



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:56 PM UTC

PDB ID : 2V64 / pdb_00002v64
Title : Crystallographic structure of the conformational dimer of the Spindle Assembly Checkpoint protein Mad2.
Authors : Mapelli, M.; Massimiliano, L.; Santaguida, S.; Musacchio, A.
Deposited on : 2007-07-13
Resolution : 2.90 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:

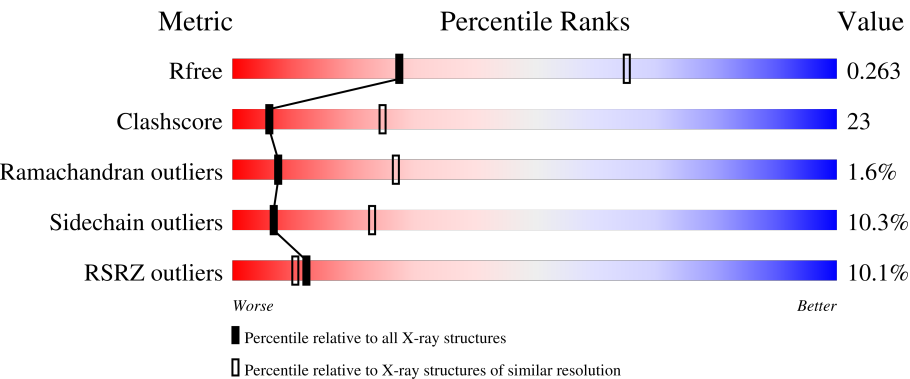
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	213	8% 63% 27% 8% ..
1	C	213	8% 59% 29% 9% ..
1	F	213	5% 65% 24% 10% .
2	B	12	58% 33% 8%
2	G	12	8% 83% 8% 8%

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Mol	Chain	Length	Quality of chain
2	I	12	8%67%25%8%
3	D	207	11%44%31%6%17%
3	E	207	11%43%29%11%15%
3	H	207	14%43%36%7%13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9648 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 MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	1
			1700	1085	287	324	4			
1	C	211	Total	C	N	O	S	0	0	1
			1700	1085	287	324	4			
1	F	211	Total	C	N	O	S	0	0	1
			1700	1085	287	324	4			

- Molecule 2 is a protein called MBP1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	0	1
			92	61	16	15			
2	G	11	Total	C	N	O	0	0	1
			92	61	16	15			
2	I	12	Total	C	N	O	0	0	1
			97	64	17	16			

- Molecule 3 is a protein called MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	172	Total	C	N	O	S	0	0	1
			1383	887	226	267	3			
3	E	176	Total	C	N	O	S	0	0	1
			1423	916	231	273	3			
3	H	181	Total	C	N	O	S	0	0	1
			1455	934	237	281	3			

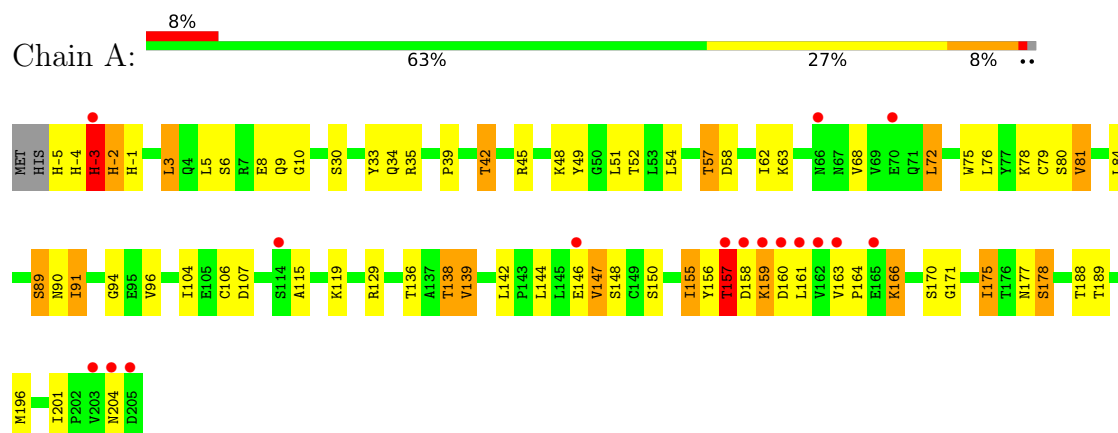
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total 3	O 3	0	0
4	F	2	Total 2	O 2	0	0
4	H	1	Total 1	O 1	0	0

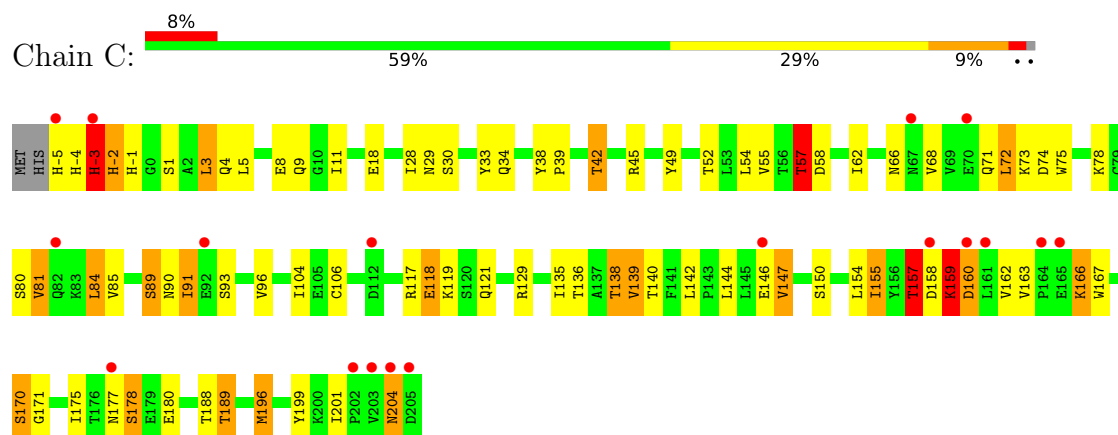
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

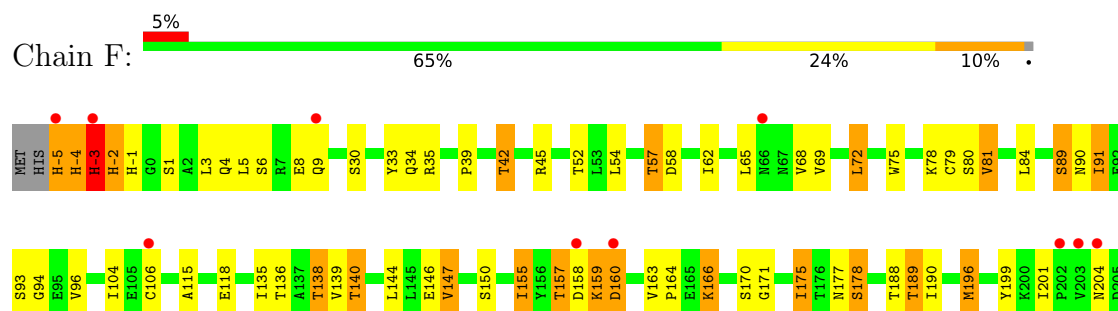
• Molecule 1: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A



• Molecule 1: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A



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The diagram illustrates a linked list structure. It consists of seven nodes arranged horizontally. Each node is represented by a rectangle divided into two parts: a top part for the data and a bottom part for the next pointer. The nodes are labeled as follows: S1 (data), W2 (data), Y5 (data), P6 (data), R10 (data), A11 (data), and VAL (data). The next pointer of S1 points to W2, W2 points to Y5, Y5 points to P6, P6 points to R10, R10 points to A11, and A11 points to VAL. The VAL node is the last node in the list, as its next pointer is null (represented by a grey box).

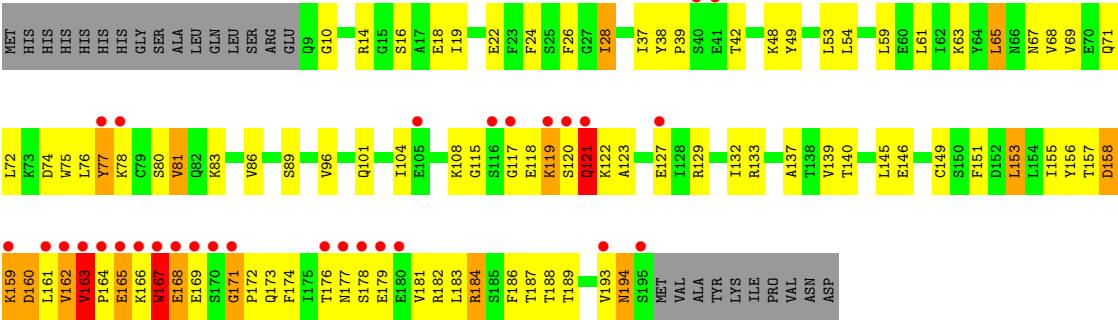
A diagram of a 4-bit register. It consists of four colored blocks: a green block labeled 'S1', an orange block labeled 'R10', a green block labeled 'A11', and a grey block labeled 'VAL'. A red dot is positioned above the 'S1' block.

A diagram of a 12-bit bus. It consists of 12 vertical bars of equal height, each labeled with a hexadecimal digit: S1, Y5, P8, Q9, R10, A11, and V12. The bars are colored in a repeating pattern: S1, Y5, and P8 are green; Q9, R10, and A11 are orange; and V12 is green. A red dot is positioned above the Q9 bar.

VAL	K78	MET
VAL	V61	HIS
PRO	Q62	HIS
GLU	K33	HIS
LYS	L94	HIS
TRP	V85	HIS
GLU	V86	GLY
GLU	V87	GLY
SER	I88	SER
GLY	S89	ALA
P172	N90	LEU
Q173	I91	CLN
F174	E92	LEU
I175	S93	SER
T176		ARG
M177	V96	E8
S178	L97	
R179	E98	T12
E180	R99	L13
V181	W100	R14
R182		
L183	I104	E18
R184	E105	I19
S185	C106	V20
F186	D107	
T187	K108	F23
	G115	R35
I190	S116	G36
H191	G117	I37
K192	E118	F38
V193	K119	P39
M194		S40
S195	Q125	E41
MET	D126	T42
VAL	E127	
ALA		K48
LYS	S130	Y49
ILE	V131	
PRO	I132	L54
VAL	R133	
ASN	Q134	D58
ASP	V139	L59
	T140	I62
	F141	K63
	L142	V64
		L65
	L145	M66
		N67
	D152	V68
	L153	V69
	I154	E70
	I155	Q71
	V156	L72
	T157	K73
	D158	D74
	K159	W75
	D160	L76
	L161	V77

E169	S170	G171	P172	Q173	F174	T175	T176	M177	S178	E179	E180	V181	R182	L183	R184	S185	F186	T187	I190	H191	K192	V193	M194	S195	MET	VAL	ALA	TYR	LYS	ILE	PRO	VAL	ASN	ASP																		
C79	S80	V81	Q82	S89	V96	W100	Q101	F102	D103	I104	E105	C106	D107	K108	GLY	SER	GLY	GLY	GLY	L13	R14	I19	P23	F26	I37	Y38	P39	S40	E41	T42	K48	L54	V55	D58	L59	E60	L61	I62	K63	Y64	L65	M66	N67	V68	V69	E70	Q71	L72	W75	L76	Y77	V78

● Molecule 3: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.58Å 111.88Å 131.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.44 – 2.90 29.44 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.8 (29.44-2.90) 94.7 (29.44-2.90)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.273 0.224 , 0.263	Depositor DCC
R_{free} test set	1766 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9648	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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	0.90	4/1733 (0.2%)	1.34	16/2350 (0.7%)
1	C	0.94	5/1733 (0.3%)	1.46	24/2350 (1.0%)
1	F	0.92	4/1733 (0.2%)	1.43	19/2350 (0.8%)
2	B	0.93	1/98 (1.0%)	1.05	1/136 (0.7%)
2	G	0.96	1/98 (1.0%)	0.98	0/136
2	I	0.99	1/103 (1.0%)	1.08	1/143 (0.7%)
3	D	1.02	6/1404 (0.4%)	1.25	11/1899 (0.6%)
3	E	1.00	9/1447 (0.6%)	1.24	14/1962 (0.7%)
3	H	1.02	7/1480 (0.5%)	1.23	14/2006 (0.7%)
All	All	0.96	38/9829 (0.4%)	1.33	100/13332 (0.8%)

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
1	C	0	1
1	F	1	3
3	E	0	1
3	H	0	4
All	All	1	11

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	-3	HIS	C-O	-12.51	1.07	1.24
1	C	-3	HIS	C-O	-12.10	1.08	1.24
1	A	-4	HIS	CB-CG	8.65	1.62	1.50
3	D	54	LEU	CG-CD1	-8.07	1.25	1.52
1	F	-4	HIS	CB-CG	7.87	1.61	1.50
1	C	-4	HIS	CB-CG	7.86	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	-1	HIS	N-CA	-7.09	1.37	1.46
3	D	54	LEU	CG-CD2	-7.06	1.29	1.52
3	H	18	GLU	CB-CG	-6.94	1.31	1.52
3	E	122	LYS	CB-CG	-6.87	1.31	1.52
1	F	-1	HIS	N-CA	-6.70	1.38	1.46
3	H	158	ASP	CB-CG	-6.55	1.35	1.52
3	H	159	LYS	CD-CE	-6.42	1.33	1.52
3	E	158	ASP	CB-CG	-6.25	1.36	1.52
1	C	11	ILE	CA-CB	6.25	1.61	1.54
1	A	-1	HIS	CA-C	6.04	1.60	1.52
1	A	157	THR	C-O	-6.02	1.17	1.24
3	H	160	ASP	CB-CG	-6.01	1.37	1.52
3	E	159	LYS	CB-CG	-5.97	1.34	1.52
2	G	10	ARG	C-N	-5.84	1.25	1.33
3	E	160	ASP	CB-CG	-5.80	1.37	1.52
3	D	194	ASN	C-N	-5.75	1.25	1.33
3	D	78	LYS	CD-CE	-5.73	1.35	1.52
3	H	159	LYS	CB-CG	-5.56	1.35	1.52
2	B	10	ARG	C-N	-5.54	1.25	1.33
3	E	122	LYS	CD-CE	-5.50	1.35	1.52
3	H	122	LYS	CB-CG	-5.48	1.36	1.52
3	D	155	ILE	CG1-CD1	-5.46	1.30	1.51
1	C	204	ASN	C-N	-5.43	1.25	1.33
3	E	158	ASP	CA-CB	-5.39	1.45	1.53
3	D	160	ASP	CB-CG	-5.38	1.38	1.52
3	E	194	ASN	C-N	-5.36	1.25	1.33
3	H	194	ASN	C-N	-5.36	1.25	1.33
2	I	11	ALA	C-N	-5.32	1.25	1.33
3	E	70	GLU	CG-CD	-5.29	1.38	1.52
1	F	204	ASN	C-N	-5.24	1.26	1.33
1	A	204	ASN	C-N	-5.13	1.26	1.33
3	E	77	TYR	CD1-CE1	-5.08	1.23	1.38

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	-3	HIS	N-CA-C	33.34	153.03	113.02
1	C	-3	HIS	N-CA-C	32.95	150.28	112.72
1	A	-3	HIS	N-CA-C	22.82	142.38	112.26
1	A	178	SER	N-CA-C	11.67	125.31	108.86
3	D	54	LEU	CD1-CG-CD2	-11.63	85.20	110.80
1	F	-2	HIS	N-CA-CB	-10.84	92.99	111.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	178	SER	N-CA-C	10.78	124.05	108.86
1	C	178	SER	N-CA-C	10.65	123.87	108.86
1	C	-4	HIS	CA-C-N	-10.63	105.61	122.73
1	C	-4	HIS	C-N-CA	-10.63	105.61	122.73
1	C	-2	HIS	N-CA-CB	-10.29	94.05	112.27
3	E	159	LYS	CB-CG-CD	-9.43	89.62	111.30
1	F	-3	HIS	O-C-N	-9.07	110.69	122.39
3	D	181	VAL	N-CA-C	8.98	118.92	110.74
3	E	70	GLU	CA-CB-CG	-8.95	96.19	114.10
1	A	-4	HIS	CA-C-N	-8.10	110.47	122.86
1	A	-4	HIS	C-N-CA	-8.10	110.47	122.86
3	E	122	LYS	CG-CD-CE	-8.03	92.83	111.30
3	H	159	LYS	CB-CG-CD	-7.90	93.12	111.30
1	C	-4	HIS	CA-C-O	7.71	129.61	121.06
3	H	158	ASP	CB-CG-OD1	-7.68	100.73	118.40
1	C	-3	HIS	CB-CA-C	-7.49	98.59	110.94
3	H	108	LYS	N-CA-C	-7.48	103.72	112.92
3	E	161	LEU	N-CA-C	7.42	118.98	108.74
1	F	118	GLU	N-CA-C	7.32	121.25	108.52
1	C	-3	HIS	O-C-N	-7.11	113.60	122.35
3	D	14	ARG	CD-NE-CZ	-7.11	114.44	124.40
1	C	139	VAL	N-CA-C	6.99	117.70	110.36
3	H	159	LYS	CA-C-N	-6.98	110.29	122.64
3	H	159	LYS	C-N-CA	-6.98	110.29	122.64
3	D	160	ASP	N-CA-CB	-6.97	99.83	110.77
3	E	158	ASP	CA-C-N	-6.96	111.74	122.05
3	E	158	ASP	C-N-CA	-6.96	111.74	122.05
1	C	157	THR	N-CA-C	6.94	117.43	108.34
3	E	177	ASN	N-CA-C	-6.92	101.95	110.61
1	F	190	ILE	N-CA-C	-6.87	106.20	111.62
1	A	175	ILE	N-CA-C	-6.86	99.84	108.89
1	A	35	ARG	N-CA-C	-6.84	104.82	113.02
3	D	78	LYS	CB-CG-CD	-6.82	95.61	111.30
1	F	-4	HIS	CA-C-N	-6.82	110.84	122.56
1	F	-4	HIS	C-N-CA	-6.82	110.84	122.56
1	C	-4	HIS	O-C-N	-6.78	117.31	123.41
1	A	10	GLY	N-CA-C	6.71	119.90	110.38
1	C	-2	HIS	CB-CA-C	-6.60	101.67	111.70
1	A	-2	HIS	N-CA-CB	-6.50	99.50	110.49
3	H	193	VAL	N-CA-C	-6.49	101.20	109.58
1	F	-3	HIS	CB-CA-C	-6.43	98.92	110.37
1	F	115	ALA	CA-C-N	6.20	126.14	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	115	ALA	C-N-CA	6.20	126.14	119.76
1	F	94	GLY	N-CA-C	-6.19	106.08	115.00
3	H	18	GLU	CG-CD-OE1	6.18	132.61	118.40
1	F	140	THR	N-CA-C	6.13	117.63	111.07
3	D	159	LYS	CA-C-N	-6.10	114.17	122.77
3	D	159	LYS	C-N-CA	-6.10	114.17	122.77
3	D	66	ASN	CB-CA-C	-6.09	101.31	110.88
3	H	67	ASN	N-CA-CB	-6.05	101.30	110.07
1	C	170	SER	N-CA-C	6.03	116.05	108.45
3	H	122	LYS	CG-CD-CE	-6.03	97.43	111.30
1	C	163	VAL	CA-C-N	5.97	127.30	119.84
1	C	163	VAL	C-N-CA	5.97	127.30	119.84
3	E	160	ASP	CB-CG-OD1	-5.85	104.94	118.40
1	A	-4	HIS	CA-C-O	5.83	128.85	120.51
1	C	57	THR	N-CA-C	-5.83	106.02	114.12
3	H	149	CYS	N-CA-C	5.79	117.03	108.86
1	A	-4	HIS	CB-CA-C	-5.75	98.97	110.42
3	H	159	LYS	N-CA-C	5.74	117.54	111.28
3	H	146	GLU	N-CA-C	5.74	120.10	112.30
1	F	-4	HIS	CA-C-O	5.73	127.42	121.06
1	A	115	ALA	N-CA-C	5.72	113.37	108.22
3	D	158	ASP	CB-CG-OD1	-5.71	105.26	118.40
1	A	157	THR	N-CA-C	5.68	119.16	108.65
1	F	175	ILE	N-CA-C	-5.68	100.40	108.58
1	C	89	SER	N-CA-C	5.54	117.40	109.14
3	E	122	LYS	N-CA-CB	-5.54	101.75	110.06
3	D	91	ILE	N-CA-C	5.53	116.92	110.62
1	C	118	GLU	N-CA-C	5.52	118.63	108.58
3	E	78	LYS	CB-CG-CD	-5.50	98.65	111.30
1	F	-4	HIS	CB-CA-C	-5.49	100.59	110.03
3	E	149	CYS	N-CA-C	5.46	116.93	109.18
1	F	-2	HIS	CB-CA-C	-5.44	102.78	111.86
2	B	6	PRO	N-CA-C	5.43	117.33	110.70
1	F	35	ARG	N-CA-C	-5.37	106.31	112.92
1	C	159	LYS	N-CA-C	5.36	122.21	110.80
1	F	-2	HIS	CB-CG-CD2	-5.33	124.27	131.20
3	H	121	GLN	N-CA-C	-5.33	102.58	111.37
1	A	-3	HIS	CB-CA-C	-5.32	102.57	111.13
1	C	-2	HIS	CB-CG-CD2	-5.30	124.31	131.20
3	D	93	SER	N-CA-C	5.30	117.86	111.40
3	E	146	GLU	N-CA-C	5.24	117.16	110.61
3	E	158	ASP	CB-CG-OD1	-5.21	106.41	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	LEU	N-CA-C	-5.17	100.02	108.76
1	A	-3	HIS	O-C-N	-5.16	115.60	122.20
1	A	139	VAL	N-CA-C	5.14	115.76	110.36
3	E	162	VAL	N-CA-C	-5.12	98.69	109.34
1	C	121	GLN	N-CA-C	-5.10	105.61	111.07
1	A	94	GLY	N-CA-C	-5.09	107.67	115.00
2	I	10	ARG	N-CA-C	5.06	119.19	112.30
1	C	38	TYR	CA-C-N	5.01	125.01	119.90
1	C	38	TYR	C-N-CA	5.01	125.01	119.90
3	H	54	LEU	CD1-CG-CD2	-5.01	99.78	110.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	-3	HIS	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-3	HIS	Sidechain,Mainchain
1	C	-3	HIS	Mainchain
3	E	184	ARG	Sidechain
1	F	-2	HIS	Sidechain
1	F	-3	HIS	Mainchain
1	F	-5	HIS	Sidechain
3	H	162	VAL	Peptide
3	H	163	VAL	Peptide
3	H	164	PRO	Peptide
3	H	184	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	1700	0	1707	62	0
1	C	1700	0	1707	64	2
1	F	1700	0	1707	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	92	0	82	2	0
2	G	92	0	82	1	0
2	I	97	0	87	5	0
3	D	1383	0	1399	78	0
3	E	1423	0	1438	99	2
3	H	1455	0	1469	92	0
4	C	3	0	0	0	0
4	F	2	0	0	0	0
4	H	1	0	0	0	0
All	All	9648	0	9678	437	2

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 23.

All (437) 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)
3:H:184:ARG:HH11	3:H:184:ARG:CB	1.39	1.34
3:H:184:ARG:HB3	3:H:184:ARG:NH1	1.44	1.28
1:A:-3:HIS:NE2	1:F:-3:HIS:CE1	2.16	1.14
1:A:-3:HIS:CE1	1:C:-5:HIS:HE1	1.67	1.12
3:D:14:ARG:HH21	3:D:14:ARG:HB3	1.10	1.09
3:H:184:ARG:HH11	3:H:184:ARG:CA	1.65	1.09
3:D:14:ARG:HB3	3:D:14:ARG:NH2	1.68	1.07
1:A:-3:HIS:CE1	1:C:-5:HIS:CE1	2.45	1.04
1:A:-3:HIS:CE1	1:C:-3:HIS:NE2	2.26	1.04
3:D:14:ARG:HH21	3:D:14:ARG:CB	1.72	1.02
1:C:-3:HIS:CE1	1:F:-3:HIS:NE2	2.30	1.00
3:D:181:VAL:O	3:D:182:ARG:HB3	1.62	0.99
3:H:184:ARG:HH11	3:H:184:ARG:HB3	1.01	0.99
3:E:166:LYS:O	3:E:167:TRP:HB2	1.60	0.98
3:H:160:ASP:O	3:H:161:LEU:HG	1.63	0.98
3:H:159:LYS:NZ	3:H:194:ASN:HD22	1.63	0.96
3:D:173:GLN:HB2	3:D:187:THR:HB	1.49	0.94
3:E:177:ASN:HA	3:E:184:ARG:NH2	1.84	0.93
1:A:-3:HIS:ND1	1:C:-5:HIS:CE1	2.38	0.92
3:E:163:VAL:HG21	3:E:190:ILE:CD1	1.99	0.91
1:A:-3:HIS:ND1	1:C:-5:HIS:HE1	1.68	0.91
1:A:-3:HIS:CE1	1:F:-3:HIS:HE1	1.91	0.89
3:D:84:LEU:HG	3:D:104:ILE:HD11	1.55	0.88
1:A:-3:HIS:HD1	1:C:-5:HIS:CE1	1.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-3:HIS:HE1	1:C:-3:HIS:CE1	1.92	0.87
1:A:-3:HIS:CE1	1:C:-3:HIS:CE1	2.63	0.87
1:C:-3:HIS:CE1	1:F:-3:HIS:CE1	2.61	0.87
3:E:14:ARG:H	3:E:14:ARG:NH2	1.73	0.86
3:H:167:TRP:CE3	3:H:168:GLU:N	2.43	0.86
3:D:176:THR:HG22	3:D:177:ASN:H	1.40	0.86
3:E:14:ARG:H	3:E:14:ARG:HH21	1.18	0.86
3:H:184:ARG:CB	3:H:184:ARG:NH1	2.15	0.86
3:E:192:LYS:H	3:E:192:LYS:HZ2	1.23	0.85
3:D:177:ASN:ND2	3:D:184:ARG:HD3	1.90	0.85
3:E:178:SER:O	3:E:179:GLU:HB2	1.76	0.85
1:A:-3:HIS:CE1	1:F:-3:HIS:CE1	2.64	0.85
3:E:160:ASP:C	3:E:161:LEU:HG	2.03	0.84
3:H:81:VAL:HG22	3:H:104:ILE:HD12	1.61	0.82
3:E:165:GLU:O	3:E:166:LYS:HB2	1.78	0.82
3:H:14:ARG:HG2	3:H:14:ARG:NH2	1.94	0.81
3:H:14:ARG:HG2	3:H:14:ARG:HH21	1.43	0.81
3:E:108:LYS:NZ	3:E:108:LYS:HB3	1.95	0.81
3:E:177:ASN:C	3:E:179:GLU:H	1.89	0.80
3:E:177:ASN:HA	3:E:184:ARG:HH21	1.46	0.80
3:D:83:LYS:HG3	3:D:156:TYR:HD1	1.47	0.79
3:H:157:THR:OG1	3:H:161:LEU:HD11	1.82	0.79
3:E:108:LYS:HB3	3:E:108:LYS:HZ3	1.48	0.78
1:F:157:THR:OG1	1:F:158:ASP:N	2.15	0.77
1:F:33:TYR:CZ	1:F:54:LEU:HD22	2.20	0.77
3:E:14:ARG:NH1	3:E:127:GLU:OE1	2.18	0.77
3:H:159:LYS:HZ1	3:H:194:ASN:HD22	1.32	0.76
3:H:59:LEU:HG	3:H:63:LYS:HE3	1.69	0.75
1:C:30:SER:O	1:C:34:GLN:HG3	1.87	0.74
1:A:96:VAL:HG12	1:A:175:ILE:HG12	1.69	0.74
3:D:174:PHE:CE1	3:D:186:PHE:HB3	2.22	0.74
3:E:163:VAL:HG21	3:E:190:ILE:HD12	1.69	0.73
3:H:24:PHE:O	3:H:28:ILE:HG22	1.88	0.73
1:C:-3:HIS:HE1	1:F:-3:HIS:CE1	2.05	0.73
1:A:39:PRO:O	1:A:42:THR:HB	1.89	0.72
3:E:166:LYS:O	3:E:167:TRP:CB	2.35	0.72
3:H:184:ARG:NH1	3:H:184:ARG:CA	2.45	0.72
3:E:145:LEU:HD22	3:E:182:ARG:HD3	1.71	0.72
3:H:89:SER:HB3	3:H:96:VAL:HA	1.71	0.72
3:D:58:ASP:O	3:D:62:ILE:HG13	1.90	0.71
1:A:80:SER:O	1:A:157:THR:HB	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:176:THR:O	3:D:177:ASN:HB2	1.89	0.71
1:F:39:PRO:O	1:F:42:THR:HB	1.91	0.71
1:A:-3:HIS:HE1	1:C:-5:HIS:CE1	2.08	0.71
1:F:80:SER:O	1:F:157:THR:HB	1.90	0.70
3:D:173:GLN:CB	3:D:187:THR:HB	2.22	0.70
3:E:14:ARG:HH21	3:E:14:ARG:N	1.89	0.70
1:C:39:PRO:O	1:C:42:THR:HB	1.92	0.70
1:A:158:ASP:O	1:A:160:ASP:N	2.23	0.70
3:E:14:ARG:NH2	3:E:14:ARG:HG2	2.06	0.70
3:H:163:VAL:HG23	3:H:165:GLU:N	2.07	0.70
3:H:167:TRP:HE3	3:H:168:GLU:H	1.35	0.69
1:A:-3:HIS:NE2	1:F:-3:HIS:HE1	1.78	0.69
3:E:177:ASN:O	3:E:179:GLU:N	2.23	0.69
3:H:159:LYS:NZ	3:H:194:ASN:ND2	2.39	0.69
1:C:96:VAL:HG12	1:C:175:ILE:HG12	1.74	0.69
1:F:135:ILE:O	1:F:138:THR:HB	1.93	0.69
1:C:166:LYS:NZ	1:C:166:LYS:HB3	2.08	0.68
1:F:96:VAL:HG12	1:F:175:ILE:HG12	1.75	0.68
1:F:158:ASP:O	1:F:160:ASP:N	2.26	0.68
3:H:160:ASP:O	3:H:161:LEU:CG	2.39	0.68
3:E:71:GLN:HG2	3:E:167:TRP:CZ2	2.28	0.67
3:H:78:LYS:HE3	3:H:80:SER:OG	1.94	0.67
1:C:80:SER:O	1:C:157:THR:HB	1.94	0.67
3:H:177:ASN:HB2	3:H:184:ARG:NH2	2.09	0.67
3:E:14:ARG:NH1	3:E:127:GLU:CD	2.53	0.66
1:F:140:THR:HB	3:H:132:ILE:HG21	1.77	0.66
1:F:-5:HIS:ND1	1:F:-4:HIS:N	2.43	0.66
3:E:14:ARG:NE	3:E:127:GLU:OE2	2.28	0.66
1:F:30:SER:O	1:F:34:GLN:HG3	1.96	0.66
1:C:188:THR:O	1:C:189:THR:HG23	1.97	0.65
3:D:174:PHE:HE1	3:D:186:PHE:HB3	1.61	0.65
3:H:39:PRO:O	3:H:42:THR:HB	1.97	0.65
3:E:39:PRO:O	3:E:42:THR:HB	1.97	0.65
3:H:153:LEU:HD22	3:H:155:ILE:HD13	1.79	0.65
3:E:173:GLN:HG3	3:E:174:PHE:N	2.11	0.64
1:C:81:VAL:HG22	1:C:104:ILE:HD12	1.79	0.64
1:C:158:ASP:O	1:C:160:ASP:N	2.29	0.64
3:H:81:VAL:HG22	3:H:104:ILE:CD1	2.26	0.64
1:C:135:ILE:O	1:C:138:THR:HB	1.97	0.64
3:H:163:VAL:O	3:H:163:VAL:HG22	1.96	0.64
3:D:39:PRO:O	3:D:42:THR:HB	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:81:VAL:HG22	3:E:104:ILE:HD12	1.79	0.63
2:I:8:PRO:C	2:I:10:ARG:H	2.04	0.63
3:E:14:ARG:HH21	3:E:14:ARG:CG	2.12	0.62
1:F:1:SER:HB3	1:F:4:GLN:HG3	1.80	0.62
1:F:188:THR:O	1:F:189:THR:HG23	2.00	0.62
3:H:176:THR:C	3:H:178:SER:H	2.07	0.62
1:A:157:THR:OG1	1:A:158:ASP:N	2.30	0.62
3:D:156:TYR:HE2	3:D:191:HIS:ND1	1.98	0.62
1:F:136:THR:O	1:F:139:VAL:HG23	1.98	0.62
3:H:184:ARG:HB3	3:H:184:ARG:CZ	2.23	0.61
1:C:42:THR:O	1:C:57:THR:HB	1.99	0.61
3:D:159:LYS:NZ	3:D:194:ASN:HB2	2.15	0.61
3:D:178:SER:O	3:D:179:GLU:HG2	2.00	0.61
1:F:42:THR:O	1:F:57:THR:HB	2.00	0.61
1:A:89:SER:HB3	1:A:96:VAL:HA	1.83	0.61
1:C:89:SER:HB3	1:C:96:VAL:HA	1.83	0.61
3:D:71:GLN:HE21	3:D:75:TRP:NE1	1.98	0.61
3:H:14:ARG:HH21	3:H:14:ARG:CG	2.05	0.61
1:F:188:THR:C	1:F:189:THR:HG23	2.25	0.61
3:H:145:LEU:CD2	3:H:182:ARG:HD3	2.31	0.61
1:F:33:TYR:CE1	1:F:54:LEU:HD22	2.36	0.60
1:C:49:TYR:O	1:C:129:ARG:HD3	2.01	0.60
3:D:173:GLN:HB2	3:D:187:THR:CB	2.28	0.60
1:A:146:GLU:CD	1:A:146:GLU:H	2.09	0.60
1:C:162:VAL:HG12	1:C:162:VAL:O	1.99	0.60
3:H:171:GLY:HA3	3:H:188:THR:O	2.00	0.60
1:C:3:LEU:CD1	3:E:10:GLY:HA2	2.30	0.60
1:F:-5:HIS:HE1	1:F:-3:HIS:CE1	2.19	0.60
3:E:58:ASP:O	3:E:62:ILE:HG13	2.02	0.59
3:H:184:ARG:HH11	3:H:184:ARG:HA	1.61	0.59
3:D:14:ARG:NH2	3:D:14:ARG:CB	2.45	0.59
1:A:33:TYR:CZ	1:A:54:LEU:HD22	2.37	0.59
1:C:178:SER:HA	1:C:201:ILE:HG13	1.85	0.59
3:E:148:SER:HB3	3:E:184:ARG:HG3	1.84	0.59
3:E:192:LYS:H	3:E:192:LYS:NZ	1.98	0.59
3:H:174:PHE:CE1	3:H:186:PHE:HB3	2.37	0.59
3:D:193:VAL:O	3:D:194:ASN:HB2	2.01	0.59
3:D:177:ASN:CG	3:D:184:ARG:CD	2.76	0.58
1:C:146:GLU:OE2	1:C:147:VAL:HG13	2.03	0.58
3:E:40:SER:C	3:E:42:THR:H	2.11	0.58
2:I:10:ARG:O	2:I:10:ARG:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:THR:O	1:C:139:VAL:HG23	2.03	0.58
3:H:22:GLU:OE1	3:H:49:TYR:HE1	1.87	0.58
1:A:-5:HIS:HE1	1:F:-3:HIS:CE1	2.22	0.58
1:F:8:GLU:O	1:F:9:GLN:HB2	2.03	0.57
3:D:89:SER:HB3	3:D:96:VAL:HA	1.86	0.57
3:H:166:LYS:O	3:H:167:TRP:CB	2.52	0.57
1:A:-2:HIS:O	1:A:119:LYS:HE3	2.05	0.57
1:C:188:THR:C	1:C:189:THR:HG23	2.28	0.57
3:D:179:GLU:HB2	3:D:181:VAL:HG23	1.86	0.57
3:H:179:GLU:HB2	3:H:181:VAL:HG23	1.86	0.57
3:E:178:SER:O	3:E:179:GLU:CB	2.49	0.57
1:F:58:ASP:O	1:F:62:ILE:HG13	2.05	0.57
1:F:166:LYS:HB3	1:F:166:LYS:NZ	2.20	0.57
3:H:14:ARG:CZ	3:H:127:GLU:OE2	2.53	0.57
3:H:120:SER:O	3:H:121:GLN:C	2.45	0.57
3:H:165:GLU:O	3:H:166:LYS:HB2	2.04	0.57
3:H:159:LYS:HZ2	3:H:194:ASN:HD22	1.52	0.57
3:H:22:GLU:OE1	3:H:49:TYR:CE1	2.57	0.57
3:D:177:ASN:CG	3:D:184:ARG:HD3	2.30	0.57
1:C:118:GLU:HG2	3:E:141:PHE:CE1	2.40	0.56
3:H:184:ARG:NH1	3:H:184:ARG:O	2.38	0.56
2:I:10:ARG:O	2:I:10:ARG:CG	2.53	0.56
1:C:138:THR:HG23	1:C:142:LEU:CD1	2.35	0.56
3:D:12:THR:HG21	3:D:14:ARG:HH22	1.71	0.56
1:F:1:SER:HB3	1:F:4:GLN:CG	2.35	0.56
1:A:90:ASN:ND2	1:A:147:VAL:HG21	2.20	0.56
3:E:37:ILE:HG22	3:E:183:LEU:HB2	1.87	0.55
1:F:178:SER:HA	1:F:201:ILE:HG13	1.88	0.55
1:F:90:ASN:ND2	1:F:147:VAL:HG21	2.21	0.55
1:F:68:VAL:HG12	1:F:72:LEU:HD22	1.88	0.55
3:H:157:THR:CB	3:H:161:LEU:HD11	2.35	0.55
1:C:157:THR:OG1	1:C:158:ASP:N	2.38	0.55
3:E:14:ARG:CZ	3:E:127:GLU:CD	2.80	0.55
3:H:167:TRP:HE3	3:H:168:GLU:N	1.97	0.55
3:E:89:SER:HB3	3:E:96:VAL:HA	1.87	0.54
1:A:51:LEU:HD11	1:A:129:ARG:HG3	1.90	0.54
3:D:193:VAL:O	3:D:193:VAL:HG23	2.06	0.54
3:E:108:LYS:NZ	3:E:108:LYS:CB	2.69	0.54
3:D:12:THR:CG2	3:D:14:ARG:HH22	2.21	0.54
3:E:14:ARG:HH21	3:E:14:ARG:HG2	1.68	0.54
3:H:38:TYR:HE1	3:H:183:LEU:HD23	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:145:LEU:HD21	3:H:182:ARG:HD3	1.90	0.54
3:H:159:LYS:HZ2	3:H:194:ASN:ND2	2.04	0.54
3:E:13:LEU:HD22	3:E:23:PHE:HB3	1.90	0.54
3:E:82:GLN:OE1	3:E:193:VAL:HG11	2.08	0.53
3:E:165:GLU:O	3:E:166:LYS:CB	2.55	0.53
1:C:177:ASN:OD1	1:C:201:ILE:HD12	2.08	0.53
3:E:177:ASN:C	3:E:179:GLU:N	2.59	0.53
1:C:45:ARG:HG2	1:C:52:THR:CG2	2.38	0.53
3:E:168:GLU:O	3:E:169:GLU:HB2	2.07	0.53
3:D:23:PHE:CE2	3:D:127:GLU:HB3	2.44	0.53
1:A:178:SER:HA	1:A:201:ILE:HG13	1.91	0.53
1:F:1:SER:CB	1:F:4:GLN:HG3	2.39	0.53
3:H:71:GLN:HE21	3:H:75:TRP:NE1	2.06	0.53
3:H:76:LEU:HD21	3:H:104:ILE:HD13	1.90	0.53
1:C:33:TYR:CZ	1:C:54:LEU:HD22	2.44	0.53
3:E:59:LEU:HG	3:E:63:LYS:HE2	1.90	0.53
1:F:45:ARG:HG2	1:F:52:THR:CG2	2.39	0.53
3:E:145:LEU:HD22	3:E:182:ARG:CD	2.37	0.52
1:A:136:THR:O	1:A:139:VAL:HG23	2.09	0.52
3:H:166:LYS:O	3:H:167:TRP:HB2	2.09	0.52
3:D:14:ARG:NH2	3:D:14:ARG:CG	2.66	0.52
3:E:163:VAL:HG21	3:E:190:ILE:HD11	1.88	0.52
3:E:173:GLN:HB2	3:E:187:THR:HB	1.91	0.52
1:A:42:THR:CG2	1:A:42:THR:O	2.55	0.52
1:C:140:THR:HB	3:D:132:ILE:HG21	1.92	0.52
3:E:64:TYR:O	3:E:68:VAL:HG12	2.09	0.52
1:F:68:VAL:O	1:F:72:LEU:HB2	2.09	0.52
3:H:174:PHE:HE1	3:H:186:PHE:HB3	1.74	0.52
3:D:160:ASP:OD2	3:D:160:ASP:C	2.53	0.52
3:H:167:TRP:CD1	3:H:172:PRO:HD2	2.45	0.52
1:A:30:SER:O	1:A:34:GLN:HG3	2.09	0.51
1:F:196:MET:HG3	1:F:196:MET:O	2.07	0.51
3:E:163:VAL:HG22	3:E:166:LYS:C	2.35	0.51
1:A:138:THR:HG23	1:A:142:LEU:HD12	1.92	0.51
3:E:14:ARG:CZ	3:E:127:GLU:OE2	2.59	0.51
1:C:146:GLU:CD	1:C:146:GLU:H	2.19	0.51
1:F:146:GLU:CD	1:F:146:GLU:H	2.18	0.51
3:D:161:LEU:HG	3:D:190:ILE:HD13	1.93	0.51
3:D:159:LYS:HZ1	3:D:194:ASN:HB2	1.75	0.51
2:I:8:PRO:C	2:I:10:ARG:N	2.69	0.51
3:H:129:ARG:O	3:H:133:ARG:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ASN:OD1	1:A:201:ILE:HD12	2.11	0.51
1:A:166:LYS:NZ	1:A:166:LYS:HB3	2.26	0.50
3:E:77:TYR:C	3:E:77:TYR:CD2	2.89	0.50
1:F:166:LYS:HB3	1:F:166:LYS:HZ3	1.77	0.50
3:D:14:ARG:HG2	3:D:127:GLU:OE2	2.12	0.50
1:F:91:ILE:HG12	1:F:150:SER:HB3	1.93	0.50
3:D:181:VAL:O	3:D:182:ARG:CB	2.44	0.50
3:H:72:LEU:HG	3:H:76:LEU:CD1	2.41	0.50
3:E:127:GLU:OE1	3:E:127:GLU:HA	2.11	0.50
3:E:168:GLU:O	3:E:169:GLU:CB	2.60	0.50
3:H:118:GLU:H	3:H:118:GLU:CD	2.20	0.50
3:H:145:LEU:HD23	3:H:145:LEU:C	2.37	0.50
3:E:38:TYR:HE1	3:E:183:LEU:HD23	1.77	0.49
1:F:65:LEU:O	1:F:69:VAL:HG23	2.12	0.49
3:E:10:GLY:N	3:E:103:ASP:OD2	2.44	0.49
3:E:163:VAL:HG21	3:E:166:LYS:O	2.12	0.49
3:H:120:SER:O	3:H:123:ALA:N	2.45	0.49
3:H:158:ASP:OD1	3:H:158:ASP:C	2.52	0.49
3:D:176:THR:O	3:D:177:ASN:CB	2.60	0.49
1:A:3:LEU:O	1:A:6:SER:OG	2.27	0.49
3:E:159:LYS:NZ	3:E:194:ASN:HB2	2.27	0.49
1:A:158:ASP:C	1:A:160:ASP:H	2.20	0.49
1:C:1:SER:HB3	1:C:4:GLN:HG3	1.94	0.49
3:E:77:TYR:HD2	3:E:77:TYR:O	1.96	0.49
1:A:146:GLU:CD	1:A:146:GLU:N	2.70	0.49
3:D:48:LYS:HG3	3:D:49:TYR:CD1	2.47	0.49
3:D:49:TYR:O	3:D:125:GLN:NE2	2.34	0.49
3:E:14:ARG:CB	3:E:105:GLU:HB3	2.43	0.49
1:F:57:THR:CG2	1:F:57:THR:O	2.60	0.49
3:D:178:SER:O	3:D:179:GLU:CG	2.61	0.48
1:F:158:ASP:C	1:F:160:ASP:H	2.21	0.48
1:A:75:TRP:NE1	1:A:161:LEU:HD21	2.28	0.48
1:C:-2:HIS:O	1:C:119:LYS:HE3	2.14	0.48
3:H:37:ILE:HG22	3:H:183:LEU:HB2	1.95	0.48
1:C:158:ASP:C	1:C:160:ASP:H	2.21	0.48
3:E:79:CYS:SG	3:E:106:CYS:HB3	2.53	0.48
3:H:26:PHE:HZ	3:H:48:LYS:HG2	1.79	0.48
3:D:174:PHE:HD1	3:D:174:PHE:H	1.61	0.48
3:E:173:GLN:CG	3:E:174:PHE:N	2.77	0.48
1:C:170:SER:OG	1:C:171:GLY:N	2.44	0.48
3:E:175:ILE:HG22	3:E:176:THR:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLU:O	1:A:9:GLN:HB2	2.13	0.48
1:A:42:THR:O	1:A:57:THR:HB	2.14	0.48
1:A:138:THR:HG23	1:A:142:LEU:CD1	2.43	0.48
1:F:177:ASN:OD1	1:F:201:ILE:HD12	2.13	0.48
3:D:178:SER:O	3:D:179:GLU:CB	2.61	0.48
3:D:186:PHE:CD2	3:D:186:PHE:C	2.92	0.48
3:E:145:LEU:CD2	3:E:182:ARG:HD3	2.41	0.48
3:D:72:LEU:HG	3:D:76:LEU:HD11	1.96	0.47
1:A:45:ARG:HG2	1:A:52:THR:CG2	2.45	0.47
1:C:167:TRP:CD2	2:I:5:TYR:HB2	2.49	0.47
3:D:74:ASP:O	3:D:77:TYR:HB3	2.14	0.47
3:E:82:GLN:HE22	3:E:193:VAL:CG1	2.27	0.47
3:D:186:PHE:C	3:D:186:PHE:HD2	2.22	0.47
3:H:159:LYS:HA	3:H:159:LYS:HD2	1.55	0.47
1:A:-5:HIS:CE1	1:F:-3:HIS:CE1	3.03	0.47
1:A:81:VAL:HG22	1:A:104:ILE:HD12	1.96	0.47
1:C:138:THR:HG23	1:C:142:LEU:HD12	1.96	0.47
1:C:166:LYS:HB3	1:C:166:LYS:HZ3	1.77	0.47
3:D:83:LYS:HG2	3:D:156:TYR:HB2	1.97	0.47
3:E:167:TRP:CD1	3:E:168:GLU:N	2.83	0.47
3:D:178:SER:C	3:D:179:GLU:HG2	2.39	0.47
3:E:72:LEU:HG	3:E:76:LEU:HD11	1.96	0.47
1:F:155:ILE:HD13	1:F:155:ILE:HA	1.65	0.47
3:H:38:TYR:CE1	3:H:61:LEU:HD22	2.50	0.47
3:D:141:PHE:CE2	1:F:6:SER:HA	2.49	0.47
3:D:161:LEU:O	3:D:161:LEU:HD12	2.15	0.47
3:D:193:VAL:O	3:D:194:ASN:CB	2.61	0.47
1:A:51:LEU:CG	1:A:129:ARG:HG3	2.45	0.47
3:E:40:SER:C	3:E:42:THR:N	2.70	0.47
3:E:77:TYR:CD2	3:E:77:TYR:O	2.67	0.47
3:D:177:ASN:ND2	3:D:184:ARG:CD	2.70	0.46
1:A:170:SER:OG	1:A:171:GLY:N	2.47	0.46
3:E:159:LYS:HZ1	3:E:194:ASN:HB2	1.80	0.46
1:A:51:LEU:CD1	1:A:129:ARG:HG3	2.46	0.46
1:A:188:THR:C	1:A:189:THR:HG23	2.39	0.46
1:A:33:TYR:CE1	1:A:54:LEU:HD22	2.51	0.46
3:E:153:LEU:HD22	3:E:155:ILE:HD13	1.97	0.46
1:A:91:ILE:HB	1:A:148:SER:O	2.15	0.46
3:D:59:LEU:HG	3:D:63:LYS:HE3	1.98	0.46
3:D:83:LYS:HG3	3:D:156:TYR:CD1	2.37	0.46
3:D:156:TYR:CE2	3:D:191:HIS:ND1	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:72:LEU:HG	3:E:76:LEU:CD1	2.46	0.46
1:F:159:LYS:HB3	1:F:159:LYS:HE2	1.79	0.46
3:E:167:TRP:CG	3:E:168:GLU:H	2.34	0.46
1:A:48:LYS:HG3	1:A:49:TYR:CD1	2.51	0.45
1:C:66:ASN:N	1:C:66:ASN:HD22	2.14	0.45
3:E:157:THR:OG1	3:E:161:LEU:HD21	2.16	0.45
3:H:14:ARG:NH1	3:H:127:GLU:OE1	2.49	0.45
1:C:155:ILE:HA	1:C:155:ILE:HD13	1.66	0.45
1:F:81:VAL:HG22	1:F:104:ILE:HD12	1.98	0.45
3:H:28:ILE:O	3:H:28:ILE:HG12	2.14	0.45
1:A:-5:HIS:HE1	1:F:-3:HIS:HE1	1.64	0.45
3:D:81:VAL:HG22	3:D:81:VAL:O	2.16	0.45
3:H:184:ARG:NH1	3:H:184:ARG:HA	2.25	0.45
1:C:58:ASP:O	1:C:62:ILE:HG13	2.15	0.45
3:E:10:GLY:HA3	3:E:101:GLN:O	2.16	0.45
3:H:10:GLY:N	3:H:101:GLN:NE2	2.65	0.45
3:H:178:SER:O	3:H:179:GLU:HB2	2.17	0.45
3:D:65:LEU:O	3:D:69:VAL:HG23	2.16	0.45
3:E:14:ARG:HA	3:E:105:GLU:HB3	1.98	0.44
3:H:14:ARG:CG	3:H:127:GLU:OE2	2.65	0.44
3:H:145:LEU:HD22	3:H:182:ARG:HD3	1.98	0.44
3:E:59:LEU:O	3:E:60:GLU:C	2.60	0.44
3:E:75:TRP:O	3:E:80:SER:HB2	2.17	0.44
1:C:18:GLU:HG2	1:C:73:LYS:HD2	1.99	0.44
1:C:146:GLU:CD	1:C:146:GLU:N	2.75	0.44
1:F:8:GLU:O	1:F:9:GLN:CB	2.65	0.44
1:F:78:LYS:HE3	1:F:78:LYS:HB2	1.74	0.44
3:E:26:PHE:HZ	3:E:48:LYS:HG2	1.82	0.44
1:F:89:SER:HB3	1:F:96:VAL:HA	1.99	0.44
2:G:10:ARG:H	2:G:10:ARG:HG3	1.51	0.44
1:C:29:ASN:OD1	1:C:55:VAL:HA	2.18	0.44
1:C:78:LYS:HE3	1:C:78:LYS:HB2	1.75	0.44
3:D:86:VAL:HB	3:D:100:TRP:HB2	2.00	0.44
3:D:157:THR:HG21	3:D:161:LEU:HD23	1.99	0.44
1:A:91:ILE:HG12	1:A:150:SER:HB3	2.00	0.44
3:H:184:ARG:NH1	3:H:184:ARG:C	2.75	0.44
3:D:177:ASN:O	3:D:178:SER:C	2.61	0.44
3:H:14:ARG:NH2	3:H:14:ARG:CG	2.62	0.44
3:E:163:VAL:CG2	3:E:167:TRP:HB2	2.48	0.43
1:A:159:LYS:HE2	1:A:159:LYS:HB3	1.80	0.43
1:F:75:TRP:HB3	1:F:81:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:GLU:CD	1:F:146:GLU:N	2.76	0.43
1:F:78:LYS:O	1:F:79:CYS:HB2	2.18	0.43
1:A:78:LYS:HE3	1:A:78:LYS:HB2	1.66	0.43
3:E:42:THR:O	3:E:42:THR:CG2	2.65	0.43
3:E:166:LYS:HB2	3:E:170:SER:HA	2.01	0.43
1:C:85:VAL:HB	1:C:154:LEU:HB2	2.00	0.43
3:E:167:TRP:CE3	3:E:172:PRO:HD2	2.54	0.43
3:D:157:THR:HG21	3:D:161:LEU:CD2	2.49	0.43
3:H:74:ASP:O	3:H:77:TYR:HD2	2.01	0.43
3:H:117:GLY:O	3:H:118:GLU:C	2.62	0.43
1:C:8:GLU:O	1:C:9:GLN:HB2	2.18	0.43
3:D:40:SER:C	3:D:42:THR:H	2.26	0.43
3:E:176:THR:HG23	3:E:178:SER:H	1.84	0.43
1:F:178:SER:HB2	1:F:199:TYR:O	2.18	0.42
3:H:42:THR:O	3:H:42:THR:CG2	2.64	0.42
3:H:42:THR:O	3:H:42:THR:HG22	2.19	0.42
1:A:51:LEU:HG	1:A:129:ARG:HG3	2.01	0.42
1:A:58:ASP:O	1:A:62:ILE:HG13	2.19	0.42
1:C:159:LYS:HE2	1:C:159:LYS:HB3	1.81	0.42
3:H:163:VAL:HG23	3:H:165:GLU:H	1.79	0.42
1:A:107:ASP:OD2	1:A:107:ASP:C	2.61	0.42
2:B:5:TYR:C	2:B:5:TYR:CD2	2.97	0.42
3:H:59:LEU:HD12	3:H:59:LEU:HA	1.70	0.42
3:H:160:ASP:OD1	3:H:160:ASP:N	2.45	0.42
3:E:82:GLN:HE22	3:E:193:VAL:HG11	1.83	0.42
3:E:175:ILE:O	3:E:176:THR:OG1	2.37	0.42
3:E:193:VAL:O	3:E:194:ASN:HB2	2.18	0.42
3:D:42:THR:O	3:D:42:THR:CG2	2.66	0.42
3:D:97:LEU:O	3:D:98:GLU:HB3	2.18	0.42
3:E:174:PHE:CE1	3:E:186:PHE:HB3	2.55	0.42
1:C:117:ARG:HD2	1:C:189:THR:OG1	2.20	0.42
3:D:130:SER:O	3:D:134:GLN:HG3	2.20	0.42
3:H:137:ALA:O	3:H:140:THR:HB	2.19	0.42
3:D:91:ILE:HG12	3:D:184:ARG:HG3	2.01	0.42
3:E:186:PHE:HD2	3:E:187:THR:N	2.17	0.42
3:H:10:GLY:H	3:H:101:GLN:NE2	2.17	0.42
1:C:68:VAL:HG12	1:C:72:LEU:HD22	2.01	0.42
1:F:-5:HIS:CE1	1:F:-3:HIS:CE1	3.03	0.42
3:H:65:LEU:HA	3:H:65:LEU:HD23	1.81	0.42
1:C:180:GLU:OE2	1:C:196:MET:HE1	2.19	0.42
3:E:190:ILE:HG22	3:E:191:HIS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:72:LEU:HG	3:H:76:LEU:HD12	2.01	0.42
3:H:176:THR:C	3:H:178:SER:N	2.74	0.42
1:A:68:VAL:O	1:A:72:LEU:HB2	2.20	0.42
3:D:75:TRP:CZ2	3:D:161:LEU:HD11	2.54	0.42
1:C:28:ILE:O	1:C:29:ASN:C	2.63	0.41
3:H:77:TYR:CD2	3:H:78:LYS:HG2	2.54	0.41
3:E:81:VAL:HG22	3:E:104:ILE:CD1	2.49	0.41
1:F:90:ASN:HB3	1:F:93:SER:OG	2.20	0.41
1:F:163:VAL:HA	1:F:164:PRO:HD3	1.89	0.41
3:H:26:PHE:CE2	3:H:53:LEU:HD13	2.55	0.41
3:E:163:VAL:CG2	3:E:166:LYS:C	2.94	0.41
3:E:166:LYS:O	3:E:190:ILE:HD12	2.20	0.41
3:E:190:ILE:CG2	3:E:191:HIS:N	2.83	0.41
1:F:170:SER:OG	1:F:171:GLY:N	2.52	0.41
3:D:72:LEU:HD11	3:D:84:LEU:HD21	2.01	0.41
3:D:176:THR:CG2	3:D:177:ASN:H	2.18	0.41
3:H:65:LEU:O	3:H:69:VAL:HG23	2.19	0.41
1:A:72:LEU:O	1:A:76:LEU:HG	2.21	0.41
1:A:78:LYS:O	1:A:79:CYS:HB2	2.21	0.41
3:D:87:VAL:HB	3:D:152:ASP:HB2	2.02	0.41
1:C:71:GLN:NE2	1:C:75:TRP:CE2	2.89	0.41
3:E:82:GLN:NE2	3:E:193:VAL:HG11	2.35	0.41
3:H:83:LYS:HG2	3:H:156:TYR:HB2	2.02	0.41
1:C:91:ILE:HG12	1:C:150:SER:HB3	2.03	0.41
3:D:19:ILE:HA	3:D:19:ILE:HD12	1.82	0.41
3:D:37:ILE:HG22	3:D:183:LEU:HB2	2.03	0.41
3:D:156:TYR:HA	3:D:191:HIS:O	2.20	0.41
3:E:136:THR:HA	3:E:139:VAL:HG13	2.02	0.41
3:D:81:VAL:HG22	3:D:104:ILE:CD1	2.51	0.41
3:E:163:VAL:CG2	3:E:166:LYS:O	2.69	0.41
3:H:178:SER:O	3:H:179:GLU:CB	2.69	0.41
1:A:163:VAL:HA	1:A:164:PRO:HD3	1.85	0.40
1:F:-5:HIS:ND1	1:F:-5:HIS:C	2.79	0.40
3:H:119:LYS:HE3	3:H:119:LYS:N	2.36	0.40
1:A:156:TYR:CD1	2:B:2:TRP:CE2	3.09	0.40
3:E:100:TRP:CZ2	3:E:142:LEU:HD11	2.56	0.40
1:C:118:GLU:HG2	3:E:141:PHE:CD1	2.55	0.40
1:C:178:SER:HB2	1:C:199:TYR:O	2.22	0.40
3:D:18:GLU:HG2	3:D:73:LYS:HE2	2.04	0.40
3:D:19:ILE:CG2	3:D:20:VAL:N	2.83	0.40
1:C:90:ASN:HB3	1:C:93:SER:OG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:86:VAL:HG11	3:H:151:PHE:CE2	2.56	0.40
1:A:155:ILE:HD13	1:A:155:ILE:HA	1.64	0.40
3:D:35:ARG:NH1	3:D:142:LEU:HB2	2.37	0.40

All (2) 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:C:204:ASN:N	3:E:78:LYS:NZ[4_545]	2.13	0.07
1:C:74:ASP:OD1	3:E:63:LYS:NZ[2_455]	2.16	0.04

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	209/213 (98%)	199 (95%)	9 (4%)	1 (0%)	24	54
1	C	209/213 (98%)	200 (96%)	8 (4%)	1 (0%)	24	54
1	F	209/213 (98%)	199 (95%)	9 (4%)	1 (0%)	24	54
2	B	9/12 (75%)	7 (78%)	2 (22%)	0	100	100
2	G	9/12 (75%)	7 (78%)	2 (22%)	0	100	100
2	I	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
3	D	168/207 (81%)	149 (89%)	14 (8%)	5 (3%)	3	14
3	E	172/207 (83%)	147 (86%)	19 (11%)	6 (4%)	3	12
3	H	179/207 (86%)	160 (89%)	14 (8%)	5 (3%)	4	15
All	All	1174/1296 (91%)	1077 (92%)	78 (7%)	19 (2%)	7	27

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	LYS
1	C	159	LYS
3	D	179	GLU
3	D	194	ASN
3	E	167	TRP
3	E	169	GLU
3	E	178	SER
3	E	179	GLU
1	F	159	LYS
3	H	167	TRP
3	D	177	ASN
3	D	182	ARG
3	E	166	LYS
3	H	115	GLY
3	H	165	GLU
3	H	168	GLU
3	E	106	CYS
3	D	115	GLY
3	H	171	GLY

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	194/197 (98%)	176 (91%)	18 (9%)	8	27
1	C	194/197 (98%)	176 (91%)	18 (9%)	8	27
1	F	194/197 (98%)	175 (90%)	19 (10%)	7	25
2	B	10/11 (91%)	10 (100%)	0	100	100
2	G	10/11 (91%)	10 (100%)	0	100	100
2	I	10/11 (91%)	10 (100%)	0	100	100
3	D	159/191 (83%)	144 (91%)	15 (9%)	8	26
3	E	164/191 (86%)	139 (85%)	25 (15%)	3	9
3	H	167/191 (87%)	149 (89%)	18 (11%)	6	21
All	All	1102/1197 (92%)	989 (90%)	113 (10%)	7	23

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	5	LEU
1	A	42	THR
1	A	57	THR
1	A	63	LYS
1	A	72	LEU
1	A	81	VAL
1	A	84	LEU
1	A	89	SER
1	A	91	ILE
1	A	106	CYS
1	A	138	THR
1	A	144	LEU
1	A	147	VAL
1	A	155	ILE
1	A	157	THR
1	A	166	LYS
1	A	196	MET
1	C	3	LEU
1	C	5	LEU
1	C	42	THR
1	C	57	THR
1	C	72	LEU
1	C	81	VAL
1	C	84	LEU
1	C	91	ILE
1	C	106	CYS
1	C	138	THR
1	C	144	LEU
1	C	147	VAL
1	C	155	ILE
1	C	157	THR
1	C	160	ASP
1	C	166	LYS
1	C	189	THR
1	C	196	MET
3	D	14	ARG
3	D	19	ILE
3	D	68	VAL
3	D	70	GLU
3	D	81	VAL
3	D	107	ASP

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Mol	Chain	Res	Type
3	D	132	ILE
3	D	139	VAL
3	D	145	LEU
3	D	153	LEU
3	D	160	ASP
3	D	173	GLN
3	D	178	SER
3	D	186	PHE
3	D	187	THR
3	E	14	ARG
3	E	19	ILE
3	E	42	THR
3	E	54	LEU
3	E	55	VAL
3	E	66	ASN
3	E	68	VAL
3	E	77	TYR
3	E	81	VAL
3	E	89	SER
3	E	107	ASP
3	E	108	LYS
3	E	139	VAL
3	E	151	PHE
3	E	153	LEU
3	E	158	ASP
3	E	159	LYS
3	E	161	LEU
3	E	165	GLU
3	E	168	GLU
3	E	169	GLU
3	E	173	GLN
3	E	179	GLU
3	E	187	THR
3	E	192	LYS
1	F	3	LEU
1	F	5	LEU
1	F	42	THR
1	F	57	THR
1	F	72	LEU
1	F	81	VAL
1	F	84	LEU
1	F	89	SER

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Mol	Chain	Res	Type
1	F	91	ILE
1	F	106	CYS
1	F	138	THR
1	F	144	LEU
1	F	147	VAL
1	F	155	ILE
1	F	157	THR
1	F	160	ASP
1	F	166	LYS
1	F	189	THR
1	F	196	MET
3	H	16	SER
3	H	19	ILE
3	H	28	ILE
3	H	65	LEU
3	H	68	VAL
3	H	77	TYR
3	H	81	VAL
3	H	119	LYS
3	H	121	GLN
3	H	139	VAL
3	H	153	LEU
3	H	162	VAL
3	H	163	VAL
3	H	167	TRP
3	H	169	GLU
3	H	173	GLN
3	H	187	THR
3	H	189	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-5	HIS
1	A	66	ASN
1	A	82	GLN
1	A	125	GLN
1	C	-5	HIS
1	C	66	ASN
1	C	125	GLN
1	C	194	ASN
3	D	66	ASN

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Mol	Chain	Res	Type
3	D	67	ASN
3	D	71	GLN
3	D	173	GLN
3	D	177	ASN
3	D	194	ASN
3	E	47	GLN
3	E	66	ASN
3	E	71	GLN
3	E	101	GLN
3	E	121	GLN
3	E	173	GLN
3	E	177	ASN
1	F	-5	HIS
1	F	-3	HIS
1	F	66	ASN
1	F	125	GLN
1	F	194	ASN
3	H	34	GLN
3	H	47	GLN
3	H	66	ASN
3	H	71	GLN
3	H	101	GLN
3	H	121	GLN
3	H	194	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	211/213 (99%)	0.27	16 (7%)	20 16	16, 31, 61, 100	0
1	C	211/213 (99%)	0.34	18 (8%)	16 14	16, 32, 61, 100	0
1	F	211/213 (99%)	0.23	10 (4%)	36 28	16, 30, 61, 100	0
2	B	11/12 (91%)	0.56	0	100 100	36, 43, 67, 69	0
2	G	11/12 (91%)	0.54	1 (9%)	15 12	37, 43, 66, 68	0
2	I	12/12 (100%)	0.94	1 (8%)	17 14	38, 42, 69, 69	0
3	D	172/207 (83%)	0.59	23 (13%)	7 5	14, 36, 88, 96	0
3	E	176/207 (85%)	0.55	22 (12%)	8 7	17, 38, 94, 98	0
3	H	181/207 (87%)	0.67	30 (16%)	4 3	15, 37, 92, 99	0
All	All	1196/1296 (92%)	0.43	121 (10%)	12 10	14, 34, 84, 100	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	205	ASP	6.2
3	D	176	THR	6.2
1	C	204	ASN	6.1
3	H	170	SER	5.9
3	H	167	TRP	5.5
3	D	160	ASP	5.2
1	F	160	ASP	5.2
1	A	158	ASP	5.1
3	D	161	LEU	5.1
3	D	177	ASN	5.1
3	E	161	LEU	5.1
1	C	67	ASN	4.6
1	C	203	VAL	4.6
3	H	164	PRO	4.6
1	A	203	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
3	D	77	TYR	4.5
1	A	66	ASN	4.4
3	D	106	CYS	4.4
3	H	168	GLU	4.3
1	A	-3	HIS	4.3
3	H	169	GLU	4.2
3	H	77	TYR	4.1
1	F	203	VAL	4.1
3	H	162	VAL	4.1
3	E	162	VAL	4.0
3	E	164	PRO	4.0
1	C	112	ASP	3.9
1	F	158	ASP	3.9
3	E	168	GLU	3.9
1	A	204	ASN	3.9
3	E	77	TYR	3.8
3	E	108	LYS	3.8
3	E	70	GLU	3.8
3	H	163	VAL	3.8
1	C	158	ASP	3.8
1	A	165	GLU	3.7
3	E	107	ASP	3.7
1	C	-5	HIS	3.6
3	D	116	SER	3.6
3	H	177	ASN	3.5
3	H	193	VAL	3.4
1	F	106	CYS	3.3
1	A	159	LYS	3.3
1	C	165	GLU	3.2
1	A	160	ASP	3.2
3	E	179	GLU	3.2
3	H	116	SER	3.1
3	H	178	SER	3.1
2	I	9	GLN	3.1
3	H	159	LYS	3.1
3	D	180	GLU	3.1
3	D	159	LYS	3.1
1	F	-3	HIS	3.1
3	D	108	LYS	3.1
3	H	165	GLU	3.0
1	A	157	THR	3.0
3	D	172	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
3	E	9	GLN	2.9
3	E	160	ASP	2.9
3	H	166	LYS	2.9
1	A	146	GLU	2.9
3	D	78	LYS	2.9
1	F	204	ASN	2.9
3	D	119	LYS	2.8
1	F	202	PRO	2.8
3	H	176	THR	2.7
3	E	159	LYS	2.7
3	H	41	GLU	2.6
3	H	180	GLU	2.6
1	A	163	VAL	2.6
3	H	121	GLN	2.6
3	E	163	VAL	2.6
3	D	179	GLU	2.6
1	C	-3	HIS	2.5
3	E	120	SER	2.5
1	C	202	PRO	2.5
1	C	92	GLU	2.5
1	C	161	LEU	2.5
3	D	174	PHE	2.5
1	C	177	ASN	2.5
3	D	178	SER	2.5
3	H	195	SER	2.4
3	E	167	TRP	2.4
3	H	179	GLU	2.4
3	H	161	LEU	2.4
3	E	180	GLU	2.4
3	D	191	HIS	2.4
1	A	161	LEU	2.4
3	H	117	GLY	2.4
3	H	120	SER	2.4
3	D	67	ASN	2.4
1	A	162	VAL	2.4
1	A	205	ASP	2.4
3	E	170	SER	2.3
3	H	78	LYS	2.3
3	E	158	ASP	2.3
3	D	195	SER	2.3
3	D	158	ASP	2.3
3	E	178	SER	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	181	VAL	2.3
3	H	171	GLY	2.3
1	C	82	GLN	2.2
3	E	166	LYS	2.2
1	C	160	ASP	2.2
1	F	-5	HIS	2.2
3	E	184	ARG	2.2
1	C	70	GLU	2.2
3	E	193	VAL	2.2
1	A	114	SER	2.2
1	F	9	GLN	2.2
3	D	117	GLY	2.2
3	H	127	GLU	2.2
1	C	146	GLU	2.1
1	A	70	GLU	2.1
3	D	193	VAL	2.1
3	H	119	LYS	2.1
1	C	164	PRO	2.1
3	H	105	GLU	2.1
2	G	1	SER	2.0
1	F	66	ASN	2.0
3	H	40	SER	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.