Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2021 – 09:02 am GMT

PDB ID	:	6Z71
Title	:	Structure of the MATE family multidrug resistance transporter Aq_128 from Aquifex aeolicus in the outward-facing state
Authors	:	Zhao, J.; Safarian, S.; Thielmann, Y.; Xie, H.; Wang, J.; Michel, H.
Deposited on	:	2020-05-29
Resolution	:	3.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

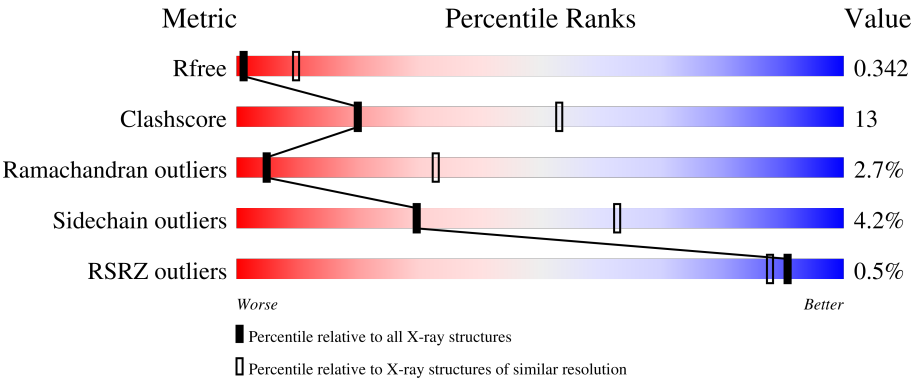
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	496	% 59% 23% · 16%
1	B	496	56% 26% · 15%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6632 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 Aq128.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3301	2232	506	549	14			
1	B	423	Total	C	N	O	S	0	0	0
			3331	2253	511	553	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	473	ARG	-	expression tag	UNP O66528
A	474	ASN	-	expression tag	UNP O66528
A	475	SER	-	expression tag	UNP O66528
A	476	GLU	-	expression tag	UNP O66528
A	477	ASN	-	expression tag	UNP O66528
A	478	LEU	-	expression tag	UNP O66528
A	479	TYR	-	expression tag	UNP O66528
A	480	PHE	-	expression tag	UNP O66528
A	481	GLN	-	expression tag	UNP O66528
A	482	GLY	-	expression tag	UNP O66528
A	483	GLY	-	expression tag	UNP O66528
A	484	ARG	-	expression tag	UNP O66528
A	485	GLY	-	expression tag	UNP O66528
A	486	SER	-	expression tag	UNP O66528
A	487	HIS	-	expression tag	UNP O66528
A	488	HIS	-	expression tag	UNP O66528
A	489	HIS	-	expression tag	UNP O66528
A	490	HIS	-	expression tag	UNP O66528
A	491	HIS	-	expression tag	UNP O66528
A	492	HIS	-	expression tag	UNP O66528
A	493	HIS	-	expression tag	UNP O66528
A	494	HIS	-	expression tag	UNP O66528
A	495	HIS	-	expression tag	UNP O66528
A	496	HIS	-	expression tag	UNP O66528
B	473	ARG	-	expression tag	UNP O66528

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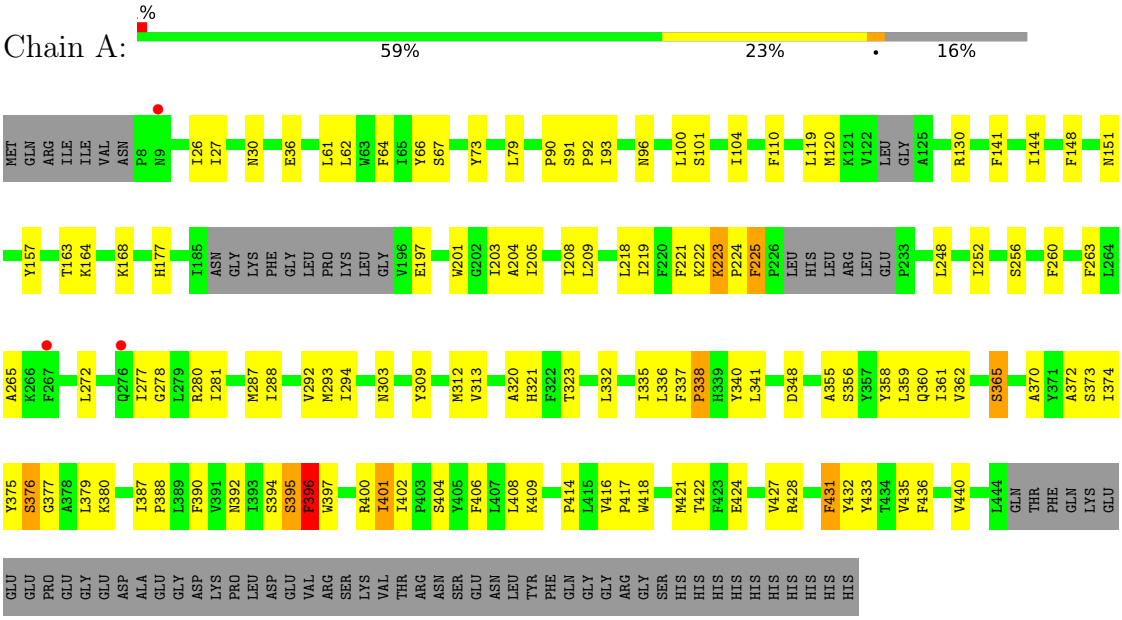
Chain	Residue	Modelled	Actual	Comment	Reference
B	474	ASN	-	expression tag	UNP O66528
B	475	SER	-	expression tag	UNP O66528
B	476	GLU	-	expression tag	UNP O66528
B	477	ASN	-	expression tag	UNP O66528
B	478	LEU	-	expression tag	UNP O66528
B	479	TYR	-	expression tag	UNP O66528
B	480	PHE	-	expression tag	UNP O66528
B	481	GLN	-	expression tag	UNP O66528
B	482	GLY	-	expression tag	UNP O66528
B	483	GLY	-	expression tag	UNP O66528
B	484	ARG	-	expression tag	UNP O66528
B	485	GLY	-	expression tag	UNP O66528
B	486	SER	-	expression tag	UNP O66528
B	487	HIS	-	expression tag	UNP O66528
B	488	HIS	-	expression tag	UNP O66528
B	489	HIS	-	expression tag	UNP O66528
B	490	HIS	-	expression tag	UNP O66528
B	491	HIS	-	expression tag	UNP O66528
B	492	HIS	-	expression tag	UNP O66528
B	493	HIS	-	expression tag	UNP O66528
B	494	HIS	-	expression tag	UNP O66528
B	495	HIS	-	expression tag	UNP O66528
B	496	HIS	-	expression tag	UNP O66528

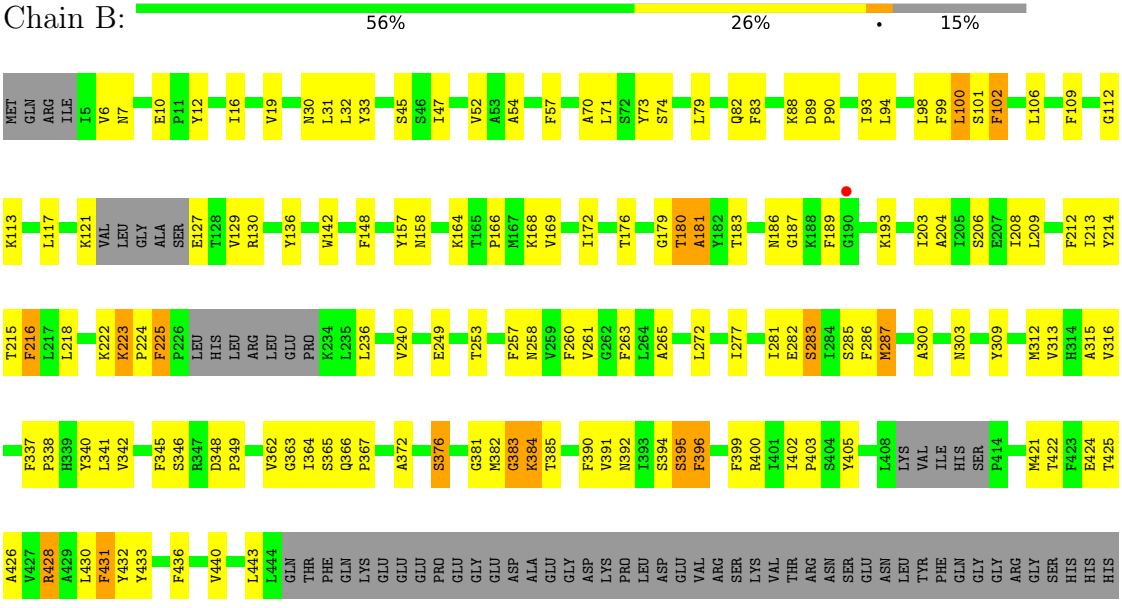
3 Residue-property plots (i)

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: Aq128



• Molecule 1: Aq128



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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.30Å 71.50Å 104.30Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	19.98 – 3.50 19.98 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.98-3.50) 99.8 (19.98-3.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.29Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.312 , 0.342 0.312 , 0.342	Depositor DCC
R_{free} test set	881 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	84.0	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	6632	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.42% 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	0.27	0/3396	0.45	0/4615
1	B	0.29	0/3426	0.51	1/4654 (0.0%)
All	All	0.28	0/6822	0.48	1/9269 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	222	LYS	C-N-CA	5.39	135.18	121.70

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	3301	0	3437	80	0
1	B	3331	0	3470	90	0
All	All	6632	0	6907	170	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 13.

All (170) 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:218:LEU:HA	1:B:223:LYS:HB2	1.48	0.95
1:B:6:VAL:HG11	1:B:315:ALA:HB2	1.52	0.90
1:B:157:TYR:HD2	1:B:166:PRO:HD3	1.41	0.83
1:A:424:GLU:OE2	1:A:428:ARG:NH2	2.16	0.78
1:B:390:PHE:O	1:B:394:SER:OG	2.02	0.76
1:B:223:LYS:HG2	1:B:224:PRO:HD3	1.70	0.73
1:B:249:GLU:O	1:B:253:THR:OG1	2.06	0.71
1:A:376:SER:HB2	1:A:432:TYR:CZ	2.27	0.70
1:B:6:VAL:HG12	1:B:303:ASN:HD21	1.58	0.69
1:A:323:THR:HG23	1:A:370:ALA:HB1	1.74	0.68
1:B:218:LEU:CA	1:B:223:LYS:HB2	2.23	0.68
1:A:79:LEU:HB3	1:A:93:ILE:HD13	1.75	0.67
1:A:141:PHE:HA	1:A:144:ILE:HG12	1.79	0.65
1:B:30:ASN:HB3	1:B:287:MET:HG3	1.78	0.65
1:B:176:THR:O	1:B:180:THR:OG1	2.14	0.64
1:B:101:SER:HB2	1:B:148:PHE:HB3	1.79	0.63
1:A:400:ARG:HD3	1:A:424:GLU:CD	2.19	0.62
1:A:36:GLU:OE2	1:A:177:HIS:ND1	2.27	0.61
1:A:281:ILE:HG21	1:A:359:LEU:HD22	1.83	0.61
1:B:164:LYS:O	1:B:168:LYS:HG2	2.01	0.61
1:B:391:VAL:HG22	1:B:431:PHE:HE2	1.65	0.61
1:A:356:SER:O	1:A:360:GLN:HG3	2.02	0.60
1:A:27:ILE:HG12	1:A:288:ILE:HA	1.83	0.60
1:B:100:LEU:HD13	1:B:236:LEU:HD23	1.82	0.60
1:A:218:LEU:HD13	1:A:224:PRO:HG2	1.84	0.59
1:B:157:TYR:CD2	1:B:166:PRO:HD3	2.30	0.59
1:A:221:PHE:O	1:A:223:LYS:N	2.36	0.59
1:B:337:PHE:O	1:B:341:LEU:HD13	2.01	0.59
1:B:281:ILE:HG23	1:B:341:LEU:HD23	1.85	0.59
1:A:397:TRP:O	1:A:402:ILE:HB	2.03	0.58
1:A:252:ILE:O	1:A:256:SER:OG	2.21	0.58
1:B:212:PHE:O	1:B:216:PHE:N	2.35	0.58
1:B:94:LEU:O	1:B:98:LEU:HG	2.03	0.57
1:B:157:TYR:HE1	1:B:223:LYS:HD2	1.69	0.57
1:B:169:VAL:HG11	1:B:214:TYR:CE1	2.40	0.57
1:B:203:ILE:O	1:B:206:SER:OG	2.21	0.57
1:A:400:ARG:NH1	1:A:421:MET:HB2	2.21	0.56
1:B:179:GLY:O	1:B:181:ALA:N	2.36	0.56
1:A:90:PRO:HG2	1:A:225:PHE:CE2	2.41	0.55
1:B:396:PHE:HA	1:B:400:ARG:HG2	1.87	0.55
1:B:287:MET:SD	1:B:287:MET:N	2.80	0.55
1:A:390:PHE:O	1:A:394:SER:OG	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PRO:O	1:A:96:ASN:ND2	2.36	0.54
1:B:421:MET:O	1:B:425:THR:HG22	2.07	0.54
1:A:404:SER:O	1:A:408:LEU:HB2	2.08	0.54
1:B:127:GLU:HA	1:B:130:ARG:HD2	1.90	0.53
1:A:303:ASN:HB2	1:A:312:MET:HB3	1.90	0.53
1:A:355:ALA:O	1:A:359:LEU:HG	2.09	0.53
1:B:82:GLN:NE2	1:B:381:GLY:O	2.42	0.52
1:A:26:ILE:HG21	1:A:294:ILE:HD12	1.91	0.52
1:A:365:SER:HB3	1:A:422:THR:HG23	1.91	0.52
1:A:424:GLU:HA	1:A:427:VAL:HG22	1.92	0.51
1:B:400:ARG:HD2	1:B:424:GLU:CD	2.31	0.51
1:B:282:GLU:OE1	1:B:362:VAL:HG11	2.10	0.51
1:B:71:LEU:HD11	1:B:240:VAL:HA	1.92	0.51
1:B:102:PHE:CE2	1:B:106:LEU:HD21	2.47	0.50
1:B:309:TYR:O	1:B:313:VAL:HG23	2.12	0.50
1:A:205:ILE:HA	1:A:208:ILE:HG12	1.92	0.50
1:A:392:ASN:OD1	1:A:432:TYR:OH	2.19	0.50
1:B:215:THR:HA	1:B:218:LEU:HD22	1.94	0.50
1:A:376:SER:O	1:A:380:LYS:HG3	2.11	0.50
1:A:400:ARG:O	1:A:401:ILE:HB	2.12	0.50
1:B:282:GLU:HB3	1:B:286:PHE:CZ	2.47	0.50
1:A:293:MET:HG2	1:A:377:GLY:HA3	1.93	0.50
1:B:94:LEU:HD22	1:B:225:PHE:HE1	1.76	0.50
1:B:395:SER:OG	1:B:428:ARG:NH1	2.45	0.49
1:B:258:ASN:O	1:B:261:VAL:HG12	2.13	0.49
1:A:100:LEU:O	1:A:104:ILE:HG13	2.12	0.49
1:B:6:VAL:HG23	1:B:10:GLU:OE2	2.11	0.49
1:B:391:VAL:HG22	1:B:431:PHE:CE2	2.47	0.49
1:B:54:ALA:HB2	1:B:129:VAL:HG13	1.93	0.49
1:B:70:ALA:HA	1:B:73:TYR:HB3	1.95	0.49
1:B:283:SER:HA	1:B:286:PHE:HB2	1.95	0.49
1:B:365:SER:HB3	1:B:422:THR:HG23	1.95	0.49
1:B:316:VAL:HG21	1:B:436:PHE:CZ	2.48	0.49
1:A:281:ILE:HG21	1:A:359:LEU:CD2	2.42	0.49
1:B:424:GLU:OE2	1:B:428:ARG:NH1	2.43	0.49
1:B:45:SER:HA	1:B:52:VAL:HG22	1.95	0.48
1:B:70:ALA:O	1:B:74:SER:N	2.39	0.48
1:B:117:LEU:HD23	1:B:130:ARG:HB3	1.95	0.48
1:B:83:PHE:HB3	1:B:90:PRO:HB3	1.95	0.48
1:B:337:PHE:HB3	1:B:340:TYR:HD1	1.78	0.48
1:A:218:LEU:HG	1:A:219:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PHE:HB2	1:A:401:ILE:HD11	1.96	0.48
1:A:293:MET:HG3	1:A:373:SER:O	2.13	0.48
1:A:436:PHE:O	1:A:440:VAL:HG23	2.13	0.48
1:B:31:LEU:O	1:B:33:TYR:N	2.41	0.48
1:A:387:ILE:N	1:A:388:PRO:HD2	2.29	0.48
1:B:260:PHE:O	1:B:263:PHE:HB2	2.14	0.48
1:B:338:PRO:O	1:B:342:VAL:HG23	2.14	0.47
1:B:169:VAL:HG22	1:B:213:ILE:HG21	1.96	0.47
1:A:120:MET:HB3	1:A:130:ARG:HG2	1.97	0.47
1:A:372:ALA:HA	1:A:432:TYR:HD1	1.80	0.47
1:B:282:GLU:O	1:B:285:SER:N	2.48	0.47
1:A:62:LEU:O	1:A:66:TYR:N	2.47	0.47
1:A:30:ASN:HB3	1:A:287:MET:SD	2.55	0.47
1:B:265:ALA:HA	1:B:272:LEU:HD21	1.96	0.47
1:A:61:LEU:HD11	1:A:119:LEU:HD23	1.98	0.46
1:A:335:ILE:HG12	1:A:360:GLN:HA	1.98	0.46
1:A:288:ILE:O	1:A:292:VAL:HG23	2.15	0.46
1:A:303:ASN:CB	1:A:312:MET:HB3	2.46	0.46
1:A:431:PHE:O	1:A:435:VAL:HG13	2.16	0.46
1:B:79:LEU:HB3	1:B:93:ILE:HD13	1.97	0.46
1:B:282:GLU:OE1	1:B:286:PHE:CE1	2.69	0.46
1:B:348:ASP:OD1	1:B:349:PRO:HD2	2.16	0.46
1:B:364:ILE:O	1:B:367:PRO:HD2	2.16	0.46
1:B:363:GLY:HA2	1:B:366:GLN:HG2	1.97	0.45
1:B:372:ALA:O	1:B:376:SER:HB3	2.16	0.45
1:A:218:LEU:HA	1:A:224:PRO:CD	2.46	0.45
1:A:260:PHE:O	1:A:263:PHE:HB2	2.16	0.45
1:B:313:VAL:HG22	1:B:440:VAL:HG21	1.98	0.45
1:A:277:ILE:HA	1:A:280:ARG:HD2	1.99	0.45
1:A:361:ILE:HG21	1:A:418:TRP:HB3	1.98	0.45
1:B:215:THR:HA	1:B:218:LEU:CD2	2.47	0.45
1:B:31:LEU:HG	1:B:32:LEU:H	1.81	0.45
1:A:204:ALA:O	1:A:208:ILE:HG23	2.18	0.44
1:B:88:LYS:HD3	1:B:89:ASP:H	1.82	0.44
1:B:168:LYS:O	1:B:172:ILE:HG13	2.17	0.44
1:A:337:PHE:O	1:A:341:LEU:HD13	2.18	0.44
1:B:277:ILE:HG23	1:B:345:PHE:HD1	1.82	0.44
1:B:402:ILE:HB	1:B:403:PRO:HD3	1.99	0.44
1:A:263:PHE:HE2	1:A:401:ILE:HG23	1.81	0.44
1:B:282:GLU:CD	1:B:362:VAL:HG11	2.38	0.44
1:A:359:LEU:HA	1:A:362:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:TYR:O	1:B:436:PHE:N	2.50	0.44
1:A:164:LYS:O	1:A:168:LYS:HG2	2.18	0.44
1:B:382:MET:O	1:B:384:LYS:N	2.51	0.43
1:A:26:ILE:HD11	1:A:163:THR:HG21	2.00	0.43
1:A:263:PHE:CE2	1:A:401:ILE:HG23	2.54	0.43
1:A:323:THR:HG21	1:A:374:ILE:HG13	1.99	0.43
1:B:396:PHE:O	1:B:400:ARG:HG2	2.18	0.43
1:A:265:ALA:HA	1:A:272:LEU:HD12	2.01	0.43
1:B:383:GLY:O	1:B:385:THR:N	2.51	0.43
1:A:101:SER:HB2	1:A:148:PHE:HB3	2.00	0.43
1:B:282:GLU:OE1	1:B:286:PHE:HE1	2.00	0.43
1:A:278:GLY:HA3	1:A:358:TYR:CE2	2.53	0.42
1:B:223:LYS:NZ	1:B:224:PRO:HD2	2.34	0.42
1:B:424:GLU:OE2	1:B:428:ARG:NH2	2.53	0.42
1:A:332:LEU:HG	1:A:336:LEU:HD13	2.01	0.42
1:A:365:SER:O	1:A:365:SER:OG	2.35	0.42
1:A:395:SER:O	1:A:396:PHE:C	2.57	0.42
1:A:416:VAL:HB	1:A:417:PRO:HD3	2.02	0.42
1:A:91:SER:N	1:A:92:PRO:HD2	2.34	0.42
1:A:177:HIS:CE1	1:A:203:ILE:HG12	2.54	0.42
1:A:208:ILE:HG13	1:A:209:LEU:N	2.33	0.42
1:A:320:ALA:HA	1:A:323:THR:HG22	2.02	0.42
1:A:375:TYR:O	1:A:379:LEU:HD13	2.20	0.42
1:B:204:ALA:O	1:B:208:ILE:HD12	2.20	0.42
1:A:197:GLU:HG2	1:A:201:TRP:CD1	2.55	0.41
1:B:183:THR:HG21	1:B:189:PHE:HB2	2.02	0.41
1:A:62:LEU:HD12	1:A:62:LEU:HA	1.86	0.41
1:A:73:TYR:HB2	1:A:151:ASN:OD1	2.20	0.41
1:A:309:TYR:O	1:A:313:VAL:HG23	2.19	0.41
1:A:408:LEU:HD12	1:A:408:LEU:HA	1.89	0.41
1:A:414:PRO:O	1:A:417:PRO:HD2	2.21	0.41
1:B:186:ASN:O	1:B:193:LYS:HG2	2.20	0.41
1:B:16:ILE:HA	1:B:19:VAL:HG12	2.03	0.41
1:A:218:LEU:HG	1:A:219:ILE:N	2.35	0.41
1:A:338:PRO:HB3	1:A:356:SER:HB2	2.03	0.41
1:A:424:GLU:HA	1:A:427:VAL:CG2	2.51	0.41
1:B:183:THR:O	1:B:187:GLY:N	2.54	0.41
1:B:209:LEU:HD12	1:B:209:LEU:HA	1.87	0.41
1:B:300:ALA:HA	1:B:312:MET:HG3	2.03	0.41
1:B:392:ASN:ND2	1:B:432:TYR:OH	2.47	0.41
1:B:402:ILE:O	1:B:405:TYR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ARG:HD2	1:B:432:TYR:HE1	1.85	0.41
1:A:157:TYR:OH	1:A:224:PRO:HG3	2.22	0.40
1:B:399:PHE:HA	1:B:403:PRO:HG2	2.03	0.40
1:B:440:VAL:HA	1:B:443:LEU:HG	2.03	0.40
1:A:248:LEU:O	1:A:252:ILE:HG13	2.21	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	411/496 (83%)	367 (89%)	36 (9%)	8 (2%)	8	40
1	B	415/496 (84%)	366 (88%)	35 (8%)	14 (3%)	3	28
All	All	826/992 (83%)	733 (89%)	71 (9%)	22 (3%)	5	33

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	LYS
1	A	396	PHE
1	B	181	ALA
1	B	223	LYS
1	B	384	LYS
1	A	64	PHE
1	A	67	SER
1	A	338	PRO
1	B	100	LEU
1	B	180	THR
1	B	383	GLY
1	B	431	PHE
1	A	395	SER

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Mol	Chain	Res	Type
1	B	12	TYR
1	B	47	ILE
1	B	136	TYR
1	B	426	ALA
1	B	112	GLY
1	B	396	PHE
1	A	110	PHE
1	B	430	LEU
1	A	401	ILE

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	357/424 (84%)	345 (97%)	12 (3%)	37 68
1	B	359/424 (85%)	341 (95%)	18 (5%)	24 58
All	All	716/848 (84%)	686 (96%)	30 (4%)	30 63

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	LYS
1	A	225	PHE
1	A	321	HIS
1	A	340	TYR
1	A	348	ASP
1	A	365	SER
1	A	376	SER
1	A	396	PHE
1	A	406	PHE
1	A	409	LYS
1	A	431	PHE
1	A	433	TYR
1	B	7	ASN
1	B	57	PHE

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Mol	Chain	Res	Type
1	B	99	PHE
1	B	102	PHE
1	B	109	PHE
1	B	113	LYS
1	B	121	LYS
1	B	142	TRP
1	B	158	ASN
1	B	216	PHE
1	B	225	PHE
1	B	257	PHE
1	B	283	SER
1	B	287	MET
1	B	346	SER
1	B	376	SER
1	B	395	SER
1	B	428	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	B	303	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 monosaccharides 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^{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	419/496 (84%)	-0.13	3 (0%)	87	83	39, 71, 108, 138	0
1	B	423/496 (85%)	-0.15	1 (0%)	95	93	37, 74, 106, 120	0
All	All	842/992 (84%)	-0.14	4 (0%)	91	88	37, 72, 107, 138	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	ASN	2.6
1	A	267	PHE	2.3
1	A	276	GLN	2.1
1	B	190	GLY	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 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.