Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2024 – 06:50 PM JST

PDB ID	:	8WDM
Title	:	Crystal structure of a novel PU plastic degradation enzyme from Thermaerobacter marianensis
Authors	:	Li, Z.S.; Wang, H.; Gao, J.; Chen, Y.Y.; Wei, H.L.; Li, Q.; Han, X.; Wei, R.; Liu, W.D.
Deposited on	:	2023-09-15
Resolution	:	2.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

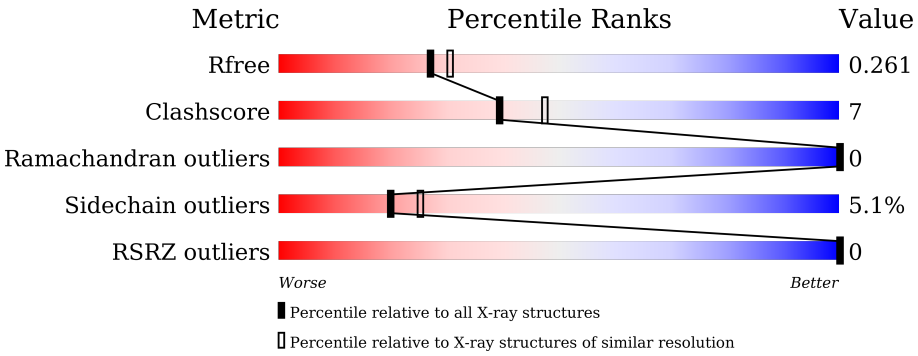
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	527	76% 17% • 6%
1	B	527	78% 16% 6%
1	C	527	75% 17% • 6%
1	D	527	79% 15% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15446 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 Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3718	2365	679	665	9			
1	B	498	Total	C	N	O	S	0	0	0
			3755	2384	684	678	9			
1	C	493	Total	C	N	O	S	0	0	0
			3721	2366	679	667	9			
1	D	496	Total	C	N	O	S	0	0	0
			3726	2371	676	670	9			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP E6SHQ4
A	-5	HIS	-	expression tag	UNP E6SHQ4
A	-4	HIS	-	expression tag	UNP E6SHQ4
A	-3	HIS	-	expression tag	UNP E6SHQ4
A	-2	HIS	-	expression tag	UNP E6SHQ4
A	-1	HIS	-	expression tag	UNP E6SHQ4
A	0	HIS	-	expression tag	UNP E6SHQ4
A	1	GLU	-	expression tag	UNP E6SHQ4
A	2	ASN	-	expression tag	UNP E6SHQ4
A	3	LEU	-	expression tag	UNP E6SHQ4
A	4	TYR	-	expression tag	UNP E6SHQ4
A	5	PHE	-	expression tag	UNP E6SHQ4
A	6	GLN	-	expression tag	UNP E6SHQ4
A	7	GLY	-	expression tag	UNP E6SHQ4
A	8	ALA	-	expression tag	UNP E6SHQ4
A	9	GLY	-	expression tag	UNP E6SHQ4
A	10	ALA	-	expression tag	UNP E6SHQ4
A	11	GLY	-	expression tag	UNP E6SHQ4
A	12	ALA	-	expression tag	UNP E6SHQ4
A	13	GLY	-	expression tag	UNP E6SHQ4
A	14	ALA	-	expression tag	UNP E6SHQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	expression tag	UNP E6SHQ4
A	16	ALA	-	expression tag	UNP E6SHQ4
B	-6	MET	-	initiating methionine	UNP E6SHQ4
B	-5	HIS	-	expression tag	UNP E6SHQ4
B	-4	HIS	-	expression tag	UNP E6SHQ4
B	-3	HIS	-	expression tag	UNP E6SHQ4
B	-2	HIS	-	expression tag	UNP E6SHQ4
B	-1	HIS	-	expression tag	UNP E6SHQ4
B	0	HIS	-	expression tag	UNP E6SHQ4
B	1	GLU	-	expression tag	UNP E6SHQ4
B	2	ASN	-	expression tag	UNP E6SHQ4
B	3	LEU	-	expression tag	UNP E6SHQ4
B	4	TYR	-	expression tag	UNP E6SHQ4
B	5	PHE	-	expression tag	UNP E6SHQ4
B	6	GLN	-	expression tag	UNP E6SHQ4
B	7	GLY	-	expression tag	UNP E6SHQ4
B	8	ALA	-	expression tag	UNP E6SHQ4
B	9	GLY	-	expression tag	UNP E6SHQ4
B	10	ALA	-	expression tag	UNP E6SHQ4
B	11	GLY	-	expression tag	UNP E6SHQ4
B	12	ALA	-	expression tag	UNP E6SHQ4
B	13	GLY	-	expression tag	UNP E6SHQ4
B	14	ALA	-	expression tag	UNP E6SHQ4
B	15	GLY	-	expression tag	UNP E6SHQ4
B	16	ALA	-	expression tag	UNP E6SHQ4
C	-6	MET	-	initiating methionine	UNP E6SHQ4
C	-5	HIS	-	expression tag	UNP E6SHQ4
C	-4	HIS	-	expression tag	UNP E6SHQ4
C	-3	HIS	-	expression tag	UNP E6SHQ4
C	-2	HIS	-	expression tag	UNP E6SHQ4
C	-1	HIS	-	expression tag	UNP E6SHQ4
C	0	HIS	-	expression tag	UNP E6SHQ4
C	1	GLU	-	expression tag	UNP E6SHQ4
C	2	ASN	-	expression tag	UNP E6SHQ4
C	3	LEU	-	expression tag	UNP E6SHQ4
C	4	TYR	-	expression tag	UNP E6SHQ4
C	5	PHE	-	expression tag	UNP E6SHQ4
C	6	GLN	-	expression tag	UNP E6SHQ4
C	7	GLY	-	expression tag	UNP E6SHQ4
C	8	ALA	-	expression tag	UNP E6SHQ4
C	9	GLY	-	expression tag	UNP E6SHQ4
C	10	ALA	-	expression tag	UNP E6SHQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	11	GLY	-	expression tag	UNP E6SHQ4
C	12	ALA	-	expression tag	UNP E6SHQ4
C	13	GLY	-	expression tag	UNP E6SHQ4
C	14	ALA	-	expression tag	UNP E6SHQ4
C	15	GLY	-	expression tag	UNP E6SHQ4
C	16	ALA	-	expression tag	UNP E6SHQ4
D	-6	MET	-	initiating methionine	UNP E6SHQ4
D	-5	HIS	-	expression tag	UNP E6SHQ4
D	-4	HIS	-	expression tag	UNP E6SHQ4
D	-3	HIS	-	expression tag	UNP E6SHQ4
D	-2	HIS	-	expression tag	UNP E6SHQ4
D	-1	HIS	-	expression tag	UNP E6SHQ4
D	0	HIS	-	expression tag	UNP E6SHQ4
D	1	GLU	-	expression tag	UNP E6SHQ4
D	2	ASN	-	expression tag	UNP E6SHQ4
D	3	LEU	-	expression tag	UNP E6SHQ4
D	4	TYR	-	expression tag	UNP E6SHQ4
D	5	PHE	-	expression tag	UNP E6SHQ4
D	6	GLN	-	expression tag	UNP E6SHQ4
D	7	GLY	-	expression tag	UNP E6SHQ4
D	8	ALA	-	expression tag	UNP E6SHQ4
D	9	GLY	-	expression tag	UNP E6SHQ4
D	10	ALA	-	expression tag	UNP E6SHQ4
D	11	GLY	-	expression tag	UNP E6SHQ4
D	12	ALA	-	expression tag	UNP E6SHQ4
D	13	GLY	-	expression tag	UNP E6SHQ4
D	14	ALA	-	expression tag	UNP E6SHQ4
D	15	GLY	-	expression tag	UNP E6SHQ4
D	16	ALA	-	expression tag	UNP E6SHQ4

- Molecule 2 is water.

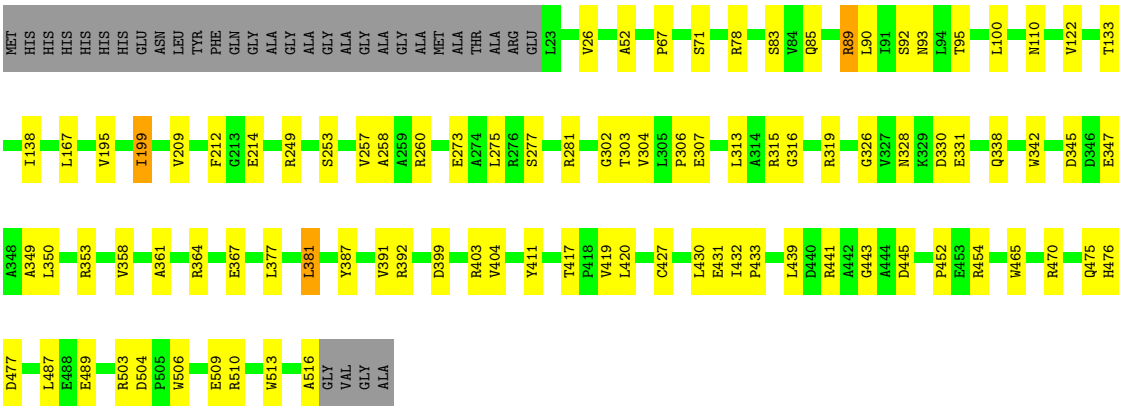
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	127	Total O 127 127	0	0
2	B	129	Total O 129 129	0	0
2	C	136	Total O 136 136	0	0
2	D	134	Total O 134 134	0	0

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.

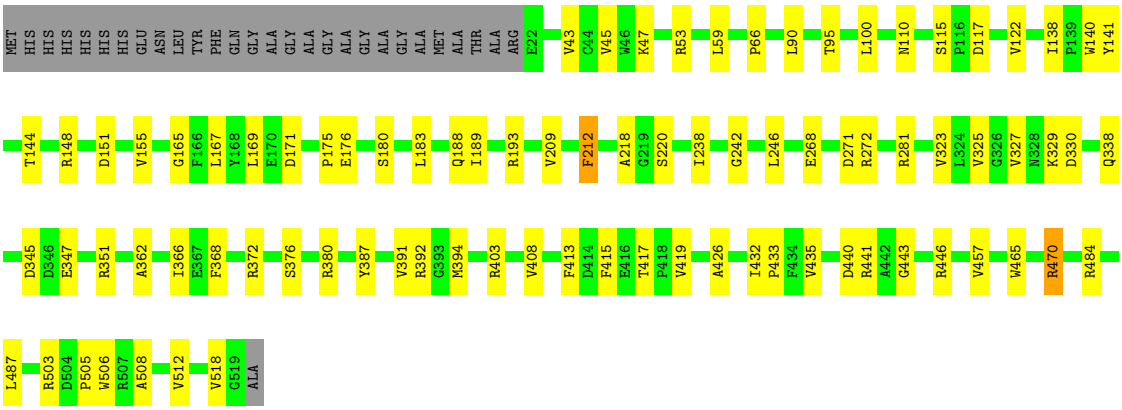
• Molecule 1: Carboxylic ester hydrolase

Chain A:



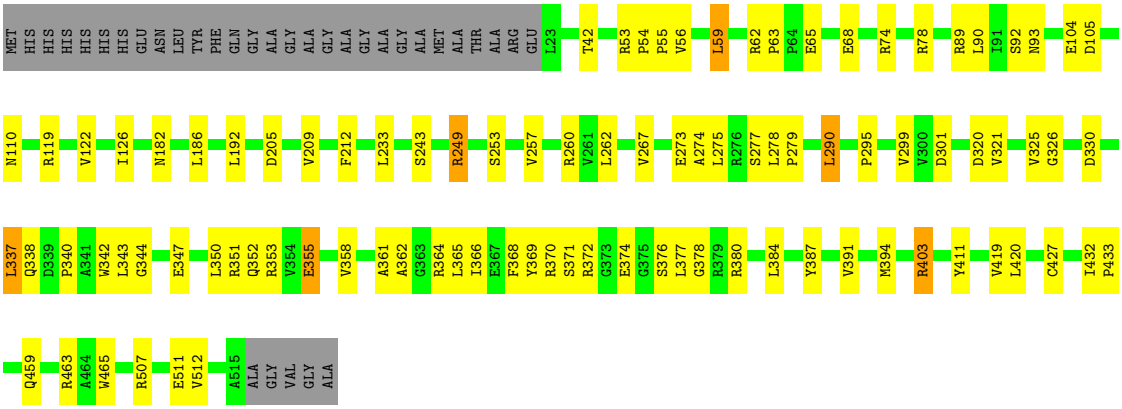
• Molecule 1: Carboxylic ester hydrolase

Chain B:



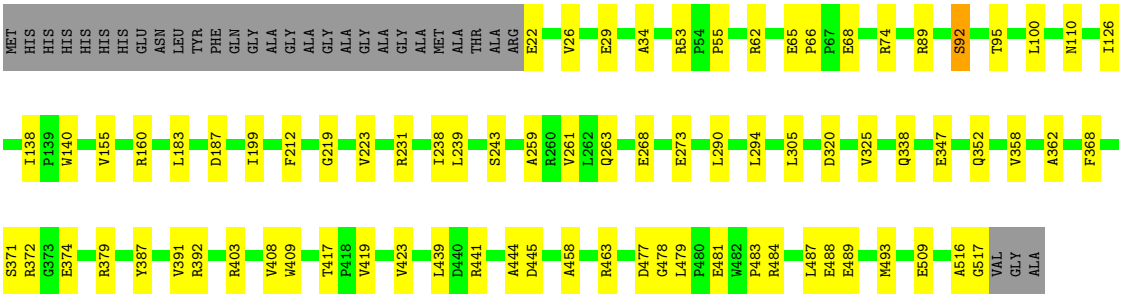
• Molecule 1: Carboxylic ester hydrolase

Chain C:



• Molecule 1: Carboxylic ester hydrolase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	81.88Å 81.88Å 667.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.58 – 2.20 41.58 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.58-2.20) 99.9 (41.58-2.20)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.231 , 0.265 0.234 , 0.261	Depositor DCC
R_{free} test set	120940 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15446	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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

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	0.37	0/3820	0.61	0/5222
1	B	0.38	0/3857	0.63	0/5270
1	C	0.38	0/3823	0.62	0/5225
1	D	0.39	0/3828	0.63	0/5233
All	All	0.38	0/15328	0.63	0/20950

There are no bond length outliers.

There are no bond angle outliers.

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	3718	0	3631	57	0
1	B	3755	0	3661	47	0
1	C	3721	0	3636	54	0
1	D	3726	0	3630	40	0
2	A	127	0	0	0	0
2	B	129	0	0	0	0
2	C	136	0	0	0	0
2	D	134	0	0	0	0
All	All	15446	0	14558	194	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 7.

All (194) 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:89:ARG:HG3	1:A:89:ARG:HH21	1.06	1.12
1:A:89:ARG:HH21	1:A:89:ARG:CG	1.88	0.85
1:A:89:ARG:HG3	1:A:89:ARG:NH2	1.86	0.83
1:B:144:THR:O	1:B:148:ARG:HG3	1.78	0.82
1:C:419:VAL:HG12	1:C:420:LEU:HG	1.67	0.76
1:A:89:ARG:HD3	1:A:92:SER:CB	2.17	0.73
1:A:89:ARG:HD3	1:A:92:SER:HB3	1.70	0.72
1:D:160:ARG:HD3	1:D:187:ASP:OD2	1.89	0.72
1:D:368:PHE:HZ	1:D:372:ARG:HH11	1.38	0.71
1:B:403:ARG:HG3	1:B:487:LEU:HD11	1.74	0.69
1:B:43:VAL:HG21	1:B:148:ARG:HG2	1.76	0.67
1:A:83:SER:O	1:A:85:GLN:HG3	1.95	0.67
1:B:446:ARG:HG3	1:B:446:ARG:HH11	1.59	0.67
1:A:89:ARG:CG	1:A:89:ARG:NH2	2.52	0.66
1:B:372:ARG:O	1:B:380:ARG:HG2	1.95	0.66
1:B:100:LEU:HD21	1:B:138:ILE:HD11	1.77	0.65
1:D:100:LEU:HD21	1:D:138:ILE:HD11	1.80	0.64
1:D:259:ALA:O	1:D:263:GLN:NE2	2.30	0.64
1:B:53:ARG:HE	1:B:59:LEU:HD11	1.62	0.64
1:B:392:ARG:NH1	1:B:518:VAL:O	2.31	0.64
1:C:249:ARG:HH11	1:C:249:ARG:HG2	1.62	0.64
1:B:43:VAL:CG2	1:B:148:ARG:HG2	2.29	0.63
1:C:89:ARG:O	1:C:93:ASN:HB2	2.00	0.62
1:B:508:ALA:O	1:B:512:VAL:HG23	1.99	0.61
1:D:89:ARG:HA	1:D:92:SER:HB3	1.82	0.61
1:B:90:LEU:HD22	1:B:338:GLN:HG2	1.82	0.60
1:C:54:PRO:HB3	1:C:105:ASP:HB2	1.84	0.60
1:A:89:ARG:HD3	1:A:92:SER:OG	2.01	0.59
1:D:358:VAL:HG23	1:D:362:ALA:HB2	1.86	0.58
1:D:403:ARG:HG3	1:D:487:LEU:HD11	1.84	0.58
1:A:364:ARG:HD3	1:A:516:ALA:HB2	1.85	0.57
1:A:316:GLY:O	1:A:319:ARG:HG2	2.04	0.57
1:C:320:ASP:OD2	1:C:320:ASP:N	2.31	0.57
1:D:212:PHE:HB2	1:D:238:ILE:HB	1.87	0.57
1:A:349:ALA:HB1	1:A:353:ARG:NH1	2.20	0.56
1:A:257:VAL:HG22	1:A:260:ARG:HH21	1.71	0.56
1:B:212:PHE:HB2	1:B:238:ILE:HB	1.88	0.56
1:B:387:TYR:HA	1:B:391:VAL:HB	1.88	0.55
1:D:387:TYR:HA	1:D:391:VAL:HB	1.87	0.55
1:B:443:GLY:HA2	1:B:446:ARG:NH1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HG23	1:A:443:GLY:HA3	1.89	0.55
1:A:273:GLU:OE2	1:A:277:SER:OG	2.26	0.54
1:C:369:TYR:CE2	1:C:384:LEU:HD23	2.43	0.54
1:D:488:GLU:OE2	1:D:489:GLU:HG2	2.07	0.54
1:C:459:GLN:OE1	1:C:463:ARG:NH1	2.41	0.54
1:A:90:LEU:HD13	1:A:338:GLN:HG2	1.90	0.53
1:C:351:ARG:O	1:C:355:GLU:HB2	2.09	0.53
1:B:151:ASP:HB3	1:B:470:ARG:HH21	1.73	0.53
1:D:372:ARG:HH12	1:D:509:GLU:HG3	1.73	0.53
1:B:45:VAL:HG21	1:B:47:LYS:HE3	1.91	0.53
1:C:89:ARG:HD2	1:C:92:SER:HB3	1.90	0.53
1:D:368:PHE:HZ	1:D:372:ARG:NH1	2.05	0.53
1:C:249:ARG:HH11	1:C:249:ARG:CG	2.20	0.53
1:C:342:TRP:O	1:C:378:GLY:HA3	2.09	0.53
1:D:53:ARG:HG3	1:D:66:PRO:O	2.09	0.53
1:C:56:VAL:HG12	1:C:104:GLU:HG2	1.91	0.52
1:C:507:ARG:O	1:C:511:GLU:HG3	2.09	0.52
1:A:347:GLU:HG3	1:A:377:LEU:CD2	2.39	0.52
1:B:413:PHE:CZ	1:B:415:PHE:HB3	2.46	0.51
1:C:326:GLY:HA3	1:C:411:TYR:CE2	2.45	0.51
1:C:253:SER:O	1:C:257:VAL:HG23	2.11	0.50
1:D:439:LEU:O	1:D:444:ALA:HB3	2.11	0.50
1:A:387:TYR:CE1	1:A:392:ARG:HG3	2.47	0.50
1:C:362:ALA:O	1:C:366:ILE:HG13	2.12	0.50
1:D:479:LEU:HD22	1:D:493:MET:HE1	1.93	0.50
1:C:62:ARG:HH11	1:C:63:PRO:HD2	1.77	0.50
1:A:307:GLU:OE1	1:A:315:ARG:NH1	2.45	0.50
1:D:223:VAL:HG13	1:D:305:LEU:HD13	1.94	0.50
1:D:53:ARG:NH1	1:D:68:GLU:HG2	2.27	0.49
1:A:85:GLN:HB3	1:A:133:THR:HG22	1.94	0.49
1:D:417:THR:OG1	1:D:419:VAL:HG22	2.13	0.49
1:A:358:VAL:HG12	1:A:361:ALA:HB3	1.95	0.49
1:C:90:LEU:HD13	1:C:338:GLN:HG2	1.95	0.49
1:C:249:ARG:CG	1:C:249:ARG:NH1	2.76	0.49
1:C:370:ARG:HG3	1:C:380:ARG:NH1	2.28	0.49
1:A:167:LEU:HD11	1:A:258:ALA:HA	1.94	0.49
1:A:350:LEU:HD12	1:A:377:LEU:HD23	1.95	0.49
1:A:432:ILE:HB	1:A:433:PRO:HD3	1.94	0.49
1:B:180:SER:HA	1:B:183:LEU:HG	1.95	0.49
1:C:63:PRO:HB3	1:C:186:LEU:HD13	1.95	0.49
1:C:358:VAL:HG12	1:C:361:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:PRO:HD2	1:D:231:ARG:NH2	2.29	0.48
1:A:249:ARG:NH2	1:A:253:SER:HB2	2.29	0.48
1:A:377:LEU:HG	1:A:381:LEU:HD22	1.95	0.48
1:C:432:ILE:HB	1:C:433:PRO:HD3	1.95	0.48
1:D:441:ARG:HD3	1:D:441:ARG:HA	1.61	0.48
1:C:387:TYR:HA	1:C:391:VAL:HB	1.96	0.47
1:A:509:GLU:O	1:A:513:TRP:HD1	1.97	0.47
1:B:325:VAL:HG22	1:B:394:MET:HG3	1.97	0.47
1:B:175:PRO:HG3	1:C:344:GLY:HA3	1.96	0.47
1:D:62:ARG:O	1:D:160:ARG:NH2	2.33	0.47
1:A:489:GLU:HB3	1:A:503:ARG:HD3	1.95	0.47
1:B:95:THR:HB	1:B:140:TRP:CH2	2.49	0.47
1:B:362:ALA:O	1:B:366:ILE:HG13	2.14	0.47
1:A:303:THR:OG1	1:A:304:VAL:N	2.46	0.47
1:A:475:GLN:NE2	1:A:476:HIS:O	2.47	0.47
1:B:327:VAL:HG21	1:B:391:VAL:HG22	1.96	0.47
1:D:55:PRO:HG3	1:D:160:ARG:HD2	1.96	0.47
1:A:419:VAL:HG12	1:A:420:LEU:HG	1.97	0.47
1:A:387:TYR:HA	1:A:391:VAL:HB	1.96	0.46
1:B:176:GLU:HA	1:C:340:PRO:HB3	1.96	0.46
1:C:122:VAL:HB	1:C:209:VAL:HG22	1.98	0.46
1:A:85:GLN:O	1:A:281:ARG:NH2	2.49	0.46
1:A:214:GLU:HG3	1:A:431:GLU:OE2	2.15	0.46
1:D:160:ARG:NH2	1:D:183:LEU:HD13	2.31	0.46
1:D:261:VAL:HG22	1:D:290:LEU:HD11	1.98	0.46
1:A:330:ASP:O	1:A:427:CYS:HA	2.16	0.46
1:C:403:ARG:HA	1:C:403:ARG:HD3	1.57	0.46
1:B:268:GLU:HG3	1:B:271:ASP:HB2	1.98	0.46
1:C:89:ARG:HD2	1:C:89:ARG:HA	1.83	0.46
1:D:53:ARG:HD3	1:D:65:GLU:HB2	1.98	0.46
1:C:182:ASN:ND2	1:C:301:ASP:OD2	2.47	0.45
1:C:358:VAL:HG11	1:C:365:LEU:CD1	2.46	0.45
1:D:516:ALA:O	1:D:517:GLY:C	2.53	0.45
1:B:329:LYS:HB3	1:B:426:ALA:HB3	1.97	0.45
1:B:368:PHE:CZ	1:B:512:VAL:HG21	2.51	0.45
1:C:249:ARG:O	1:C:299:VAL:HA	2.16	0.45
1:B:441:ARG:HH11	1:B:441:ARG:HD3	1.57	0.45
1:C:352:GLN:HA	1:C:355:GLU:OE1	2.16	0.45
1:A:342:TRP:HZ3	1:A:381:LEU:HB3	1.81	0.45
1:C:260:ARG:HB2	1:C:290:LEU:HD11	1.99	0.45
1:D:239:LEU:HB2	1:D:325:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:GLU:O	1:D:483:PRO:HD3	2.17	0.45
1:B:100:LEU:HD12	1:B:100:LEU:H	1.81	0.45
1:B:175:PRO:HB2	1:C:343:LEU:HB2	1.99	0.45
1:C:273:GLU:O	1:C:277:SER:HB3	2.17	0.45
1:D:477:ASP:OD2	1:D:478:GLY:N	2.50	0.44
1:A:504:ASP:OD2	1:A:510:ARG:NH2	2.49	0.44
1:A:506:TRP:O	1:A:510:ARG:HB3	2.16	0.44
1:B:188:GLN:OE1	1:B:220:SER:HB3	2.17	0.44
1:C:325:VAL:HG22	1:C:394:MET:HG3	1.99	0.44
1:D:110:ASN:O	1:D:155:VAL:HA	2.18	0.44
1:A:439:LEU:HD13	1:A:454:ARG:HG3	1.99	0.44
1:B:212:PHE:CB	1:B:238:ILE:HB	2.48	0.44
1:B:110:ASN:O	1:B:155:VAL:HA	2.17	0.44
1:D:219:GLY:HA2	1:D:243:SER:O	2.18	0.44
1:C:53:ARG:HH11	1:C:68:GLU:CG	2.31	0.43
1:D:320:ASP:OD1	1:D:320:ASP:N	2.38	0.43
1:A:89:ARG:HB3	1:A:93:ASN:ND2	2.33	0.43
1:C:350:LEU:HD12	1:C:377:LEU:HD23	2.00	0.43
1:C:59:LEU:HD11	1:C:65:GLU:HG3	2.01	0.43
1:C:267:VAL:HG13	1:C:274:ALA:HB3	1.99	0.43
1:D:95:THR:HB	1:D:140:TRP:CH2	2.54	0.43
1:A:326:GLY:HA3	1:A:411:TYR:CE2	2.53	0.43
1:B:122:VAL:HB	1:B:209:VAL:HG22	2.01	0.43
1:D:409:TRP:CE2	1:D:484:ARG:HG2	2.54	0.43
1:B:140:TRP:CD1	1:B:433:PRO:HG3	2.54	0.43
1:C:337:LEU:HD11	1:C:420:LEU:HD13	2.01	0.43
1:C:368:PHE:CE1	1:C:512:VAL:HG11	2.54	0.43
1:B:417:THR:OG1	1:B:419:VAL:HG22	2.19	0.43
1:A:100:LEU:HD11	1:A:138:ILE:HD11	2.01	0.42
1:B:218:ALA:HB3	1:B:242:GLY:HA3	2.01	0.42
1:C:290:LEU:HD22	1:C:295:PRO:HB3	2.01	0.42
1:A:328:ASN:O	1:A:331:GLU:HG2	2.19	0.42
1:B:432:ILE:O	1:B:435:VAL:HG22	2.20	0.42
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.76	0.42
1:C:54:PRO:HB3	1:C:105:ASP:CB	2.49	0.42
1:B:189:ILE:O	1:B:193:ARG:HG3	2.20	0.42
1:D:439:LEU:HD11	1:D:458:ALA:CB	2.50	0.42
1:A:313:LEU:HD23	1:A:313:LEU:HA	1.85	0.42
1:B:167:LEU:HD23	1:B:169:LEU:HD21	2.02	0.41
1:B:505:PRO:HG2	1:B:506:TRP:CE3	2.55	0.41
1:C:330:ASP:O	1:C:427:CYS:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:GLU:HA	1:D:34:ALA:HA	2.01	0.41
1:A:275:LEU:HA	1:A:275:LEU:HD12	1.86	0.41
1:B:53:ARG:HG3	1:B:66:PRO:O	2.20	0.41
1:B:144:THR:HG22	1:B:148:ARG:HD3	2.02	0.41
1:B:329:LYS:HE3	1:B:330:ASP:OD2	2.20	0.41
1:A:122:VAL:HB	1:A:209:VAL:HG22	2.02	0.41
1:A:399:ASP:HB3	1:A:403:ARG:NH2	2.36	0.41
1:C:262:LEU:HD23	1:C:262:LEU:HA	1.79	0.41
1:D:368:PHE:CZ	1:D:372:ARG:NH1	2.80	0.41
1:C:337:LEU:HD12	1:C:337:LEU:HA	1.77	0.41
1:D:212:PHE:CB	1:D:238:ILE:HB	2.48	0.41
1:A:316:GLY:HA2	1:A:404:VAL:HG11	2.03	0.41
1:A:433:PRO:HB2	1:A:439:LEU:HD23	2.02	0.41
1:A:195:VAL:O	1:A:199:ILE:HB	2.21	0.41
1:C:105:ASP:OD2	1:C:105:ASP:O	2.39	0.41
1:A:52:ALA:HA	1:A:67:PRO:HD3	2.01	0.41
1:B:138:ILE:HB	1:B:141:TYR:CD2	2.56	0.41
1:C:119:ARG:HB3	1:C:205:ASP:HB2	2.02	0.41
1:D:379:ARG:HH21	1:D:423:VAL:HG12	1.86	0.41
1:A:347:GLU:HG3	1:A:377:LEU:HD22	2.02	0.40
1:C:368:PHE:CD1	1:C:512:VAL:HG11	2.56	0.40
1:D:445:ASP:OD1	1:D:445:ASP:N	2.54	0.40
1:B:165:GLY:O	1:B:183:LEU:HB2	2.21	0.40
1:A:89:ARG:O	1:A:90:LEU:C	2.59	0.40
1:A:403:ARG:HG3	1:A:487:LEU:HD11	2.02	0.40
1:B:323:VAL:O	1:B:408:VAL:HA	2.20	0.40
1:C:54:PRO:HA	1:C:55:PRO:HD3	1.97	0.40
1:C:192:LEU:HB3	1:C:233:LEU:HB3	2.04	0.40
1:A:302:GLY:HA2	1:A:306:PRO:HA	2.04	0.40
1:A:430:LEU:O	1:A:433:PRO:HD2	2.21	0.40
1:C:278:LEU:HA	1:C:279:PRO:HD3	1.93	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	492/527 (93%)	483 (98%)	9 (2%)	0	100	100
1	B	496/527 (94%)	484 (98%)	12 (2%)	0	100	100
1	C	491/527 (93%)	479 (98%)	12 (2%)	0	100	100
1	D	494/527 (94%)	480 (97%)	14 (3%)	0	100	100
All	All	1973/2108 (94%)	1926 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	358/383 (94%)	342 (96%)	16 (4%)	23	30
1	B	363/383 (95%)	346 (95%)	17 (5%)	22	29
1	C	360/383 (94%)	337 (94%)	23 (6%)	14	17
1	D	358/383 (94%)	341 (95%)	17 (5%)	22	29
All	All	1439/1532 (94%)	1366 (95%)	73 (5%)	20	25

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	71	SER
1	A	78	ARG
1	A	89	ARG
1	A	110	ASN
1	A	199	ILE
1	A	212	PHE
1	A	345	ASP
1	A	367	GLU
1	A	381	LEU

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Mol	Chain	Res	Type
1	A	417	THR
1	A	441	ARG
1	A	445	ASP
1	A	465	TRP
1	A	470	ARG
1	A	477	ASP
1	B	115	SER
1	B	117	ASP
1	B	171	ASP
1	B	212	PHE
1	B	246	LEU
1	B	272	ARG
1	B	281	ARG
1	B	345	ASP
1	B	347	GLU
1	B	351	ARG
1	B	376	SER
1	B	440	ASP
1	B	457	VAL
1	B	465	TRP
1	B	470	ARG
1	B	484	ARG
1	B	503	ARG
1	C	42	THR
1	C	59	LEU
1	C	74	ARG
1	C	78	ARG
1	C	110	ASN
1	C	126	ILE
1	C	212	PHE
1	C	243	SER
1	C	249	ARG
1	C	275	LEU
1	C	290	LEU
1	C	321	VAL
1	C	337	LEU
1	C	347	GLU
1	C	353	ARG
1	C	355	GLU
1	C	364	ARG
1	C	371	SER
1	C	372	ARG

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Mol	Chain	Res	Type
1	C	374	GLU
1	C	376	SER
1	C	403	ARG
1	C	465	TRP
1	D	22	GLU
1	D	26	VAL
1	D	74	ARG
1	D	92	SER
1	D	126	ILE
1	D	199	ILE
1	D	268	GLU
1	D	273	GLU
1	D	294	LEU
1	D	338	GLN
1	D	347	GLU
1	D	352	GLN
1	D	371	SER
1	D	374	GLU
1	D	392	ARG
1	D	408	VAL
1	D	463	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	459	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 oligosaccharides 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

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^{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	A	494/527 (93%)	-1.44	0	100	100	31, 43, 70, 89	0
1	B	498/527 (94%)	-1.42	0	100	100	29, 44, 67, 81	0
1	C	493/527 (93%)	-1.44	0	100	100	30, 43, 73, 93	0
1	D	496/527 (94%)	-1.44	0	100	100	29, 44, 67, 83	0
All	All	1981/2108 (93%)	-1.43	0	100	100	29, 44, 69, 93	0

There are no RSRZ outliers to report.

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.