



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:22 AM UTC

PDB ID : 3OHN / pdb\_00003ohn  
Title : Crystal structure of the FimD translocation domain  
Authors : Wang, T.; Li, H.  
Deposited on : 2010-08-17  
Resolution : 3.01 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

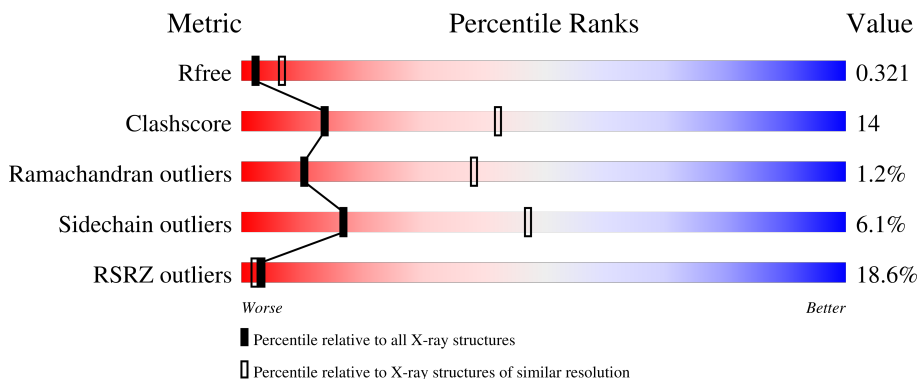
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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  $\geq 3$ , 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	558	
1	B	558	

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 7246 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 Outer membrane usher protein FimD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	468	3636	2271	640	719	6	0	0	0
1	B	463	3610	2259	634	711	6	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	664	GLY	-	expression tag	UNP C8U0R5
A	665	GLY	-	expression tag	UNP C8U0R5
A	666	PRO	-	expression tag	UNP C8U0R5
A	667	VAL	-	expression tag	UNP C8U0R5
A	668	ALA	-	expression tag	UNP C8U0R5
A	669	THR	-	expression tag	UNP C8U0R5
A	670	LEU	-	expression tag	UNP C8U0R5
A	671	VAL	-	expression tag	UNP C8U0R5
A	672	PRO	-	expression tag	UNP C8U0R5
A	673	ARG	-	expression tag	UNP C8U0R5
A	674	GLY	-	expression tag	UNP C8U0R5
A	675	SER	-	expression tag	UNP C8U0R5
A	676	HIS	-	expression tag	UNP C8U0R5
A	677	HIS	-	expression tag	UNP C8U0R5
A	678	HIS	-	expression tag	UNP C8U0R5
A	679	HIS	-	expression tag	UNP C8U0R5
A	680	HIS	-	expression tag	UNP C8U0R5
A	681	HIS	-	expression tag	UNP C8U0R5
B	664	GLY	-	expression tag	UNP C8U0R5
B	665	GLY	-	expression tag	UNP C8U0R5
B	666	PRO	-	expression tag	UNP C8U0R5
B	667	VAL	-	expression tag	UNP C8U0R5
B	668	ALA	-	expression tag	UNP C8U0R5
B	669	THR	-	expression tag	UNP C8U0R5
B	670	LEU	-	expression tag	UNP C8U0R5

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<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
B	671	VAL	-	expression tag	UNP C8U0R5
B	672	PRO	-	expression tag	UNP C8U0R5
B	673	ARG	-	expression tag	UNP C8U0R5
B	674	GLY	-	expression tag	UNP C8U0R5
B	675	SER	-	expression tag	UNP C8U0R5
B	676	HIS	-	expression tag	UNP C8U0R5
B	677	HIS	-	expression tag	UNP C8U0R5
B	678	HIS	-	expression tag	UNP C8U0R5
B	679	HIS	-	expression tag	UNP C8U0R5
B	680	HIS	-	expression tag	UNP C8U0R5
B	681	HIS	-	expression tag	UNP C8U0R5





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.02Å 87.13Å 95.88Å 63.92° 88.43° 76.94°	Depositor
Resolution (Å)	28.89 – 3.01 28.89 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.0 (28.89-3.01) 98.1 (28.89-3.01)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 3.00Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.230 , 0.305 0.310 , 0.321	Depositor DCC
$R_{free}$ test set	1371 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.4	Xtrriage
Anisotropy	0.629	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 27.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	7246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.70	4/3715 (0.1%)	0.82	7/5038 (0.1%)
1	B	0.91	15/3689 (0.4%)	0.86	8/5002 (0.2%)
All	All	0.81	19/7404 (0.3%)	0.84	15/10040 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	434	TYR	C-O	-7.72	1.15	1.24
1	B	414	VAL	C-O	-7.32	1.16	1.24
1	B	435	ARG	C-O	-7.06	1.16	1.24
1	A	515	GLU	CA-C	-6.47	1.44	1.52
1	A	347	LYS	CA-C	-6.45	1.45	1.52
1	A	515	GLU	C-O	-6.35	1.16	1.24
1	B	436	TYR	C-O	-6.16	1.16	1.24
1	B	432	VAL	CA-CB	-6.08	1.46	1.54
1	B	432	VAL	C-O	-6.07	1.17	1.24
1	B	433	GLY	C-O	-5.80	1.16	1.23
1	B	381	GLY	C-O	-5.70	1.18	1.23
1	B	414	VAL	CA-CB	-5.50	1.47	1.54
1	B	377	ALA	CA-CB	-5.35	1.44	1.53
1	B	415	ARG	C-O	-5.34	1.17	1.24
1	B	411	GLY	C-O	-5.24	1.17	1.23
1	B	416	PHE	C-O	-5.19	1.17	1.24
1	A	485	GLN	CA-C	-5.13	1.46	1.52
1	B	377	ALA	C-O	-5.08	1.17	1.23
1	B	142	LEU	C-O	-5.05	1.17	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	THR	N-CA-C	13.57	129.55	108.79
1	A	309	SER	N-CA-C	11.58	123.91	111.28
1	B	307	ASP	N-CA-C	-11.15	95.81	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	GLY	N-CA-C	10.24	125.02	112.73
1	B	612	GLY	N-CA-C	-9.06	91.71	113.18
1	A	309	SER	CA-C-N	-7.79	107.36	121.62
1	A	309	SER	C-N-CA	-7.79	107.36	121.62
1	B	140	GLY	N-CA-C	-7.17	96.19	113.18
1	A	448	THR	CB-CA-C	-7.12	99.20	111.30
1	B	613	GLY	N-CA-C	-6.61	97.51	113.18
1	B	453	ASN	N-CA-C	6.58	119.32	108.99
1	B	141	LEU	N-CA-C	-5.91	100.56	109.95
1	B	414	VAL	CB-CA-C	-5.73	102.09	110.62
1	B	379	ASN	N-CA-C	5.16	117.23	109.23
1	A	347	LYS	CB-CA-C	-5.07	103.34	110.13

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	3636	0	3426	71	0
1	B	3610	0	3402	134	0
All	All	7246	0	6828	204	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 14.

All (204) 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:628:TYR:CE2	1:B:630:GLY:N	1.87	1.38
1:B:142:LEU:HD12	1:B:143:ASN:N	1.39	1.36
1:B:141:LEU:HD12	1:B:142:LEU:N	1.43	1.30
1:B:141:LEU:HD12	1:B:141:LEU:C	1.53	1.26
1:B:365:ILE:HD12	1:B:365:ILE:O	1.35	1.24
1:B:142:LEU:HD12	1:B:142:LEU:C	1.53	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ILE:HD12	1:B:365:ILE:C	1.68	1.17
1:B:451:ARG:HA	1:B:451:ARG:HE	1.02	1.10
1:B:403:LEU:HB3	1:B:404:PRO:CD	1.83	1.06
1:A:583:ASN:C	1:A:583:ASN:HD22	1.60	1.06
1:B:389:LEU:O	1:B:420:LYS:HD2	1.56	1.05
1:A:521:LEU:CD2	1:A:521:LEU:C	2.29	1.04
1:B:365:ILE:C	1:B:365:ILE:CD1	2.30	1.03
1:B:403:LEU:HB3	1:B:404:PRO:HD2	1.38	1.03
1:B:455:TYR:HE2	1:B:472:ASP:HB2	1.20	1.02
1:B:141:LEU:HB2	1:B:657:LEU:CD2	1.90	1.01
1:B:141:LEU:C	1:B:141:LEU:CD1	2.30	1.01
1:B:628:TYR:HD2	1:B:628:TYR:C	1.70	1.00
1:B:295:ASN:HB2	1:B:317:TYR:OH	1.60	1.00
1:B:628:TYR:CD2	1:B:629:ARG:N	2.30	0.99
1:B:587:THR:H	1:B:613:GLY:HA2	1.25	0.98
1:A:521:LEU:C	1:A:521:LEU:HD22	1.88	0.98
1:B:142:LEU:C	1:B:142:LEU:CD1	2.29	0.98
1:B:586:MET:HE2	1:B:612:GLY:O	1.64	0.97
1:B:628:TYR:C	1:B:628:TYR:CD2	2.36	0.97
1:B:454:GLY:O	1:B:455:TYR:HB3	1.59	0.96
1:B:141:LEU:CD1	1:B:142:LEU:N	2.30	0.95
1:B:141:LEU:HB2	1:B:657:LEU:HD23	1.46	0.95
1:B:628:TYR:HE2	1:B:630:GLY:N	1.52	0.95
1:B:455:TYR:CE2	1:B:472:ASP:HB2	2.01	0.94
1:B:455:TYR:C	1:B:455:TYR:HD2	1.74	0.94
1:A:448:THR:HG23	1:A:448:THR:O	1.68	0.94
1:B:451:ARG:HA	1:B:451:ARG:NE	1.84	0.93
1:B:450:SER:O	1:B:451:ARG:HB2	1.70	0.92
1:B:141:LEU:HD12	1:B:142:LEU:CA	2.01	0.90
1:A:521:LEU:CD2	1:A:522:ASN:N	2.34	0.90
1:A:309:SER:O	1:A:310:THR:HG23	1.73	0.88
1:B:159:SER:C	1:B:160:HIS:HD2	1.80	0.88
1:A:521:LEU:HD23	1:A:522:ASN:N	1.88	0.88
1:A:583:ASN:C	1:A:583:ASN:ND2	2.30	0.87
1:B:455:TYR:C	1:B:455:TYR:CD2	2.47	0.86
1:A:592:VAL:HG11	1:A:607:GLN:HA	1.55	0.86
1:B:159:SER:C	1:B:160:HIS:CD2	2.57	0.82
1:B:628:TYR:O	1:B:634:ASN:HB2	1.79	0.82
1:B:142:LEU:CD1	1:B:143:ASN:N	2.34	0.82
1:B:451:ARG:HE	1:B:451:ARG:CA	1.85	0.82
1:B:601:ASN:O	1:B:629:ARG:NE	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:MET:O	1:B:452:MET:HG2	1.81	0.79
1:A:521:LEU:C	1:A:521:LEU:HD23	2.06	0.79
1:A:499:TYR:CZ	1:A:520:GLY:HA3	2.18	0.78
1:B:403:LEU:HD22	1:B:476:LEU:HD23	1.64	0.78
1:B:405:ASP:OD1	1:B:451:ARG:NH2	2.16	0.78
1:B:601:ASN:O	1:B:629:ARG:CZ	2.31	0.78
1:B:414:VAL:CG1	1:B:414:VAL:O	2.30	0.77
1:B:454:GLY:O	1:B:455:TYR:CB	2.32	0.77
1:B:612:GLY:HA2	1:B:618:SER:HA	1.65	0.77
1:B:379:ASN:C	1:B:379:ASN:OD1	2.29	0.76
1:B:629:ARG:N	1:B:629:ARG:HD3	2.00	0.75
1:B:450:SER:O	1:B:451:ARG:CB	2.33	0.74
1:B:414:VAL:O	1:B:414:VAL:HG13	1.83	0.74
1:B:586:MET:CE	1:B:612:GLY:O	2.37	0.73
1:A:592:VAL:HG22	1:A:593:TYR:H	1.54	0.73
1:B:657:LEU:O	1:B:658:ALA:HB3	1.89	0.72
1:B:403:LEU:CB	1:B:404:PRO:CD	2.62	0.72
1:B:210:ILE:HG13	1:B:211:PRO:HD3	1.71	0.71
1:A:521:LEU:HD23	1:A:522:ASN:H	1.56	0.71
1:A:640:SER:HB3	1:A:647:GLN:HB2	1.71	0.70
1:B:628:TYR:CE2	1:B:630:GLY:CA	2.75	0.70
1:A:521:LEU:HD22	1:A:522:ASN:N	2.04	0.69
1:A:499:TYR:CE2	1:A:520:GLY:HA3	2.28	0.69
1:B:159:SER:O	1:B:160:HIS:CD2	2.47	0.67
1:B:628:TYR:HD2	1:B:629:ARG:N	1.80	0.67
1:B:356:LEU:HG	1:B:366:TYR:HB3	1.78	0.66
1:B:628:TYR:OH	1:B:630:GLY:HA3	1.96	0.66
1:B:601:ASN:HA	1:B:629:ARG:HE	1.61	0.65
1:B:529:ASN:HB3	1:B:554:ASN:HB2	1.78	0.65
1:B:627:ASN:OD1	1:B:628:TYR:N	2.30	0.65
1:B:453:ASN:OD1	1:B:454:GLY:N	2.30	0.65
1:A:346:GLU:OE1	1:A:347:LYS:N	2.29	0.65
1:B:379:ASN:OD1	1:B:380:PHE:N	2.30	0.64
1:A:309:SER:O	1:A:310:THR:CG2	2.44	0.64
1:A:287:ILE:HD12	1:A:288:ASN:H	1.63	0.63
1:B:629:ARG:HD3	1:B:629:ARG:H	1.62	0.63
1:B:579:SER:C	1:B:580:HIS:ND1	2.57	0.63
1:B:142:LEU:HD12	1:B:143:ASN:CA	2.25	0.63
1:A:261:ARG:HB2	1:A:305:GLU:OE2	1.99	0.63
1:A:264:ALA:HB2	1:A:305:GLU:OE1	1.98	0.62
1:B:586:MET:HG2	1:B:613:GLY:HA3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:LYS:HZ1	1:A:485:GLN:HG2	1.63	0.61
1:B:614:GLY:O	1:B:616:GLY:N	2.33	0.61
1:A:306:ALA:O	1:A:307:ASP:CB	2.48	0.61
1:A:583:ASN:ND2	1:A:583:ASN:O	2.30	0.61
1:A:483:LYS:HZ1	1:A:485:GLN:CG	2.13	0.60
1:A:483:LYS:NZ	1:A:485:GLN:HG2	2.17	0.60
1:A:261:ARG:NE	1:A:583:ASN:OD1	2.35	0.60
1:B:657:LEU:O	1:B:658:ALA:CB	2.49	0.59
1:B:628:TYR:CZ	1:B:630:GLY:N	2.61	0.59
1:B:629:ARG:N	1:B:629:ARG:CD	2.66	0.58
1:A:529:ASN:HB3	1:A:554:ASN:HB2	1.85	0.58
1:B:287:ILE:HD12	1:B:288:ASN:H	1.67	0.58
1:A:306:ALA:O	1:A:307:ASP:HB2	2.03	0.58
1:B:581:ASP:HB3	1:B:588:ASN:HB3	1.86	0.57
1:B:379:ASN:HB2	1:B:397:THR:HG23	1.86	0.57
1:B:587:THR:N	1:B:613:GLY:HA2	2.09	0.57
1:B:517:PHE:HB3	1:B:536:LEU:HB3	1.87	0.57
1:B:295:ASN:HB2	1:B:317:TYR:CZ	2.39	0.57
1:A:483:LYS:NZ	1:A:485:GLN:CG	2.67	0.57
1:A:430:GLN:HG2	1:A:488:VAL:HG12	1.86	0.56
1:B:403:LEU:HB3	1:B:404:PRO:HD3	1.81	0.56
1:A:384:LYS:HG2	1:A:385:ASN:N	2.22	0.55
1:B:404:PRO:HB3	1:B:450:SER:HA	1.87	0.55
1:B:628:TYR:CZ	1:B:630:GLY:CA	2.90	0.55
1:B:322:LEU:HD23	1:B:356:LEU:HD21	1.89	0.54
1:B:403:LEU:HD22	1:B:476:LEU:CD2	2.37	0.54
1:B:168:SER:HB3	1:B:179:ASP:HB3	1.89	0.54
1:A:517:PHE:HB3	1:A:536:LEU:HB3	1.90	0.54
1:B:629:ARG:HA	1:B:634:ASN:HB3	1.91	0.52
1:B:257:HIS:HB2	1:B:518:GLN:HG2	1.92	0.52
1:B:628:TYR:OH	1:B:630:GLY:CA	2.58	0.52
1:B:145:ASN:HB3	1:B:165:ASN:HB2	1.92	0.51
1:B:397:THR:O	1:B:412:GLN:HA	2.10	0.51
1:B:170:LEU:HB3	1:B:177:LEU:HB3	1.93	0.51
1:B:343:ALA:O	1:B:344:GLN:HG2	2.10	0.51
1:A:583:ASN:O	1:A:584:GLY:C	2.50	0.51
1:B:580:HIS:ND1	1:B:580:HIS:N	2.58	0.51
1:B:628:TYR:CD2	1:B:629:ARG:CA	2.93	0.51
1:B:519:ALA:HB3	1:B:534:TYR:HB3	1.92	0.51
1:B:590:ALA:HA	1:B:609:GLY:HA3	1.94	0.50
1:B:160:HIS:CD2	1:B:160:HIS:N	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:LEU:HB2	1:B:496:SER:HB2	1.94	0.50
1:B:338:TYR:HB3	1:B:348:PRO:HD2	1.93	0.50
1:B:628:TYR:CZ	1:B:630:GLY:HA3	2.45	0.50
1:B:453:ASN:OD1	1:B:454:GLY:O	2.30	0.49
1:B:603:SER:OG	1:B:629:ARG:NH1	2.45	0.49
1:A:402:THR:HG22	1:A:408:GLN:HG2	1.94	0.49
1:B:141:LEU:HD12	1:B:141:LEU:O	2.02	0.49
1:A:500:LEU:HD12	1:A:519:ALA:HB2	1.94	0.49
1:B:628:TYR:CE2	1:B:629:ARG:C	2.82	0.49
1:B:656:VAL:CG1	1:B:657:LEU:N	2.72	0.49
1:A:445:ALA:O	1:A:448:THR:HG23	2.12	0.48
1:A:581:ASP:HB2	1:A:588:ASN:HB3	1.95	0.48
1:B:151:VAL:HG12	1:B:647:GLN:HG2	1.96	0.48
1:B:597:LEU:C	1:B:599:ASP:H	2.21	0.48
1:B:232:ASN:HD22	1:B:271:ASN:HD22	1.62	0.48
1:B:413:SER:HB2	1:B:441:TYR:CZ	2.48	0.48
1:A:154:ARG:O	1:A:155:ILE:HG13	2.14	0.48
1:B:579:SER:O	1:B:579:SER:OG	2.30	0.48
1:A:448:THR:O	1:A:448:THR:CG2	2.38	0.47
1:A:515:GLU:HB2	1:A:538:LYS:HB3	1.95	0.47
1:A:262:GLY:N	1:A:305:GLU:OE2	2.41	0.47
1:B:365:ILE:C	1:B:365:ILE:HD13	2.34	0.47
1:B:656:VAL:HG13	1:B:657:LEU:N	2.28	0.47
1:A:261:ARG:CZ	1:A:583:ASN:OD1	2.62	0.47
1:A:388:ALA:O	1:A:389:LEU:HB2	2.13	0.47
1:A:533:SER:HB2	1:A:550:ALA:HB3	1.95	0.47
1:A:610:TYR:HA	1:A:620:SER:HA	1.96	0.47
1:A:415:ARG:HD2	1:A:435:ARG:HH21	1.78	0.47
1:B:420:LYS:O	1:B:421:SER:OG	2.30	0.47
1:B:628:TYR:O	1:B:634:ASN:CB	2.57	0.47
1:A:352:GLN:HG3	1:A:370:GLN:HB3	1.97	0.46
1:B:628:TYR:CD2	1:B:630:GLY:N	2.61	0.46
1:A:420:LYS:HB3	1:A:430:GLN:HB3	1.98	0.46
1:A:621:THR:OG1	1:A:642:SER:OG	2.31	0.46
1:A:196:ASN:HD21	1:B:196:ASN:HB3	1.82	0.45
1:B:495:THR:HG22	1:B:525:PHE:HB3	1.98	0.45
1:B:162:ALA:HB3	1:B:185:TYR:HB3	1.99	0.45
1:A:322:LEU:HD23	1:A:356:LEU:HD21	1.99	0.44
1:A:445:ALA:O	1:A:448:THR:CG2	2.65	0.44
1:A:483:LYS:NZ	1:A:485:GLN:HG3	2.33	0.44
1:A:262:GLY:HA2	1:A:282:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:THR:HG22	1:B:312:ILE:HG12	1.99	0.43
1:A:516:GLN:HE21	1:A:518:GLN:HG2	1.83	0.43
1:B:455:TYR:HE2	1:B:472:ASP:CB	2.09	0.43
1:B:614:GLY:O	1:B:615:ASP:C	2.60	0.43
1:A:403:LEU:HB3	1:A:404:PRO:HD2	2.00	0.43
1:A:256:ILE:H	1:A:287:ILE:HD11	1.84	0.43
1:B:576:TYR:HE2	1:B:578:MET:HE2	1.84	0.43
1:B:601:ASN:HA	1:B:629:ARG:NE	2.31	0.42
1:A:525:PHE:CE2	1:A:527:ASP:HB2	2.54	0.42
1:B:164:LEU:HB3	1:B:183:TRP:HB3	2.02	0.42
1:A:576:TYR:HE2	1:A:578:MET:HE2	1.84	0.42
1:B:451:ARG:NE	1:B:451:ARG:CA	2.57	0.42
1:A:592:VAL:HG13	1:A:593:TYR:N	2.35	0.42
1:A:145:ASN:HB3	1:A:165:ASN:HB2	2.01	0.42
1:A:448:THR:O	1:A:448:THR:OG1	2.30	0.42
1:B:287:ILE:H	1:B:287:ILE:HG13	1.63	0.42
1:A:531:THR:HG23	1:A:552:ASN:HB2	2.01	0.41
1:A:234:ARG:HE	1:A:339:ARG:HD3	1.85	0.41
1:A:540:ALA:C	1:A:542:GLN:H	2.28	0.41
1:B:402:THR:O	1:B:402:THR:OG1	2.30	0.41
1:A:214:SER:HA	1:A:240:SER:HA	2.03	0.41
1:B:230:GLY:HA3	1:B:296:SER:HB2	2.02	0.41
1:B:505:GLN:HB3	1:B:514:ASP:HB3	2.03	0.41
1:A:154:ARG:C	1:A:156:GLY:H	2.28	0.41
1:A:175:TRP:CE3	1:A:205:LEU:HG	2.55	0.41
1:A:483:LYS:HZ3	1:A:503:SER:HB2	1.85	0.41
1:B:146:PHE:HD1	1:B:164:LEU:HD13	1.86	0.41
1:B:525:PHE:O	1:B:526:GLU:HG2	2.20	0.41
1:B:525:PHE:C	1:B:527:ASP:H	2.28	0.41
1:A:302:THR:HB	1:A:312:ILE:HG23	2.03	0.41
1:B:510:THR:HG22	1:B:512:ASN:H	1.86	0.41
1:B:203:THR:H	1:B:220:ASP:HB2	1.86	0.40
1:B:604:TYR:HB3	1:B:626:LEU:HD23	2.02	0.40
1:B:141:LEU:CD1	1:B:142:LEU:CA	2.86	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	456/558 (82%)	422 (92%)	29 (6%)	5 (1%)	11	41
1	B	449/558 (80%)	409 (91%)	34 (8%)	6 (1%)	9	36
All	All	905/1116 (81%)	831 (92%)	63 (7%)	11 (1%)	10	38

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ILE
1	A	592	VAL
1	B	451	ARG
1	A	348	PRO
1	A	541	TRP
1	B	592	VAL
1	B	615	ASP
1	B	325	ARG
1	B	405	ASP
1	B	526	GLU
1	A	612	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	381/457 (83%)	365 (96%)	16 (4%)	26	59
1	B	378/457 (83%)	348 (92%)	30 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	759/914 (83%)	713 (94%)	46 (6%)	17 47

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	ILE
1	A	287	ILE
1	A	301	VAL
1	A	307	ASP
1	A	310	THR
1	A	346	GLU
1	A	347	LYS
1	A	448	THR
1	A	449	TYR
1	A	514	ASP
1	A	515	GLU
1	A	521	LEU
1	A	545	ARG
1	A	583	ASN
1	A	596	LEU
1	A	642	SER
1	B	141	LEU
1	B	142	LEU
1	B	172	ILE
1	B	200	HIS
1	B	205	LEU
1	B	256	ILE
1	B	287	ILE
1	B	301	VAL
1	B	309	SER
1	B	356	LEU
1	B	359	LEU
1	B	364	THR
1	B	365	ILE
1	B	379	ASN
1	B	386	MET
1	B	397	THR
1	B	415	ARG
1	B	420	LYS
1	B	430	GLN
1	B	435	ARG
1	B	451	ARG

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Mol	Chain	Res	Type
1	B	452	MET
1	B	455	TYR
1	B	480	LYS
1	B	518	GLN
1	B	580	HIS
1	B	596	LEU
1	B	628	TYR
1	B	629	ARG
1	B	656	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	149	ASN
1	A	167	GLN
1	A	186	ASN
1	A	196	ASN
1	A	199	GLN
1	A	271	ASN
1	A	311	GLN
1	A	379	ASN
1	A	400	ASN
1	A	479	ASN
1	A	491	GLN
1	A	505	GLN
1	A	518	GLN
1	A	580	HIS
1	A	627	ASN
1	B	145	ASN
1	B	153	ASN
1	B	160	HIS
1	B	165	ASN
1	B	167	GLN
1	B	171	ASN
1	B	180	ASN
1	B	232	ASN
1	B	311	GLN
1	B	345	GLN
1	B	479	ASN
1	B	485	GLN
1	B	491	GLN

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Mol	Chain	Res	Type
1	B	505	GLN
1	B	518	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	468/558 (83%)	1.30	87 (18%) <b>3</b> <b>2</b>	20, 58, 96, 124	0
1	B	463/558 (82%)	1.29	86 (18%) <b>3</b> <b>2</b>	22, 62, 105, 128	0
All	All	931/1116 (83%)	1.29	173 (18%) <b>3</b> <b>2</b>	20, 60, 101, 128	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	591	GLY	7.3
1	B	327	GLY	5.7
1	A	593	TYR	5.5
1	B	292	ALA	5.3
1	B	341	GLY	5.2
1	A	155	ILE	5.0
1	A	341	GLY	4.5
1	B	319	SER	4.5
1	B	295	ASN	4.5
1	A	450	SER	4.4
1	A	576	TYR	4.4
1	A	295	ASN	4.3
1	B	289	ASP	4.3
1	B	576	TYR	4.3
1	A	541	TRP	4.1
1	B	635	ALA	4.1
1	A	526	GLU	3.9
1	B	325	ARG	3.9
1	B	298	ASP	3.9
1	A	142	LEU	3.8
1	B	294	GLY	3.8
1	B	593	TYR	3.7
1	B	287	ILE	3.7
1	B	637	ILE	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	293	ALA	3.6
1	B	293	ALA	3.5
1	A	389	LEU	3.4
1	B	573	SER	3.4
1	B	315	VAL	3.4
1	A	454	GLY	3.4
1	B	572	ALA	3.4
1	A	650	TYR	3.4
1	B	582	LEU	3.4
1	B	286	THR	3.4
1	B	650	TYR	3.3
1	A	453	ASN	3.3
1	A	590	ALA	3.3
1	A	581	ASP	3.2
1	B	347	LYS	3.2
1	B	581	ASP	3.2
1	A	181	THR	3.2
1	A	292	ALA	3.2
1	A	451	ARG	3.2
1	B	526	GLU	3.2
1	A	572	ALA	3.1
1	B	318	SER	3.1
1	A	592	VAL	3.1
1	B	291	TYR	3.1
1	B	421	SER	3.1
1	B	578	MET	3.1
1	A	319	SER	3.0
1	A	291	TYR	3.0
1	B	611	ALA	3.0
1	A	290	ILE	3.0
1	B	343	ALA	3.0
1	B	494	ARG	3.0
1	A	471	THR	3.0
1	A	229	ASP	2.9
1	B	146	PHE	2.9
1	A	574	ALA	2.9
1	B	592	VAL	2.9
1	A	584	GLY	2.9
1	A	296	SER	2.8
1	A	263	THR	2.8
1	A	342	ASN	2.8
1	A	422	LEU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	443	ASN	2.8
1	A	578	MET	2.8
1	B	657	LEU	2.8
1	B	473	TYR	2.7
1	A	160	HIS	2.7
1	A	524	ALA	2.7
1	B	406	ASP	2.7
1	A	148	GLY	2.7
1	B	261	ARG	2.7
1	A	607	GLN	2.7
1	B	630	GLY	2.6
1	A	164	LEU	2.6
1	A	318	SER	2.6
1	B	241	ASP	2.6
1	A	430	GLN	2.6
1	B	263	THR	2.6
1	B	296	SER	2.6
1	A	426	GLY	2.6
1	A	289	ASP	2.6
1	A	373	ASP	2.6
1	A	343	ALA	2.5
1	B	326	GLU	2.5
1	B	537	THR	2.5
1	A	545	ARG	2.5
1	A	613	GLY	2.5
1	A	188	SER	2.5
1	A	547	GLN	2.5
1	B	265	GLN	2.5
1	B	187	SER	2.4
1	B	340	SER	2.4
1	A	427	THR	2.4
1	B	173	GLY	2.4
1	B	623	TYR	2.4
1	B	515	GLU	2.4
1	B	557	PHE	2.4
1	A	279	THR	2.4
1	B	196	ASN	2.4
1	A	256	ILE	2.4
1	A	372	ALA	2.4
1	B	658	ALA	2.4
1	A	647	GLN	2.4
1	B	596	LEU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	254	PRO	2.4
1	B	183	TRP	2.4
1	B	493	GLY	2.4
1	B	648	LEU	2.4
1	B	328	HIS	2.3
1	A	644	ASP	2.3
1	A	536	LEU	2.3
1	B	225	GLY	2.3
1	B	574	ALA	2.3
1	A	549	LEU	2.3
1	B	216	LEU	2.3
1	A	294	GLY	2.3
1	B	342	ASN	2.3
1	A	226	ASP	2.3
1	A	140	GLY	2.3
1	A	302	THR	2.3
1	A	476	LEU	2.3
1	B	271	ASN	2.3
1	B	305	GLU	2.3
1	B	290	ILE	2.3
1	B	634	ASN	2.3
1	A	643	ASP	2.3
1	A	340	SER	2.2
1	A	656	VAL	2.2
1	A	582	LEU	2.2
1	A	588	ASN	2.2
1	A	586	MET	2.2
1	A	648	LEU	2.2
1	B	316	PRO	2.2
1	A	621	THR	2.2
1	A	641	HIS	2.2
1	A	639	TYR	2.1
1	B	589	LEU	2.1
1	A	211	PRO	2.1
1	B	297	GLY	2.1
1	B	529	ASN	2.1
1	B	226	ASP	2.1
1	A	500	LEU	2.1
1	A	543	LYS	2.1
1	B	267	THR	2.1
1	B	455	TYR	2.1
1	B	492	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	311	GLN	2.1
1	B	518	GLN	2.1
1	B	513	VAL	2.1
1	B	323	LEU	2.1
1	A	329	THR	2.1
1	A	344	GLN	2.1
1	A	231	ILE	2.1
1	A	287	ILE	2.1
1	A	317	TYR	2.1
1	A	604	TYR	2.1
1	B	616	GLY	2.1
1	B	166	LEU	2.0
1	A	527	ASP	2.0
1	B	220	ASP	2.0
1	B	430	GLN	2.0
1	A	172	ILE	2.0
1	A	419	ASN	2.0
1	A	452	MET	2.0
1	B	198	TRP	2.0
1	B	329	THR	2.0
1	B	632	TYR	2.0
1	B	647	GLN	2.0
1	A	585	ARG	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 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.