



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:37 AM EDT

PDB ID : 2DEO / pdb_00002deo
Title : 1510-N membrane protease specific for a stomatin homolog from *Pyrococcus horikoshii*
Authors : Yokoyama, H.; Matsui, I.
Deposited on : 2006-02-16
Resolution : 3.00 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

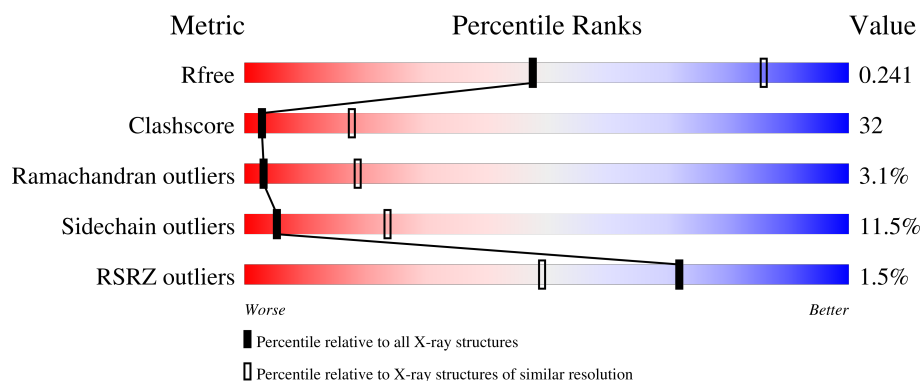
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 ≥ 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	230	
1	B	230	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3124 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 441aa long hypothetical nfeD protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	Se	88	0	0
			1542	986	255	296	1	4			
1	B	200	Total	C	N	O	S	Se	88	0	0
			1550	994	256	295	1	4			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MSE	-	initiating methionine	UNP O59179
A	70	MSE	MET	modified residue	UNP O59179
A	71	MSE	MET	modified residue	UNP O59179
A	111	MSE	MET	modified residue	UNP O59179
A	199	MSE	MET	modified residue	UNP O59179
A	237	LEU	-	cloning artifact	UNP O59179
A	238	GLU	-	cloning artifact	UNP O59179
A	239	HIS	-	expression tag	UNP O59179
A	240	HIS	-	expression tag	UNP O59179
A	241	HIS	-	expression tag	UNP O59179
A	242	HIS	-	expression tag	UNP O59179
A	243	HIS	-	expression tag	UNP O59179
A	244	HIS	-	expression tag	UNP O59179
B	15	MSE	-	initiating methionine	UNP O59179
B	70	MSE	MET	modified residue	UNP O59179
B	71	MSE	MET	modified residue	UNP O59179
B	111	MSE	MET	modified residue	UNP O59179
B	199	MSE	MET	modified residue	UNP O59179
B	237	LEU	-	cloning artifact	UNP O59179
B	238	GLU	-	cloning artifact	UNP O59179
B	239	HIS	-	expression tag	UNP O59179
B	240	HIS	-	expression tag	UNP O59179
B	241	HIS	-	expression tag	UNP O59179
B	242	HIS	-	expression tag	UNP O59179
B	243	HIS	-	expression tag	UNP O59179

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Chain	Residue	Modelled	Actual	Comment	Reference
B	244	HIS	-	expression tag	UNP O59179

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	12	Total O 12 12	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.21Å 108.40Å 59.34Å 90.00° 110.06° 90.00°	Depositor
Resolution (Å)	19.76 – 3.00 19.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.76-3.00) 99.6 (19.76-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.85 (at 2.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.242 0.197 , 0.241	Depositor DCC
R_{free} test set	1263 reflections (10.19%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3124	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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

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	1.31	9/1563 (0.6%)	1.61	30/2113 (1.4%)
1	B	1.38	10/1571 (0.6%)	1.58	29/2124 (1.4%)
All	All	1.35	19/3134 (0.6%)	1.60	59/4237 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	THR	CA-CB	-8.37	1.42	1.53
1	B	24	VAL	CA-CB	-7.50	1.45	1.54
1	B	185	VAL	CA-CB	-7.20	1.45	1.54
1	B	112	ALA	CA-CB	-6.86	1.41	1.52
1	A	24	VAL	CA-CB	-6.21	1.46	1.54
1	B	223	ALA	CA-CB	-6.19	1.44	1.53
1	A	172	THR	CA-CB	-6.12	1.45	1.53
1	A	223	ALA	CA-CB	-6.00	1.42	1.53
1	A	112	ALA	CA-CB	-5.96	1.42	1.53
1	A	56	ILE	CA-CB	-5.87	1.46	1.54
1	A	93	ALA	CA-CB	5.55	1.61	1.53
1	A	177	LEU	CA-C	-5.31	1.46	1.52
1	A	58	ILE	CA-CB	5.30	1.60	1.54
1	B	77	ILE	CA-CB	-5.28	1.48	1.54
1	B	196	SER	CA-C	-5.19	1.45	1.52
1	A	98	ALA	CA-CB	-5.15	1.44	1.53
1	B	102	ILE	CA-CB	-5.05	1.48	1.54
1	B	74	VAL	CA-CB	-5.04	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	20	ALA	N-CA	5.03	1.52	1.46

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ALA	N-CA-C	-15.29	95.49	114.75
1	B	21	LYS	N-CA-C	11.23	122.78	107.73
1	A	62	THR	CA-C-N	10.90	132.11	119.47
1	A	62	THR	C-N-CA	10.90	132.11	119.47
1	B	62	THR	CA-C-N	-9.43	108.05	119.84
1	B	62	THR	C-N-CA	-9.43	108.05	119.84
1	B	69	ALA	N-CA-C	-9.33	101.16	112.54
1	A	181	VAL	N-CA-C	-9.09	103.99	111.81
1	B	181	VAL	N-CA-C	-8.68	104.34	111.81
1	A	21	LYS	N-CA-C	8.11	118.67	108.45
1	A	184	VAL	N-CA-C	7.83	118.69	108.35
1	B	59	GLU	N-CA-C	-7.83	97.28	109.25
1	B	64	GLY	N-CA-C	7.65	124.91	111.14
1	B	184	VAL	N-CA-C	7.42	119.43	108.45
1	A	64	GLY	N-CA-C	7.37	125.00	110.77
1	B	172	THR	N-CA-C	-7.08	100.54	110.31
1	A	166	THR	N-CA-C	7.04	121.72	113.20
1	B	92	GLY	N-CA-C	-6.91	106.47	114.69
1	B	63	PRO	N-CA-C	6.84	126.55	112.47
1	A	59	GLU	N-CA-C	-6.76	98.91	109.25
1	A	54	GLU	N-CA-C	-6.75	104.30	112.54
1	B	72	ASN	N-CA-C	-6.73	104.02	111.36
1	A	60	LEU	N-CA-C	6.62	119.71	107.99
1	A	210	VAL	CA-C-N	-6.49	114.14	122.77
1	A	210	VAL	C-N-CA	-6.49	114.14	122.77
1	B	56	ILE	CA-C-N	-6.27	115.42	123.19
1	B	56	ILE	C-N-CA	-6.27	115.42	123.19
1	B	54	GLU	N-CA-C	-6.22	104.95	112.54
1	A	96	ALA	N-CA-C	5.96	119.20	109.24
1	B	159	THR	N-CA-C	-5.90	104.93	111.36
1	B	60	LEU	N-CA-C	5.89	118.01	108.41
1	A	227	LYS	N-CA-C	-5.85	104.81	111.07
1	B	141	ASN	N-CA-C	-5.79	104.82	112.34
1	B	85	ILE	CA-C-N	-5.68	115.26	122.37
1	B	85	ILE	C-N-CA	-5.68	115.26	122.37
1	A	205	VAL	N-CA-C	-5.65	98.30	107.28
1	B	166	THR	N-CA-C	5.62	120.00	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ILE	N-CA-C	-5.62	105.03	110.42
1	B	164	PHE	N-CA-C	-5.61	104.85	110.97
1	B	210	VAL	CA-C-N	-5.58	115.35	122.77
1	B	210	VAL	C-N-CA	-5.58	115.35	122.77
1	A	89	TYR	CA-C-N	5.56	140.34	127.00
1	A	89	TYR	C-N-CA	5.56	140.34	127.00
1	A	89	TYR	C-N-CD	-5.46	108.59	120.60
1	B	101	TYR	N-CA-C	-5.39	105.32	111.14
1	A	217	VAL	N-CA-C	5.27	116.97	108.85
1	A	58	ILE	N-CA-C	-5.27	100.16	107.80
1	A	156	ARG	N-CA-C	-5.25	101.71	110.17
1	A	33	ILE	CB-CA-C	-5.25	104.61	110.96
1	B	96	ALA	N-CA-C	5.20	117.58	109.52
1	A	159	THR	N-CA-C	-5.19	105.70	111.36
1	B	205	VAL	N-CA-C	-5.12	98.64	107.24
1	B	217	VAL	N-CA-C	5.09	116.69	108.85
1	A	23	ILE	N-CA-C	5.09	116.29	108.71
1	A	209	TYR	N-CA-C	-5.08	102.76	110.28
1	A	154	SER	N-CA-C	-5.05	105.82	112.94
1	B	209	TYR	N-CA-C	-5.03	102.84	110.28
1	A	95	ALA	CA-C-N	-5.02	114.60	122.73
1	A	95	ALA	C-N-CA	-5.02	114.60	122.73

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	TYR	Sidechain
1	A	89	TYR	Sidechain

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	1542	0	1569	89	0
1	B	1550	0	1587	101	0
2	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	0	0	0
All	All	3124	0	3156	188	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 32.

All (188) 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:111:MSE:HE2	1:A:173:PRO:HG3	1.47	0.94
1:B:192:LEU:HD12	1:B:192:LEU:O	1.72	0.89
1:A:62:THR:HG22	1:A:62:THR:O	1.72	0.87
1:B:84:VAL:H	1:B:107:HIS:CD2	1.96	0.84
1:A:213:ASN:OD1	1:A:215:THR:HB	1.78	0.84
1:B:52:ASN:HD22	1:B:52:ASN:N	1.76	0.80
1:B:21:LYS:HG3	1:B:218:GLU:HG3	1.65	0.79
1:B:148:LYS:NZ	1:B:162:GLU:HB2	1.98	0.79
1:A:148:LYS:O	1:A:152:GLN:HG3	1.82	0.78
1:B:201:THR:HG23	1:B:203:ILE:O	1.85	0.77
1:A:84:VAL:H	1:A:107:HIS:CD2	2.03	0.76
1:B:70:MSE:SE	1:B:71:MSE:H	2.18	0.75
1:B:230:LEU:C	1:B:232:SER:H	1.93	0.75
1:B:111:MSE:HE2	1:B:173:PRO:HG3	1.70	0.73
1:A:201:THR:HG23	1:A:203:ILE:O	1.90	0.71
1:A:21:LYS:HG3	1:A:218:GLU:HG3	1.73	0.71
1:A:140:THR:C	1:A:142:TYR:H	1.98	0.70
1:A:229:LYS:O	1:A:232:SER:HB3	1.90	0.70
1:B:52:ASN:N	1:B:52:ASN:ND2	2.37	0.70
1:B:70:MSE:SE	1:B:71:MSE:N	2.75	0.70
1:A:21:LYS:HD2	1:B:220:ARG:HD3	1.73	0.70
1:A:21:LYS:NZ	1:A:216:ASN:HB3	2.08	0.69
1:B:192:LEU:HD12	1:B:192:LEU:C	2.17	0.68
1:B:29:ILE:HD12	1:B:41:PHE:CE1	2.29	0.67
1:B:18:ILE:O	1:B:19:LEU:HB2	1.93	0.67
1:B:84:VAL:H	1:B:107:HIS:HD2	1.38	0.67
1:B:230:LEU:O	1:B:232:SER:N	2.29	0.65
1:B:66:ARG:HA	1:B:97:SER:HB3	1.76	0.65
1:A:157:ASN:OD1	1:A:157:ASN:C	2.40	0.65
1:A:70:MSE:HG3	1:A:71:MSE:H	1.60	0.64
1:B:148:LYS:HZ2	1:B:162:GLU:HB2	1.63	0.64
1:A:230:LEU:C	1:A:232:SER:H	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:CD2	1:A:183:GLU:HG2	2.27	0.63
1:B:229:LYS:O	1:B:232:SER:HB3	1.98	0.63
1:A:100:THR:HG21	1:A:118:GLY:H	1.63	0.63
1:B:23:ILE:HD11	1:B:220:ARG:HH11	1.64	0.63
1:B:232:SER:O	1:B:235:THR:N	2.32	0.63
1:A:140:THR:O	1:A:142:TYR:N	2.26	0.62
1:A:167:LYS:O	1:A:168:ASP:C	2.41	0.62
1:A:140:THR:C	1:A:142:TYR:N	2.57	0.62
1:B:21:LYS:HB2	1:B:216:ASN:O	2.00	0.62
1:B:172:THR:HG23	1:B:174:GLU:OE2	1.99	0.62
1:B:100:THR:HG21	1:B:118:GLY:O	2.00	0.61
1:B:230:LEU:C	1:B:232:SER:N	2.54	0.61
1:A:62:THR:O	1:A:62:THR:CG2	2.47	0.61
1:B:38:TYR:CD2	1:B:38:TYR:C	2.78	0.61
1:B:148:LYS:HZ1	1:B:162:GLU:HB2	1.64	0.60
1:A:73:ILE:CG2	1:A:102:ILE:HG12	2.30	0.60
1:B:140:THR:C	1:B:142:TYR:N	2.56	0.60
1:B:148:LYS:HZ1	1:B:162:GLU:CB	2.15	0.60
1:B:33:ILE:HD11	1:B:62:THR:OG1	2.02	0.60
1:B:232:SER:O	1:B:234:ILE:N	2.35	0.59
1:A:159:THR:O	1:A:163:GLU:HG3	2.03	0.59
1:A:100:THR:CG2	1:A:118:GLY:H	2.15	0.58
1:B:174:GLU:H	1:B:174:GLU:CD	2.10	0.58
1:A:230:LEU:O	1:A:232:SER:N	2.36	0.58
1:B:172:THR:HB	1:B:175:GLU:HG3	1.85	0.58
1:B:156:ARG:HD3	1:B:181:VAL:O	2.04	0.58
1:B:148:LYS:NZ	1:B:162:GLU:CB	2.67	0.57
1:A:54:GLU:O	1:A:55:ALA:HB2	2.03	0.57
1:A:230:LEU:C	1:A:232:SER:N	2.61	0.57
1:B:149:SER:O	1:B:153:GLU:HG2	2.03	0.57
1:B:201:THR:CG2	1:B:203:ILE:O	2.51	0.57
1:A:70:MSE:HG3	1:A:71:MSE:N	2.18	0.57
1:A:36:TYR:C	1:A:36:TYR:CD1	2.83	0.56
1:B:172:THR:HG22	1:B:175:GLU:H	1.71	0.56
1:A:234:ILE:C	1:A:236:ASP:H	2.15	0.55
1:B:173:PRO:HD2	1:B:174:GLU:OE2	2.05	0.55
1:B:233:TYR:C	1:B:235:THR:H	2.14	0.55
1:A:21:LYS:HZ2	1:A:216:ASN:HB3	1.71	0.55
1:B:140:THR:HG22	1:B:141:ASN:N	2.21	0.55
1:B:223:ALA:HB1	1:B:224:PRO:HD2	1.88	0.55
1:B:73:ILE:O	1:B:76:ARG:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ALA:O	1:A:70:MSE:HE3	2.07	0.54
1:A:74:VAL:O	1:A:78:GLN:HG3	2.07	0.54
1:B:21:LYS:HG3	1:B:218:GLU:CG	2.36	0.54
1:A:73:ILE:HG21	1:A:102:ILE:HG12	1.90	0.53
1:B:84:VAL:N	1:B:107:HIS:CD2	2.72	0.53
1:B:174:GLU:CD	1:B:174:GLU:N	2.65	0.53
1:B:232:SER:O	1:B:233:TYR:C	2.50	0.53
1:A:73:ILE:HG21	1:A:102:ILE:CD1	2.39	0.53
1:B:65:GLY:O	1:B:67:ALA:N	2.42	0.53
1:A:172:THR:O	1:A:173:PRO:C	2.50	0.52
1:B:160:ILE:O	1:B:161:ALA:C	2.51	0.52
1:B:144:ILE:O	1:B:145:ALA:C	2.49	0.51
1:B:232:SER:C	1:B:234:ILE:N	2.67	0.51
1:A:144:ILE:O	1:A:145:ALA:C	2.52	0.51
1:B:68:ASP:C	1:B:70:MSE:N	2.66	0.51
1:A:21:LYS:CG	1:A:218:GLU:HG3	2.40	0.51
1:A:225:SER:OG	1:A:228:ASP:OD2	2.28	0.51
1:A:157:ASN:HD21	1:A:160:ILE:HG12	1.76	0.50
1:B:29:ILE:CD1	1:B:41:PHE:CE1	2.95	0.50
1:A:73:ILE:HG22	1:A:102:ILE:HG12	1.93	0.50
1:A:84:VAL:H	1:A:107:HIS:HD2	1.52	0.50
1:B:96:ALA:HA	1:B:100:THR:HG22	1.94	0.50
1:A:29:ILE:HG22	1:A:29:ILE:O	2.12	0.50
1:A:43:ARG:HH12	1:A:228:ASP:CG	2.18	0.49
1:B:68:ASP:HA	1:B:70:MSE:CE	2.42	0.49
1:B:140:THR:C	1:B:142:TYR:H	2.19	0.49
1:B:23:ILE:CD1	1:B:220:ARG:HH11	2.25	0.49
1:B:108:LEU:CD2	1:B:183:GLU:HG2	2.42	0.49
1:B:52:ASN:HD22	1:B:52:ASN:H	1.56	0.49
1:B:20:ALA:C	1:B:21:LYS:HG2	2.36	0.49
1:A:88:VAL:HB	1:A:111:MSE:HG2	1.94	0.49
1:A:154:SER:OG	1:A:156:ARG:HG3	2.13	0.48
1:B:98:ALA:O	1:B:102:ILE:HD12	2.13	0.48
1:B:43:ARG:HH12	1:B:228:ASP:CG	2.22	0.48
1:A:230:LEU:O	1:A:233:TYR:N	2.46	0.48
1:B:110:ALA:HA	1:B:184:VAL:O	2.14	0.48
1:A:21:LYS:CD	1:A:218:GLU:HG3	2.44	0.47
1:A:160:ILE:O	1:A:161:ALA:C	2.57	0.47
1:B:86:ILE:HG13	1:B:103:ALA:HA	1.97	0.47
1:A:37:THR:O	1:A:38:TYR:C	2.55	0.47
1:A:157:ASN:ND2	1:A:160:ILE:HG12	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:HIS:CE1	1:A:205:VAL:HG22	2.49	0.47
1:B:37:THR:O	1:B:38:TYR:C	2.57	0.47
1:B:70:MSE:HB3	1:B:98:ALA:HB1	1.97	0.47
1:A:201:THR:CG2	1:A:203:ILE:O	2.61	0.47
1:B:161:ALA:O	1:B:164:PHE:HB2	2.14	0.47
1:A:40:GLN:O	1:A:41:PHE:C	2.58	0.47
1:B:71:MSE:O	1:B:75:GLN:HG3	2.15	0.47
1:B:84:VAL:N	1:B:107:HIS:HD2	2.08	0.47
1:A:77:ILE:O	1:A:80:SER:HB3	2.15	0.46
1:B:86:ILE:HG12	1:B:106:SER:CB	2.45	0.46
1:A:142:TYR:CD2	1:A:142:TYR:C	2.94	0.46
1:B:68:ASP:HA	1:B:70:MSE:HG3	1.96	0.46
1:B:70:MSE:O	1:B:73:ILE:N	2.49	0.46
1:A:172:THR:HG23	1:A:173:PRO:HD2	1.97	0.46
1:A:110:ALA:HA	1:A:184:VAL:O	2.16	0.46
1:B:74:VAL:O	1:B:75:GLN:C	2.56	0.46
1:B:140:THR:O	1:B:143:PHE:N	2.49	0.46
1:A:218:GLU:OE1	1:B:220:ARG:CZ	2.64	0.46
1:B:109:ILE:HG21	1:B:182:ILE:HG22	1.98	0.46
1:A:108:LEU:HD22	1:A:183:GLU:HG2	1.98	0.45
1:B:21:LYS:NZ	1:B:216:ASN:HB3	2.30	0.45
1:A:100:THR:HG21	1:A:118:GLY:N	2.28	0.45
1:B:45:ILE:O	1:B:49:GLU:HG3	2.16	0.45
1:B:97:SER:O	1:B:100:THR:HG23	2.17	0.45
1:A:140:THR:O	1:A:144:ILE:HG13	2.16	0.45
1:A:97:SER:O	1:A:98:ALA:C	2.56	0.45
1:A:28:GLN:O	1:A:29:ILE:CG1	2.64	0.45
1:A:36:TYR:O	1:A:39:ASP:HB2	2.17	0.45
1:B:54:GLU:O	1:B:55:ALA:HB2	2.16	0.45
1:A:228:ASP:OD2	1:A:228:ASP:N	2.50	0.44
1:A:90:PRO:O	1:A:91:PRO:C	2.60	0.44
1:B:21:LYS:CG	1:B:218:GLU:HG3	2.39	0.44
1:B:101:TYR:N	1:B:101:TYR:CD1	2.86	0.44
1:B:88:VAL:HB	1:B:111:MSE:HG2	1.98	0.44
1:A:225:SER:HG	1:A:228:ASP:CG	2.26	0.44
1:A:28:GLN:O	1:A:29:ILE:HG13	2.18	0.43
1:B:68:ASP:CA	1:B:70:MSE:HG3	2.48	0.43
1:B:140:THR:O	1:B:141:ASN:C	2.61	0.43
1:B:172:THR:CG2	1:B:175:GLU:HG3	2.48	0.43
1:A:160:ILE:HD13	1:A:160:ILE:HA	1.72	0.43
1:A:177:LEU:HD22	1:A:185:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:THR:HA	1:A:63:PRO:HD2	1.62	0.43
1:A:38:TYR:C	1:A:38:TYR:CD2	2.96	0.43
1:A:41:PHE:O	1:A:42:ASP:C	2.58	0.43
1:A:184:VAL:HG22	1:A:199:MSE:HE1	2.00	0.43
1:A:54:GLU:O	1:A:54:GLU:HG3	2.18	0.43
1:A:156:ARG:HD3	1:A:181:VAL:O	2.19	0.43
1:A:117:ILE:CG2	1:A:171:LEU:HB2	2.49	0.42
1:A:174:GLU:H	1:A:174:GLU:CD	2.27	0.42
1:A:188:ASP:O	1:A:189:ILE:C	2.60	0.42
1:B:95:ALA:O	1:B:100:THR:HG22	2.19	0.42
1:A:71:MSE:O	1:A:75:GLN:HG3	2.19	0.42
1:B:171:LEU:HA	1:B:171:LEU:HD23	1.75	0.42
1:B:25:TYR:CE1	1:B:222:LEU:HD21	2.55	0.42
1:A:43:ARG:NH1	1:A:228:ASP:OD1	2.35	0.42
1:A:231:ILE:O	1:A:235:THR:CB	2.67	0.42
1:B:68:ASP:HA	1:B:70:MSE:HE2	2.01	0.42
1:B:213:ASN:OD1	1:B:215:THR:HB	2.20	0.42
1:A:74:VAL:O	1:A:75:GLN:C	2.63	0.41
1:B:68:ASP:C	1:B:70:MSE:H	2.24	0.41
1:A:143:PHE:HD2	1:A:143:PHE:HA	1.75	0.41
1:B:188:ASP:O	1:B:189:ILE:C	2.61	0.41
1:A:234:ILE:C	1:A:236:ASP:N	2.76	0.41
1:A:227:LYS:O	1:A:228:ASP:C	2.64	0.41
1:B:18:ILE:O	1:B:19:LEU:CB	2.66	0.41
1:B:37:THR:O	1:B:40:GLN:N	2.54	0.41
1:A:71:MSE:HB3	1:A:71:MSE:HE2	1.66	0.40
1:B:109:ILE:CG2	1:B:182:ILE:HG22	2.51	0.40
1:B:154:SER:OG	1:B:156:ARG:HG3	2.21	0.40
1:A:21:LYS:HB2	1:A:216:ASN:O	2.21	0.40
1:B:96:ALA:O	1:B:97:SER:HB2	2.21	0.40
1:B:144:ILE:C	1:B:146:TYR:N	2.79	0.40
1:A:157:ASN:OD1	1:A:159:THR:N	2.55	0.40
1:B:23:ILE:HD11	1:B:220:ARG:NH1	2.33	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	195/230 (85%)	176 (90%)	15 (8%)	4 (2%)	5	27
1	B	196/230 (85%)	171 (87%)	17 (9%)	8 (4%)	2	13
All	All	391/460 (85%)	347 (89%)	32 (8%)	12 (3%)	3	19

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	B	66	ARG
1	B	67	ALA
1	A	231	ILE
1	B	63	PRO
1	B	231	ILE
1	B	233	TYR
1	B	234	ILE
1	A	29	ILE
1	B	19	LEU
1	A	142	TYR
1	B	29	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	165/188 (88%)	148 (90%)	17 (10%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	166/188 (88%)	145 (87%)	21 (13%)	4	20
All	All	331/376 (88%)	293 (88%)	38 (12%)	5	24

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	29	ILE
1	A	71	MSE
1	A	73	ILE
1	A	82	ILE
1	A	94	SER
1	A	108	LEU
1	A	150	LEU
1	A	157	ASN
1	A	170	SER
1	A	172	THR
1	A	182	ILE
1	A	192	LEU
1	A	201	THR
1	A	215	THR
1	A	217	VAL
1	A	228	ASP
1	B	19	LEU
1	B	21	LYS
1	B	29	ILE
1	B	52	ASN
1	B	56	ILE
1	B	60	LEU
1	B	78	GLN
1	B	82	ILE
1	B	85	ILE
1	B	91	PRO
1	B	94	SER
1	B	100	THR
1	B	108	LEU
1	B	120	CYS
1	B	140	THR
1	B	144	ILE
1	B	172	THR
1	B	178	LYS
1	B	201	THR

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Mol	Chain	Res	Type
1	B	215	THR
1	B	217	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	50	GLN
1	A	75	GLN
1	A	107	HIS
1	B	52	ASN
1	B	79	GLN
1	B	107	HIS

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	195/230 (84%)	-0.58	3 (1%)	72 49	18, 44, 106, 141	22 (11%)
1	B	196/230 (85%)	-0.52	3 (1%)	72 49	17, 44, 101, 138	22 (11%)
All	All	391/460 (85%)	-0.55	6 (1%)	72 49	17, 44, 103, 141	44 (11%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	GLY	3.3
1	A	236	ASP	2.4
1	B	233	TYR	2.1
1	A	142	TYR	2.1
1	B	64	GLY	2.1
1	B	65	GLY	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.