



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:46 AM GMT

PDB ID : 1LP9
Title : Xenoreactive complex AHIII 12.2 TCR bound to p1049/HLA-A2.1
Authors : Buslepp, J.; Wang, H.; Biddison, W.E.; Appella, E.; Collins, E.J.
Deposited on : 2002-05-07
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

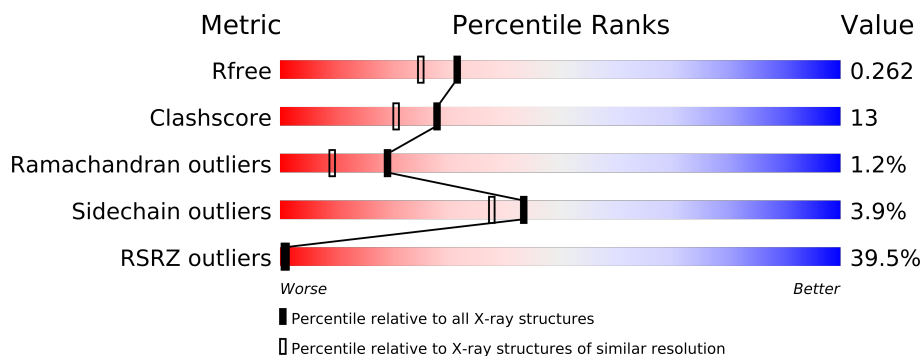
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	275	
1	H	275	
2	B	100	
2	I	100	
3	C	9	
3	J	9	
4	E	194	
4	L	194	
5	F	238	
5	M	238	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13552 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	14	0	0
			2247	1403	409	426	9			
1	H	275	Total	C	N	O	S	18	0	0
			2247	1403	409	426	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	9	0	0
			837	533	141	159	4			
2	I	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING MET	UNP P61769
I	0	MET	-	INITIATING MET	UNP P61769

- Molecule 3 is a protein called self-peptide P1049.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			76	56	10	10			
3	J	9	Total	C	N	O	0	0	0
			76	56	10	10			

- Molecule 4 is a protein called T-cell Receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	194	Total	C	N	O	S	102	0	0
			1521	965	245	302	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	194	Total	C	N	O	S	96	0	0
			1521	965	245	302	9			

- Molecule 5 is a protein called T-cell Receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	237	Total	C	N	O	S	27	0	0
			1887	1192	331	359	5			
5	M	237	Total	C	N	O	S	25	0	0
			1887	1192	331	359	5			

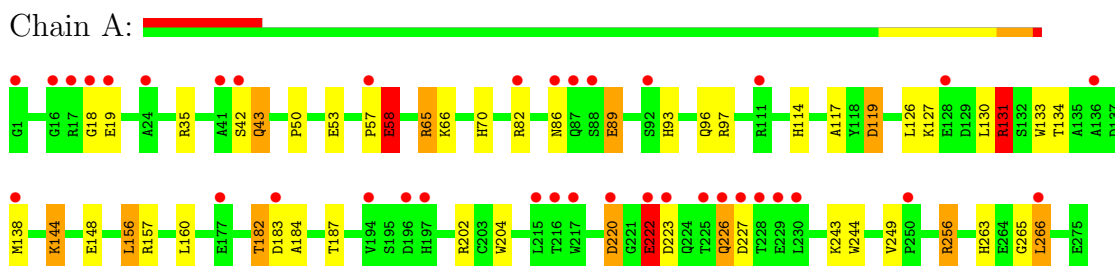
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total	O	0	0
			79	79		
6	B	20	Total	O	0	0
			20	20		
6	C	3	Total	O	0	0
			3	3		
6	E	47	Total	O	0	0
			47	47		
6	F	46	Total	O	0	0
			46	46		
6	H	64	Total	O	0	0
			64	64		
6	I	28	Total	O	0	0
			28	28		
6	J	2	Total	O	0	0
			2	2		
6	L	53	Total	O	0	0
			53	53		
6	M	74	Total	O	0	0
			74	74		

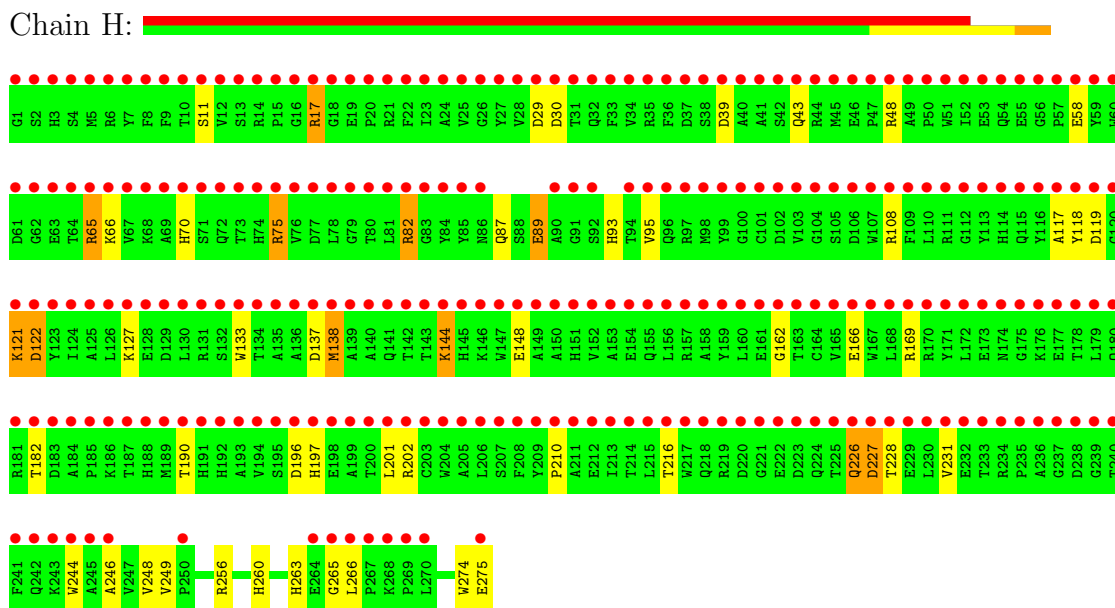
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

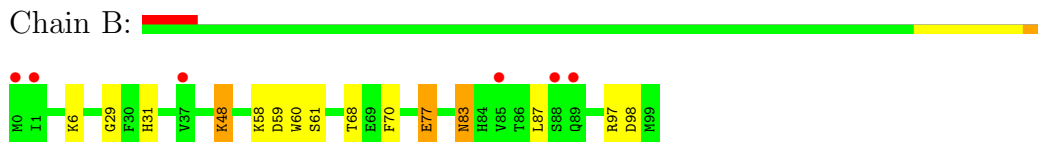
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



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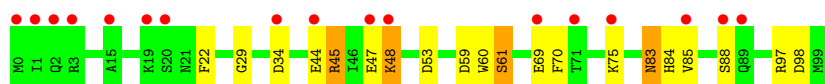


- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin





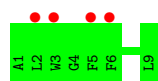
- Molecule 3: self-peptide P1049

Chain C:



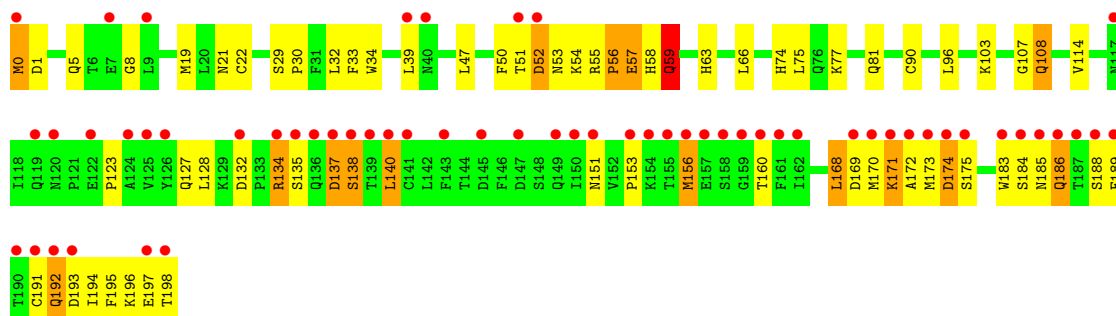
- Molecule 3: self-peptide P1049

Chain J:



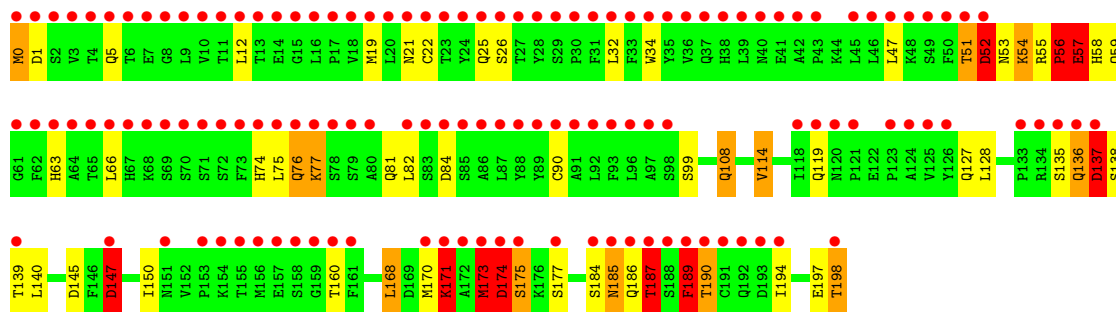
- Molecule 4: T-cell Receptor alpha chain

Chain E:



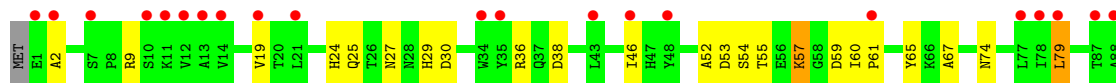
- Molecule 4: T-cell Receptor alpha chain

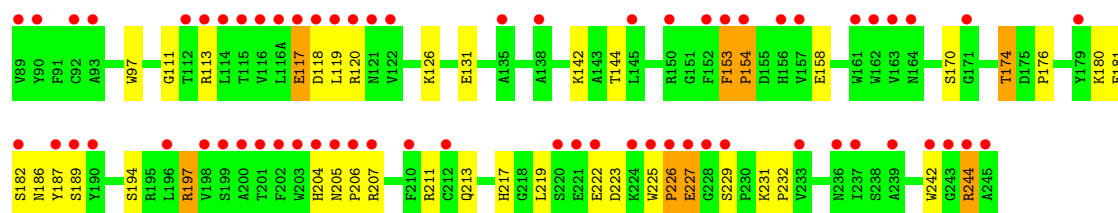
Chain L:



- Molecule 5: T-cell Receptor beta chain

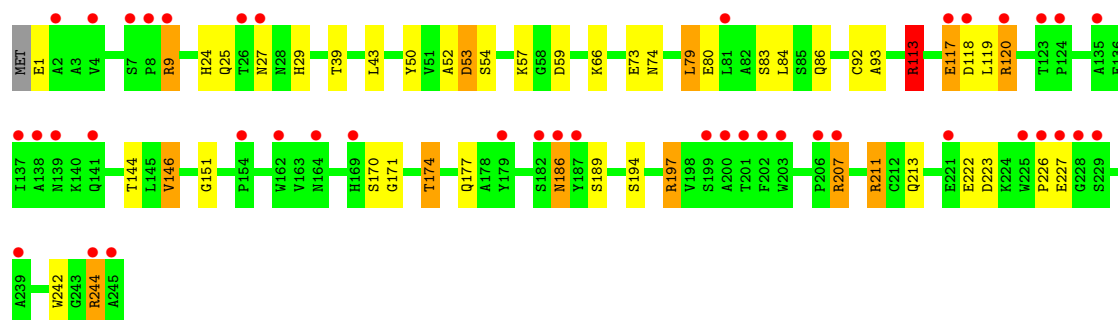
Chain F:





• Molecule 5: T-cell Receptor beta chain

Chain M:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.71Å 84.47Å 121.34Å 90.00° 92.13° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.00) 100.0 (29.96-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.219 , 0.253 0.230 , 0.262	Depositor DCC
R_{free} test set	6421 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.7	EDS
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 127789 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	13552	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.70 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2719e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	2.22	13/2312 (0.6%)	1.24	20/3137 (0.6%)
1	H	1.24	9/2312 (0.4%)	2.48	26/3137 (0.8%)
2	B	1.93	4/860 (0.5%)	1.59	7/1162 (0.6%)
2	I	3.59	7/860 (0.8%)	0.96	7/1162 (0.6%)
3	C	0.67	0/80	0.73	0/108
3	J	0.64	0/80	0.67	0/108
4	E	2.39	21/1557 (1.3%)	1.67	35/2112 (1.7%)
4	L	1.78	20/1557 (1.3%)	1.94	38/2112 (1.8%)
5	F	2.34	17/1943 (0.9%)	2.17	24/2644 (0.9%)
5	M	2.36	13/1943 (0.7%)	2.47	24/2644 (0.9%)
All	All	2.19	104/13504 (0.8%)	1.96	181/18326 (1.0%)

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	4
1	H	0	2
2	B	0	1
4	E	1	4
4	L	0	7
5	F	0	4
5	M	0	4
All	All	1	26

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	GLU	CG-CD	87.36	2.83	1.51
2	I	44	GLU	CD-OE1	68.60	2.01	1.25
2	I	44	GLU	CD-OE2	61.19	1.93	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	117	GLU	CG-CD	59.87	2.41	1.51
5	F	222	GLU	CG-CD	48.99	2.25	1.51
5	F	113	ARG	NE-CZ	45.96	1.92	1.33
5	M	117	GLU	CB-CG	44.54	2.36	1.52
4	E	192	GLN	CD-OE1	43.78	2.20	1.24
2	B	58	LYS	CD-CE	43.38	2.59	1.51
5	F	126	LYS	CE-NZ	37.84	2.43	1.49
4	E	108	GLN	CG-CD	34.66	2.30	1.51
4	E	192	GLN	CB-CG	34.26	2.45	1.52
2	I	48	LYS	CE-NZ	33.29	2.32	1.49
5	M	113	ARG	NE-CZ	32.53	1.75	1.33
4	L	171	LYS	CE-NZ	32.35	2.29	1.49
5	M	120	ARG	CZ-NH1	30.45	1.72	1.33
1	H	138	MET	CG-SD	-29.83	1.03	1.81
1	A	65	ARG	CZ-NH1	29.68	1.71	1.33
5	M	9	ARG	CZ-NH1	-28.42	0.96	1.33
4	E	137	ASP	CG-OD1	28.36	1.90	1.25
4	E	192	GLN	C-O	27.15	1.75	1.23
4	L	171	LYS	CB-CG	-25.56	0.83	1.52
5	F	207	ARG	NE-CZ	24.94	1.65	1.33
2	B	6	LYS	CE-NZ	23.77	2.08	1.49
2	I	48	LYS	CD-CE	23.47	2.10	1.51
1	H	144	LYS	CE-NZ	23.28	2.07	1.49
5	F	117	GLU	CB-CG	23.23	1.96	1.52
4	L	137	ASP	CB-CG	23.10	2.00	1.51
5	F	227	GLU	CD-OE2	-22.82	1.00	1.25
1	A	58	GLU	CD-OE1	22.72	1.50	1.25
5	M	222	GLU	CD-OE2	22.64	1.50	1.25
4	L	189	PHE	CE2-CZ	22.51	1.80	1.37
4	E	59	GLN	C-N	-21.31	0.94	1.33
2	I	61	SER	CB-OG	21.25	1.69	1.42
4	E	137	ASP	CG-OD2	20.91	1.73	1.25
5	F	120	ARG	CG-CD	20.82	2.04	1.51
1	A	131	ARG	CZ-NH1	20.56	1.59	1.33
2	B	48	LYS	CD-CE	19.41	1.99	1.51
5	M	50	TYR	CE2-CZ	18.84	1.63	1.38
5	F	126	LYS	CD-CE	18.79	1.98	1.51
5	F	227	GLU	CB-CG	18.57	1.87	1.52
4	E	59	GLN	CA-CB	18.41	1.94	1.53
1	H	121	LYS	CD-CE	18.20	1.96	1.51
5	F	154	PRO	N-CD	-18.02	1.22	1.47
1	H	58	GLU	CD-OE2	-17.76	1.06	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	113	ARG	CZ-NH1	-17.61	1.10	1.33
4	L	136	GLN	CD-NE2	17.14	1.75	1.32
1	A	222	GLU	CG-CD	16.98	1.77	1.51
1	H	89	GLU	CD-OE1	15.44	1.42	1.25
5	F	222	GLU	CD-OE2	-15.22	1.08	1.25
5	F	57	LYS	CD-CE	14.94	1.88	1.51
4	E	156	MET	CG-SD	14.93	2.19	1.81
1	A	144	LYS	CE-NZ	14.86	1.86	1.49
4	E	56	PRO	CG-CD	-14.71	1.02	1.50
2	I	48	LYS	CG-CD	14.41	2.01	1.52
5	M	207	ARG	CZ-NH2	-13.87	1.15	1.33
5	M	113	ARG	CZ-NH2	13.86	1.51	1.33
1	A	226	GLN	CB-CG	13.67	1.89	1.52
4	L	174	ASP	CG-OD2	13.33	1.56	1.25
4	L	56	PRO	CA-CB	13.19	1.79	1.53
4	E	192	GLN	CG-CD	12.66	1.80	1.51
5	F	222	GLU	CB-CG	-12.30	1.28	1.52
1	A	89	GLU	CD-OE1	11.87	1.38	1.25
4	L	76	GLN	CD-NE2	11.85	1.62	1.32
5	F	207	ARG	CG-CD	11.23	1.80	1.51
1	H	227	ASP	CG-OD2	11.12	1.50	1.25
4	L	189	PHE	CG-CD2	10.98	1.55	1.38
4	L	108	GLN	CD-NE2	10.91	1.60	1.32
5	M	207	ARG	CZ-NH1	10.81	1.47	1.33
5	F	227	GLU	CA-CB	10.71	1.77	1.53
1	H	17	ARG	NE-CZ	10.51	1.46	1.33
2	B	58	LYS	CG-CD	9.44	1.84	1.52
4	E	186	GLN	CD-OE1	-9.17	1.03	1.24
1	A	256	ARG	CZ-NH1	-8.99	1.21	1.33
1	A	249	VAL	CB-CG1	-8.44	1.35	1.52
4	L	136	GLN	CD-OE1	8.31	1.42	1.24
1	A	243	LYS	CE-NZ	8.09	1.69	1.49
4	E	114	VAL	CB-CG1	-7.92	1.36	1.52
4	E	140	LEU	CG-CD2	7.92	1.81	1.51
5	F	2	ALA	C-O	7.58	1.37	1.23
1	H	226	GLN	CA-CB	-7.58	1.37	1.53
4	L	185	ASN	CG-OD1	-7.40	1.07	1.24
4	E	58	HIS	N-CA	7.10	1.60	1.46
5	M	119	LEU	CG-CD2	-6.95	1.26	1.51
4	L	119	GLN	CD-NE2	-6.84	1.15	1.32
4	E	57	GLU	N-CA	6.80	1.59	1.46
4	L	56	PRO	C-O	6.77	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	32	LEU	CG-CD1	-6.55	1.27	1.51
4	L	137	ASP	CA-CB	6.21	1.67	1.53
5	F	207	ARG	CZ-NH1	-6.11	1.25	1.33
4	E	58	HIS	CA-C	6.04	1.68	1.52
1	H	249	VAL	CB-CG1	-6.00	1.40	1.52
4	E	57	GLU	CA-C	5.96	1.68	1.52
4	L	57	GLU	N-CA	5.88	1.58	1.46
2	I	44	GLU	CG-CD	5.85	1.60	1.51
1	A	226	GLN	CA-CB	5.81	1.66	1.53
4	E	134	ARG	CZ-NH2	5.66	1.40	1.33
1	A	226	GLN	C-O	5.50	1.33	1.23
4	L	171	LYS	CG-CD	5.38	1.70	1.52
4	E	56	PRO	CA-C	5.38	1.63	1.52
4	L	57	GLU	CA-C	5.30	1.66	1.52
5	M	227	GLU	CA-CB	5.30	1.65	1.53
4	E	137	ASP	CB-CG	5.21	1.62	1.51
4	L	66	LEU	CG-CD2	5.17	1.71	1.51

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	17	ARG	NE-CZ-NH1	-101.59	69.50	120.30
5	M	207	ARG	NE-CZ-NH1	-65.69	87.46	120.30
5	M	207	ARG	NE-CZ-NH2	-56.78	91.91	120.30
1	H	17	ARG	NE-CZ-NH2	51.09	145.84	120.30
5	F	207	ARG	NE-CZ-NH1	-50.50	95.05	120.30
5	M	9	ARG	NE-CZ-NH1	45.61	143.11	120.30
5	M	120	ARG	NE-CZ-NH1	-44.06	98.27	120.30
5	F	222	GLU	OE1-CD-OE2	37.19	167.92	123.30
5	F	113	ARG	NE-CZ-NH2	-36.59	102.00	120.30
1	H	17	ARG	CD-NE-CZ	-35.46	73.96	123.60
5	F	113	ARG	NE-CZ-NH1	34.79	137.69	120.30
1	A	58	GLU	CG-CD-OE1	-32.92	52.45	118.30
2	B	77	GLU	OE1-CD-OE2	-32.83	83.90	123.30
5	F	207	ARG	NH1-CZ-NH2	30.59	153.05	119.40
4	L	174	ASP	CB-CG-OD2	-29.29	91.94	118.30
2	B	58	LYS	CD-CE-NZ	-28.98	45.04	111.70
4	E	59	GLN	O-C-N	-27.89	75.79	123.20
4	L	137	ASP	CB-CG-OD1	-26.20	94.72	118.30
4	L	76	GLN	OE1-CD-NE2	-26.04	62.02	121.90
5	F	113	ARG	CD-NE-CZ	-25.33	88.14	123.60
1	H	256	ARG	NE-CZ-NH2	24.86	132.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	227	GLU	OE1-CD-OE2	-24.66	93.71	123.30
1	H	58	GLU	OE1-CD-OE2	-24.56	93.82	123.30
5	F	153	PHE	C-N-CD	-24.29	67.16	120.60
4	L	194	ILE	CG1-CB-CG2	-24.23	58.09	111.40
5	M	113	ARG	NE-CZ-NH2	-22.33	109.13	120.30
4	L	174	ASP	OD1-CG-OD2	-22.28	80.96	123.30
4	E	59	GLN	CA-C-N	20.98	158.17	116.20
4	L	137	ASP	CB-CG-OD2	20.66	136.90	118.30
5	M	9	ARG	NH1-CZ-NH2	-20.39	96.97	119.40
5	M	120	ARG	NH1-CZ-NH2	20.03	141.43	119.40
1	A	131	ARG	NE-CZ-NH1	-19.73	110.44	120.30
1	H	121	LYS	CD-CE-NZ	19.16	155.77	111.70
5	M	113	ARG	CD-NE-CZ	-18.01	98.38	123.60
5	M	207	ARG	CG-CD-NE	17.35	148.24	111.80
5	F	207	ARG	NE-CZ-NH2	-16.99	111.80	120.30
4	L	136	GLN	OE1-CD-NE2	-16.43	84.12	121.90
5	F	222	GLU	CA-CB-CG	15.71	147.96	113.40
4	E	66	LEU	CD1-CG-CD2	-15.49	64.02	110.50
4	L	171	LYS	CA-CB-CG	15.33	147.13	113.40
4	L	189	PHE	CB-CG-CD2	-15.31	110.08	120.80
4	E	134	ARG	NE-CZ-NH2	-14.86	112.87	120.30
1	A	58	GLU	OE1-CD-OE2	-14.76	105.58	123.30
4	E	56	PRO	N-CA-CB	-14.74	85.62	103.30
5	M	50	TYR	CG-CD1-CE1	14.47	132.88	121.30
4	E	59	GLN	N-CA-CB	14.08	135.94	110.60
1	H	75	ARG	NE-CZ-NH1	14.02	127.31	120.30
1	A	58	GLU	CB-CG-CD	-13.81	76.91	114.20
1	H	58	GLU	CG-CD-OE2	13.20	144.69	118.30
4	E	192	GLN	CA-CB-CG	-12.94	84.93	113.40
4	E	192	GLN	CG-CD-OE1	12.80	147.20	121.60
2	I	45	ARG	NE-CZ-NH1	12.60	126.60	120.30
5	M	117	GLU	CG-CD-OE2	-12.51	93.28	118.30
4	E	186	GLN	OE1-CD-NE2	-12.35	93.50	121.90
1	H	121	LYS	CG-CD-CE	12.35	148.94	111.90
4	L	56	PRO	N-CA-C	12.30	144.09	112.10
5	M	50	TYR	CB-CG-CD1	12.23	128.34	121.00
5	F	222	GLU	CG-CD-OE1	-11.94	94.42	118.30
2	I	48	LYS	CG-CD-CE	-11.88	76.27	111.90
4	L	137	ASP	CA-CB-CG	11.69	139.11	113.40
1	H	89	GLU	OE1-CD-OE2	11.60	137.22	123.30
4	E	192	GLN	O-C-N	-11.59	104.16	122.70
4	E	57	GLU	N-CA-C	11.55	142.19	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	222	GLU	CG-CD-OE2	-11.36	95.58	118.30
1	H	256	ARG	NH1-CZ-NH2	-11.36	106.91	119.40
4	E	58	HIS	CA-CB-CG	11.01	132.31	113.60
1	A	89	GLU	OE1-CD-OE2	10.73	136.17	123.30
5	F	57	LYS	CD-CE-NZ	10.58	136.03	111.70
1	A	65	ARG	NE-CZ-NH1	10.54	125.57	120.30
5	F	2	ALA	O-C-N	-10.05	106.62	122.70
4	E	59	GLN	C-N-CA	9.82	142.92	122.30
5	F	227	GLU	N-CA-CB	-9.76	93.04	110.60
1	A	249	VAL	CA-CB-CG1	9.74	125.51	110.90
2	B	6	LYS	CD-CE-NZ	9.63	133.85	111.70
1	A	222	GLU	CG-CD-OE2	-9.48	99.34	118.30
5	M	117	GLU	CA-CB-CG	-9.32	92.89	113.40
4	L	32	LEU	CB-CG-CD1	9.27	126.75	111.00
1	A	65	ARG	NH1-CZ-NH2	-9.17	109.32	119.40
4	E	140	LEU	CB-CG-CD2	-9.13	95.48	111.00
4	E	58	HIS	N-CA-C	9.10	135.57	111.00
5	F	2	ALA	CA-C-O	9.09	139.18	120.10
4	L	119	GLN	CG-CD-NE2	8.98	138.26	116.70
5	F	222	GLU	CB-CG-CD	8.85	138.09	114.20
1	A	226	GLN	CA-CB-CG	8.84	132.86	113.40
2	B	58	LYS	CB-CG-CD	-8.74	88.88	111.60
1	H	144	LYS	CD-CE-NZ	-8.74	91.61	111.70
2	B	48	LYS	CD-CE-NZ	-8.62	91.88	111.70
4	L	174	ASP	CB-CG-OD1	-8.59	110.57	118.30
4	E	59	GLN	CB-CA-C	-8.51	93.37	110.40
5	F	126	LYS	CD-CE-NZ	8.50	131.24	111.70
4	L	119	GLN	OE1-CD-NE2	-8.48	102.39	121.90
4	E	57	GLU	N-CA-CB	-8.38	95.51	110.60
5	M	113	ARG	NE-CZ-NH1	-8.32	116.14	120.30
4	L	137	ASP	N-CA-CB	-8.26	95.74	110.60
4	L	66	LEU	CD1-CG-CD2	-8.22	85.84	110.50
5	F	120	ARG	CB-CG-CD	-8.18	90.33	111.60
4	E	156	MET	CG-SD-CE	-8.14	87.17	100.20
4	L	58	HIS	O-C-N	-8.13	109.68	122.70
4	L	187	THR	OG1-CB-CG2	-8.07	91.43	110.00
1	H	65	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	H	89	GLU	CG-CD-OE1	-7.99	102.32	118.30
4	L	171	LYS	N-CA-CB	-7.99	96.22	110.60
1	A	256	ARG	NE-CZ-NH1	7.86	124.23	120.30
4	E	56	PRO	N-CD-CG	7.60	114.61	103.20
5	F	126	LYS	CG-CD-CE	-7.59	89.13	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	57	GLU	CA-C-N	7.45	133.59	117.20
4	L	58	HIS	CA-C-N	7.40	133.48	117.20
4	L	190	THR	OG1-CB-CG2	7.36	126.92	110.00
4	E	140	LEU	CD1-CG-CD2	-7.17	88.97	110.50
4	E	192	GLN	OE1-CD-NE2	-7.07	105.64	121.90
4	L	57	GLU	N-CA-C	7.07	130.07	111.00
1	A	249	VAL	CG1-CB-CG2	7.02	122.13	110.90
4	E	53	ASN	C-N-CA	-7.00	104.21	121.70
4	L	56	PRO	CA-C-O	-6.93	103.57	120.20
4	L	187	THR	CA-CB-CG2	-6.91	102.72	112.40
1	H	249	VAL	CA-CB-CG1	6.85	121.17	110.90
4	E	56	PRO	N-CA-C	6.74	129.63	112.10
5	M	197	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	H	182	THR	OG1-CB-CG2	-6.50	95.04	110.00
2	I	45	ARG	NH1-CZ-NH2	-6.48	112.27	119.40
2	B	98	ASP	CB-CG-OD2	6.47	124.12	118.30
4	E	54	LYS	CB-CA-C	6.47	123.34	110.40
4	E	108	GLN	CG-CD-OE1	-6.47	108.66	121.60
5	M	50	TYR	CE1-CZ-CE2	-6.31	109.70	119.80
5	M	59	ASP	CB-CG-OD2	6.29	123.97	118.30
5	M	227	GLU	CA-CB-CG	6.24	127.14	113.40
4	E	134	ARG	NH1-CZ-NH2	6.24	126.26	119.40
1	H	249	VAL	CG1-CB-CG2	6.22	120.86	110.90
5	F	223	ASP	CB-CG-OD2	6.17	123.85	118.30
5	M	53	ASP	CB-CG-OD2	6.12	123.81	118.30
4	L	189	PHE	CD1-CG-CD2	6.09	126.22	118.30
4	E	193	ASP	CB-CG-OD2	5.99	123.69	118.30
4	E	156	MET	CA-CB-CG	5.98	123.46	113.30
1	A	144	LYS	CD-CE-NZ	-5.94	98.04	111.70
1	H	30	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	226	GLN	CB-CG-CD	5.88	126.90	111.60
4	L	84	ASP	CB-CG-OD2	5.86	123.57	118.30
4	L	189	PHE	CZ-CE2-CD2	-5.85	113.08	120.10
5	M	211	ARG	NE-CZ-NH2	-5.83	117.38	120.30
4	L	190	THR	CA-CB-CG2	5.80	120.52	112.40
4	L	56	PRO	CA-C-N	5.79	129.93	117.20
1	A	119	ASP	CB-CG-OD2	5.78	123.50	118.30
4	E	192	GLN	CA-C-O	5.77	132.21	120.10
1	H	138	MET	CB-CA-C	5.74	121.87	110.40
1	A	89	GLU	CG-CD-OE1	-5.67	106.97	118.30
5	M	207	ARG	CB-CG-CD	5.64	126.27	111.60
1	H	75	ARG	NH1-CZ-NH2	-5.64	113.20	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	50	TYR	CD1-CG-CD2	-5.62	111.72	117.90
4	E	66	LEU	CB-CG-CD2	-5.61	101.47	111.00
2	I	34	ASP	CB-CG-OD2	5.53	123.28	118.30
2	I	53	ASP	CB-CG-OD2	5.53	123.27	118.30
4	E	55	ARG	N-CA-C	5.52	125.92	111.00
5	F	154	PRO	N-CD-CG	5.51	111.46	103.20
4	E	137	ASP	CB-CG-OD2	5.49	123.24	118.30
4	L	57	GLU	O-C-N	-5.46	113.96	122.70
4	L	52	ASP	C-N-CA	-5.46	108.06	121.70
5	F	30	ASP	CB-CG-OD2	5.42	123.18	118.30
4	E	57	GLU	CB-CA-C	5.42	121.23	110.40
1	H	227	ASP	CB-CG-OD2	5.42	123.17	118.30
4	E	57	GLU	CA-CB-CG	5.41	125.30	113.40
1	H	226	GLN	CB-CG-CD	5.41	125.67	111.60
2	I	44	GLU	OE1-CD-OE2	5.39	129.77	123.30
1	H	39	ASP	CB-CG-OD2	5.38	123.14	118.30
5	M	223	ASP	CB-CG-OD2	5.37	123.13	118.30
2	I	98	ASP	CB-CG-OD2	5.33	123.10	118.30
4	L	194	ILE	CB-CG1-CD1	-5.28	99.11	113.90
5	M	211	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	227	ASP	CB-CG-OD2	5.24	123.02	118.30
4	L	171	LYS	CB-CG-CD	-5.23	98.01	111.60
1	A	183	ASP	CB-CG-OD2	5.22	123.00	118.30
1	H	137	ASP	CB-CG-OD2	5.21	122.98	118.30
1	H	29	ASP	CB-CG-OD2	5.19	122.97	118.30
4	L	56	PRO	CB-CA-C	-5.17	99.06	112.00
4	L	145	ASP	CB-CG-OD2	5.14	122.93	118.30
5	F	38	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	223	ASP	CB-CG-OD2	5.12	122.91	118.30
4	L	147	ASP	CB-CG-OD2	5.12	122.90	118.30
1	H	122	ASP	CB-CG-OD2	5.09	122.88	118.30
2	B	59	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	220	ASP	CB-CG-OD2	5.03	122.83	118.30
4	E	192	GLN	CG-CD-NE2	-5.01	104.68	116.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	57	GLU	CA

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Sidechain
1	A	222	GLU	Sidechain
1	A	58	GLU	Sidechain
1	A	65	ARG	Sidechain
2	B	77	GLU	Sidechain
4	E	108	GLN	Sidechain
4	E	186	GLN	Sidechain
4	E	192	GLN	Mainchain
4	E	59	GLN	Mainchain
5	F	117	GLU	Sidechain
5	F	153	PHE	Mainchain,Peptide
5	F	227	GLU	Sidechain
1	H	17	ARG	Sidechain
1	H	65	ARG	Sidechain
4	L	108	GLN	Sidechain
4	L	136	GLN	Sidechain
4	L	137	ASP	Sidechain
4	L	174	ASP	Sidechain
4	L	189	PHE	Sidechain
4	L	56	PRO	Mainchain
4	L	76	GLN	Sidechain
5	M	1	GLU	Mainchain
5	M	113	ARG	Sidechain
5	M	117	GLU	Sidechain
5	M	207	ARG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2247	0	2096	49	0
1	H	2247	0	2096	38	4
2	B	837	0	803	11	0
2	I	837	0	803	16	1
3	C	76	0	76	1	0
3	J	76	0	76	0	0
4	E	1521	0	1473	63	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1521	0	1475	63	0
5	F	1887	0	1790	58	0
5	M	1887	0	1790	45	1
6	A	79	0	0	7	0
6	B	20	0	0	4	0
6	C	3	0	0	0	0
6	E	47	0	0	8	0
6	F	46	0	0	4	0
6	H	64	0	0	3	0
6	I	28	0	0	9	0
6	J	2	0	0	0	0
6	L	53	0	0	9	0
6	M	74	0	0	14	0
All	All	13552	0	12478	316	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (316) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:M:244:ARG:HG2	6:M:306:HOH:O	1.35	1.24
1:A:138:MET:HG3	6:A:336:HOH:O	1.39	1.19
4:L:99:SER:CB	6:L:250:HOH:O	1.87	1.19
4:L:0:MET:CE	4:L:1:ASP:H	1.56	1.18
5:M:244:ARG:CG	6:M:306:HOH:O	1.84	1.18
4:L:99:SER:HB2	6:L:250:HOH:O	1.43	1.16
4:L:171:LYS:CG	4:L:171:LYS:CA	2.24	1.16
2:B:48:LYS:HA	6:B:119:HOH:O	1.50	1.10
4:L:0:MET:HE2	4:L:1:ASP:H	1.17	1.08
5:M:242:TRP:O	6:M:306:HOH:O	1.71	1.07
1:A:43:GLN:HA	1:A:43:GLN:HE21	1.12	1.07
1:A:86:ASN:ND2	6:A:342:HOH:O	1.88	1.04
4:L:0:MET:HE2	4:L:1:ASP:N	1.72	1.03
5:F:242:TRP:O	5:F:244:ARG:NH1	1.91	1.02
4:E:140:LEU:HD12	4:E:183:TRP:HB3	1.38	1.02
4:E:198:THR:HG21	6:E:228:HOH:O	1.59	1.02
1:A:82:ARG:HE	1:A:89:GLU:HG2	1.23	1.01
5:M:66:LYS:NZ	5:M:80:GLU:OE2	1.94	1.01
2:I:85:VAL:HG23	6:I:110:HOH:O	1.62	1.00
4:L:99:SER:OG	6:L:250:HOH:O	1.73	1.00
4:E:151:ASN:H	4:E:198:THR:HG23	1.25	0.98
4:E:196:LYS:O	4:E:197:GLU:HG2	1.63	0.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:211:ARG:NH2	5:F:213:GLN:OE1	1.97	0.98
4:E:8:GLY:O	6:E:239:HOH:O	1.81	0.97
4:L:52:ASP:N	6:L:241:HOH:O	1.90	0.95
5:M:24:HIS:HD2	5:M:74:ASN:HD21	1.08	0.95
4:E:0:MET:HG3	4:E:1:ASP:H	1.33	0.94
4:L:0:MET:HE3	4:L:0:MET:HA	1.52	0.92
1:A:43:GLN:HA	1:A:43:GLN:NE2	1.80	0.92
2:B:48:LYS:O	2:B:48:LYS:HG3	1.67	0.91
1:H:48:ARG:HD3	6:H:322:HOH:O	1.69	0.91
4:E:140:LEU:CD1	4:E:183:TRP:HB3	2.01	0.91
4:L:171:LYS:CD	4:L:171:LYS:CA	2.48	0.90
5:F:244:ARG:HG2	5:F:244:ARG:HH11	1.33	0.90
5:F:187:TYR:OH	4:L:171:LYS:HG3	1.72	0.90
5:M:177:GLN:HB2	6:M:316:HOH:O	1.72	0.89
4:L:171:LYS:CA	4:L:171:LYS:HD2	2.02	0.89
4:L:51:THR:HA	6:L:251:HOH:O	1.74	0.88
4:L:0:MET:CE	4:L:1:ASP:N	2.30	0.87
4:L:171:LYS:HA	4:L:171:LYS:HD2	1.57	0.87
5:F:244:ARG:CG	5:F:244:ARG:HH11	1.87	0.87
5:M:211:ARG:NH2	5:M:213:GLN:OE1	2.09	0.86
4:E:77:LYS:NZ	4:E:81:GLN:HE21	1.74	0.86
4:E:151:ASN:HD22	4:E:198:THR:HG22	1.39	0.86
4:L:186:GLN:HB3	4:L:189:PHE:HB2	1.57	0.84
5:F:55:THR:HG22	6:F:280:HOH:O	1.76	0.84
4:E:151:ASN:N	4:E:198:THR:HG23	1.92	0.83
1:A:182:THR:HG21	1:A:265:GLY:HA2	1.59	0.83
5:M:113:ARG:HG2	6:M:304:HOH:O	1.77	0.82
5:F:25:GLN:HE21	5:F:27:ASN:H	1.27	0.82
5:M:113:ARG:CG	6:M:304:HOH:O	2.26	0.81
1:A:182:THR:CG2	1:A:265:GLY:HA2	2.11	0.81
4:L:0:MET:HE3	4:L:1:ASP:H	1.43	0.81
5:M:144:THR:OG1	5:M:197:ARG:HD3	1.82	0.80
5:F:54:SER:HB3	6:F:282:HOH:O	1.82	0.79
4:E:8:GLY:N	6:E:243:HOH:O	1.95	0.79
5:M:24:HIS:HD2	5:M:74:ASN:ND2	1.80	0.79
1:A:43:GLN:CA	1:A:43:GLN:HE21	1.92	0.78
1:A:97:ARG:HH21	1:A:114:HIS:HE1	1.32	0.78
4:E:77:LYS:HZ1	4:E:81:GLN:HE21	1.30	0.77
4:L:22:CYS:H	4:L:74:HIS:HD2	1.33	0.76
5:F:180:LYS:HG2	5:F:182:SER:O	1.86	0.76
2:I:69:GLU:OE2	6:I:121:HOH:O	2.03	0.76
5:M:174:THR:HB	5:M:194:SER:HB2	1.66	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:M:174:THR:HG21	6:M:265:HOH:O	1.85	0.75
5:F:186:ASN:CB	4:L:171:LYS:O	2.34	0.75
5:F:24:HIS:HD2	5:F:74:ASN:HD21	1.36	0.74
1:A:42:SER:HB2	1:H:138:MET:HE3	1.69	0.74
1:H:138:MET:CA	1:H:138:MET:SD	2.76	0.74
4:E:22:CYS:H	4:E:74:HIS:HD2	1.35	0.73
1:A:93:HIS:HE1	6:A:326:HOH:O	1.70	0.73
4:E:151:ASN:H	4:E:198:THR:CG2	2.00	0.73
5:F:244:ARG:HG2	5:F:244:ARG:NH1	1.99	0.71
4:E:103:LYS:NZ	5:F:59:ASP:OD1	2.24	0.71
4:L:0:MET:HE1	4:L:25:GLN:C	2.10	0.71
1:A:182:THR:CG2	1:A:265:GLY:CA	2.69	0.71
5:M:24:HIS:CD2	5:M:74:ASN:HD21	2.00	0.71
4:L:174:ASP:CG	4:L:174:ASP:O	2.28	0.70
4:E:151:ASN:HD22	4:E:198:THR:CG2	2.04	0.70
1:A:53:GLU:OE2	6:A:304:HOH:O	2.08	0.69
2:B:87:LEU:O	6:B:115:HOH:O	2.08	0.69
4:E:198:THR:CB	6:E:228:HOH:O	2.40	0.69
5:M:25:GLN:HE22	5:M:29:HIS:H	1.38	0.69
4:L:171:LYS:HG2	5:M:170:SER:OG	1.93	0.69
1:A:42:SER:HB2	1:H:138:MET:CE	2.23	0.69
5:M:83:SER:H	5:M:86:GLN:HE21	1.40	0.69
1:H:43:GLN:NE2	1:H:43:GLN:HA	2.07	0.68
6:A:284:HOH:O	1:H:144:LYS:CE	2.40	0.68
1:H:216:THR:HG22	6:H:308:HOH:O	1.94	0.67
5:F:25:GLN:HE21	5:F:27:ASN:N	1.92	0.67
4:E:0:MET:CG	4:E:1:ASP:H	2.08	0.67
4:L:186:GLN:OE1	4:L:189:PHE:CD1	2.48	0.67
4:L:51:THR:N	6:L:241:HOH:O	2.26	0.67
4:E:0:MET:HG3	4:E:1:ASP:N	2.10	0.66
1:H:138:MET:HA	1:H:138:MET:SD	2.35	0.66
5:M:113:ARG:CD	6:M:304:HOH:O	2.43	0.65
4:E:153:PRO:HG3	4:E:196:LYS:O	1.97	0.65
1:H:263:HIS:CD2	1:H:265:GLY:H	2.15	0.65
1:A:127:LYS:HE3	1:A:134:THR:OG1	1.97	0.65
2:I:85:VAL:CG2	6:I:103:HOH:O	2.44	0.64
5:F:186:ASN:HB2	4:L:171:LYS:O	1.97	0.64
5:M:25:GLN:HE21	5:M:27:ASN:H	1.45	0.64
4:E:198:THR:CG2	6:E:228:HOH:O	2.27	0.64
5:F:52:ALA:O	5:F:53:ASP:HB2	1.96	0.64
1:A:82:ARG:NE	1:A:89:GLU:HG2	2.06	0.64
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.80	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:L:186:GLN:O	4:L:187:THR:C	2.36	0.63
2:I:69:GLU:CD	6:I:121:HOH:O	2.37	0.63
5:F:60:ILE:N	5:F:61:PRO:CD	2.61	0.63
6:A:284:HOH:O	1:H:144:LYS:HE3	1.97	0.63
4:L:0:MET:O	4:L:1:ASP:HB2	1.99	0.62
5:F:187:TYR:CE1	4:L:171:LYS:HG3	2.34	0.62
5:F:187:TYR:CZ	4:L:171:LYS:HG3	2.34	0.62
1:H:263:HIS:HD2	1:H:265:GLY:H	1.47	0.62
5:F:25:GLN:HE22	5:F:29:HIS:H	1.47	0.62
1:A:58:GLU:CD	1:A:58:GLU:HB3	2.20	0.62
5:F:204:HIS:HA	5:F:244:ARG:O	2.00	0.62
5:F:144:THR:OG1	5:F:197:ARG:HD3	2.00	0.62
4:E:188:SER:O	4:E:189:PHE:CD1	2.52	0.62
5:M:118:ASP:OD2	5:M:120:ARG:HB2	2.00	0.62
1:A:50:PRO:O	1:H:127:LYS:NZ	2.33	0.61
2:I:29:GLY:HA2	2:I:61:SER:HB2	1.81	0.61
5:F:24:HIS:HD2	5:F:74:ASN:ND2	1.98	0.61
1:H:196:ASP:OD1	1:H:197:HIS:ND1	2.31	0.61
4:L:82:LEU:HA	4:L:114:VAL:HG22	1.82	0.61
1:H:43:GLN:HE21	1:H:43:GLN:HA	1.66	0.61
4:L:63:HIS:HE1	6:L:248:HOH:O	1.83	0.61
5:F:131:GLU:OE2	5:F:244:ARG:NH2	2.34	0.61
4:E:140:LEU:HD12	4:E:183:TRP:CB	2.21	0.61
4:E:151:ASN:ND2	4:E:198:THR:CG2	2.64	0.61
2:B:83:ASN:ND2	6:B:115:HOH:O	2.31	0.60
4:L:127:GLN:C	4:L:128:LEU:HD23	2.23	0.59
1:A:263:HIS:CD2	1:A:265:GLY:H	2.20	0.59
1:H:227:ASP:OD2	1:H:248:VAL:O	2.20	0.59
5:F:25:GLN:NE2	5:F:27:ASN:H	1.99	0.59
5:M:244:ARG:NE	6:M:317:HOH:O	1.67	0.59
1:A:202:ARG:HD3	1:A:244:TRP:CD2	2.38	0.59
5:M:113:ARG:NE	6:M:304:HOH:O	2.36	0.58
4:E:151:ASN:CB	4:E:198:THR:HG23	2.34	0.58
2:I:83:ASN:HD22	2:I:84:HIS:H	1.51	0.58
4:L:0:MET:CE	4:L:0:MET:HA	2.24	0.57
2:I:83:ASN:ND2	6:I:117:HOH:O	2.35	0.57
4:L:0:MET:CA	4:L:0:MET:HE3	2.29	0.57
4:E:197:GLU:O	4:E:197:GLU:HG3	2.05	0.57
4:E:51:THR:HG23	4:E:51:THR:O	2.04	0.57
4:L:34:TRP:HD1	4:L:47:LEU:HD11	1.69	0.56
5:F:118:ASP:O	6:F:283:HOH:O	2.18	0.56
5:F:9:ARG:NH1	5:F:111:GLY:O	2.38	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:82:ARG:HE	1:H:89:GLU:HG2	1.69	0.56
1:H:202:ARG:HD3	1:H:244:TRP:CD2	2.40	0.56
4:E:151:ASN:ND2	4:E:198:THR:HG22	2.13	0.56
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.88	0.56
5:M:151:GLY:HA2	5:M:189:SER:OG	2.06	0.56
1:A:263:HIS:HD2	1:A:265:GLY:H	1.52	0.56
5:F:65:TYR:CD1	5:F:79:LEU:HD22	2.41	0.56
5:M:118:ASP:OD1	5:M:120:ARG:HG3	2.05	0.56
4:L:198:THR:OG1	4:L:198:THR:O	2.22	0.56
4:E:160:THR:HA	4:E:184:SER:HB2	1.87	0.55
4:E:50:PHE:O	4:E:51:THR:HG22	2.07	0.55
4:L:47:LEU:HD12	4:L:47:LEU:C	2.26	0.55
1:A:130:LEU:O	1:A:157:ARG:NH1	2.36	0.55
5:F:186:ASN:HB3	4:L:171:LYS:O	2.05	0.55
1:H:93:HIS:HD2	1:H:119:ASP:OD2	1.89	0.55
1:H:93:HIS:HE1	6:H:325:HOH:O	1.89	0.55
5:M:244:ARG:NE	6:M:306:HOH:O	2.39	0.54
4:L:77:LYS:NZ	4:L:81:GLN:HE21	2.06	0.54
1:A:126:LEU:HD22	1:A:156:LEU:HD13	1.90	0.54
4:L:168:LEU:HD21	5:M:171:GLY:O	2.07	0.54
4:L:135:SER:HB3	4:L:138:SER:HB3	1.89	0.54
5:F:174:THR:HB	5:F:194:SER:HB2	1.89	0.54
1:H:66:LYS:O	1:H:70:HIS:HD2	1.91	0.54
2:B:48:LYS:CE	2:B:48:LYS:CG	2.86	0.54
4:L:147:ASP:OD1	4:L:150:ILE:HG23	2.08	0.54
2:I:45:ARG:NH2	2:I:47:GLU:OE2	2.40	0.54
4:L:0:MET:CA	4:L:0:MET:CE	2.85	0.53
4:L:5:GLN:NE2	4:L:90:CYS:H	2.07	0.53
1:A:97:ARG:HH21	1:A:114:HIS:CE1	2.19	0.53
4:E:168:LEU:HD12	4:E:169:ASP:N	2.23	0.53
5:F:57:LYS:HB3	5:F:61:PRO:CG	2.38	0.53
4:L:128:LEU:HD12	5:M:146:VAL:HG13	1.90	0.53
4:L:0:MET:HE1	4:L:26:SER:N	2.24	0.52
4:E:77:LYS:HZ1	4:E:81:GLN:NE2	2.03	0.52
4:E:128:LEU:N	4:E:128:LEU:HD23	2.24	0.52
5:M:52:ALA:O	5:M:53:ASP:HB2	2.09	0.52
4:L:22:CYS:H	4:L:74:HIS:CD2	2.22	0.52
4:E:127:GLN:C	4:E:128:LEU:HD23	2.29	0.52
4:L:160:THR:HG23	4:L:184:SER:HB2	1.92	0.52
5:M:25:GLN:HE21	5:M:27:ASN:N	2.06	0.52
5:M:79:LEU:N	5:M:79:LEU:HD23	2.24	0.52
4:E:168:LEU:C	4:E:168:LEU:HD12	2.31	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:59:ASP:O	2:I:60:TRP:HB2	2.09	0.51
4:L:0:MET:HE3	4:L:1:ASP:N	2.13	0.51
2:B:48:LYS:HG3	2:B:68:THR:HG1	1.76	0.51
4:E:0:MET:HE2	4:E:0:MET:HA	1.93	0.51
1:A:42:SER:CB	1:H:138:MET:CE	2.87	0.51
5:M:24:HIS:CD2	5:M:74:ASN:ND2	2.69	0.51
4:E:63:HIS:HE1	6:E:244:HOH:O	1.94	0.51
5:F:57:LYS:HB3	5:F:61:PRO:HG3	1.92	0.50
5:F:186:ASN:HB2	4:L:173:MET:H	1.76	0.50
1:A:18:GLY:O	1:A:19:GLU:HG3	2.11	0.50
1:A:66:LYS:O	1:A:70:HIS:HD2	1.95	0.50
2:I:48:LYS:CB	2:I:48:LYS:CD	2.90	0.50
1:H:117:ALA:HB2	2:I:60:TRP:CE2	2.46	0.50
4:E:5:GLN:NE2	4:E:90:CYS:H	2.10	0.50
5:M:174:THR:HB	5:M:194:SER:CB	2.38	0.49
2:B:97:ARG:NH1	6:B:111:HOH:O	2.25	0.49
4:E:170:MET:SD	5:F:197:ARG:HG2	2.52	0.49
5:F:55:THR:HG21	5:F:67:ALA:HB3	1.95	0.49
1:A:182:THR:HG23	1:A:265:GLY:CA	2.42	0.49
2:I:69:GLU:HG3	6:I:121:HOH:O	2.12	0.49
1:A:82:ARG:NH1	1:A:82:ARG:HG2	2.27	0.48
5:M:25:GLN:NE2	5:M:27:ASN:H	2.09	0.48
4:E:151:ASN:HB2	4:E:198:THR:HG23	1.93	0.48
4:L:170:MET:HB2	4:L:175:SER:OG	2.13	0.48
1:A:114:HIS:CB	1:A:156:LEU:HD11	2.44	0.48
5:F:25:GLN:NE2	5:F:27:ASN:N	2.60	0.48
5:F:187:TYR:HE1	4:L:171:LYS:CG	2.27	0.48
4:L:12:LEU:O	4:L:114:VAL:HA	2.14	0.48
5:F:219:LEU:HD12	5:F:232:PRO:HD2	1.96	0.47
5:M:73:GLU:CD	5:M:73:GLU:H	2.18	0.47
4:L:171:LYS:HG2	5:M:170:SER:CB	2.44	0.47
5:M:174:THR:CG2	6:M:265:HOH:O	2.55	0.47
5:M:25:GLN:HE21	5:M:27:ASN:HB2	1.79	0.47
5:F:65:TYR:HD1	5:F:79:LEU:HD22	1.78	0.47
1:H:274:TRP:O	1:H:275:GLU:O	2.32	0.47
4:E:194:ILE:HG13	4:E:195:PHE:CD1	2.50	0.47
2:I:85:VAL:HG21	6:I:103:HOH:O	2.10	0.47
4:L:137:ASP:O	4:L:139:THR:HG23	2.14	0.47
5:F:60:ILE:N	5:F:61:PRO:HD3	2.30	0.47
1:A:156:LEU:HD22	1:A:160:LEU:HG	1.96	0.46
1:A:184:ALA:HB1	1:A:266:LEU:HD13	1.97	0.46
4:E:77:LYS:HZ3	4:E:81:GLN:HE21	1.55	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:11:SER:OG	1:H:95:VAL:HB	2.15	0.46
4:E:1:ASP:HB3	4:E:96:LEU:HD11	1.96	0.46
1:A:42:SER:CB	1:H:138:MET:HE2	2.46	0.46
1:A:133:TRP:HB2	1:A:144:LYS:HE3	1.98	0.46
2:B:48:LYS:CG	2:B:48:LYS:O	2.44	0.46
2:I:97:ARG:NH1	6:I:127:HOH:O	2.31	0.46
2:B:29:GLY:HA2	2:B:61:SER:OG	2.16	0.46
4:E:5:GLN:HE21	4:E:107:GLY:HA3	1.80	0.46
5:F:36:ARG:HB3	5:F:46:ILE:HD11	1.98	0.45
4:E:0:MET:CG	4:E:1:ASP:N	2.75	0.45
4:E:188:SER:O	4:E:189:PHE:CG	2.69	0.45
1:A:148:GLU:OE1	6:A:330:HOH:O	2.21	0.45
5:M:83:SER:H	5:M:86:GLN:NE2	2.11	0.45
1:H:121:LYS:HG3	1:H:122:ASP:N	2.29	0.45
5:M:244:ARG:CD	6:M:306:HOH:O	2.40	0.45
1:H:227:ASP:OD2	1:H:248:VAL:HB	2.17	0.45
4:E:77:LYS:NZ	4:E:81:GLN:NE2	2.55	0.45
2:I:69:GLU:CG	6:I:121:HOH:O	2.65	0.45
1:A:127:LYS:CE	1:A:134:THR:OG1	2.65	0.45
4:E:171:LYS:HG2	5:F:170:SER:OG	2.17	0.45
1:A:57:PRO:HG3	1:H:148:GLU:OE1	2.17	0.44
4:L:175:SER:HB2	6:L:211:HOH:O	2.16	0.44
5:M:186:ASN:HD22	5:M:186:ASN:HA	1.63	0.44
4:E:197:GLU:CG	4:E:197:GLU:O	2.65	0.44
4:L:34:TRP:CE2	4:L:75:LEU:HB2	2.53	0.44
4:E:32:LEU:C	4:E:33:PHE:CD1	2.91	0.44
5:M:244:ARG:HG3	6:M:306:HOH:O	1.84	0.44
1:A:82:ARG:HH11	1:A:82:ARG:HG2	1.83	0.44
4:E:34:TRP:CE2	4:E:75:LEU:HB2	2.52	0.44
5:F:187:TYR:CE1	4:L:171:LYS:CG	3.00	0.43
4:E:29:SER:HA	4:E:30:PRO:HD3	1.84	0.43
4:E:63:HIS:CE1	6:E:244:HOH:O	2.70	0.43
1:H:228:THR:HA	1:H:246:ALA:O	2.18	0.43
4:L:186:GLN:OE1	4:L:189:PHE:HD1	1.98	0.43
4:E:34:TRP:HD1	4:E:47:LEU:HD11	1.81	0.43
4:E:19:MET:HE2	4:E:21:ASN:OD1	2.19	0.43
1:A:182:THR:CG2	1:A:265:GLY:HA3	2.48	0.43
4:L:51:THR:CA	6:L:251:HOH:O	2.48	0.43
1:A:220:ASP:OD2	1:A:256:ARG:NH2	2.50	0.43
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.53	0.43
4:L:128:LEU:HD23	4:L:128:LEU:N	2.34	0.43
4:E:171:LYS:O	4:E:172:ALA:C	2.57	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:19:MET:CE	4:E:21:ASN:OD1	2.67	0.43
1:H:190:THR:OG1	1:H:202:ARG:HB3	2.18	0.42
1:A:157:ARG:CZ	1:A:157:ARG:HB2	2.49	0.42
1:H:162:GLY:O	1:H:166:GLU:HG3	2.18	0.42
5:F:59:ASP:C	5:F:61:PRO:HD2	2.40	0.42
5:M:92:CYS:SG	5:M:93:ALA:N	2.92	0.42
1:A:42:SER:HB2	1:H:138:MET:HE2	2.02	0.42
4:E:170:MET:SD	5:F:142:LYS:HE2	2.60	0.42
4:E:47:LEU:C	4:E:47:LEU:HD12	2.39	0.42
1:H:43:GLN:HE21	1:H:43:GLN:CA	2.26	0.42
4:L:171:LYS:CG	4:L:171:LYS:N	2.80	0.42
3:C:7:PRO:HA	5:F:97:TRP:CE3	2.53	0.42
2:I:22:PHE:CZ	2:I:69:GLU:HG2	2.55	0.42
1:A:222:GLU:CD	1:A:222:GLU:CB	2.88	0.42
4:L:21:ASN:HA	4:L:74:HIS:CD2	2.55	0.42
1:A:58:GLU:CB	1:A:58:GLU:CD	2.87	0.42
4:E:135:SER:HB2	4:E:138:SER:HB2	2.01	0.42
5:F:119:LEU:HD22	5:F:219:LEU:HD21	2.02	0.41
5:F:225:TRP:CD2	5:F:226:PRO:HD2	2.55	0.41
5:M:43:LEU:HD12	5:M:43:LEU:HA	1.98	0.41
5:F:19:VAL:HB	5:F:79:LEU:HG	2.02	0.41
5:F:174:THR:HG22	5:F:194:SER:OG	2.21	0.41
4:E:132:ASP:O	4:E:135:SER:O	2.38	0.41
1:A:131:ARG:HG2	1:A:157:ARG:NH2	2.36	0.41
1:H:87:GLN:HE22	1:H:118:TYR:HE2	1.67	0.41
5:F:176:PRO:HD2	6:F:275:HOH:O	2.20	0.41
5:F:60:ILE:N	5:F:61:PRO:HD2	2.35	0.41
1:H:210:PRO:O	1:H:263:HIS:HE1	2.03	0.41
5:F:158:GLU:CD	5:F:217:HIS:HE2	2.23	0.41
5:F:205:ASN:HA	5:F:206:PRO:HD3	1.92	0.41
5:F:24:HIS:CD2	5:F:74:ASN:HD21	2.26	0.41
1:H:216:THR:CG2	1:H:260:HIS:HB2	2.51	0.41
5:F:181:GLU:HG2	5:F:189:SER:O	2.21	0.41
5:F:79:LEU:N	5:F:79:LEU:HD23	2.36	0.40
4:E:123:PRO:HG3	6:E:205:HOH:O	2.20	0.40
1:A:187:THR:HA	1:A:204:TRP:O	2.20	0.40
5:M:57:LYS:HB2	5:M:57:LYS:HZ3	1.87	0.40
4:E:50:PHE:O	4:E:51:THR:CG2	2.69	0.40
1:H:133:TRP:HB2	1:H:144:LYS:HE3	2.04	0.40
1:H:231:VAL:HG13	1:H:244:TRP:CZ2	2.56	0.40
5:F:231:LYS:HA	5:F:232:PRO:HD3	1.81	0.40
5:M:39:THR:O	5:M:39:THR:HG22	2.22	0.40

All (5) 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	Distance(Å)	Clash(Å)
4:E:198:THR:OG1	1:H:108:ARG:NE[2_645]	1.92	0.28
4:E:198:THR:O	1:H:169:ARG:NH1[2_645]	2.03	0.17
1:H:226:GLN:NE2	2:I:75:LYS:NZ[2_546]	2.15	0.05
4:E:198:THR:O	1:H:169:ARG:NH2[2_645]	2.16	0.04
4:E:59:GLN:NE2	5:M:84:LEU:CB[1_545]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	273/275 (99%)	266 (97%)	6 (2%)	1 (0%)	43	36
1	H	273/275 (99%)	269 (98%)	4 (2%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	I	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	J	7/9 (78%)	7 (100%)	0	0	100	100
4	E	192/194 (99%)	170 (88%)	17 (9%)	5 (3%)	8	2
4	L	192/194 (99%)	172 (90%)	9 (5%)	11 (6%)	3	0
5	F	235/238 (99%)	223 (95%)	10 (4%)	2 (1%)	25	14
5	M	235/238 (99%)	225 (96%)	9 (4%)	1 (0%)	43	36
All	All	1610/1632 (99%)	1533 (95%)	57 (4%)	20 (1%)	19	9

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	39	LEU
4	E	52	ASP
4	E	56	PRO
5	F	154	PRO
4	L	51	THR

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Mol	Chain	Res	Type
4	L	52	ASP
4	L	53	ASN
4	L	55	ARG
4	L	56	PRO
4	L	59	GLN
4	L	57	GLU
4	L	187	THR
5	M	226	PRO
4	E	174	ASP
4	L	173	MET
1	A	226	GLN
4	E	191	CYS
4	L	54	LYS
4	L	197	GLU
5	F	226	PRO

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	231/231 (100%)	226 (98%)	5 (2%)	64	65
1	H	231/231 (100%)	227 (98%)	4 (2%)	73	75
2	B	95/95 (100%)	93 (98%)	2 (2%)	66	67
2	I	95/95 (100%)	92 (97%)	3 (3%)	51	47
3	C	7/7 (100%)	7 (100%)	0	100	100
3	J	7/7 (100%)	7 (100%)	0	100	100
4	E	177/177 (100%)	164 (93%)	13 (7%)	20	13
4	L	177/177 (100%)	161 (91%)	16 (9%)	14	8
5	F	204/206 (99%)	199 (98%)	5 (2%)	60	59
5	M	204/206 (99%)	197 (97%)	7 (3%)	49	45
All	All	1428/1432 (100%)	1373 (96%)	55 (4%)	43	38

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	43	GLN
1	A	156	LEU
1	A	182	THR
1	A	266	LEU
2	B	70	PHE
2	B	83	ASN
4	E	0	MET
4	E	52	ASP
4	E	57	GLU
4	E	134	ARG
4	E	137	ASP
4	E	138	SER
4	E	156	MET
4	E	168	LEU
4	E	171	LYS
4	E	173	MET
4	E	174	ASP
4	E	175	SER
4	E	185	ASN
5	F	79	LEU
5	F	174	THR
5	F	197	ARG
5	F	229	SER
5	F	244	ARG
1	H	75	ARG
1	H	82	ARG
1	H	201	LEU
1	H	266	LEU
2	I	70	PHE
2	I	83	ASN
2	I	88	SER
4	L	0	MET
4	L	19	MET
4	L	54	LYS
4	L	57	GLU
4	L	77	LYS
4	L	114	VAL
4	L	140	LEU
4	L	147	ASP
4	L	168	LEU
4	L	171	LYS
4	L	173	MET

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Mol	Chain	Res	Type
4	L	175	SER
4	L	177	SER
4	L	185	ASN
4	L	190	THR
4	L	198	THR
5	M	9	ARG
5	M	54	SER
5	M	79	LEU
5	M	146	VAL
5	M	174	THR
5	M	186	ASN
5	M	244	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	70	HIS
1	A	87	GLN
1	A	93	HIS
1	A	114	HIS
1	A	263	HIS
2	B	2	GLN
2	B	31	HIS
2	B	51	HIS
2	B	83	ASN
4	E	5	GLN
4	E	38	HIS
4	E	63	HIS
4	E	74	HIS
4	E	81	GLN
4	E	151	ASN
5	F	24	HIS
5	F	25	GLN
5	F	74	ASN
5	F	186	ASN
1	H	43	GLN
1	H	70	HIS
1	H	87	GLN
1	H	93	HIS
1	H	141	GLN
1	H	263	HIS

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Mol	Chain	Res	Type
2	I	2	GLN
2	I	83	ASN
2	I	89	GLN
4	L	5	GLN
4	L	38	HIS
4	L	63	HIS
4	L	74	HIS
4	L	81	GLN
5	M	24	HIS
5	M	25	GLN
5	M	74	ASN
5	M	86	GLN
5	M	186	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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 ⓘ

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	275/275 (100%)	0.96	37 (13%) 4 4	9, 15, 20, 24	8 (2%)
1	H	275/275 (100%)	6.68	251 (91%) 0 1	11, 15, 20, 26	11 (4%)
2	B	100/100 (100%)	0.76	6 (6%) 21 20	11, 15, 22, 25	6 (6%)
2	I	100/100 (100%)	1.03	17 (17%) 2 2	11, 15, 20, 25	3 (3%)
3	C	9/9 (100%)	1.86	5 (55%) 0 1	13, 13, 14, 15	0
3	J	9/9 (100%)	1.70	4 (44%) 1 1	13, 14, 15, 16	0
4	E	187/194 (96%)	1.80	59 (31%) 1 1	10, 15, 21, 29	19 (10%)
4	L	187/194 (96%)	4.21	131 (70%) 0 1	10, 15, 21, 31	22 (11%)
5	F	237/238 (99%)	1.79	86 (36%) 1 1	11, 15, 19, 23	11 (4%)
5	M	237/238 (99%)	1.05	42 (17%) 2 2	11, 15, 19, 24	13 (5%)
All	All	1616/1632 (99%)	2.54	638 (39%) 1 1	9, 15, 20, 31	93 (5%)

All (638) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	217	TRP	16.6
1	H	159	TYR	16.6
1	H	213	ILE	14.9
1	H	167	TRP	14.2
1	H	204	TRP	14.2
1	H	7	TYR	14.1
1	H	201	LEU	13.9
4	L	20	LEU	13.7
1	H	235	PRO	13.5
1	H	203	CYS	13.4
1	H	25	VAL	13.1
1	H	163	THR	13.1
1	H	236	ALA	12.9

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Mol	Chain	Res	Type	RSRZ
1	H	215	LEU	12.8
1	H	214	THR	12.7
1	H	171	TYR	12.7
1	H	231	VAL	12.6
1	H	99	TYR	12.5
4	L	10	VAL	12.5
1	H	220	ASP	12.4
1	H	200	THR	12.3
1	H	67	VAL	12.2
1	H	69	ALA	12.1
1	H	193	ALA	12.0
1	H	164	CYS	12.0
1	H	33	PHE	12.0
1	H	234	ARG	11.9
1	H	179	LEU	11.8
1	H	191	HIS	11.7
1	H	8	PHE	11.7
1	H	241	PHE	11.7
1	H	209	TYR	11.6
1	H	156	LEU	11.4
1	H	230	LEU	11.4
1	H	31	THR	11.4
1	H	194	VAL	11.3
1	H	27	TYR	11.3
1	H	192	HIS	11.2
1	H	199	ALA	11.2
1	H	147	TRP	11.1
4	L	74	HIS	11.1
1	H	245	ALA	11.0
1	H	168	LEU	11.0
1	H	196	ASP	10.9
1	H	187	THR	10.9
1	H	216	THR	10.9
4	L	19	MET	10.9
4	L	12	LEU	10.8
1	H	9	PHE	10.8
4	L	21	ASN	10.8
1	H	34	VAL	10.7
1	H	202	ARG	10.7
1	H	160	LEU	10.6
1	H	165	VAL	10.6
1	H	28	VAL	10.5

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Mol	Chain	Res	Type	RSRZ
4	L	18	VAL	10.5
1	H	205	ALA	10.5
1	H	59	TYR	10.5
1	H	5	MET	10.5
1	H	206	LEU	10.5
4	L	22	CYS	10.4
1	H	45	MET	10.3
1	H	221	GLY	10.2
1	H	172	LEU	10.2
1	H	239	GLY	10.2
1	H	65	ARG	10.2
1	H	158	ALA	10.2
1	H	107	TRP	10.2
1	H	30	ASP	10.1
1	H	189	MET	10.1
1	H	16	GLY	10.1
1	H	190	THR	10.0
4	L	52	ASP	10.0
1	H	188	HIS	10.0
4	L	75	LEU	10.0
1	H	155	GLN	9.9
1	H	244	TRP	9.8
1	H	24	ALA	9.7
4	L	72	SER	9.7
1	H	218	GLN	9.7
1	H	52	ILE	9.6
1	H	152	VAL	9.6
1	H	242	GLN	9.6
1	H	26	GLY	9.6
1	H	211	ALA	9.6
1	H	62	GLY	9.5
4	L	11	THR	9.5
4	L	66	LEU	9.5
1	H	195	SER	9.4
4	E	172	ALA	9.4
1	H	208	PHE	9.3
1	H	207	SER	9.2
1	H	124	ILE	9.1
1	H	182	THR	9.1
1	H	51	TRP	9.1
4	L	6	THR	9.1
1	H	233	THR	9.0

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Mol	Chain	Res	Type	RSRZ
1	H	123	TYR	8.9
1	H	197	HIS	8.9
1	H	169	ARG	8.8
4	E	187	THR	8.8
4	L	97	ALA	8.7
1	H	219	ARG	8.7
1	H	120	GLY	8.7
1	H	125	ALA	8.6
4	L	88	TYR	8.6
1	H	180	GLN	8.6
4	L	156	MET	8.5
1	H	232	GLU	8.4
1	H	198	GLU	8.4
1	H	23	ILE	8.4
4	L	67	HIS	8.3
1	H	210	PRO	8.3
4	L	33	PHE	8.3
4	L	73	PHE	8.3
1	H	162	GLY	8.3
1	H	22	PHE	8.3
1	H	73	THR	8.2
4	L	87	LEU	8.2
1	H	185	PRO	8.2
4	L	91	ALA	8.2
1	H	238	ASP	8.2
4	L	188	SER	8.2
1	H	243	LYS	8.1
4	L	96	LEU	8.1
4	L	86	ALA	8.0
1	H	64	THR	8.0
1	H	133	TRP	8.0
4	L	70	SER	8.0
1	H	237	GLY	8.0
1	H	212	GLU	7.9
1	H	66	LYS	7.9
4	L	93	PHE	7.8
4	L	90	CYS	7.8
1	H	97	ARG	7.8
1	H	178	THR	7.8
4	E	155	THR	7.8
1	H	117	ALA	7.8
4	L	9	LEU	7.8

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Mol	Chain	Res	Type	RSRZ
1	H	240	THR	7.8
1	A	225	THR	7.7
1	H	71	SER	7.7
4	E	156	MET	7.6
1	H	4	SER	7.6
4	L	23	THR	7.6
4	L	32	LEU	7.5
1	H	227	ASP	7.5
4	L	3	VAL	7.5
1	H	98	MET	7.4
4	L	34	TRP	7.4
1	H	60	TRP	7.4
1	H	114	HIS	7.4
1	H	68	LYS	7.4
4	L	187	THR	7.4
1	H	70	HIS	7.4
4	L	17	PRO	7.3
1	H	184	ALA	7.3
4	L	5	GLN	7.3
1	H	122	ASP	7.3
1	H	32	GLN	7.2
4	L	76	GLN	7.2
4	L	198	THR	7.2
4	E	198	THR	7.2
1	H	36	PHE	7.2
1	H	228	THR	7.2
4	E	189	PHE	7.2
1	H	57	PRO	7.2
1	H	63	GLU	7.1
1	H	10	THR	7.1
1	H	101	CYS	7.1
4	L	89	TYR	7.0
4	L	65	THR	7.0
1	H	1	GLY	7.0
1	H	121	LYS	7.0
4	L	92	LEU	7.0
4	L	13	THR	6.9
1	H	150	ALA	6.8
1	H	126	LEU	6.8
4	E	188	SER	6.8
4	E	174	ASP	6.8
1	H	76	VAL	6.8

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Mol	Chain	Res	Type	RSRZ
4	E	135	SER	6.7
4	L	69	SER	6.7
1	H	186	LYS	6.7
4	L	189	PHE	6.7
4	L	4	THR	6.6
4	L	82	LEU	6.6
1	H	174	ASN	6.6
1	H	229	GLU	6.6
5	M	228	GLY	6.6
4	E	173	MET	6.5
4	L	64	ALA	6.5
4	L	35	TYR	6.5
1	H	2	SER	6.5
1	H	151	HIS	6.4
4	E	190	THR	6.4
4	L	174	ASP	6.4
1	H	118	TYR	6.4
1	H	116	TYR	6.4
4	L	137	ASP	6.4
1	H	225	THR	6.4
1	H	226	GLN	6.3
4	L	24	TYR	6.3
1	H	35	ARG	6.3
1	H	72	GLN	6.2
1	H	157	ARG	6.2
1	H	100	GLY	6.2
4	E	0	MET	6.2
4	L	158	SER	6.2
1	H	183	ASP	6.1
4	L	85	SER	6.1
1	H	47	PRO	6.1
1	H	96	GLN	6.1
4	L	184	SER	6.1
1	H	166	GLU	6.1
1	H	3	HIS	6.0
1	H	11	SER	6.0
1	H	20	PRO	6.0
4	L	71	SER	6.0
4	L	190	THR	6.0
2	I	0	MET	6.0
4	L	173	MET	6.0
1	H	113	TYR	5.9

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Mol	Chain	Res	Type	RSRZ
1	H	61	ASP	5.9
1	H	95	VAL	5.9
4	L	186	GLN	5.9
4	L	155	THR	5.9
1	H	161	GLU	5.9
1	H	50	PRO	5.8
5	M	227	GLU	5.8
5	F	226	PRO	5.8
4	E	52	ASP	5.7
4	E	185	ASN	5.7
1	H	78	LEU	5.7
4	L	98	SER	5.7
4	E	40	ASN	5.6
1	H	153	ALA	5.6
4	L	68	LYS	5.6
4	E	51	THR	5.6
4	L	8	GLY	5.6
5	F	245	ALA	5.6
4	E	119	GLN	5.6
1	H	170	ARG	5.5
1	H	224	GLN	5.5
4	L	185	ASN	5.5
4	L	31	PHE	5.5
5	F	228	GLY	5.5
1	H	18	GLY	5.5
4	E	158	SER	5.4
4	L	47	LEU	5.4
1	H	38	SER	5.4
4	E	192	GLN	5.4
1	H	109	PHE	5.4
1	H	154	GLU	5.3
4	L	16	LEU	5.3
4	L	36	VAL	5.2
4	E	184	SER	5.2
4	E	136	GLN	5.1
1	H	6	ARG	5.1
1	H	130	LEU	5.1
4	L	136	GLN	5.1
5	M	206	PRO	5.1
1	H	103	VAL	5.1
4	L	192	GLN	5.0
4	E	191	CYS	5.0

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Mol	Chain	Res	Type	RSRZ
4	L	63	HIS	5.0
1	H	222	GLU	5.0
2	I	85	VAL	5.0
4	L	46	LEU	4.9
1	H	56	GLY	4.9
4	L	62	PHE	4.9
1	H	181	ARG	4.9
1	H	29	ASP	4.9
1	H	175	GLY	4.9
1	H	149	ALA	4.9
4	L	119	GLN	4.9
5	M	186	ASN	4.8
4	E	161	PHE	4.8
1	H	143	THR	4.8
1	H	223	ASP	4.8
1	H	136	ALA	4.8
1	H	173	GLU	4.8
4	L	30	PRO	4.7
4	E	157	GLU	4.7
4	L	7	GLU	4.7
2	I	1	ILE	4.7
1	H	115	GLN	4.7
4	L	135	SER	4.7
1	H	140	ALA	4.7
1	H	105	SER	4.6
4	E	120	ASN	4.6
2	B	1	ILE	4.6
4	E	186	GLN	4.6
1	H	134	THR	4.6
5	M	182	SER	4.5
1	H	110	LEU	4.5
1	H	21	ARG	4.5
5	F	201	THR	4.4
5	M	138	ALA	4.4
2	I	88	SER	4.4
4	E	134	ARG	4.4
1	H	138	MET	4.4
5	F	2	ALA	4.4
4	L	49	SER	4.4
4	L	191	CYS	4.4
1	H	135	ALA	4.4
5	F	202	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
4	E	137	ASP	4.3
1	H	176	LYS	4.3
4	L	77	LYS	4.3
5	F	198	VAL	4.3
1	H	74	HIS	4.3
1	H	17	ARG	4.2
4	L	80	ALA	4.2
1	H	119	ASP	4.2
1	A	227	ASP	4.2
4	L	45	LEU	4.2
5	F	138	ALA	4.1
5	F	114	LEU	4.1
2	B	88	SER	4.1
1	H	55	GLU	4.1
1	H	12	VAL	4.1
1	H	40	ALA	4.1
5	F	34	TRP	4.1
4	L	61	GLY	4.1
4	L	38	HIS	4.1
1	H	112	GLY	4.1
1	H	46	GLU	4.1
1	H	129	ASP	4.1
1	H	49	ALA	4.0
5	M	187	TYR	4.0
1	H	84	TYR	4.0
4	L	0	MET	4.0
1	H	275	GLU	4.0
1	H	145	HIS	4.0
4	L	2	SER	4.0
4	L	124	ALA	3.9
1	H	41	ALA	3.9
5	F	224	LYS	3.8
1	A	88	SER	3.8
4	L	39	LEU	3.8
5	M	226	PRO	3.8
1	H	141	GLN	3.8
4	L	37	GLN	3.8
5	F	21	LEU	3.8
5	M	120	ARG	3.8
1	H	58	GLU	3.8
1	H	132	SER	3.8
5	F	156	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
4	L	139	THR	3.8
4	L	134	ARG	3.8
4	E	153	PRO	3.8
5	F	1	GLU	3.8
4	E	175	SER	3.8
4	L	42	ALA	3.8
1	A	41	ALA	3.7
4	L	157	GLU	3.7
1	H	177	GLU	3.7
1	H	94	THR	3.7
4	L	43	PRO	3.7
1	H	48	ARG	3.7
4	L	171	LYS	3.7
5	F	182	SER	3.7
4	E	141	CYS	3.7
1	A	194	VAL	3.7
5	F	200	ALA	3.6
1	H	86	ASN	3.6
2	B	0	MET	3.6
4	L	50	PHE	3.6
5	F	225	TRP	3.6
5	M	118	ASP	3.6
4	E	183	TRP	3.6
1	A	196	ASP	3.6
4	E	39	LEU	3.6
5	M	229	SER	3.5
5	F	79	LEU	3.5
4	E	139	THR	3.5
4	L	125	VAL	3.5
5	F	239	ALA	3.5
4	E	138	SER	3.5
5	F	154	PRO	3.5
1	A	222	GLU	3.5
1	H	104	GLY	3.5
4	L	83	SER	3.5
1	H	144	LYS	3.5
1	H	53	GLU	3.4
4	L	51	THR	3.4
5	F	10	SER	3.4
1	H	137	ASP	3.4
4	L	79	SER	3.4
5	M	239	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
4	E	154	LYS	3.4
4	L	154	LYS	3.4
1	A	223	ASP	3.4
5	F	163	VAL	3.4
1	H	42	SER	3.4
4	L	29	SER	3.3
5	F	116(A)	LEU	3.3
4	E	171	LYS	3.3
5	F	12	VAL	3.3
5	F	122	VAL	3.3
1	H	44	ARG	3.3
5	F	113	ARG	3.3
1	H	268	LYS	3.3
1	A	86	ASN	3.3
5	F	90	TYR	3.3
5	F	187	TYR	3.3
4	L	26	SER	3.3
1	H	75	ARG	3.3
2	I	48	LYS	3.3
4	L	14	GLU	3.3
4	L	161	PHE	3.3
5	F	153	PHE	3.3
4	E	140	LEU	3.3
1	H	267	PRO	3.2
5	F	115	THR	3.2
4	L	120	ASN	3.2
4	L	172	ALA	3.2
1	H	39	ASP	3.2
4	E	169	ASP	3.2
4	L	170	MET	3.2
2	B	85	VAL	3.2
4	E	150	ILE	3.2
4	E	160	THR	3.2
1	H	108	ARG	3.2
5	M	245	ALA	3.2
4	E	159	GLY	3.1
1	A	82	ARG	3.1
5	M	141	GLN	3.1
1	H	13	SER	3.1
1	H	92	SER	3.1
2	I	20	SER	3.1
4	L	28	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
4	L	78	SER	3.1
1	A	226	GLN	3.1
1	H	82	ARG	3.1
5	F	46	ILE	3.1
5	F	145	LEU	3.1
4	L	40	ASN	3.1
5	M	139	ASN	3.1
4	E	147	ASP	3.1
5	F	118	ASP	3.1
5	F	206	PRO	3.1
5	F	116	VAL	3.1
1	H	37	ASP	3.0
1	A	197	HIS	3.0
5	F	204	HIS	3.0
1	H	81	LEU	3.0
1	H	111	ARG	3.0
4	L	151	ASN	3.0
5	F	161	TRP	3.0
1	H	77	ASP	3.0
4	E	7	GLU	3.0
4	L	159	GLY	3.0
1	A	183	ASP	3.0
1	A	229	GLU	3.0
1	H	15	PRO	3.0
1	H	102	ASP	3.0
4	E	117	ASN	3.0
1	A	138	MET	2.9
5	M	26	THR	2.9
1	H	128	GLU	2.9
5	F	152	PHE	2.9
5	F	237	ILE	2.9
4	E	193	ASP	2.9
1	A	128	GLU	2.9
1	A	228	THR	2.9
1	H	131	ARG	2.9
1	H	264	GLU	2.9
5	F	162	TRP	2.9
5	M	8	PRO	2.9
4	E	145	ASP	2.9
1	A	215	LEU	2.9
1	H	80	THR	2.9
5	M	27	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
4	E	126	TYR	2.8
5	F	189	SER	2.8
1	A	220	ASP	2.8
1	H	85	TYR	2.8
5	M	169	HIS	2.8
5	F	120	ARG	2.8
5	F	212	CYS	2.8
1	H	19	GLU	2.8
5	M	4	VAL	2.8
5	M	81	LEU	2.8
1	A	19	GLU	2.8
2	I	69	GLU	2.8
4	L	48	LYS	2.8
5	F	93	ALA	2.8
3	C	6	PHE	2.8
4	L	25	GLN	2.8
5	M	202	PHE	2.7
2	I	34	ASP	2.7
1	A	42	SER	2.7
1	H	14	ARG	2.7
5	M	200	ALA	2.7
4	E	149	GLN	2.7
1	A	230	LEU	2.7
5	F	77	LEU	2.7
5	F	229	SER	2.7
4	L	194	ILE	2.7
4	L	123	PRO	2.7
5	F	220	SER	2.7
4	L	84	ASP	2.7
5	M	221	GLU	2.7
5	M	244	ARG	2.7
4	E	170	MET	2.7
4	L	177	SER	2.7
1	H	83	GLY	2.7
1	H	266	LEU	2.7
5	F	119	LEU	2.7
1	H	146	LYS	2.7
5	F	19	VAL	2.7
4	L	15	GLY	2.6
4	L	41	GLU	2.6
5	M	137	ILE	2.6
5	M	162	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	44	GLU	2.6
4	E	125	VAL	2.6
4	L	153	PRO	2.6
5	F	236	ASN	2.6
4	L	126	TYR	2.6
5	F	190	TYR	2.6
1	H	79	GLY	2.6
5	F	157	VAL	2.6
1	H	43	GLN	2.6
5	F	11	LYS	2.6
4	L	133	PRO	2.6
4	L	193	ASP	2.6
2	I	75	LYS	2.6
1	H	148	GLU	2.5
2	I	89	GLN	2.5
3	J	5	PHE	2.5
4	L	160	THR	2.5
5	F	196	LEU	2.5
5	F	227	GLU	2.5
5	M	207	ARG	2.5
1	A	18	GLY	2.5
1	H	142	THR	2.5
4	E	124	ALA	2.5
1	H	54	GLN	2.5
3	C	2	LEU	2.5
5	F	243	GLY	2.5
4	E	122	GLU	2.5
1	A	111	ARG	2.5
5	F	117	GLU	2.5
5	F	89	VAL	2.4
1	H	127	LYS	2.4
5	F	221	GLU	2.4
1	A	216	THR	2.4
4	E	151	ASN	2.4
5	F	207	ARG	2.4
5	M	164	ASN	2.4
1	A	217	TRP	2.4
4	E	197	GLU	2.4
5	F	222	GLU	2.4
1	H	139	ALA	2.4
1	H	270	LEU	2.4
5	F	43	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
4	L	147	ASP	2.4
5	F	242	TRP	2.4
5	M	154	PRO	2.4
5	M	225	TRP	2.4
1	H	250	PRO	2.3
3	C	5	PHE	2.3
4	L	118	ILE	2.3
4	E	9	LEU	2.3
4	E	143	PHE	2.3
4	L	175	SER	2.3
5	M	117	GLU	2.3
5	F	35	TYR	2.3
5	F	88	ALA	2.3
4	E	162	ILE	2.3
5	F	112	THR	2.3
5	F	164	ASN	2.3
1	H	265	GLY	2.3
2	I	19	LYS	2.3
5	M	179	TYR	2.3
5	F	13	ALA	2.3
1	A	1	GLY	2.3
1	H	91	GLY	2.3
1	A	266	LEU	2.3
2	I	2	GLN	2.2
2	B	37	VAL	2.2
5	F	14	VAL	2.2
5	F	199	SER	2.2
5	F	244	ARG	2.2
5	M	135	ALA	2.2
1	A	92	SER	2.2
5	F	121	ASN	2.2
5	M	199	SER	2.2
2	I	15	ALA	2.2
1	A	177	GLU	2.2
5	F	87	THR	2.2
5	M	124	PRO	2.2
2	I	47	GLU	2.2
5	F	210	PHE	2.2
5	F	7	SER	2.2
3	C	3	TRP	2.2
5	F	135	ALA	2.2
1	H	106	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	17	ARG	2.2
5	F	150	ARG	2.2
3	J	2	LEU	2.2
1	A	136	ALA	2.2
5	F	233	VAL	2.2
5	F	179	TYR	2.1
5	F	92	CYS	2.1
2	I	71	THR	2.1
5	M	123	THR	2.1
4	L	27	THR	2.1
1	H	269	PRO	2.1
5	F	78	ILE	2.1
5	F	171	GLY	2.1
1	A	250	PRO	2.1
4	L	121	PRO	2.1
5	M	7	SER	2.1
1	A	24	ALA	2.1
5	M	201	THR	2.1
3	J	6	PHE	2.1
5	M	203	TRP	2.1
5	F	48	TYR	2.1
4	E	132	ASP	2.1
1	A	16	GLY	2.1
5	F	203	TRP	2.1
4	L	1	ASP	2.1
1	A	87	GLN	2.0
2	B	89	GLN	2.0
3	J	3	TRP	2.0
1	H	246	ALA	2.0
3	C	1	ALA	2.0
5	M	2	ALA	2.0
2	I	3	ARG	2.0
5	F	205	ASN	2.0
1	H	90	ALA	2.0
5	M	9	ARG	2.0
1	A	57	PRO	2.0
5	F	61	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.