



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:29 AM UTC

PDB ID : 2QR4 / pdb_00002qr4
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

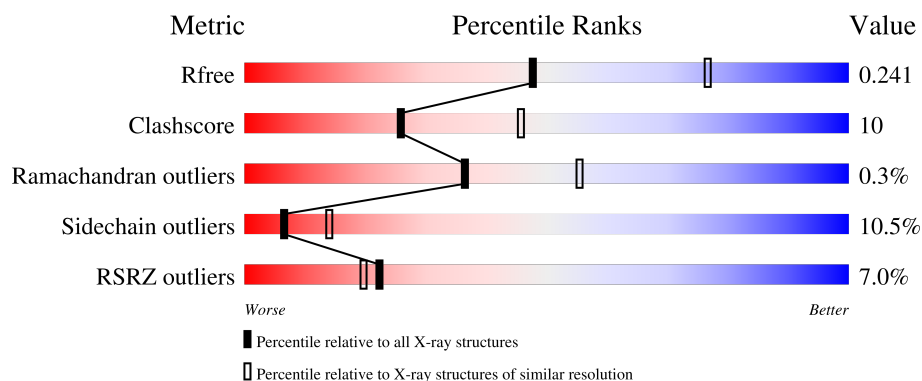
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	3% 68% 18% • 11%
1	B	587	9% 65% 17% • 14%

2 Entry composition

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.

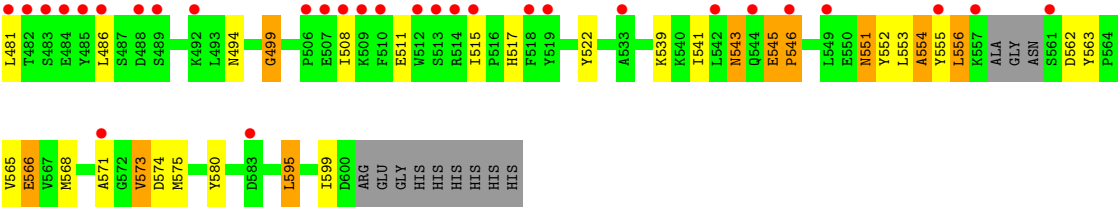
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	Se	0	4	0
			4265	2723	700	832	10			
1	B	506	Total	C	N	O	Se	0	2	0
			4096	2612	675	800	9			

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
2	A	99	Total	O	0	0
			99	99		
2	B	89	Total	O	0	0
			89	89		



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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)	0.32 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

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.

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	0.53	0/4351	0.84	5/5872 (0.1%)
1	B	0.67	12/4176 (0.3%)	0.87	9/5632 (0.2%)
All	All	0.60	12/8527 (0.1%)	0.86	14/11504 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	436	THR	CB-OG1	-9.60	1.28	1.43
1	B	438	LYS	C-O	9.29	1.35	1.24
1	B	437	GLU	CD-OE1	8.12	1.40	1.25
1	B	437	GLU	CD-OE2	7.69	1.40	1.25
1	B	438	LYS	CA-C	7.45	1.62	1.52
1	B	436	THR	CA-CB	6.65	1.64	1.53
1	B	442	VAL	C-O	6.31	1.31	1.24
1	B	551	ASN	CG-OD1	6.17	1.35	1.23
1	B	439	ASP	C-O	5.68	1.31	1.24
1	B	551	ASN	CG-ND2	5.54	1.44	1.33
1	B	435	GLU	CD-OE1	5.46	1.35	1.25
1	B	442	VAL	C-N	5.32	1.40	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	499	GLY	CA-C-N	9.60	130.26	119.32
1	B	499	GLY	C-N-CA	9.60	130.26	119.32
1	B	436	THR	CA-CB-OG1	7.47	120.80	109.60
1	A	478	GLY	CA-C-N	-7.19	117.41	122.59
1	A	478	GLY	C-N-CA	-7.19	117.41	122.59
1	B	439	ASP	CA-C-O	6.85	126.27	119.49
1	B	554	ALA	N-CA-C	-6.50	105.98	114.04
1	B	437	GLU	CG-CD-OE2	6.03	132.26	118.40
1	A	185	PHE	CA-C-N	-5.59	114.98	120.52
1	A	185	PHE	C-N-CA	-5.59	114.98	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	545	GLU	CA-C-N	5.49	126.71	119.84
1	B	545	GLU	C-N-CA	5.49	126.71	119.84
1	A	524	VAL	N-CA-C	5.43	117.84	111.05
1	B	551	ASN	OD1-CG-ND2	5.04	127.64	122.60

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	4265	0	4074	72	0
1	B	4096	0	3863	87	0
2	A	99	0	0	5	0
2	B	89	0	0	3	0
All	All	8549	0	7937	155	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 (155) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:416:PHE:CD2	1:A:416:PHE:C	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:552:TYR:C	1:B:554:ALA:H	2.25	0.43
1:B:563:TYR:HB3	1:B:566:GLU:HG2	2.00	0.43
1:B:192:ASN:C	1:B:194:GLU:H	2.26	0.43
1:B:574:ASP:C	1:B:574:ASP:OD1	2.62	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:64:PHE:CD2	1:B:64:PHE:C	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:GLU:HB3	1:A:548:ALA:HB2	2.02	0.41
1:B:41:LEU:C	1:B:43:GLN:H	2.28	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:B:415:ILE:O	1:B:416:PHE:C	2.62	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	43	63
1	B	498/587 (85%)	476 (96%)	20 (4%)	2 (0%)	30	49
All	All	1015/1174 (86%)	981 (97%)	31 (3%)	3 (0%)	36	55

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 ⓘ

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%)	408 (90%)	46 (10%)	7	15
1	B	430/504 (85%)	383 (89%)	47 (11%)	6	13
All	All	884/1008 (88%)	791 (90%)	93 (10%)	6	14

All (93) 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
1	A	65	VAL
1	A	66	LEU
1	A	85[A]	GLN
1	A	85[B]	GLN
1	A	87	THR
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	184	VAL
1	A	187	THR

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Mol	Chain	Res	Type
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	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	555	TYR
1	A	565	VAL
1	A	566	GLU
1	B	25	LEU
1	B	35	LEU
1	B	37	LEU
1	B	42	LYS
1	B	44	SER
1	B	51	LEU
1	B	65	VAL
1	B	66	LEU
1	B	87	THR
1	B	95	LEU
1	B	102	LEU
1	B	110	VAL
1	B	144	GLN
1	B	146	VAL
1	B	148	ASN
1	B	161	LEU
1	B	169	ASP

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Mol	Chain	Res	Type
1	B	177	VAL
1	B	184	VAL
1	B	187	THR
1	B	198	LEU
1	B	202	VAL
1	B	235	SER
1	B	270	VAL
1	B	285	LEU
1	B	311	LEU
1	B	334	MSE
1	B	339	MSE
1	B	385	GLN
1	B	386	LEU
1	B	429	LEU
1	B	434	LEU
1	B	438	LYS
1	B	446	VAL
1	B	447	LEU
1	B	458	VAL
1	B	473	THR
1	B	476	GLU
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	566	GLU
1	B	573	VAL
1	B	595	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	83	ASN
1	A	127	GLN
1	A	148	ASN
1	A	179	ASN
1	A	192	ASN
1	A	228	GLN
1	A	231	ASN

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Mol	Chain	Res	Type
1	A	281	HIS
1	A	385	GLN
1	A	391	HIS
1	A	395	HIS
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	228	GLN
1	B	265	HIS
1	B	281	HIS
1	B	427	ASN
1	B	448	ASN
1	B	463	GLN
1	B	469	HIS
1	B	521	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 oligosaccharides 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, 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%)	0.29	15 (2%) 53 49	17, 45, 68, 123	4 (0%)
1	B	496/587 (84%)	0.68	55 (11%) 10 8	20, 45, 66, 91	2 (0%)
All	All	1007/1174 (85%)	0.48	70 (6%) 22 20	17, 45, 68, 123	6 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	415	ILE	6.0
1	B	400	TYR	5.1
1	B	312	GLY	5.1
1	A	316	ILE	4.7
1	B	519	TYR	4.3
1	B	383	LEU	4.3
1	B	481	LEU	4.1
1	B	512	TRP	4.0
1	B	542	LEU	3.8
1	B	483	SER	3.7
1	B	193	GLY	3.6
1	B	515	ILE	3.6
1	A	25	LEU	3.5
1	B	544	GLN	3.4
1	B	327	ALA	3.4
1	B	479	VAL	3.4
1	B	510	PHE	3.3
1	B	513	SER	3.3
1	B	555	TYR	3.2
1	B	430	THR	3.2
1	A	322	GLU	3.2
1	B	484	GLU	3.0
1	B	485	TYR	3.0
1	A	546	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	324	LYS	3.0
1	B	482	THR	2.9
1	B	546	PRO	2.9
1	B	508	ILE	2.9
1	A	555	TYR	2.9
1	B	514	ARG	2.9
1	A	141	TYR	2.9
1	B	478	GLY	2.8
1	B	507	GLU	2.8
1	B	489	SER	2.8
1	B	98[A]	ARG	2.8
1	B	486	LEU	2.7
1	A	382	THR	2.7
1	A	315	PRO	2.6
1	B	480	PRO	2.6
1	B	328	LEU	2.6
1	A	313	GLU	2.6
1	A	394	GLY	2.6
1	B	506	PRO	2.6
1	B	340	ALA	2.6
1	B	533	ALA	2.5
1	B	561	SER	2.5
1	B	428	ILE	2.4
1	B	571	ALA	2.4
1	B	509	LYS	2.4
1	B	488	ASP	2.4
1	A	560	ASN	2.4
1	B	467	PHE	2.3
1	A	415	ILE	2.3
1	A	336	GLU	2.3
1	B	424	THR	2.3
1	A	558	ALA	2.2
1	B	338	TYR	2.2
1	B	583	ASP	2.2
1	B	141	TYR	2.2
1	B	137	VAL	2.2
1	B	492	LYS	2.2
1	B	557	LYS	2.2
1	B	473	THR	2.1
1	B	332	LYS	2.1
1	B	416	PHE	2.1
1	B	330	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	518	PHE	2.1
1	A	26	SER	2.1
1	B	549	LEU	2.1
1	B	477	LYS	2.1

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 oligosaccharides 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.