Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 03:53 AM EDT

PDB ID	:	2QR4
Title	:	Crystal structure of oligoendopeptidase-F from Enterococcus faecium
Authors	:	Ramagopal, U.A.; Toro, R.; Meyer, A.J.; Freeman, J.; Bain, K.; Rodgers, L.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-07-27
Resolution	:	2.50 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 (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 (i)) were used in the production of this report:

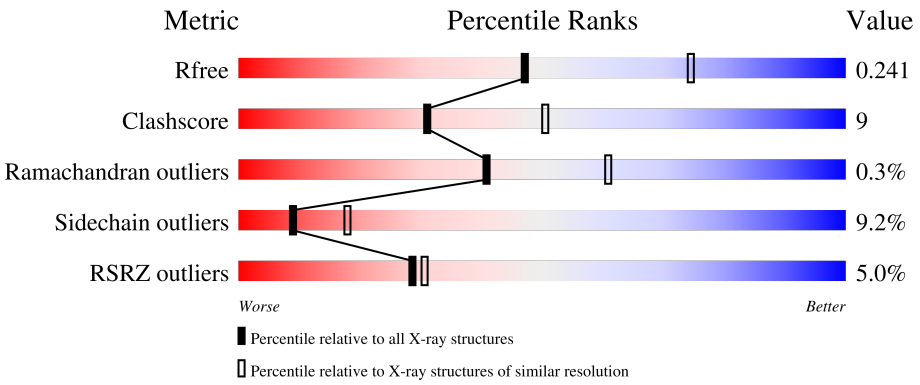
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	587	4% 68% 18% • 11%
1	B	587	4% 68% 15% • 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8549 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 Peptidase M3B, oligoendopeptidase F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	521	4265	2723	700	832	10	0	4	0
1	B	506	4096	2612	675	800	9	0	2	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MSE	-	expression tag	UNP Q3XYC8
A	24	SER	-	expression tag	UNP Q3XYC8
A	25	LEU	-	expression tag	UNP Q3XYC8
A	602	GLU	-	expression tag	UNP Q3XYC8
A	603	GLY	-	expression tag	UNP Q3XYC8
A	604	HIS	-	expression tag	UNP Q3XYC8
A	605	HIS	-	expression tag	UNP Q3XYC8
A	606	HIS	-	expression tag	UNP Q3XYC8
A	607	HIS	-	expression tag	UNP Q3XYC8
A	608	HIS	-	expression tag	UNP Q3XYC8
A	609	HIS	-	expression tag	UNP Q3XYC8
B	23	MSE	-	expression tag	UNP Q3XYC8
B	24	SER	-	expression tag	UNP Q3XYC8
B	25	LEU	-	expression tag	UNP Q3XYC8
B	602	GLU	-	expression tag	UNP Q3XYC8
B	603	GLY	-	expression tag	UNP Q3XYC8
B	604	HIS	-	expression tag	UNP Q3XYC8
B	605	HIS	-	expression tag	UNP Q3XYC8
B	606	HIS	-	expression tag	UNP Q3XYC8
B	607	HIS	-	expression tag	UNP Q3XYC8
B	608	HIS	-	expression tag	UNP Q3XYC8
B	609	HIS	-	expression tag	UNP Q3XYC8

- Molecule 2 is water.

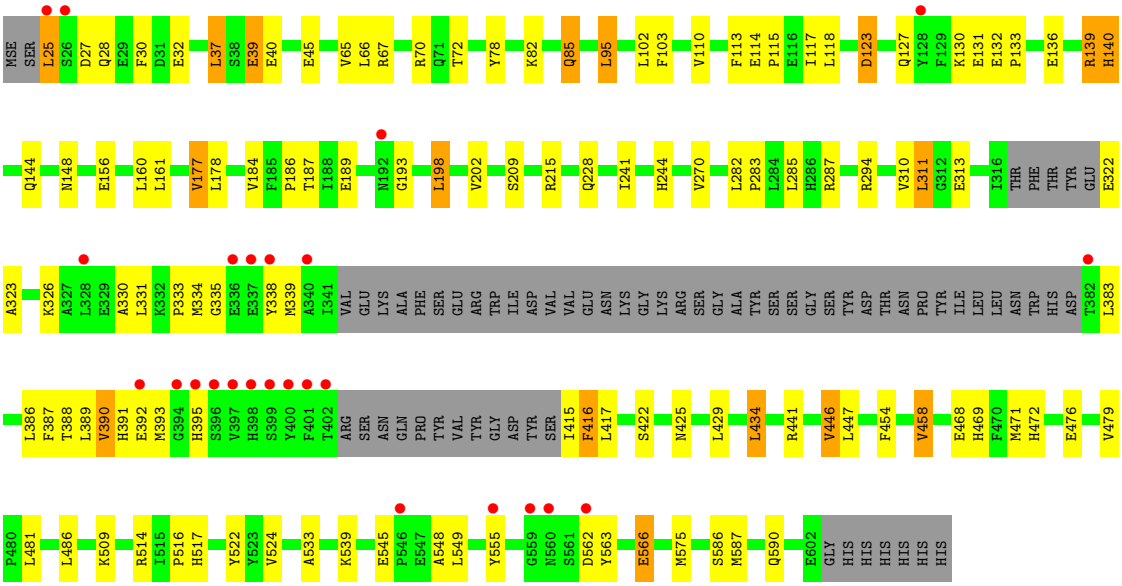
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	99	99	99	0	0
			Total	O		
2	B	89	89	89	0	0

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.

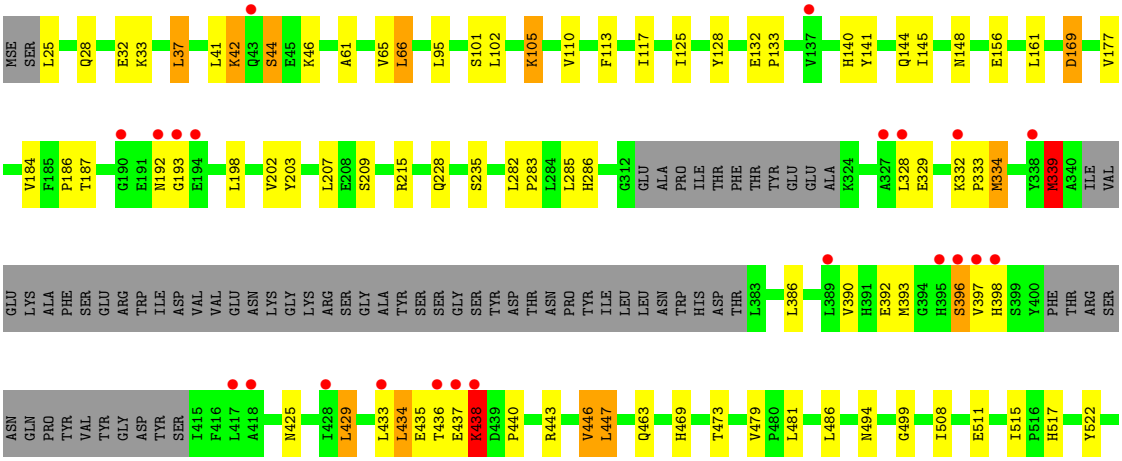
• Molecule 1: Peptidase M3B, oligoendopeptidase F

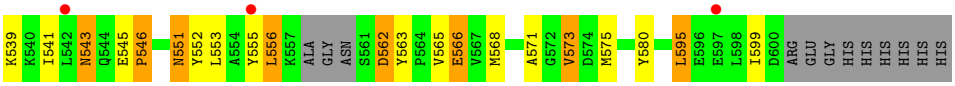
Chain A:



• Molecule 1: Peptidase M3B, oligoendopeptidase F

Chain B:




K539
K540
I541
L542
N543
Q544
E545
P546
N551
Y552
L553
A554
Y555
L556
K557
ALA
GLY
ASN
S561
D562
Y563
P564
V565
E566
V567
M568
A571
G572
V573
D574
M575
Y580
L595
E596
E597
L598
I599
D600
ARG
GLU
GLY
HIS
HIS
HIS
HIS
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HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	133.14Å 133.14Å 171.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 2.50 39.04 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.04-2.50) 99.9 (39.04-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.244 0.186 , 0.241	Depositor DCC
R_{free} test set	2726 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	46.5	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8549	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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	0.43	0/4351	0.55	0/5872
1	B	0.61	8/4176 (0.2%)	0.60	4/5632 (0.1%)
All	All	0.53	8/8527 (0.1%)	0.57	4/11504 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	437	GLU	CD-OE1	13.75	1.40	1.25
1	B	437	GLU	CD-OE2	13.01	1.40	1.25
1	B	435	GLU	CD-OE1	9.15	1.35	1.25
1	B	436	THR	CB-OG1	-7.43	1.28	1.43
1	B	435	GLU	CD-OE2	6.90	1.33	1.25
1	B	438	LYS	C-O	6.62	1.35	1.23
1	B	437	GLU	CG-CD	6.57	1.61	1.51
1	B	551	ASN	CG-OD1	5.15	1.35	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	437	GLU	OE1-CD-OE2	-8.59	113.00	123.30
1	B	437	GLU	CG-CD-OE2	6.98	132.26	118.30
1	B	436	THR	CA-CB-OG1	5.62	120.80	109.00
1	B	436	THR	CA-CB-CG2	-5.41	104.83	112.40

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	4265	0	4074	72	0
1	B	4096	0	3863	81	0
2	A	99	0	0	5	0
2	B	89	0	0	3	0
All	All	8549	0	7937	149	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 9.

All (149) 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:228:GLN:NE2	1:B:184:VAL:HG12	1.62	1.11
1:B:438:LYS:H	1:B:438:LYS:HD2	1.35	0.90
1:A:533:ALA:HB2	1:A:575:MSE:HE3	1.53	0.90
1:A:228:GLN:HE22	1:B:184:VAL:HG12	1.37	0.90
1:B:463:GLN:HE22	1:B:494:ASN:HD22	1.20	0.86
1:B:553:LEU:HA	1:B:556:LEU:HD13	1.57	0.86
1:B:390:VAL:HG12	1:B:425:ASN:HB3	1.66	0.76
1:B:434:LEU:HD11	1:B:447:LEU:HD13	1.67	0.75
1:B:517:HIS:HD2	2:B:622:HOH:O	1.69	0.74
1:B:553:LEU:HA	1:B:556:LEU:CD1	2.16	0.74
1:A:28:GLN:NE2	1:A:32:GLU:OE2	2.22	0.71
1:A:389:LEU:O	1:A:393:MSE:HG3	1.91	0.70
1:A:70:ARG:HD2	2:A:644:HOH:O	1.91	0.69
1:B:334:MSE:CE	1:B:541:ILE:HD13	2.23	0.69
1:B:334:MSE:HE1	1:B:541:ILE:HD13	1.74	0.69
1:A:509:LYS:HD3	2:A:679:HOH:O	1.92	0.68
1:A:563:TYR:HB3	1:A:566:GLU:HG2	1.73	0.68
1:B:434:LEU:HD13	1:B:446:VAL:CG2	2.23	0.68
1:A:123:ASP:OD2	1:A:123:ASP:N	2.27	0.67
1:B:140:HIS:HE1	1:B:562:ASP:HB2	1.60	0.67
1:B:141:TYR:CZ	1:B:145:ILE:HD11	2.29	0.67
1:B:140:HIS:CE1	1:B:562:ASP:HB2	2.32	0.65
1:A:25:LEU:HA	1:A:28:GLN:HB3	1.79	0.64
1:A:39:GLU:HG3	1:A:40:GLU:N	2.13	0.63
1:B:398:HIS:HD2	1:B:556:LEU:HB2	1.65	0.62
1:A:587:MSE:HG3	2:A:686:HOH:O	2.00	0.61
1:B:42:LYS:HD3	1:B:42:LYS:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:N	1:A:25:LEU:HD23	2.16	0.61
1:B:392:GLU:O	1:B:396:SER:HB2	2.02	0.60
1:B:425:ASN:O	1:B:429:LEU:HD23	2.02	0.59
1:B:438:LYS:H	1:B:438:LYS:CD	2.12	0.59
1:A:563:TYR:HB3	1:A:566:GLU:CG	2.30	0.59
1:B:438:LYS:HD2	1:B:438:LYS:N	2.15	0.58
1:A:434:LEU:CD1	1:A:446:VAL:HG22	2.33	0.58
1:A:127:GLN:O	1:A:131:GLU:HG3	2.04	0.58
1:A:323:ALA:HB1	1:A:386:LEU:HD13	1.86	0.58
1:B:42:LYS:N	1:B:42:LYS:CD	2.67	0.57
1:B:192:ASN:OD1	1:B:193:GLY:N	2.31	0.55
1:A:27:ASP:HB3	1:A:95:LEU:HD23	1.89	0.55
1:A:177:VAL:CG1	1:A:178:LEU:N	2.70	0.55
1:A:241:ILE:HD13	1:A:471:MSE:HB3	1.88	0.55
1:A:113:PHE:CZ	1:A:117:ILE:HD11	2.41	0.55
1:B:144:GLN:HA	1:B:144:GLN:OE1	2.07	0.54
1:A:228:GLN:NE2	1:B:184:VAL:CG1	2.54	0.54
1:B:539:LYS:O	1:B:543:ASN:HB2	2.08	0.54
1:B:101:SER:O	1:B:105:LYS:HE2	2.07	0.54
1:A:209:SER:O	1:A:215:ARG:HD3	2.07	0.53
1:B:434:LEU:HD13	1:B:446:VAL:HG21	1.90	0.53
1:A:244:HIS:ND1	1:A:472:HIS:HE1	2.07	0.53
1:A:469:HIS:HD2	1:A:522:TYR:OH	1.91	0.53
1:B:334:MSE:HE3	1:B:541:ILE:HG21	1.90	0.53
1:B:463:GLN:HE22	1:B:494:ASN:ND2	1.99	0.53
1:B:113:PHE:CZ	1:B:117:ILE:HD11	2.44	0.52
1:B:186:PRO:O	1:B:198:LEU:HB2	2.10	0.51
1:A:533:ALA:HB2	1:A:575:MSE:CE	2.36	0.51
1:A:45:GLU:HA	1:A:45:GLU:OE1	2.11	0.51
1:B:125:ILE:O	1:B:128:TYR:HB2	2.11	0.51
1:B:575:MSE:HA	1:B:580:TYR:CE1	2.45	0.51
1:A:434:LEU:HD13	1:A:446:VAL:HG22	1.93	0.50
1:A:40:GLU:OE2	1:A:67:ARG:HD2	2.11	0.50
1:B:334:MSE:CE	1:B:334:MSE:HA	2.42	0.50
1:B:568:MSE:HG3	1:B:573:VAL:HG13	1.93	0.50
1:B:156:GLU:HG3	2:B:635:HOH:O	2.11	0.50
1:B:393:MSE:O	1:B:397:VAL:HG23	2.11	0.50
1:B:599:ILE:HG22	1:B:599:ILE:O	2.12	0.49
1:B:429:LEU:HD23	1:B:429:LEU:H	1.78	0.49
1:B:545:GLU:CB	1:B:546:PRO:HD2	2.43	0.49
1:B:61:ALA:O	1:B:65:VAL:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASP:HA	1:A:30:PHE:HB3	1.95	0.48
1:A:310:VAL:HG23	1:A:311:LEU:HD22	1.96	0.48
1:A:416:PHE:CD2	1:A:416:PHE:C	2.85	0.48
1:A:72:THR:HG22	1:A:103:PHE:HD1	1.78	0.48
1:B:565:VAL:HA	1:B:575:MSE:CE	2.43	0.48
1:A:136:GLU:OE2	1:A:139:ARG:NE	2.39	0.48
1:A:434:LEU:HD11	1:A:446:VAL:HG22	1.96	0.48
1:A:468:GLU:O	1:A:472:HIS:HD2	1.97	0.48
1:A:156:GLU:HG3	2:A:696:HOH:O	2.13	0.48
1:A:282:LEU:N	1:A:283:PRO:CD	2.77	0.48
1:B:433:LEU:HD23	1:B:446:VAL:HG11	1.96	0.48
1:B:113:PHE:CE2	1:B:117:ILE:HD11	2.49	0.47
1:A:27:ASP:HB3	1:A:95:LEU:CD2	2.45	0.47
1:B:334:MSE:HA	1:B:334:MSE:HE2	1.96	0.47
1:A:390:VAL:HG13	1:A:425:ASN:HB3	1.96	0.47
1:A:434:LEU:HD13	1:A:446:VAL:CG2	2.45	0.47
1:B:440:PRO:HA	1:B:443:ARG:HB2	1.95	0.47
1:A:25:LEU:N	1:A:25:LEU:CD2	2.77	0.47
1:A:189:GLU:OE1	1:A:193:GLY:HA2	2.15	0.47
1:A:586:SER:O	1:A:590:GLN:HG2	2.16	0.46
1:A:140:HIS:HE1	1:A:562:ASP:OD2	1.97	0.46
1:B:46:LYS:HG2	1:B:46:LYS:O	2.15	0.46
1:B:469:HIS:HD2	1:B:522:TYR:OH	1.98	0.46
1:B:511:GLU:HG2	1:B:515:ILE:HD11	1.98	0.46
1:B:332:LYS:N	1:B:333:PRO:CD	2.79	0.46
1:A:330:ALA:O	1:A:333:PRO:HD2	2.15	0.45
1:A:454:PHE:CD1	1:A:458:VAL:HG13	2.52	0.45
1:A:177:VAL:HG12	1:A:178:LEU:N	2.31	0.45
1:B:65:VAL:HB	1:B:110:VAL:HG22	1.98	0.45
1:A:186:PRO:O	1:A:198:LEU:HB2	2.16	0.45
1:A:294:ARG:NH2	2:A:683:HOH:O	2.43	0.45
1:B:434:LEU:HD13	1:B:446:VAL:HG22	1.96	0.44
1:B:545:GLU:HB3	1:B:546:PRO:HD2	1.99	0.44
1:A:391:HIS:CD2	1:A:422:SER:HB3	2.53	0.44
1:A:514:ARG:O	1:A:516:PRO:HD3	2.18	0.44
1:B:66:LEU:HD12	1:B:66:LEU:HA	1.66	0.44
1:B:434:LEU:CD1	1:B:446:VAL:HG22	2.48	0.44
1:B:140:HIS:CE1	1:B:144:GLN:HE21	2.36	0.44
1:B:203:TYR:CE1	1:B:207:LEU:HD21	2.52	0.44
1:B:438:LYS:CD	1:B:438:LYS:N	2.79	0.44
1:A:114:GLU:HB2	1:A:115:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:MSE:HE3	1:B:541:ILE:HD13	1.97	0.43
1:A:334:MSE:HE2	1:A:338:TYR:CD1	2.53	0.43
1:B:140:HIS:HE1	1:B:562:ASP:CB	2.29	0.43
1:B:209:SER:O	1:B:215:ARG:HD3	2.18	0.43
1:B:169:ASP:HA	2:B:684:HOH:O	2.18	0.43
1:B:563:TYR:HB3	1:B:566:GLU:HG2	2.00	0.43
1:B:282:LEU:N	1:B:283:PRO:CD	2.81	0.43
1:A:78:TYR:OH	1:A:82:LYS:HE2	2.19	0.43
1:B:329:GLU:O	1:B:332:LYS:HB2	2.18	0.43
1:B:434:LEU:HD12	1:B:434:LEU:HA	1.74	0.43
1:B:37:LEU:HD12	1:B:37:LEU:HA	1.77	0.42
1:A:326:LYS:HE3	1:A:326:LYS:HB2	1.82	0.42
1:A:387:PHE:CD2	1:A:429:LEU:HD23	2.55	0.42
1:B:286:HIS:CD2	1:B:499:GLY:HA3	2.54	0.42
1:A:132:GLU:HA	1:A:133:PRO:HD2	1.77	0.42
1:A:388:THR:HG22	1:A:392:GLU:OE1	2.19	0.42
1:B:552:TYR:O	1:B:556:LEU:HD13	2.20	0.42
1:A:130:LYS:HE2	1:A:130:LYS:HB3	1.78	0.42
1:A:517:HIS:HB3	1:A:524:VAL:HG13	2.02	0.42
1:B:41:LEU:O	1:B:44:SER:OG	2.37	0.41
1:B:132:GLU:HA	1:B:133:PRO:HD2	1.88	0.41
1:B:328:LEU:O	1:B:339:MSE:HE2	2.20	0.41
1:A:545:GLU:HB3	1:A:548:ALA:HB2	2.02	0.41
1:B:595:LEU:O	1:B:599:ILE:HG12	2.20	0.41
1:A:335:GLY:O	1:A:339:MSE:HG2	2.21	0.41
1:A:82:LYS:O	1:A:85[B]:GLN:HB3	2.20	0.41
1:A:416:PHE:HZ	1:A:575:MSE:HE1	1.86	0.41
1:B:42:LYS:H	1:B:42:LYS:CD	2.28	0.41
1:B:398:HIS:CD2	1:B:556:LEU:HB2	2.51	0.41
1:B:508:ILE:HA	1:B:508:ILE:HD12	1.85	0.41
1:A:25:LEU:HA	1:A:28:GLN:CB	2.48	0.41
1:B:553:LEU:HA	1:B:556:LEU:HD11	2.01	0.41
1:A:184:VAL:HG13	1:B:228:GLN:NE2	2.37	0.40
1:B:551:ASN:HB3	1:B:571:ALA:HA	2.02	0.40
1:A:95:LEU:HD22	1:A:95:LEU:HA	1.93	0.40
1:A:549:LEU:HD13	1:A:549:LEU:HA	1.95	0.40
1:A:37:LEU:HD12	1:A:37:LEU:HA	1.81	0.40
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.89	0.40
1:A:533:ALA:CB	1:A:575:MSE:HE3	2.37	0.40
1:B:28:GLN:O	1:B:32:GLU:HG3	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	517/587 (88%)	505 (98%)	11 (2%)	1 (0%)	47	68
1	B	498/587 (85%)	476 (96%)	20 (4%)	2 (0%)	34	54
All	All	1015/1174 (86%)	981 (97%)	31 (3%)	3 (0%)	41	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	GLU
1	B	546	PRO
1	B	339	MSE

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	454/504 (90%)	409 (90%)	45 (10%)	8	15
1	B	430/504 (85%)	393 (91%)	37 (9%)	10	20
All	All	884/1008 (88%)	802 (91%)	82 (9%)	9	17

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	37	LEU
1	A	39	GLU

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Mol	Chain	Res	Type
1	A	65	VAL
1	A	66	LEU
1	A	85[A]	GLN
1	A	85[B]	GLN
1	A	95	LEU
1	A	102	LEU
1	A	110	VAL
1	A	123	ASP
1	A	139	ARG
1	A	140	HIS
1	A	144	GLN
1	A	148	ASN
1	A	160	LEU
1	A	161	LEU
1	A	177	VAL
1	A	187	THR
1	A	198	LEU
1	A	202	VAL
1	A	270	VAL
1	A	285	LEU
1	A	287	ARG
1	A	311	LEU
1	A	322	GLU
1	A	331	LEU
1	A	383	LEU
1	A	390	VAL
1	A	395	HIS
1	A	415	ILE
1	A	416	PHE
1	A	417	LEU
1	A	434	LEU
1	A	441	ARG
1	A	446	VAL
1	A	447	LEU
1	A	458	VAL
1	A	476	GLU
1	A	479	VAL
1	A	481	LEU
1	A	486	LEU
1	A	539	LYS
1	A	555	TYR
1	A	566	GLU

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Mol	Chain	Res	Type
1	B	25	LEU
1	B	33	LYS
1	B	37	LEU
1	B	42	LYS
1	B	44	SER
1	B	66	LEU
1	B	95	LEU
1	B	102	LEU
1	B	105	LYS
1	B	148	ASN
1	B	161	LEU
1	B	169	ASP
1	B	177	VAL
1	B	187	THR
1	B	202	VAL
1	B	235	SER
1	B	285	LEU
1	B	334	MSE
1	B	339	MSE
1	B	386	LEU
1	B	396	SER
1	B	429	LEU
1	B	434	LEU
1	B	438	LYS
1	B	446	VAL
1	B	447	LEU
1	B	473	THR
1	B	479	VAL
1	B	481	LEU
1	B	486	LEU
1	B	543	ASN
1	B	555	TYR
1	B	556	LEU
1	B	562	ASP
1	B	566	GLU
1	B	573	VAL
1	B	595	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN

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Mol	Chain	Res	Type
1	A	53	GLN
1	A	148	ASN
1	A	179	ASN
1	A	192	ASN
1	A	228	GLN
1	A	231	ASN
1	A	281	HIS
1	A	385	GLN
1	A	448	ASN
1	A	469	HIS
1	A	472	HIS
1	A	543	ASN
1	B	53	GLN
1	B	140	HIS
1	B	148	ASN
1	B	197	GLN
1	B	265	HIS
1	B	281	HIS
1	B	395	HIS
1	B	398	HIS
1	B	427	ASN
1	B	448	ASN
1	B	469	HIS
1	B	494	ASN

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	511/587 (87%)	0.28	25 (4%)	29	31	28, 45, 68, 123	0
1	B	496/587 (84%)	0.16	25 (5%)	28	30	33, 45, 66, 91	0
All	All	1007/1174 (85%)	0.22	50 (4%)	28	30	28, 45, 68, 123	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	GLY	6.2
1	A	400	TYR	5.0
1	A	402	THR	4.5
1	A	340	ALA	4.4
1	A	395	HIS	4.3
1	B	397	VAL	4.2
1	A	25	LEU	4.2
1	B	542	LEU	4.0
1	B	395	HIS	3.8
1	A	392	GLU	3.8
1	A	26	SER	3.8
1	B	327	ALA	3.7
1	A	560	ASN	3.7
1	A	336	GLU	3.6
1	A	398	HIS	3.6
1	B	389	LEU	3.5
1	A	328	LEU	3.5
1	A	396	SER	3.5
1	A	399	SER	3.5
1	A	401	PHE	3.5
1	B	396	SER	3.4
1	B	43	GLN	3.3
1	A	338	TYR	3.3
1	B	338	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	397	VAL	3.2
1	A	555	TYR	3.1
1	B	418	ALA	3.0
1	A	394	GLY	2.9
1	B	192	ASN	2.7
1	B	194	GLU	2.7
1	B	555	TYR	2.7
1	A	337	GLU	2.5
1	B	437	GLU	2.5
1	A	382	THR	2.5
1	B	417	LEU	2.4
1	A	546	PRO	2.4
1	B	332	LYS	2.3
1	A	559	GLY	2.3
1	B	190	GLY	2.2
1	B	433	LEU	2.2
1	B	398	HIS	2.2
1	A	192	ASN	2.2
1	B	328	LEU	2.2
1	B	428	ILE	2.1
1	A	128	TYR	2.1
1	B	137	VAL	2.1
1	B	597	GLU	2.1
1	B	438	LYS	2.1
1	A	562	ASP	2.1
1	B	436	THR	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.