	296/305~(97%)	292~(99%)	4 (1%)	67 81
1	В	296/305~(97%)	288~(97%)	8(3%)	44 61
1	С	296/305~(97%)	288~(97%)	8(3%)	44 61
1	D	296/305~(97%)	289~(98%)	7~(2%)	49 66
All	All	1184/1220~(97%)	1157 (98%)	27 (2%)	50 67

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	158	HIS
1	D	195	ARG
1	D	224	MET
1	D	266	ARG
1	D	296	SER
1	D	328	ARG
1	D	354	MET
1	А	68	SER
1	А	107	ARG
1	А	195	ARG
1	А	354	MET
1	В	16	LYS
1	В	54	HIS
1	В	158	HIS
1	В	195	ARG
1	В	225	ASP
1	В	296	SER
1	В	338	SER
1	В	354	MET
1	С	28	ASP



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Mol	Chain	Res	Type
1	С	65	ASN
1	С	127	PHE
1	С	181	PHE
1	С	195	ARG
1	С	283	LEU
1	С	284	SER
1	C	354	MET

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	D	125	GLN
1	А	112	GLN
1	А	256	ASN
1	С	125	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	< RSRZ >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	377/387~(97%)	0.56	30 (7%) 12 16	54, 73, 95, 110	0
1	В	377/387~(97%)	1.07	61 (16%) 1 2	63, 92, 124, 145	0
1	С	377/387~(97%)	1.15	75~(19%) 1 1	69, 105, 131, 149	0
1	D	377/387~(97%)	0.58	21 (5%) 24 30	52, 73, 95, 141	0
All	All	1508/1548~(97%)	0.84	187 (12%) 4 5	52, 84, 123, 149	0

All (187) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	D	222	LEU	9.1
1	В	220	ALA	7.8
1	С	277	VAL	6.6
1	С	377	ALA	5.8
1	С	280	VAL	5.4
1	А	234	ALA	5.4
1	С	222	LEU	5.3
1	В	279	ASP	5.2
1	С	198	LEU	5.0
1	С	287	THR	5.0
1	В	4	ILE	4.8
1	В	49	TRP	4.8
1	D	224	MET	4.7
1	А	280	VAL	4.5
1	С	178	LEU	4.4
1	В	18	ALA	4.4
1	С	31	ALA	4.3
1	С	250	ALA	4.3
1	D	223	GLY	4.3
1	С	264	LEU	4.2
1	С	278	GLY	4.2



7Y3Z

Mol	Chain	Res	Type	RSRZ
1	С	12	PHE	4.1
1	С	347	ARG	4.1
1	С	273	CYS	4.0
1	С	199	PRO	3.9
1	В	8	CYS	3.9
1	В	126	PRO	3.9
1	С	82	VAL	3.9
1	С	132	ILE	3.8
1	С	266	ARG	3.7
1	В	34	ALA	3.7
1	В	55	THR	3.7
1	В	7	VAL	3.7
1	С	46	TRP	3.7
1	В	277	VAL	3.7
1	С	271	ILE	3.6
1	D	229	VAL	3.6
1	D	234	ALA	3.5
1	С	47	GLY	3.5
1	А	222	LEU	3.5
1	А	125	GLN	3.5
1	С	234	ALA	3.4
1	В	24	ASP	3.4
1	С	169	VAL	3.4
1	А	224	MET	3.4
1	А	223	GLY	3.3
1	В	5	GLU	3.3
1	В	146	ALA	3.3
1	В	234	ALA	3.3
1	С	138	ALA	3.3
1	А	126	PRO	3.3
1	С	181	PHE	3.3
1	В	56	ALA	3.3
1	С	288	ILE	3.3
1	А	233	THR	3.3
1	В	280	VAL	3.2
1	С	183	ASP	3.2
1	С	4	ILE	3.1
1	В	103	ALA	3.1
1	В	66	VAL	3.1
1	В	17	GLU	3.1
1	С	190	LEU	3.1
1	С	229	VAL	3.0



Mol	Chain	Res	Type	RSRZ
1	D	225	ASP	2.9
1	В	50	VAL	2.9
1	С	247	TRP	2.9
1	С	173	ILE	2.9
1	С	270	VAL	2.9
1	В	276	LYS	2.9
1	В	104	GLY	2.9
1	А	235	PRO	2.8
1	С	284	SER	2.8
1	А	146	ALA	2.8
1	С	226	ASN	2.8
1	С	182	ILE	2.8
1	D	219	ILE	2.8
1	В	148	TRP	2.8
1	С	79	LEU	2.8
1	С	80	MET	2.8
1	С	196	LEU	2.8
1	С	345	GLU	2.8
1	С	282	LEU	2.8
1	В	227	ILE	2.8
1	С	66	VAL	2.7
1	В	342	ILE	2.7
1	С	223	GLY	2.7
1	D	226	ASN	2.7
1	В	57	PRO	2.7
1	В	143	ALA	2.7
1	В	127	PHE	2.7
1	D	227	ILE	2.7
1	С	81	LEU	2.7
1	D	46	TRP	2.6
1	С	194	PHE	2.6
1	С	289	ASP	2.6
1	C	35	LEU	2.5
1	В	235	PRO	2.5
1	D	190	LEU	2.5
1	D	215	LEU	2.5
1	А	148	TRP	2.5
1	А	218	ASP	2.5
1	В	15	LEU	2.5
1	В	39	GLY	2.5
1	С	228	MET	2.5
1	С	18	ALA	2.5



7Y3Z

Mol	Chain	Res	Type	RSRZ
1	А	228	MET	2.5
1	В	233	THR	2.5
1	В	33	ILE	2.5
1	В	142	LEU	2.5
1	А	229	VAL	2.4
1	В	270	VAL	2.4
1	С	192	ALA	2.4
1	С	283	LEU	2.4
1	В	12	PHE	2.4
1	С	302	VAL	2.4
1	С	88	ASP	2.4
1	А	63	VAL	2.4
1	В	160	LEU	2.4
1	В	217	ILE	2.4
1	В	278	GLY	2.4
1	А	129	LEU	2.4
1	В	284	SER	2.4
1	В	147	PRO	2.3
1	С	148	TRP	2.3
1	В	225	ASP	2.3
1	В	144	THR	2.3
1	А	225	ASP	2.3
1	В	10	GLN	2.3
1	С	180	ARG	2.3
1	В	158	HIS	2.3
1	А	227	ILE	2.3
1	А	103	ALA	2.3
1	С	7	VAL	2.3
1	С	276	LYS	2.3
1	А	220	ALA	2.3
1	В	9	ASP	2.3
1	D	153	THR	2.2
1	D	231	THR	2.2
1	А	198	LEU	2.2
1	В	190	LEU	2.2
1	D	148	TRP	2.2
1	В	340	ILE	2.2
1	C	15	LEU	2.2
1	В	370	TYR	2.2
1	С	216	PRO	2.2
1	С	63	VAL	2.2
1	А	217	ILE	2.2



Mol	Chain	Res	Type	RSRZ
1	А	120	VAL	2.2
1	В	46	TRP	2.2
1	В	123	TRP	2.2
1	С	58	TRP	2.2
1	С	186	ILE	2.2
1	В	180	ARG	2.2
1	D	280	VAL	2.2
1	В	129	LEU	2.2
1	D	233	THR	2.1
1	А	221	ALA	2.1
1	В	125	GLN	2.1
1	С	73	VAL	2.1
1	D	126	PRO	2.1
1	С	64	THR	2.1
1	С	342	ILE	2.1
1	А	215	LEU	2.1
1	А	206	VAL	2.1
1	С	257	GLY	2.1
1	D	103	ALA	2.1
1	В	120	VAL	2.1
1	В	223	GLY	2.1
1	А	219	ILE	2.1
1	С	340	ILE	2.1
1	В	231	THR	2.1
1	С	20	ALA	2.1
1	В	353	VAL	2.1
1	С	149	TRP	2.1
1	С	219	ILE	2.0
1	С	341	ILE	2.0
1	A	226	ASN	2.0
1	А	20	ALA	2.0
1	С	249	ALA	2.0
1	С	311	VAL	2.0
1	В	21	ARG	2.0
1	С	133	CYS	2.0
1	С	281	ARG	2.0
1	D	220	ALA	2.0
1	А	147	PRO	2.0
1	В	29	VAL	2.0
1	D	249	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

