Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2024 – 01:48 AM EST

PDB ID	:	3WZL
Title	:	ZEN lactonase
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Deposited on	:	2014-10-01
Resolution	:	2.60 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:

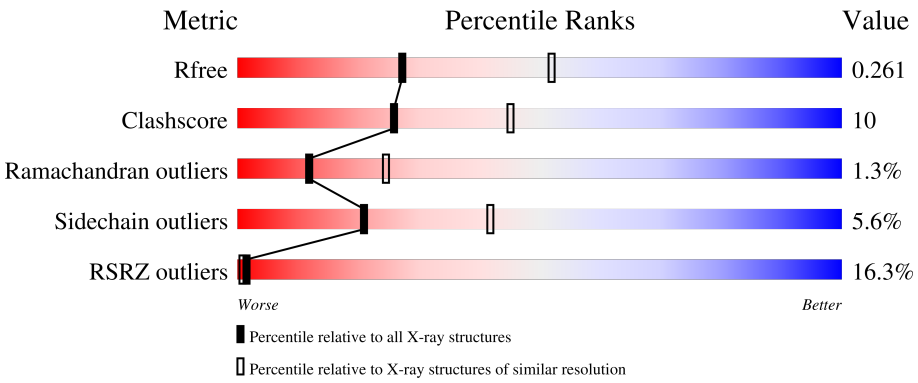
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	278	78% 16% • 5%
1	B	278	% 76% 18% • 5%
1	C	278	45% 55% 36% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6301 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 Zearalenone hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2022	1282	341	388	11	0	0	0
1	B	264	2022	1282	341	388	11	0	0	0
1	C	264	2022	1282	341	388	11	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q8NKB0
A	-12	ALA	-	expression tag	UNP Q8NKB0
A	-11	HIS	-	expression tag	UNP Q8NKB0
A	-10	HIS	-	expression tag	UNP Q8NKB0
A	-9	HIS	-	expression tag	UNP Q8NKB0
A	-8	HIS	-	expression tag	UNP Q8NKB0
A	-7	HIS	-	expression tag	UNP Q8NKB0
A	-6	HIS	-	expression tag	UNP Q8NKB0
A	-5	VAL	-	expression tag	UNP Q8NKB0
A	-4	ASP	-	expression tag	UNP Q8NKB0
A	-3	ASP	-	expression tag	UNP Q8NKB0
A	-2	ASP	-	expression tag	UNP Q8NKB0
A	-1	ASP	-	expression tag	UNP Q8NKB0
A	0	LYS	-	expression tag	UNP Q8NKB0
B	-13	MET	-	expression tag	UNP Q8NKB0
B	-12	ALA	-	expression tag	UNP Q8NKB0
B	-11	HIS	-	expression tag	UNP Q8NKB0
B	-10	HIS	-	expression tag	UNP Q8NKB0
B	-9	HIS	-	expression tag	UNP Q8NKB0
B	-8	HIS	-	expression tag	UNP Q8NKB0
B	-7	HIS	-	expression tag	UNP Q8NKB0
B	-6	HIS	-	expression tag	UNP Q8NKB0
B	-5	VAL	-	expression tag	UNP Q8NKB0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ASP	-	expression tag	UNP Q8NKB0
B	-3	ASP	-	expression tag	UNP Q8NKB0
B	-2	ASP	-	expression tag	UNP Q8NKB0
B	-1	ASP	-	expression tag	UNP Q8NKB0
B	0	LYS	-	expression tag	UNP Q8NKB0
C	-13	MET	-	expression tag	UNP Q8NKB0
C	-12	ALA	-	expression tag	UNP Q8NKB0
C	-11	HIS	-	expression tag	UNP Q8NKB0
C	-10	HIS	-	expression tag	UNP Q8NKB0
C	-9	HIS	-	expression tag	UNP Q8NKB0
C	-8	HIS	-	expression tag	UNP Q8NKB0
C	-7	HIS	-	expression tag	UNP Q8NKB0
C	-6	HIS	-	expression tag	UNP Q8NKB0
C	-5	VAL	-	expression tag	UNP Q8NKB0
C	-4	ASP	-	expression tag	UNP Q8NKB0
C	-3	ASP	-	expression tag	UNP Q8NKB0
C	-2	ASP	-	expression tag	UNP Q8NKB0
C	-1	ASP	-	expression tag	UNP Q8NKB0
C	0	LYS	-	expression tag	UNP Q8NKB0

- Molecule 2 is water.

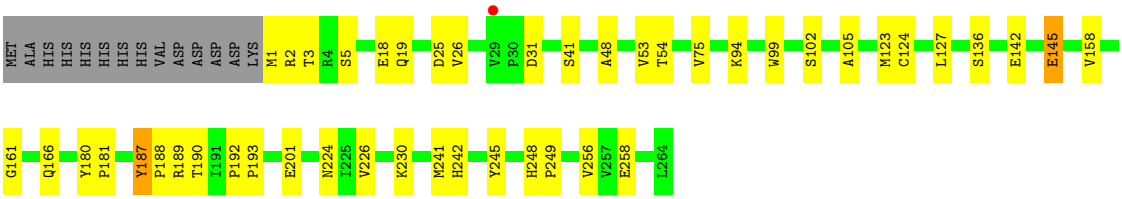
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	105	105	105	0	0
			Total	O		
2	B	99	99	99	0	0
			Total	O		
2	C	31	31	31	0	0

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.

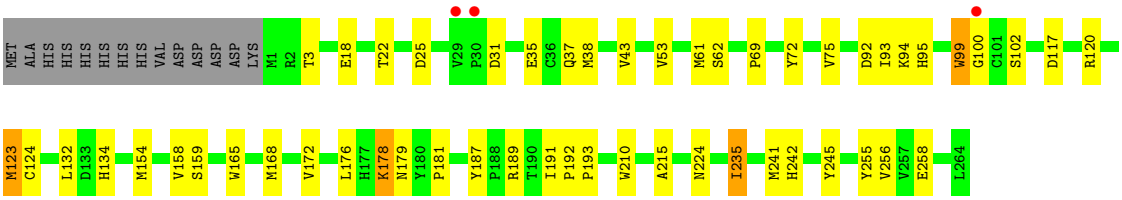
• Molecule 1: Zearalenone hydrolase

Chain A: 78% 16% • 5%



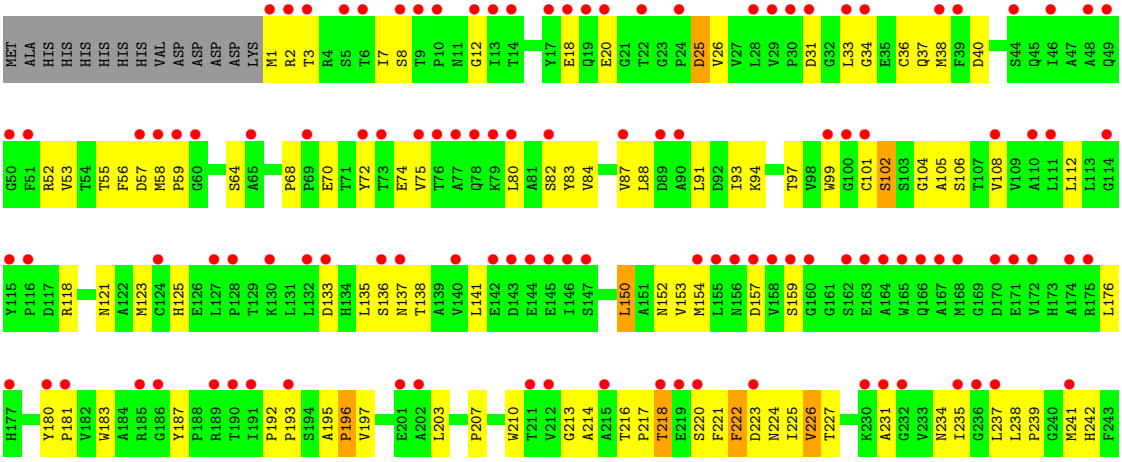
• Molecule 1: Zearalenone hydrolase

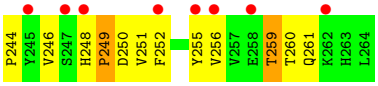
Chain B: % 76% 18% • 5%



• Molecule 1: Zearalenone hydrolase

Chain C: 45% 55% 36% • 5%




P244
Y245
V246
S247
H248
P249
D250
V251
F252
Y255
V256
V257
E258
T259
T260
Q261
K262
H263
L264

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	86.64Å 86.64Å 474.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.98 – 2.60 24.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.9 (24.98-2.60) 96.8 (24.98-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.68 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.210 , 0.266 0.208 , 0.261	Depositor DCC
R_{free} test set	1635 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.836	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 35.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6301	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.88	0/2073	0.82	1/2830 (0.0%)
1	B	0.92	3/2073 (0.1%)	0.84	0/2830
1	C	0.68	0/2073	0.72	0/2830
All	All	0.83	3/6219 (0.0%)	0.79	1/8490 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	CYS	CB-SG	-6.18	1.71	1.82
1	B	215	ALA	CA-CB	5.72	1.64	1.52
1	B	258	GLU	CG-CD	5.54	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2	ARG	NE-CZ-NH1	-6.29	117.16	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2022	0	1991	26	0
1	B	2022	0	1991	32	0
1	C	2022	0	1991	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	105	0	0	3	0
2	B	99	0	0	1	0
2	C	31	0	0	0	0
All	All	6301	0	5973	126	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 10.

All (126) 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:123:MET:HE1	1:B:256:VAL:HA	1.28	1.10
1:C:123:MET:HE1	1:C:256:VAL:HA	1.46	0.97
1:A:123:MET:HE1	1:A:256:VAL:HG22	1.53	0.90
1:A:158:VAL:HA	1:A:241:MET:HE2	1.51	0.89
1:C:99:TRP:CH2	1:C:125:HIS:HB2	2.12	0.85
1:A:1:MET:N	2:A:333:HOH:O	2.13	0.78
1:C:72:TYR:HA	1:C:75:VAL:CG2	2.13	0.78
1:C:239:PRO:HG2	1:C:251:VAL:HG11	1.67	0.77
1:A:189:ARG:NH2	2:A:318:HOH:O	2.20	0.75
1:C:192:PRO:HB2	1:C:193:PRO:HD3	1.75	0.68
1:C:213:GLY:HA2	1:C:238:LEU:O	1.95	0.66
1:C:197:VAL:HG12	1:C:203:LEU:HD21	1.79	0.65
1:B:158:VAL:HA	1:B:241:MET:HE2	1.79	0.64
1:C:99:TRP:CE2	1:C:252:PHE:HE1	2.16	0.63
1:C:25:ASP:OD1	1:C:93:ILE:HG12	1.98	0.62
1:C:38:MET:HG2	1:C:246:VAL:CG2	2.29	0.62
1:C:84:VAL:O	1:C:88:LEU:HG	1.98	0.62
1:C:18:GLU:HB2	1:C:55:THR:HG22	1.81	0.61
1:C:102:SER:HB2	1:C:242:HIS:NE2	2.15	0.61
1:C:57:ASP:HB2	1:C:64:SER:OG	2.01	0.61
1:C:218:THR:O	1:C:222:PHE:HB3	2.01	0.60
1:A:123:MET:HE3	1:A:256:VAL:HA	1.85	0.59
1:C:91:LEU:O	1:C:93:ILE:HD12	2.04	0.58
1:B:99:TRP:C	1:B:99:TRP:CD1	2.77	0.58
1:A:123:MET:CE	1:A:256:VAL:HA	2.35	0.57
1:C:150:LEU:HD21	1:C:183:TRP:CZ3	2.40	0.56
1:B:123:MET:CE	1:B:255:TYR:CE2	2.89	0.56
1:B:75:VAL:HG21	1:B:187:TYR:CE2	2.40	0.56
1:C:138:THR:HA	1:C:141:LEU:HD12	1.87	0.55
1:C:2:ARG:HH22	1:C:40:ASP:CG	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:MET:O	1:B:159:SER:HB3	2.07	0.55
1:C:31:ASP:HB3	1:C:101:CYS:HB3	1.87	0.55
1:B:123:MET:HE2	1:B:255:TYR:CE2	2.42	0.54
1:C:1:MET:O	1:C:20:GLU:HG3	2.09	0.53
1:C:112:LEU:HD11	1:C:207:PRO:HG2	1.90	0.52
1:A:105:ALA:HB1	1:A:124:CYS:HB2	1.92	0.51
1:A:25:ASP:OD2	2:A:343:HOH:O	2.18	0.51
1:C:248:HIS:HB3	1:C:251:VAL:HG21	1.93	0.51
1:B:120:ARG:NH2	2:B:326:HOH:O	2.40	0.51
1:B:192:PRO:HB2	1:B:193:PRO:HD3	1.92	0.51
1:B:3:THR:O	1:B:18:GLU:HA	2.11	0.50
1:A:102:SER:O	1:A:105:ALA:N	2.45	0.50
1:C:125:HIS:NE2	1:C:241:MET:O	2.42	0.49
1:A:142:GLU:O	1:A:145:GLU:HB2	2.12	0.49
1:A:187:TYR:H	1:A:188:PRO:HD2	1.78	0.49
1:B:154:MET:HB3	1:B:165:TRP:CZ2	2.47	0.49
1:B:117:ASP:OD2	1:B:117:ASP:N	2.46	0.49
1:C:38:MET:HG2	1:C:246:VAL:HG22	1.94	0.48
1:B:35:GLU:OE2	1:B:37:GLN:HB3	2.13	0.48
1:C:226:VAL:O	1:C:226:VAL:CG1	2.62	0.48
1:A:127:LEU:C	1:A:127:LEU:HD23	2.33	0.48
1:C:33:LEU:HD13	1:C:176:LEU:HD22	1.96	0.48
1:C:248:HIS:HB3	1:C:251:VAL:CG2	2.45	0.47
1:C:150:LEU:O	1:C:154:MET:HG2	2.15	0.47
1:B:210:TRP:O	1:B:235:ILE:HA	2.15	0.47
1:C:125:HIS:CE1	1:C:244:PRO:HG3	2.50	0.47
1:A:31:ASP:OD1	1:A:245:TYR:OH	2.33	0.47
1:C:135:LEU:HD22	1:C:183:TRP:HH2	1.79	0.47
1:B:191:ILE:HB	1:B:192:PRO:HD3	1.96	0.46
1:C:18:GLU:HB2	1:C:55:THR:CG2	2.46	0.46
1:B:61:MET:O	1:B:62:SER:C	2.54	0.46
1:A:158:VAL:HA	1:A:241:MET:CE	2.36	0.46
1:B:43:VAL:HA	1:B:53:VAL:HG11	1.97	0.46
1:B:123:MET:HE3	1:B:255:TYR:CE2	2.51	0.46
1:C:59:PRO:HG2	1:C:83:TYR:CD2	2.50	0.46
1:C:248:HIS:HA	1:C:249:PRO:HD3	1.83	0.45
1:A:3:THR:O	1:A:18:GLU:HA	2.15	0.45
1:C:52:ARG:HH11	1:C:93:ILE:HG13	1.81	0.45
1:C:94:LYS:O	1:C:118:ARG:HA	2.15	0.45
1:C:203:LEU:HB2	1:C:231:ALA:HB1	1.98	0.45
1:B:132:LEU:HD22	1:B:134:HIS:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:HG21	1:A:187:TYR:CE2	2.51	0.45
1:C:239:PRO:HB2	1:C:248:HIS:HB2	1.98	0.45
1:B:25:ASP:OD2	1:B:93:ILE:HG23	2.17	0.45
1:C:12:GLY:HA3	1:C:68:PRO:HD3	1.98	0.45
1:C:239:PRO:CG	1:C:251:VAL:HG11	2.45	0.45
1:C:153:VAL:HG13	1:C:157:ASP:HB2	1.98	0.44
1:C:226:VAL:O	1:C:226:VAL:HG13	2.17	0.44
1:A:248:HIS:N	1:A:249:PRO:HD3	2.31	0.44
1:C:195:ALA:HA	1:C:196:PRO:HD2	1.84	0.44
1:B:92:ASP:OD1	1:B:94:LYS:NZ	2.47	0.44
1:C:105:ALA:HA	1:C:108:VAL:HG22	2.00	0.44
1:C:34:GLY:O	1:C:57:ASP:HA	2.17	0.44
1:C:26:VAL:O	1:C:53:VAL:HA	2.17	0.44
1:C:216:THR:HG22	1:C:217:PRO:O	2.18	0.44
1:A:99:TRP:CD1	1:A:99:TRP:C	2.92	0.43
1:C:197:VAL:O	1:C:197:VAL:HG23	2.18	0.43
1:C:102:SER:O	1:C:105:ALA:HB3	2.18	0.43
1:C:255:TYR:O	1:C:259:THR:OG1	2.23	0.43
1:A:19:GLN:HG3	1:A:54:THR:OG1	2.18	0.43
1:C:210:TRP:O	1:C:235:ILE:HA	2.18	0.43
1:B:99:TRP:CG	1:B:100:GLY:N	2.86	0.43
1:B:102:SER:HB2	1:B:242:HIS:NE2	2.34	0.43
1:C:58:MET:CE	1:C:80:LEU:HD22	2.48	0.43
1:C:72:TYR:HA	1:C:75:VAL:HG21	1.96	0.43
1:A:26:VAL:O	1:A:53:VAL:HA	2.18	0.42
1:C:56:PHE:HZ	1:C:84:VAL:HG13	1.83	0.42
1:C:222:PHE:CD2	1:C:222:PHE:C	2.92	0.42
1:C:136:SER:C	1:C:138:THR:H	2.22	0.42
1:B:178:LYS:O	1:B:181:PRO:HD2	2.19	0.42
1:C:180:TYR:HB2	1:C:181:PRO:HD3	2.02	0.42
1:C:225:ILE:HG12	1:C:235:ILE:CD1	2.49	0.42
1:C:97:THR:HG23	1:C:121:ASN:ND2	2.35	0.42
1:B:176:LEU:O	1:B:179:ASN:N	2.52	0.42
1:C:101:CYS:O	1:C:104:GLY:N	2.53	0.42
1:A:180:TYR:HB2	1:A:181:PRO:HD3	2.01	0.42
1:A:224:ASN:HD22	1:A:224:ASN:N	2.18	0.41
1:B:31:ASP:OD1	1:B:245:TYR:OH	2.38	0.41
1:B:123:MET:HE1	1:B:256:VAL:CA	2.20	0.41
1:A:102:SER:HB2	1:A:242:HIS:NE2	2.36	0.41
1:C:104:GLY:O	1:C:108:VAL:HG22	2.20	0.41
1:C:221:PHE:O	1:C:224:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PRO:HD2	1:A:193:PRO:HD3	2.01	0.41
1:B:69:PRO:HA	1:B:72:TYR:CE2	2.56	0.41
1:C:37:GLN:HG3	1:C:37:GLN:O	2.20	0.41
1:A:201:GLU:HB3	1:C:234:ASN:HD21	1.85	0.41
1:C:84:VAL:HA	1:C:87:VAL:HG12	2.02	0.41
1:B:25:ASP:HB2	1:B:95:HIS:O	2.20	0.41
1:B:102:SER:HB2	1:B:242:HIS:CE1	2.56	0.41
1:C:97:THR:HG21	1:C:260:THR:OG1	2.21	0.41
1:C:99:TRP:CE2	1:C:252:PHE:CE1	3.05	0.41
1:A:226:VAL:HG12	1:A:230:LYS:HE2	2.03	0.41
1:B:37:GLN:HG2	1:B:172:VAL:CG2	2.52	0.40
1:C:99:TRP:CH2	1:C:125:HIS:CB	2.95	0.40
1:B:38:MET:HG2	1:B:168:MET:SD	2.61	0.40
1:C:221:PHE:O	1:C:225:ILE:HG13	2.22	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	262/278 (94%)	247 (94%)	12 (5%)	3 (1%)	14	30
1	B	262/278 (94%)	251 (96%)	11 (4%)	0	100	100
1	C	262/278 (94%)	221 (84%)	34 (13%)	7 (3%)	5	8
All	All	786/834 (94%)	719 (92%)	57 (7%)	10 (1%)	12	24

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ALA
1	C	214	ALA
1	C	102	SER

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Mol	Chain	Res	Type
1	C	137	ASN
1	A	187	TYR
1	C	159	SER
1	C	187	TYR
1	C	196	PRO
1	C	249	PRO
1	A	161	GLY

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	221/234 (94%)	213 (96%)	8 (4%)	35	61
1	B	221/234 (94%)	214 (97%)	7 (3%)	39	65
1	C	221/234 (94%)	199 (90%)	22 (10%)	7	14
All	All	663/702 (94%)	626 (94%)	37 (6%)	21	42

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	41	SER
1	A	94	LYS
1	A	136	SER
1	A	145	GLU
1	A	166	GLN
1	A	190	THR
1	A	258	GLU
1	B	22	THR
1	B	99	TRP
1	B	123	MET
1	B	178	LYS
1	B	189	ARG
1	B	224	ASN
1	B	235	ILE

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Mol	Chain	Res	Type
1	C	3	THR
1	C	7	ILE
1	C	8	SER
1	C	25	ASP
1	C	36	CYS
1	C	70	GLU
1	C	74	GLU
1	C	82	SER
1	C	106	SER
1	C	133	ASP
1	C	150	LEU
1	C	152	ASN
1	C	218	THR
1	C	220	SER
1	C	222	PHE
1	C	223	ASP
1	C	226	VAL
1	C	227	THR
1	C	237	LEU
1	C	250	ASP
1	C	259	THR
1	C	261	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	156	ASN
1	A	261	GLN
1	B	134	HIS
1	B	234	ASN
1	B	261	GLN
1	C	156	ASN
1	C	166	GLN
1	C	173	HIS
1	C	261	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, 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(Å^2)	Q<0.9
1	A	264/278 (94%)	-0.39	1 (0%)	92	91	31, 46, 76, 94	0
1	B	264/278 (94%)	-0.42	3 (1%)	80	78	30, 48, 75, 98	0
1	C	264/278 (94%)	2.23	125 (47%)	0	0	90, 116, 181, 219	0
All	All	792/834 (94%)	0.47	129 (16%)	1	1	30, 56, 153, 219	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	165	TRP	15.3
1	C	155	LEU	10.3
1	C	168	MET	9.4
1	C	177	HIS	8.7
1	C	5	SER	8.4
1	C	219	GLU	8.1
1	C	158	VAL	8.1
1	C	174	ALA	8.0
1	C	28	LEU	7.4
1	C	241	MET	7.2
1	C	145	GLU	7.0
1	C	164	ALA	6.5
1	C	156	ASN	6.4
1	C	34	GLY	6.4
1	C	236	GLY	6.0
1	C	3	THR	5.8
1	C	29	VAL	5.7
1	C	147	SER	5.6
1	C	142	GLU	5.5
1	C	247	SER	5.2
1	C	159	SER	5.2
1	C	232	GLY	5.0
1	C	245	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	212	VAL	4.7
1	C	24	PRO	4.7
1	C	167	ALA	4.7
1	C	143	ASP	4.6
1	C	80	LEU	4.6
1	C	166	GLN	4.5
1	C	218	THR	4.5
1	C	154	MET	4.5
1	C	110	ALA	4.4
1	C	171	GLU	4.4
1	C	69	PRO	4.4
1	C	44	SER	4.3
1	C	65	ALA	4.3
1	C	146	ILE	4.3
1	C	136	SER	4.3
1	C	137	ASN	4.1
1	C	30	PRO	4.0
1	C	101	CYS	4.0
1	C	33	LEU	3.9
1	C	114	GLY	3.9
1	C	78	GLN	3.8
1	C	90	ALA	3.7
1	C	99	TRP	3.6
1	C	39	PHE	3.6
1	C	76	THR	3.6
1	C	235	ILE	3.6
1	C	115	TYR	3.6
1	C	60	GLY	3.6
1	C	75	VAL	3.5
1	C	22	THR	3.5
1	C	186	GLY	3.5
1	C	132	LEU	3.4
1	C	17	TYR	3.4
1	C	6	THR	3.3
1	C	170	ASP	3.3
1	C	172	VAL	3.3
1	C	87	VAL	3.3
1	C	231	ALA	3.2
1	C	248	HIS	3.2
1	C	133	ASP	3.1
1	C	82	SER	3.1
1	C	31	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	19	GLN	3.1
1	C	9	THR	3.0
1	C	215	ALA	3.0
1	A	29	VAL	3.0
1	C	189	ARG	3.0
1	C	127	LEU	2.9
1	C	8	SER	2.9
1	C	51	PHE	2.9
1	C	144	GLU	2.9
1	C	185	ARG	2.9
1	C	46	ILE	2.9
1	C	108	VAL	2.8
1	C	180	TYR	2.8
1	C	57	ASP	2.8
1	C	111	LEU	2.8
1	C	72	TYR	2.8
1	C	258	GLU	2.7
1	C	48	ALA	2.7
1	C	77	ALA	2.7
1	C	255	TYR	2.7
1	C	79	LYS	2.7
1	C	89	ASP	2.7
1	C	38	MET	2.6
1	C	49	GLN	2.6
1	C	162	SER	2.6
1	C	220	SER	2.6
1	C	181	PRO	2.6
1	C	230	LYS	2.6
1	C	14	THR	2.5
1	C	157	ASP	2.5
1	C	128	PRO	2.5
1	C	211	THR	2.5
1	C	1	MET	2.5
1	C	163	GLU	2.5
1	C	140	VAL	2.5
1	C	223	ASP	2.5
1	C	59	PRO	2.4
1	C	50	GLY	2.4
1	C	160	GLY	2.4
1	C	116	PRO	2.4
1	C	175	ARG	2.4
1	C	262	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	30	PRO	2.4
1	B	29	VAL	2.3
1	B	100	GLY	2.3
1	C	252	PHE	2.3
1	C	73	THR	2.3
1	C	191	ILE	2.3
1	C	2	ARG	2.3
1	C	20	GLU	2.3
1	C	100	GLY	2.2
1	C	130	LYS	2.2
1	C	18	GLU	2.2
1	C	13	ILE	2.2
1	C	10	PRO	2.2
1	C	12	GLY	2.1
1	C	124	CYS	2.1
1	C	58	MET	2.1
1	C	256	VAL	2.1
1	C	190	THR	2.1
1	C	237	LEU	2.0
1	C	201	GLU	2.0
1	C	202	ALA	2.0
1	C	193	PRO	2.0

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.