



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:15 PM UTC

PDB ID : 8SSG / pdb_00008ssg
Title : Minimal protein-only/RNA-free Ribonuclease P from *Hydrogenobacter thermophilus*
Authors : Mendoza, J.; Wilhelm, C.A.; Mallik, L.; Koutmos, M.
Deposited on : 2023-05-08
Resolution : 3.20 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
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

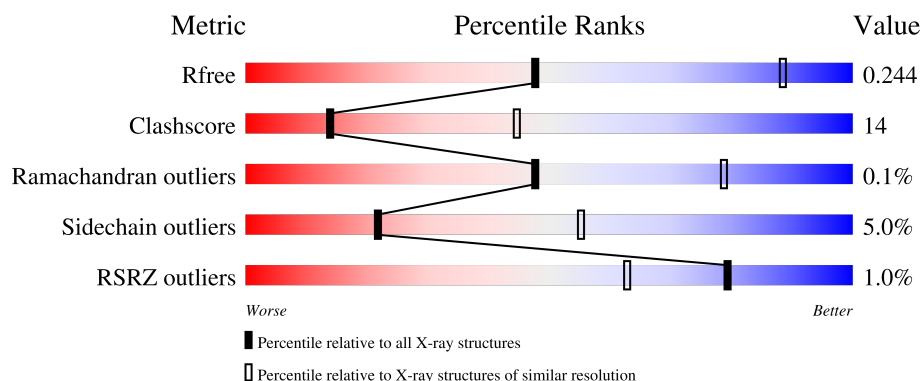
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	194	% 64% 21% 5% 10%
1	B	194	% 70% 15% • 11%
1	C	194	% 66% 22% 5% 6%
1	D	194	% 69% 18% 5% 8%
1	E	194	% 71% 13% • 13%

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Mol	Chain	Length	Quality of chain
1	F	194	% 61% 19% 5% • 14%
1	G	194	% 70% 14% • • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10146 atoms, of which 0 are hydrogens and 0 are deuteriums.

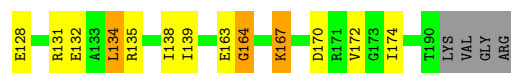
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-free ribonuclease P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	1	0
			1454	938	243	268	5			
1	B	173	Total	C	N	O	S	0	1	0
			1435	928	240	262	5			
1	C	183	Total	C	N	O	S	0	1	0
			1517	977	256	279	5			
1	D	179	Total	C	N	O	S	0	1	0
			1483	955	250	273	5			
1	E	169	Total	C	N	O	S	0	1	0
			1399	905	228	261	5			
1	F	167	Total	C	N	O	S	0	2	0
			1391	901	229	256	5			
1	G	173	Total	C	N	O	S	0	1	0
			1437	927	239	266	5			

- Molecule 2 is water.

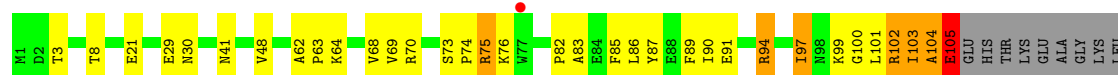
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	7	Total	O	0	0
			7	7		
2	C	5	Total	O	0	0
			5	5		
2	D	3	Total	O	0	0
			3	3		
2	E	3	Total	O	0	0
			3	3		
2	F	3	Total	O	0	0
			3	3		
2	G	1	Total	O	0	0
			1	1		



- Molecule 1: RNA-free ribonuclease P



- Molecule 1: RNA-free ribonuclease P



- Molecule 1: RNA-free ribonuclease P



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.32Å 113.76Å 155.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 3.20 29.74 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.74-3.20) 99.8 (29.74-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.198 , 0.248 0.194 , 0.244	Depositor DCC
R_{free} test set	1524 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	113.7	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 87.4	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	0.96	EDS
Total number of atoms	10146	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.15% 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	0.66	1/1485 (0.1%)	1.41	18/2007 (0.9%)
1	B	0.64	0/1465	1.30	6/1979 (0.3%)
1	C	0.75	3/1548 (0.2%)	1.42	16/2090 (0.8%)
1	D	0.63	0/1514	1.52	23/2046 (1.1%)
1	E	0.61	1/1429 (0.1%)	1.35	12/1932 (0.6%)
1	F	0.74	4/1424 (0.3%)	1.44	11/1924 (0.6%)
1	G	0.67	1/1467 (0.1%)	1.36	13/1982 (0.7%)
All	All	0.67	10/10332 (0.1%)	1.40	99/13960 (0.7%)

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	5
1	B	0	6
1	C	0	5
1	D	0	3
1	E	0	5
1	F	0	6
1	G	0	6
All	All	0	36

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	102	ARG	CD-NE	7.79	1.57	1.46
1	C	102	ARG	NE-CZ	7.71	1.41	1.33
1	F	102	ARG	C-O	7.52	1.32	1.24
1	A	107	HIS	CG-CD2	-5.76	1.29	1.35
1	F	135	ARG	NE-CZ	5.64	1.39	1.33
1	F	135	ARG	CD-NE	5.64	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	131	ARG	NE-CZ	-5.38	1.27	1.33
1	G	60	ASP	CG-OD1	-5.26	1.15	1.25
1	F	105	GLU	C-O	5.16	1.33	1.23
1	E	37	HIS	CG-CD2	-5.13	1.30	1.35

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	76	LYS	CA-C-O	18.79	141.86	121.19
1	E	23	ASP	CA-CB-CG	17.32	129.91	112.60
1	D	76	LYS	O-C-N	-13.86	105.83	122.87
1	A	190	THR	CA-CB-OG1	-13.19	89.82	109.60
1	C	107	HIS	CA-C-O	-12.27	107.42	120.42
1	D	76	LYS	CA-C-N	-12.24	103.98	120.63
1	D	76	LYS	C-N-CA	-12.24	103.98	120.63
1	C	102	ARG	CD-NE-CZ	12.18	141.44	124.40
1	G	171	ARG	CG-CD-NE	11.52	137.34	112.00
1	C	94	ARG	CG-CD-NE	11.27	136.79	112.00
1	E	132	GLU	CB-CG-CD	-11.18	93.59	112.60
1	D	76	LYS	CB-CG-CD	10.89	136.34	111.30
1	E	190	THR	CA-CB-OG1	-10.85	93.32	109.60
1	C	131	ARG	NE-CZ-NH1	-10.62	110.88	121.50
1	F	135	ARG	CD-NE-CZ	10.61	139.25	124.40
1	F	102	ARG	CA-C-O	10.57	132.05	120.63
1	F	135	ARG	NE-CZ-NH2	10.23	128.41	119.20
1	G	124	ASN	CA-CB-CG	-9.86	102.74	112.60
1	D	76	LYS	N-CA-C	9.85	124.51	110.23
1	C	107	HIS	O-C-N	9.76	133.28	122.15
1	C	131	ARG	CD-NE-CZ	-9.44	111.18	124.40
1	F	135	ARG	CG-CD-NE	8.82	131.41	112.00
1	E	70	ARG	CG-CD-NE	8.20	130.04	112.00
1	C	102	ARG	CB-CG-CD	8.08	129.89	111.30
1	F	104	ALA	CA-C-N	-7.99	107.31	121.70
1	F	104	ALA	C-N-CA	-7.99	107.31	121.70
1	G	103	ILE	CA-C-O	7.40	128.69	120.85
1	E	105	GLU	CB-CA-C	-7.36	99.43	111.50
1	D	105	GLU	CB-CA-C	-7.18	98.64	110.85
1	F	94	ARG	CG-CD-NE	7.13	127.70	112.00
1	C	102	ARG	NE-CZ-NH1	7.13	128.63	121.50
1	A	128	GLU	CB-CA-C	-7.11	95.38	109.67
1	C	106	GLU	CB-CG-CD	-7.11	100.51	112.60
1	B	129	LYS	CA-C-N	7.08	129.76	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	LYS	C-N-CA	7.08	129.76	120.28
1	B	22	GLU	CB-CG-CD	6.81	124.17	112.60
1	G	94	ARG	CB-CG-CD	-6.79	95.69	111.30
1	E	23	ASP	CB-CA-C	-6.69	98.07	109.51
1	F	146	ASP	CA-CB-CG	6.61	119.21	112.60
1	C	105	GLU	CB-CA-C	-6.58	100.50	110.90
1	A	190	THR	CA-C-O	-6.48	109.78	120.80
1	E	135	ARG	CB-CG-CD	6.45	126.14	111.30
1	D	84	GLU	O-C-N	6.41	128.92	122.12
1	G	59	GLY	CA-C-N	6.26	129.52	120.38
1	G	59	GLY	C-N-CA	6.26	129.52	120.38
1	C	109	LYS	N-CA-C	-6.22	103.81	111.33
1	A	23	ASP	N-CA-CB	-6.16	100.76	110.06
1	A	102	ARG	CB-CG-CD	6.15	125.45	111.30
1	D	164	GLY	O-C-N	6.13	128.07	122.18
1	A	172	VAL	N-CA-C	-6.12	101.66	109.80
1	G	125	ARG	CA-C-N	-6.12	112.48	120.44
1	G	125	ARG	C-N-CA	-6.12	112.48	120.44
1	B	102	ARG	CB-CG-CD	6.08	125.28	111.30
1	E	166	ARG	CB-CG-CD	6.08	125.28	111.30
1	D	127	ARG	CB-CA-C	-6.06	100.55	110.85
1	A	125	ARG	CB-CG-CD	6.02	125.14	111.30
1	C	94	ARG	CB-CG-CD	-5.97	97.57	111.30
1	E	70	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	G	106	GLU	CA-C-O	-5.92	110.74	120.80
1	C	110	GLU	CB-CG-CD	5.76	122.40	112.60
1	D	29	GLU	CB-CA-C	-5.64	99.84	110.67
1	A	76	LYS	CA-C-O	5.63	127.63	121.27
1	A	172	VAL	CA-C-O	-5.63	115.79	121.59
1	E	190	THR	CA-C-O	-5.62	111.25	120.80
1	D	125	ARG	CG-CD-NE	-5.57	99.75	112.00
1	A	106	GLU	CB-CA-C	-5.56	99.97	109.65
1	G	125	ARG	CD-NE-CZ	5.53	132.14	124.40
1	B	124	ASN	CB-CA-C	5.51	120.11	110.64
1	F	135	ARG	CB-CG-CD	5.50	123.95	111.30
1	D	122	VAL	CA-C-N	5.46	129.26	120.30
1	D	122	VAL	C-N-CA	5.46	129.26	120.30
1	A	22	GLU	CA-C-N	5.45	129.22	121.42
1	A	22	GLU	C-N-CA	5.45	129.22	121.42
1	A	76	LYS	CB-CA-C	-5.44	97.50	110.02
1	G	94	ARG	CB-CA-C	-5.43	102.35	110.88
1	A	75	ARG	CB-CG-CD	5.40	123.71	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	171	ARG	CB-CG-CD	-5.39	98.89	111.30
1	F	97	ILE	CB-CG1-CD1	-5.37	102.52	113.80
1	D	77[A]	TRP	N-CA-C	5.37	116.99	111.03
1	D	77[B]	TRP	N-CA-C	5.37	116.99	111.03
1	G	131	ARG	CB-CA-C	-5.36	101.73	110.85
1	B	128	GLU	CB-CG-CD	-5.34	103.52	112.60
1	E	70	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	D	106	GLU	CB-CG-CD	-5.27	103.64	112.60
1	D	134	LEU	CB-CA-C	-5.25	102.60	110.90
1	A	129	LYS	CG-CD-CE	5.25	123.36	111.30
1	C	84	GLU	CB-CG-CD	5.24	121.51	112.60
1	D	128	GLU	CB-CG-CD	5.22	121.48	112.60
1	D	94	ARG	CG-CD-NE	-5.18	100.59	112.00
1	D	22	GLU	CB-CG-CD	5.16	121.38	112.60
1	D	8	THR	CB-CA-C	5.13	119.31	110.79
1	C	102	ARG	NH1-CZ-NH2	-5.11	112.66	119.30
1	D	124	ASN	N-CA-CB	-5.10	102.67	110.33
1	C	75	ARG	CG-CD-NE	-5.10	100.78	112.00
1	E	166	ARG	CD-NE-CZ	-5.08	117.28	124.40
1	A	177	ILE	CB-CA-C	5.05	119.75	110.71
1	F	135	ARG	NH1-CZ-NH2	-5.05	112.74	119.30
1	A	132	GLU	CA-C-N	5.04	127.04	120.28
1	A	132	GLU	C-N-CA	5.04	127.04	120.28

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	127	ARG	Sidechain
1	A	70	ARG	Sidechain
1	A	75	ARG	Sidechain
1	A	96	ARG	Sidechain
1	B	102	ARG	Sidechain
1	B	125	ARG	Sidechain
1	B	127	ARG	Sidechain
1	B	135	ARG	Sidechain
1	B	171	ARG	Sidechain
1	B	94	ARG	Sidechain
1	C	102	ARG	Sidechain
1	C	127	ARG	Sidechain
1	C	135	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	70	ARG	Sidechain
1	C	94	ARG	Sidechain
1	D	125	ARG	Sidechain
1	D	127	ARG	Sidechain
1	D	131	ARG	Sidechain
1	E	102	ARG	Sidechain
1	E	131	ARG	Sidechain
1	E	135	ARG	Sidechain
1	E	166	ARG	Sidechain
1	E	70	ARG	Sidechain
1	F	131	ARG	Sidechain
1	F	166	ARG	Sidechain
1	F	70	ARG	Sidechain
1	F	75[A]	ARG	Sidechain
1	F	75[B]	ARG	Sidechain
1	F	94	ARG	Sidechain
1	G	102	ARG	Sidechain
1	G	131	ARG	Sidechain
1	G	171	ARG	Sidechain
1	G	70	ARG	Sidechain
1	G	94	ARG	Sidechain
1	G	96	ARG	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	1454	0	1446	40	0
1	B	1435	0	1440	52	1
1	C	1517	0	1519	92	1
1	D	1483	0	1478	96	0
1	E	1399	0	1387	58	0
1	F	1391	0	1387	78	0
1	G	1437	0	1430	26	0
2	A	8	0	0	0	0
2	B	7	0	0	2	0
2	C	5	0	0	0	0
2	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	1	0	0	0	0
All	All	10146	0	10087	291	1

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 (291) 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:D:77[A]:TRP:HH2	1:F:85:PHE:CD1	1.66	1.11
1:D:77[A]:TRP:CH2	1:F:85:PHE:CD1	2.40	1.09
1:D:77[A]:TRP:HE1	1:F:172:VAL:HB	1.16	1.07
1:B:77[A]:TRP:HZ3	1:D:82:PRO:HG2	1.11	1.07
1:C:85:PHE:CD1	1:E:77[A]:TRP:HH2	1.71	1.06
1:B:77[A]:TRP:CZ3	1:D:82:PRO:CG	2.39	1.05
1:C:85:PHE:CD1	1:E:77[A]:TRP:CH2	2.46	1.04
1:C:85:PHE:CG	1:E:77[A]:TRP:HH2	1.75	1.03
1:C:108:THR:HG21	1:C:126:LEU:CD1	1.88	1.03
1:D:77[A]:TRP:NE1	1:F:172:VAL:HB	1.73	1.03
1:B:77[A]:TRP:CE3	1:D:82:PRO:HG3	1.92	1.02
1:E:85:PHE:CD1	1:G:77[A]:TRP:HH2	1.78	1.02
1:C:85:PHE:HB2	1:E:77[A]:TRP:CH2	1.95	1.01
1:A:77[A]:TRP:HA	1:A:77[A]:TRP:CE3	1.93	1.00
1:A:172:VAL:HG13	1:C:77[A]:TRP:CZ2	1.97	1.00
1:B:77[A]:TRP:HZ3	1:D:82:PRO:CG	1.73	0.98
1:B:77[A]:TRP:CZ3	1:D:82:PRO:HG2	2.00	0.97
1:D:77[B]:TRP:CH2	1:F:85:PHE:CD1	2.54	0.95
1:D:77[A]:TRP:HE1	1:F:172:VAL:CB	1.81	0.94
1:D:20:PHE:O	1:D:21:GLU:HG2	1.66	0.94
1:D:77[A]:TRP:HZ2	1:F:172:VAL:CG1	1.81	0.94
1:E:85:PHE:CD1	1:G:77[A]:TRP:CH2	2.55	0.94
1:A:172:VAL:HG13	1:C:77[A]:TRP:CE2	2.04	0.93
1:F:100:GLY:O	1:F:103:ILE:HG12	1.68	0.92
1:D:77[B]:TRP:HH2	1:F:85:PHE:CD1	1.88	0.91
1:A:77[A]:TRP:HA	1:A:77[A]:TRP:HE3	1.35	0.90
1:F:105:GLU:HG3	1:F:105:GLU:O	1.68	0.88
1:D:77[A]:TRP:CH2	1:F:85:PHE:HD1	1.86	0.87
1:B:77[A]:TRP:HE3	1:D:82:PRO:HG3	1.39	0.87
1:D:77[A]:TRP:CH2	1:F:85:PHE:HB2	2.09	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77[B]:TRP:CE3	1:G:77[B]:TRP:HA	2.07	0.86
1:D:77[A]:TRP:HH2	1:F:85:PHE:HD1	1.21	0.86
1:C:108:THR:HG21	1:C:126:LEU:HD11	1.58	0.86
1:E:101:LEU:HD21	1:F:131:ARG:HG3	1.59	0.84
1:C:108:THR:HG21	1:C:126:LEU:HD12	1.59	0.83
1:D:77[A]:TRP:HE1	1:F:172:VAL:CA	1.90	0.82
1:C:85:PHE:CB	1:E:77[A]:TRP:HH2	1.91	0.82
1:D:77[A]:TRP:CZ3	1:F:85:PHE:HB2	2.14	0.82
1:C:85:PHE:CG	1:E:77[A]:TRP:CH2	2.65	0.82
1:G:77[B]:TRP:HA	1:G:77[B]:TRP:HE3	1.41	0.81
1:A:20:PHE:O	1:A:21:GLU:HG2	1.82	0.80
1:D:77[A]:TRP:CZ2	1:F:172:VAL:CG1	2.65	0.80
1:D:77[A]:TRP:HH2	1:F:85:PHE:CG	2.00	0.79
1:C:85:PHE:CB	1:E:77[A]:TRP:CH2	2.66	0.79
1:C:89:PHE:CE2	1:D:90:ILE:HG12	2.17	0.78
1:C:77[A]:TRP:CE3	1:C:77[A]:TRP:HA	2.18	0.78
1:B:77[A]:TRP:CE3	1:D:82:PRO:CG	2.63	0.77
1:B:77[A]:TRP:CZ3	1:D:82:PRO:HG3	2.13	0.76
1:D:77[A]:TRP:CZ2	1:F:172:VAL:HG12	2.23	0.74
1:C:89:PHE:HE2	1:D:90:ILE:HG12	1.52	0.73
1:A:89:PHE:CE2	1:B:90:ILE:HG12	2.24	0.73
1:A:90:ILE:HG12	1:B:89:PHE:CE2	2.24	0.73
1:C:62:ALA:HB3	1:C:63:PRO:HD3	1.69	0.72
1:C:109:LYS:O	1:C:110:GLU:C	2.32	0.72
1:D:77[A]:TRP:CD1	1:F:172:VAL:O	2.43	0.72
1:D:77[A]:TRP:CE3	1:F:82:PRO:HG3	2.27	0.70
1:C:77[A]:TRP:HA	1:C:77[A]:TRP:HE3	1.57	0.70
1:D:77[A]:TRP:CE2	1:F:172:VAL:HB	2.27	0.70
1:C:172:VAL:HB	1:E:77[A]:TRP:HE1	1.56	0.69
1:C:172:VAL:HB	1:E:77[A]:TRP:NE1	2.06	0.69
1:C:85:PHE:CD1	1:E:77[B]:TRP:CZ2	2.81	0.69
1:D:77[B]:TRP:CZ2	1:F:85:PHE:CD1	2.77	0.68
1:G:181:ASN:O	1:G:185:ILE:HG12	1.93	0.68
1:C:85:PHE:HB2	1:E:77[A]:TRP:CZ3	2.27	0.68
1:D:77[A]:TRP:CZ3	1:F:82:PRO:CG	2.76	0.68
1:B:77[A]:TRP:HH2	1:D:85:PHE:CD1	2.10	0.68
1:C:181:ASN:O	1:C:185:ILE:HG12	1.93	0.68
1:F:160:SER:O	1:F:166:ARG:HD3	1.94	0.67
1:C:108:THR:CG2	1:C:126:LEU:CD1	2.71	0.67
1:F:101:LEU:C	1:F:101:LEU:HD12	2.19	0.67
1:D:77[A]:TRP:HH2	1:F:85:PHE:CB	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:VAL:HG22	1:C:77[A]:TRP:CH2	2.31	0.66
1:C:172:VAL:CG1	1:E:77[A]:TRP:HZ2	2.09	0.66
1:A:172:VAL:HG22	1:C:77[A]:TRP:CZ2	2.31	0.66
1:E:85:PHE:CG	1:G:77[A]:TRP:HH2	2.15	0.65
1:E:172:VAL:HG23	1:E:174:ILE:HG12	1.79	0.65
1:B:77[A]:TRP:CH2	1:D:85:PHE:HB2	2.31	0.65
1:D:77[A]:TRP:CZ3	1:F:82:PRO:HG2	2.32	0.65
1:D:77[B]:TRP:CZ2	1:F:85:PHE:HD1	2.13	0.65
1:D:77[A]:TRP:CH2	1:F:85:PHE:CB	2.80	0.64
1:A:85:PHE:CD1	1:C:77[B]:TRP:CH2	2.85	0.64
1:A:90:ILE:HG12	1:B:89:PHE:CZ	2.32	0.64
1:D:77[A]:TRP:HZ2	1:F:172:VAL:HG11	1.59	0.64
1:C:119:VAL:HG12	1:C:120:GLY:H	1.63	0.64
1:D:164:GLY:HA2	1:D:167:LYS:HE2	1.80	0.64
1:C:101:LEU:O	1:C:105:GLU:HG3	1.98	0.64
1:A:62:ALA:HB3	1:A:63:PRO:HD3	1.80	0.63
1:F:105:GLU:O	1:F:105:GLU:CG	2.45	0.63
1:A:85:PHE:CD1	1:C:77[B]:TRP:CZ2	2.86	0.63
1:D:76:LYS:O	1:D:77[A]:TRP:C	2.36	0.63
1:C:86:LEU:O	1:C:90:ILE:HG13	1.98	0.63
1:F:104:ALA:HB1	1:F:130:TYR:CE1	2.34	0.63
1:B:77[A]:TRP:CH2	1:D:85:PHE:CD1	2.87	0.62
1:E:101:LEU:CD2	1:F:131:ARG:HG3	2.29	0.62
1:C:172:VAL:CA	1:E:77[A]:TRP:HE1	2.12	0.62
1:F:103:ILE:O	1:F:105:GLU:O	2.17	0.62
1:C:90:ILE:HG12	1:D:89:PHE:CZ	2.35	0.62
1:C:131:ARG:O	1:C:135:ARG:HG2	1.99	0.62
1:A:89:PHE:CZ	1:B:90:ILE:HG12	2.35	0.62
1:C:85:PHE:CD1	1:E:77[B]:TRP:CH2	2.88	0.62
1:D:77[A]:TRP:HZ3	1:F:82:PRO:HG2	1.62	0.62
1:A:93:VAL:O	1:A:97:ILE:HG12	2.00	0.62
1:C:85:PHE:CD1	1:E:77[A]:TRP:CZ2	2.88	0.61
1:C:134:LEU:HD21	1:D:101:LEU:HD22	1.83	0.61
1:B:125:ARG:H	1:B:125:ARG:HD3	1.66	0.61
1:D:77[A]:TRP:CH2	1:F:85:PHE:CG	2.83	0.61
1:A:126:LEU:CD2	1:B:127:ARG:HH21	2.14	0.61
1:C:20:PHE:O	1:C:21:GLU:HG2	2.01	0.60
1:C:85:PHE:HD1	1:E:77[A]:TRP:CH2	2.17	0.60
1:D:77[A]:TRP:NE1	1:F:172:VAL:O	2.34	0.60
1:C:172:VAL:CB	1:E:77[A]:TRP:HE1	2.14	0.60
1:D:77[A]:TRP:CE3	1:F:82:PRO:CG	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD21	1:B:127:ARG:HD2	1.83	0.60
1:G:96:ARG:NH1	1:G:162:ASP:OD2	2.32	0.59
1:C:125:ARG:O	1:C:129:LYS:HG3	2.03	0.59
1:D:77[B]:TRP:HH2	1:F:85:PHE:CE1	2.18	0.59
1:F:99:LYS:O	1:F:103:ILE:HG23	2.02	0.59
1:A:172:VAL:CG1	1:C:77[A]:TRP:CZ2	2.82	0.58
1:B:77[A]:TRP:CZ2	1:D:172:VAL:HB	2.38	0.58
1:F:3:THR:HG22	1:F:41:ASN:HB2	1.85	0.58
1:C:93:VAL:O	1:C:97:ILE:HG12	2.04	0.58
1:B:93:VAL:O	1:B:97:ILE:HG12	2.04	0.58
1:C:134:LEU:HD12	1:C:135:ARG:N	2.17	0.58
1:C:134:LEU:CD1	1:C:135:ARG:HD3	2.34	0.57
1:E:134:LEU:HD22	1:F:134:LEU:HD11	1.86	0.57
1:D:77[A]:TRP:HZ3	1:F:82:PRO:CG	2.17	0.57
1:E:85:PHE:CD1	1:G:77[A]:TRP:CZ2	2.92	0.57
1:C:82:PRO:CG	1:E:77[A]:TRP:CE3	2.88	0.57
1:B:123:VAL:HG12	1:B:124:ASN:N	2.18	0.56
1:C:108:THR:CG2	1:C:126:LEU:HD11	2.32	0.56
1:A:157:ILE:HG21	1:A:177:ILE:HD12	1.86	0.56
1:C:20:PHE:C	1:C:21:GLU:HG2	2.30	0.56
1:E:62:ALA:HB3	1:E:63:PRO:HD3	1.87	0.56
1:B:77[A]:TRP:HH2	1:D:85:PHE:HB2	1.71	0.56
1:C:86:LEU:HD21	1:D:85:PHE:HE2	1.71	0.56
1:B:181:ASN:O	1:B:185:ILE:HG12	2.06	0.56
1:C:105:GLU:HA	1:C:108:THR:HG22	1.86	0.56
1:C:172:VAL:HG23	1:C:174:ILE:HG12	1.87	0.56
1:B:21:GLU:HB3	1:B:23:ASP:OD1	2.06	0.56
1:D:62:ALA:HB3	1:D:63:PRO:HD3	1.87	0.56
1:E:89:PHE:CZ	1:F:90:ILE:HG12	2.41	0.56
1:A:50:TYR:CZ	1:A:54:LYS:HD2	2.40	0.56
1:C:77[A]:TRP:CE3	1:C:77[A]:TRP:CA	2.88	0.56
1:E:69:VAL:O	1:E:69:VAL:HG23	2.06	0.55
1:D:77[B]:TRP:HZ2	1:F:85:PHE:HD1	1.54	0.55
1:B:125:ARG:O	1:B:129:LYS:HD3	2.06	0.55
1:A:126:LEU:HD21	1:B:127:ARG:HH21	1.70	0.55
1:F:101:LEU:HD12	1:F:102:ARG:N	2.22	0.55
1:C:89:PHE:CE1	1:C:145:VAL:HG23	2.42	0.54
1:C:102:ARG:O	1:C:106:GLU:HB2	2.08	0.54
1:C:90:ILE:HG12	1:D:89:PHE:CE2	2.42	0.54
1:D:23:ASP:OD1	1:D:23:ASP:N	2.40	0.54
1:D:77[A]:TRP:CZ2	1:F:85:PHE:HD1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:TYR:CE2	1:F:75[B]:ARG:HD2	2.43	0.54
1:E:172:VAL:HG12	1:G:77[A]:TRP:HZ2	1.73	0.54
1:D:132:GLU:OE2	1:D:132:GLU:HA	2.08	0.53
1:E:172:VAL:CG1	1:G:77[A]:TRP:HZ2	2.21	0.53
1:C:100:GLY:O	1:C:103:ILE:HG12	2.08	0.53
1:A:101:LEU:HD11	1:B:134:LEU:HD21	1.90	0.53
1:B:83:ALA:O	1:B:86:LEU:HB3	2.09	0.53
1:D:76:LYS:O	1:D:77[B]:TRP:C	2.35	0.53
1:D:77[A]:TRP:CZ2	1:F:172:VAL:HB	2.44	0.53
1:B:77[A]:TRP:CE2	1:D:172:VAL:HB	2.43	0.53
1:B:86:LEU:O	1:B:90:ILE:HG13	2.09	0.53
1:E:89:PHE:CE2	1:F:90:ILE:HG12	2.43	0.53
1:B:62:ALA:HB3	1:B:63:PRO:HD3	1.91	0.52
1:B:77[A]:TRP:NE1	1:D:172:VAL:HB	2.23	0.52
1:C:82:PRO:HG2	1:E:77[A]:TRP:CZ3	2.44	0.52
1:C:85:PHE:CD1	1:E:77[B]:TRP:HZ2	2.26	0.52
1:B:68:VAL:HG23	1:B:69:VAL:HG23	1.90	0.52
1:C:172:VAL:HA	1:E:77[A]:TRP:HE1	1.73	0.52
1:A:128:GLU:HA	1:A:131:ARG:NH1	2.24	0.52
1:D:77[A]:TRP:HE3	1:F:82:PRO:HG3	1.72	0.52
1:F:68:VAL:HG23	1:F:69:VAL:HG23	1.91	0.52
1:G:102:ARG:HA	1:G:105:GLU:OE1	2.10	0.52
1:A:128:GLU:HA	1:A:131:ARG:HH11	1.75	0.52
1:D:68:VAL:HG23	1:D:69:VAL:HG23	1.92	0.52
1:E:172:VAL:CG1	1:G:77[A]:TRP:CZ2	2.94	0.51
1:F:172:VAL:HG23	1:F:174:ILE:HG12	1.93	0.51
1:A:68:VAL:HG23	1:A:69:VAL:HG23	1.92	0.51
1:A:85:PHE:HD1	1:C:77[B]:TRP:HZ2	1.58	0.51
1:F:73:SER:OG	1:F:74:PRO:HD2	2.11	0.51
1:F:101:LEU:O	1:F:102:ARG:C	2.51	0.51
1:D:77[A]:TRP:HE1	1:F:172:VAL:C	2.17	0.51
1:A:85:PHE:CD1	1:C:77[B]:TRP:HH2	2.26	0.50
1:G:103:ILE:O	1:G:106:GLU:HB2	2.11	0.50
1:A:77[A]:TRP:CE3	1:A:77[A]:TRP:CA	2.80	0.50
1:A:172:VAL:HG13	1:C:77[B]:TRP:CZ2	2.45	0.50
1:C:82:PRO:CG	1:E:77[A]:TRP:CZ3	2.95	0.49
1:C:89:PHE:CD1	1:C:145:VAL:HG23	2.47	0.49
1:D:77[A]:TRP:HZ3	1:F:85:PHE:HB2	1.70	0.49
1:D:134:LEU:O	1:D:138:ILE:HG12	2.12	0.49
1:C:121:ARG:HA	1:C:124:ASN:ND2	2.28	0.49
1:E:96:ARG:HE	1:E:140:ASP:HB3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ASP:OD1	1:B:23:ASP:N	2.46	0.49
1:D:77[A]:TRP:CZ2	1:F:85:PHE:CD1	2.92	0.49
1:A:99:LYS:O	1:A:103:ILE:HG12	2.13	0.49
1:C:124:ASN:O	1:C:128:GLU:HG3	2.12	0.49
1:E:87:TYR:CE2	1:F:75[A]:ARG:HG3	2.48	0.49
1:B:76:LYS:NZ	2:B:201:HOH:O	2.46	0.48
1:E:90:ILE:HG12	1:F:89:PHE:CE2	2.47	0.48
1:G:62:ALA:HB3	1:G:63:PRO:HD3	1.95	0.48
1:B:125:ARG:H	1:B:125:ARG:CD	2.26	0.48
1:C:82:PRO:HG3	1:E:77[A]:TRP:CE3	2.49	0.48
1:E:85:PHE:CG	1:G:77[A]:TRP:CH2	2.97	0.48
1:B:127:ARG:HA	1:B:130:TYR:HB2	1.95	0.48
1:A:172:VAL:HG12	1:A:174:ILE:HD12	1.95	0.48
1:G:77[B]:TRP:CE3	1:G:77[B]:TRP:CA	2.91	0.48
1:B:125:ARG:CD	1:B:125:ARG:N	2.76	0.48
1:E:93:VAL:O	1:E:97:ILE:HG12	2.14	0.48
1:E:172:VAL:HG12	1:G:77[A]:TRP:CZ2	2.49	0.48
1:F:62:ALA:HB3	1:F:63:PRO:HD3	1.96	0.47
1:F:101:LEU:C	1:F:103:ILE:N	2.69	0.47
1:A:85:PHE:CD1	1:C:77[B]:TRP:HZ2	2.31	0.47
1:B:126:LEU:O	1:B:130:TYR:CD1	2.68	0.47
1:E:85:PHE:HD1	1:G:77[A]:TRP:CZ2	2.32	0.47
1:E:90:ILE:HG12	1:F:89:PHE:CZ	2.49	0.47
1:F:8:THR:HG23	1:F:48:VAL:HG13	1.96	0.47
1:A:172:VAL:HG13	1:C:77[B]:TRP:CE2	2.48	0.47
1:B:77[A]:TRP:CZ3	1:D:85:PHE:HB2	2.49	0.47
1:C:89:PHE:CZ	1:D:90:ILE:HG12	2.49	0.47
1:G:68:VAL:HG23	1:G:69:VAL:HG23	1.97	0.47
1:G:83:ALA:O	1:G:86:LEU:HB3	2.14	0.47
1:A:90:ILE:HG12	1:B:89:PHE:HE2	1.77	0.46
1:C:134:LEU:HD11	1:C:135:ARG:HD3	1.97	0.46
1:D:172:VAL:HG23	1:D:174:ILE:HG12	1.96	0.46
1:B:18:HIS:CD2	1:B:22:GLU:HA	2.50	0.46
1:B:77[B]:TRP:CZ2	1:D:85:PHE:CD1	3.03	0.46
1:D:77[A]:TRP:CZ2	1:F:172:VAL:CB	2.99	0.46
1:C:172:VAL:HG12	1:E:77[A]:TRP:HZ2	1.80	0.45
1:C:172:VAL:CG1	1:E:77[A]:TRP:CZ2	2.96	0.45
1:F:177:ILE:HG12	1:F:185:ILE:CD1	2.46	0.45
1:C:134:LEU:HD21	1:D:101:LEU:CD2	2.46	0.45
1:G:8:THR:HG23	1:G:48:VAL:HG13	1.98	0.45
1:C:68:VAL:HG23	1:C:69:VAL:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ARG:HH11	1:C:131:ARG:HD2	1.01	0.45
1:C:85:PHE:HD1	1:E:77[A]:TRP:CZ2	2.31	0.44
1:B:46:THR:HG21	1:D:170:ASP:OD1	2.16	0.44
1:F:103:ILE:HG21	1:F:103:ILE:HD13	1.55	0.44
1:C:104:ALA:O	1:C:108:THR:HG22	2.17	0.44
1:C:85:PHE:HD1	1:E:77[B]:TRP:HZ2	1.63	0.44
1:A:123:VAL:HG13	1:A:124:ASN:N	2.31	0.44
1:F:104:ALA:CB	1:F:130:TYR:CE1	3.01	0.44
1:B:77[B]:TRP:CH2	1:D:85:PHE:CD1	3.05	0.43
1:C:134:LEU:HD12	1:C:135:ARG:HD3	2.00	0.43
1:C:101:LEU:O	1:C:102:ARG:C	2.59	0.43
1:D:77[A]:TRP:NE1	1:F:172:VAL:CB	2.54	0.43
1:D:93:VAL:O	1:D:97:ILE:HG12	2.18	0.43
1:D:135:ARG:O	1:D:139:ILE:HG12	2.19	0.43
1:C:103:ILE:O	1:C:104:ALA:C	2.60	0.43
1:E:131:ARG:HD3	1:E:135:ARG:NH2	2.33	0.43
1:G:93:VAL:O	1:G:97:ILE:HG12	2.19	0.43
1:A:13:ASN:OD1	1:A:15:ASP:HB2	2.19	0.43
1:B:77[A]:TRP:CZ3	1:D:82:PRO:CD	3.02	0.43
1:D:120:GLY:O	1:D:123:VAL:HG22	2.19	0.43
1:A:50:TYR:CE2	1:A:54:LYS:HD2	2.54	0.43
1:A:95:TYR:CZ	1:A:164:GLY:HA3	2.54	0.42
1:C:108:THR:HB	1:C:129:LYS:CE	2.49	0.42
1:A:168:TRP:C	1:A:170:ASP:H	2.27	0.42
1:D:77[A]:TRP:NE1	1:F:172:VAL:CA	2.71	0.42
1:E:85:PHE:HE2	1:F:86:LEU:HD21	1.85	0.42
1:E:131:ARG:HD3	1:E:135:ARG:HH21	1.85	0.42
1:B:77[A]:TRP:HH2	1:D:85:PHE:CB	2.31	0.42
1:B:175:LYS:HA	2:B:204:HOH:O	2.20	0.42
1:C:127:ARG:NH2	1:D:108:THR:OG1	2.53	0.42
1:G:97:ILE:HG13	1:G:98:ASN:H	1.84	0.42
1:D:29:GLU:HG2	1:D:61:LEU:HD21	2.02	0.41
1:F:83:ALA:O	1:F:86:LEU:HB3	2.19	0.41
1:E:75:ARG:HG2	1:F:87:TYR:CE2	2.55	0.41
1:G:97:ILE:HG21	1:G:97:ILE:HD13	1.90	0.41
1:C:172:VAL:HG12	1:E:77[A]:TRP:CZ2	2.56	0.41
1:A:127:ARG:HH21	1:B:126:LEU:CD1	2.33	0.41
1:C:50:TYR:CZ	1:C:54:LYS:HD2	2.56	0.41
1:C:105:GLU:O	1:C:109:LYS:N	2.54	0.41
1:B:77[A]:TRP:HH2	1:D:85:PHE:HD1	1.63	0.41
1:C:86:LEU:HD21	1:D:85:PHE:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:ILE:HG13	1:G:98:ASN:N	2.35	0.41
1:B:77[A]:TRP:HH2	1:D:85:PHE:CG	2.38	0.41
1:D:77[A]:TRP:HE1	1:F:172:VAL:HA	1.79	0.41
1:F:103:ILE:O	1:F:104:ALA:C	2.64	0.41
1:F:97:ILE:HG21	1:F:97:ILE:HD13	1.40	0.41
1:C:87:TYR:CE2	1:D:75:ARG:HG2	2.56	0.40
1:C:108:THR:HG23	1:D:127:ARG:HH12	1.85	0.40
1:G:57:SER:O	1:G:58:LEU:CB	2.68	0.40
1:D:20:PHE:C	1:D:21:GLU:HG2	2.40	0.40
1:E:83:ALA:O	1:E:86:LEU:HB3	2.21	0.40
1:B:77[A]:TRP:NE1	1:D:172:VAL:O	2.53	0.40
1:C:101:LEU:HD22	1:D:134:LEU:CD2	2.52	0.40
1:D:105:GLU:O	1:D:108:THR:HB	2.20	0.40
1:E:69:VAL:O	1:E:69:VAL:CG2	2.69	0.40
1:F:163:GLU:O	1:F:167:LYS:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:SER:OG	1:C:24:GLN:OE1[3_465]	2.17	0.03

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	172/194 (89%)	168 (98%)	4 (2%)	0	100	100
1	B	170/194 (88%)	166 (98%)	4 (2%)	0	100	100
1	C	180/194 (93%)	174 (97%)	6 (3%)	0	100	100
1	D	176/194 (91%)	173 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	166/194 (86%)	161 (97%)	3 (2%)	2 (1%)	10	42
1	F	165/194 (85%)	163 (99%)	2 (1%)	0	100	100
1	G	170/194 (88%)	166 (98%)	4 (2%)	0	100	100
All	All	1199/1358 (88%)	1171 (98%)	26 (2%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	77[A]	TRP
1	E	77[B]	TRP

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	158/171 (92%)	148 (94%)	10 (6%)	16	48
1	B	156/171 (91%)	150 (96%)	6 (4%)	29	62
1	C	165/171 (96%)	154 (93%)	11 (7%)	15	47
1	D	161/171 (94%)	158 (98%)	3 (2%)	50	73
1	E	152/171 (89%)	148 (97%)	4 (3%)	40	69
1	F	151/171 (88%)	140 (93%)	11 (7%)	13	43
1	G	156/171 (91%)	143 (92%)	13 (8%)	10	38
All	All	1099/1197 (92%)	1041 (95%)	58 (5%)	22	53

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	36	SER
1	A	76	LYS
1	A	77[A]	TRP
1	A	77[B]	TRP

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Mol	Chain	Res	Type
1	A	138	ILE
1	A	166	ARG
1	A	170	ASP
1	A	174	ILE
1	A	177	ILE
1	B	30	ASN
1	B	76	LYS
1	B	125	ARG
1	B	138	ILE
1	B	170	ASP
1	B	171	ARG
1	C	36	SER
1	C	77[A]	TRP
1	C	77[B]	TRP
1	C	102	ARG
1	C	103	ILE
1	C	106	GLU
1	C	119	VAL
1	C	138	ILE
1	C	139	ILE
1	C	146	ASP
1	C	188	ASN
1	D	23	ASP
1	D	163	GLU
1	D	167	LYS
1	E	21	GLU
1	E	23	ASP
1	E	29	GLU
1	E	30	ASN
1	F	21	GLU
1	F	29	GLU
1	F	30	ASN
1	F	64	LYS
1	F	76	LYS
1	F	91	GLU
1	F	103	ILE
1	F	105	GLU
1	F	128	GLU
1	F	146	ASP
1	F	163	GLU
1	G	10	VAL
1	G	25	LEU

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Mol	Chain	Res	Type
1	G	30	ASN
1	G	76	LYS
1	G	77[A]	TRP
1	G	77[B]	TRP
1	G	103	ILE
1	G	106	GLU
1	G	124	ASN
1	G	125	ARG
1	G	138	ILE
1	G	146	ASP
1	G	167	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	188	ASN
1	B	18	HIS
1	C	107	HIS
1	C	188	ASN
1	D	37	HIS
1	D	41	ASN
1	E	41	ASN
1	E	188	ASN
1	F	24	GLN
1	F	188	ASN
1	G	41	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 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	175/194 (90%)	-0.56	2 (1%) 78 61	63, 103, 187, 262	1 (0%)
1	B	173/194 (89%)	-0.52	2 (1%) 76 58	63, 100, 171, 252	1 (0%)
1	C	183/194 (94%)	-0.46	2 (1%) 78 61	55, 114, 166, 218	1 (0%)
1	D	179/194 (92%)	-0.59	1 (0%) 85 73	59, 102, 169, 235	1 (0%)
1	E	169/194 (87%)	-0.49	2 (1%) 76 58	75, 128, 186, 226	1 (0%)
1	F	167/194 (86%)	-0.50	1 (0%) 85 73	61, 115, 181, 242	2 (1%)
1	G	173/194 (89%)	-0.40	2 (1%) 76 58	62, 135, 190, 243	1 (0%)
All	All	1219/1358 (89%)	-0.50	12 (0%) 79 63	55, 114, 183, 262	8 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77[A]	TRP	3.7
1	G	133	ALA	3.6
1	A	77[A]	TRP	3.4
1	C	77[A]	TRP	3.1
1	G	77[A]	TRP	3.0
1	B	126	LEU	2.5
1	E	77[A]	TRP	2.4
1	C	156	ALA	2.3
1	D	77[A]	TRP	2.3
1	E	134	LEU	2.3
1	F	77[A]	TRP	2.2
1	A	104	ALA	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.