



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 03:29 AM UTC

PDB ID : 1LP9 / pdb_00001lp9
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

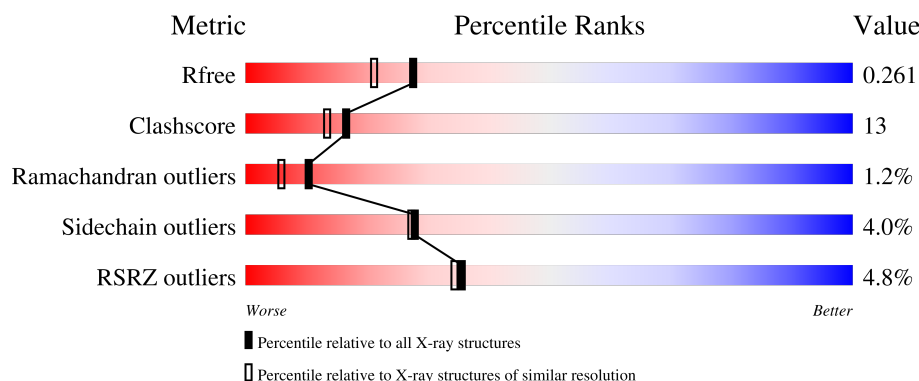
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	275	82% 13% • •
1	H	275	4% 81% 16% •
2	B	100	8% 87% 11% •
2	I	100	5% 84% 13% •
3	C	9	89% 11%

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Mol	Chain	Length	Quality of chain
3	J	9	100%
4	E	194	8% 61% 28% 9%
4	L	194	10% 68% 17% 10% 5%
5	F	238	4% 73% 22%
5	M	238	2% 79% 16%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13552 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 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 methionine	UNP P61769
I	0	MET	-	initiating methionine	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			

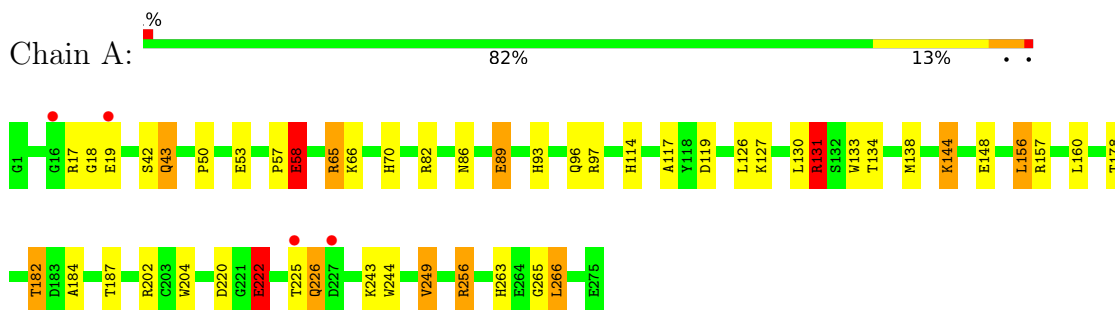
- Molecule 6 is water.

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, 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.

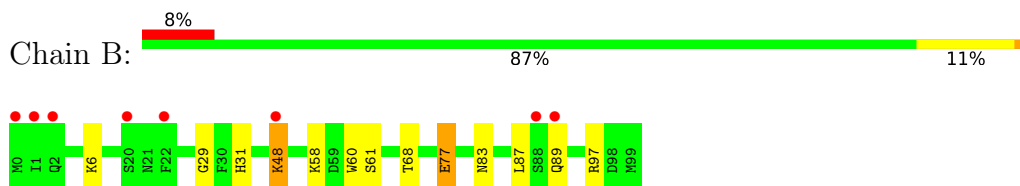
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



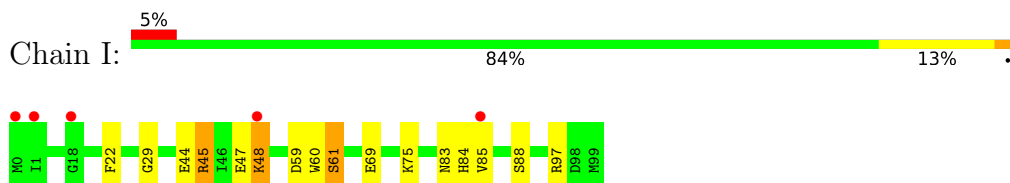
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

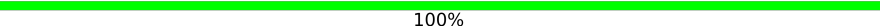


- Molecule 3: self-peptide P1049

Chain C:  89% 11%



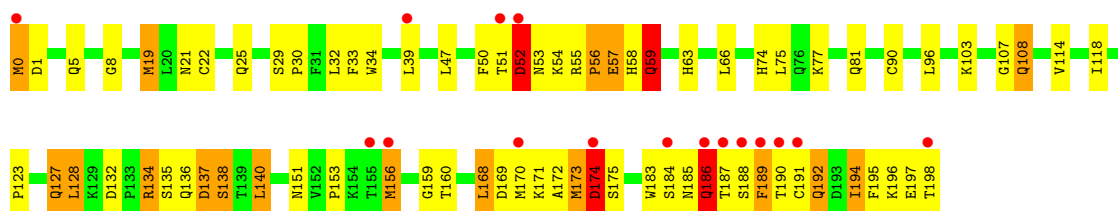
- Molecule 3: self-peptide P1049

Chain J:  100%

There are no outlier residues recorded for this chain.

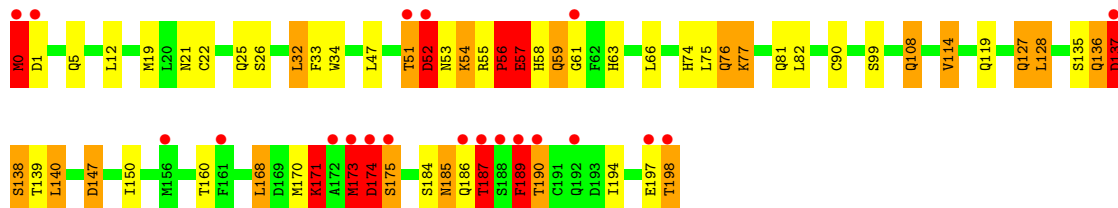
- Molecule 4: T-cell Receptor alpha chain

Chain E:  8% 61% 28% 9%



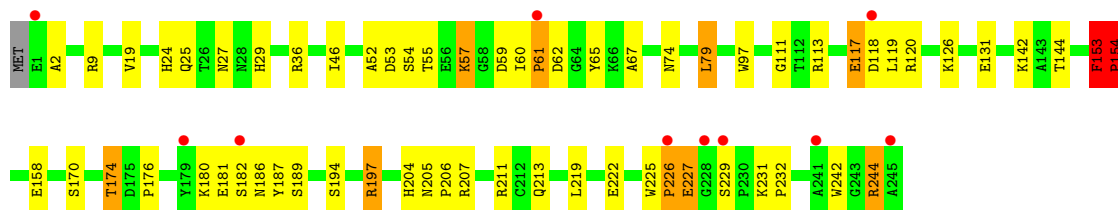
- Molecule 4: T-cell Receptor alpha chain

Chain L:  10% 68% 17% 10% 5%



- Molecule 5: T-cell Receptor beta chain

Chain F:  4% 73% 22%



- Molecule 5: T-cell Receptor beta chain

Chain M:  2% 79% 16%





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 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.00) 100.0 (30.00-2.00)	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 5.0	Depositor
R, R_{free}	0.219 , 0.253 0.230 , 0.261	Depositor DCC
R_{free} test set	6421 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.60	14/2312 (0.6%)	1.21	11/3137 (0.4%)
1	H	1.22	9/2312 (0.4%)	1.70	17/3137 (0.5%)
2	B	1.67	4/860 (0.5%)	1.26	7/1162 (0.6%)
2	I	2.38	6/860 (0.7%)	1.00	3/1162 (0.3%)
3	C	0.72	0/80	1.02	0/108
3	J	0.76	0/80	0.81	0/108
4	E	2.78	25/1557 (1.6%)	2.07	49/2112 (2.3%)
4	L	1.84	27/1557 (1.7%)	2.39	43/2112 (2.0%)
5	F	2.11	18/1943 (0.9%)	1.70	27/2644 (1.0%)
5	M	1.92	14/1943 (0.7%)	1.68	21/2644 (0.8%)
All	All	1.92	117/13504 (0.9%)	1.70	178/18326 (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 (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	113	ARG	NE-CZ	54.31	1.92	1.33
1	A	58	GLU	CG-CD	52.38	2.83	1.52
4	E	192	GLN	CD-OE1	50.90	2.20	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	192	GLN	C-O	43.43	1.75	1.24
2	I	44	GLU	CD-OE1	39.88	2.01	1.25
5	M	113	ARG	NE-CZ	38.45	1.75	1.33
5	M	117	GLU	CG-CD	35.88	2.41	1.52
2	B	58	LYS	CD-CE	35.75	2.59	1.52
2	I	44	GLU	CD-OE2	35.59	1.93	1.25
4	E	137	ASP	CG-OD1	34.33	1.90	1.25
4	E	108	GLN	CG-CD	31.49	2.30	1.52
5	F	126	LYS	CE-NZ	31.43	2.43	1.49
4	E	192	GLN	CB-CG	30.87	2.45	1.52
1	H	138	MET	CG-SD	-30.86	1.03	1.80
5	F	207	ARG	NE-CZ	29.48	1.65	1.33
5	F	222	GLU	CG-CD	29.35	2.25	1.52
5	M	120	ARG	CZ-NH1	28.49	1.72	1.32
5	M	117	GLU	CB-CG	28.11	2.36	1.52
1	A	65	ARG	CZ-NH1	27.77	1.71	1.32
2	I	48	LYS	CE-NZ	27.64	2.32	1.49
4	E	59	GLN	C-N	-27.61	0.94	1.33
4	L	171	LYS	CE-NZ	26.86	2.29	1.49
5	M	9	ARG	CZ-NH1	-26.17	0.96	1.32
4	E	137	ASP	CG-OD2	25.31	1.73	1.25
4	L	171	LYS	CB-CG	-22.97	0.83	1.52
4	L	136	GLN	CD-NE2	20.21	1.75	1.33
2	B	6	LYS	CE-NZ	19.70	2.08	1.49
1	A	131	ARG	CZ-NH1	19.31	1.59	1.32
1	H	144	LYS	CE-NZ	19.30	2.07	1.49
4	L	137	ASP	CB-CG	19.29	2.00	1.52
2	I	48	LYS	CD-CE	19.16	2.10	1.52
4	E	59	GLN	CA-CB	18.63	1.94	1.53
4	L	56	PRO	CA-CB	18.42	1.79	1.53
5	F	154	PRO	N-CD	-17.95	1.22	1.47
5	F	120	ARG	CG-CD	17.18	2.04	1.52
2	I	48	LYS	CG-CD	16.33	2.01	1.52
5	M	113	ARG	CZ-NH1	-16.14	1.10	1.32
4	L	174	ASP	CG-OD2	16.13	1.56	1.25
2	B	48	LYS	CD-CE	15.77	1.99	1.52
4	E	156	MET	CG-SD	15.68	2.19	1.80
5	F	126	LYS	CD-CE	15.26	1.98	1.52
1	H	121	LYS	CD-CE	14.77	1.96	1.52
5	F	117	GLU	CB-CG	14.62	1.96	1.52
5	F	227	GLU	CA-CB	14.48	1.77	1.53
4	E	56	PRO	CG-CD	-14.31	1.02	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	207	ARG	CZ-NH2	-14.18	1.15	1.33
4	L	76	GLN	CD-NE2	13.91	1.62	1.33
2	I	61	SER	CB-OG	13.86	1.69	1.42
4	L	189	PHE	CE2-CZ	13.82	1.80	1.38
5	M	113	ARG	CZ-NH2	13.55	1.51	1.33
1	H	227	ASP	CG-OD2	13.46	1.50	1.25
1	A	58	GLU	CD-OE1	13.31	1.50	1.25
5	M	222	GLU	CD-OE2	13.27	1.50	1.25
5	F	227	GLU	CD-OE2	-13.05	1.00	1.25
4	L	108	GLN	CD-NE2	12.80	1.60	1.33
1	H	17	ARG	NE-CZ	12.42	1.46	1.33
1	A	226	GLN	CB-CG	12.34	1.89	1.52
1	A	144	LYS	CE-NZ	12.28	1.86	1.49
5	F	57	LYS	CD-CE	12.05	1.88	1.52
4	E	58	HIS	CA-C	11.86	1.68	1.52
4	E	57	GLU	CA-C	11.71	1.68	1.52
5	F	227	GLU	CB-CG	11.66	1.87	1.52
4	E	19	MET	SD-CE	-11.61	1.50	1.79
5	F	2	ALA	C-O	11.39	1.37	1.23
4	E	192	GLN	CG-CD	11.25	1.80	1.52
4	E	58	HIS	N-CA	11.13	1.60	1.46
2	B	58	LYS	CG-CD	10.70	1.84	1.52
4	E	57	GLU	N-CA	10.67	1.59	1.46
4	L	57	GLU	CA-C	10.43	1.66	1.52
4	E	186	GLN	CD-OE1	-10.41	1.03	1.23
5	M	50	TYR	CE2-CZ	10.33	1.63	1.38
5	M	207	ARG	CZ-NH1	10.26	1.47	1.32
1	A	222	GLU	CG-CD	10.15	1.77	1.52
1	H	58	GLU	CD-OE2	-10.13	1.06	1.25
1	H	226	GLN	CA-CB	-9.91	1.37	1.53
4	L	56	PRO	C-O	9.88	1.36	1.24
4	L	136	GLN	CD-OE1	9.84	1.42	1.23
4	L	57	GLU	N-CA	9.24	1.58	1.46
4	L	137	ASP	CA-CB	9.21	1.67	1.53
5	F	207	ARG	CG-CD	9.19	1.80	1.52
1	H	89	GLU	CD-OE1	9.10	1.42	1.25
4	E	140	LEU	CG-CD2	8.67	1.81	1.52
5	F	222	GLU	CD-OE2	-8.66	1.08	1.25
4	L	185	ASN	CG-OD1	-8.36	1.07	1.23
4	L	119	GLN	CD-NE2	-8.34	1.15	1.33
1	A	256	ARG	CZ-NH1	-8.13	1.21	1.32
5	M	119	LEU	CG-CD2	-8.01	1.26	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	56	PRO	CA-C	7.89	1.63	1.52
5	F	222	GLU	CB-CG	-7.89	1.28	1.52
1	A	226	GLN	CA-CB	7.84	1.66	1.53
1	A	226	GLN	C-O	7.80	1.33	1.24
4	L	189	PHE	CG-CD2	7.79	1.55	1.38
4	L	0	MET	SD-CE	-7.59	1.60	1.79
4	L	32	LEU	CG-CD1	-7.55	1.27	1.52
4	L	57	GLU	C-N	7.50	1.44	1.33
5	M	227	GLU	CA-CB	7.38	1.65	1.53
1	A	89	GLU	CD-OE1	7.03	1.38	1.25
1	A	243	LYS	CE-NZ	6.64	1.69	1.49
5	M	237	ILE	CG1-CD1	-6.50	1.26	1.51
4	L	58	HIS	C-N	6.28	1.42	1.33
4	L	171	LYS	CG-CD	6.10	1.70	1.52
4	E	53	ASN	CA-C	-5.97	1.44	1.52
4	L	56	PRO	C-N	5.83	1.41	1.33
4	L	56	PRO	CA-C	-5.69	1.44	1.52
5	F	154	PRO	C-N	-5.67	1.27	1.33
4	L	66	LEU	CG-CD2	5.59	1.71	1.52
1	H	121	LYS	CG-CD	5.48	1.68	1.52
4	E	58	HIS	CB-CG	5.48	1.57	1.50
5	F	207	ARG	CZ-NH1	-5.46	1.25	1.32
1	A	225	THR	CB-OG1	-5.41	1.35	1.43
4	E	57	GLU	C-N	5.36	1.41	1.33
4	E	134	ARG	CZ-NH2	5.35	1.40	1.33
4	L	187	THR	CB-OG1	5.31	1.52	1.43
1	A	249	VAL	CB-CG1	-5.28	1.35	1.52
4	E	118	ILE	CG1-CD1	-5.26	1.31	1.51
4	L	61	GLY	C-N	-5.21	1.26	1.33
4	E	53	ASN	C-N	-5.05	1.26	1.33

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	76	GLN	OE1-CD-NE2	-60.58	62.02	122.60
1	H	17	ARG	NE-CZ-NH1	-52.00	69.50	121.50
4	L	136	GLN	OE1-CD-NE2	-38.48	84.12	122.60
1	H	17	ARG	CD-NE-CZ	-36.03	73.96	124.40
5	M	207	ARG	NE-CZ-NH1	-34.04	87.46	121.50
4	E	59	GLN	O-C-N	-30.40	75.79	122.61
5	M	207	ARG	NE-CZ-NH2	-30.32	91.91	119.20
1	H	17	ARG	NE-CZ-NH2	29.61	145.84	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	186	GLN	OE1-CD-NE2	-29.09	93.50	122.60
1	A	58	GLU	CG-CD-OE1	-28.67	52.45	118.40
4	L	137	ASP	CA-CB-CG	26.51	139.11	112.60
5	F	207	ARG	NE-CZ-NH1	-26.45	95.05	121.50
5	F	207	ARG	NH1-CZ-NH2	25.96	153.05	119.30
5	F	113	ARG	CD-NE-CZ	-25.90	88.14	124.40
5	M	120	ARG	NE-CZ-NH1	-23.23	98.27	121.50
5	M	9	ARG	NE-CZ-NH1	21.61	143.11	121.50
4	E	66	LEU	CD1-CG-CD2	-21.26	64.02	110.80
1	A	58	GLU	CB-CG-CD	-21.00	76.91	112.60
2	B	58	LYS	CD-CE-NZ	-20.89	45.04	111.90
4	L	119	GLN	OE1-CD-NE2	-20.21	102.39	122.60
5	F	113	ARG	NE-CZ-NH2	-19.11	102.00	119.20
5	F	222	GLU	OE1-CD-OE2	18.76	167.92	122.90
5	M	113	ARG	CD-NE-CZ	-18.59	98.38	124.40
4	E	58	HIS	CA-CB-CG	18.52	132.31	113.80
4	L	194	ILE	CG1-CB-CG2	-17.54	58.09	110.70
4	L	174	ASP	OD1-CG-OD2	-17.47	80.96	122.90
5	M	9	ARG	NH1-CZ-NH2	-17.18	96.97	119.30
5	M	120	ARG	NH1-CZ-NH2	17.02	141.43	119.30
4	E	192	GLN	OE1-CD-NE2	-16.96	105.64	122.60
4	E	192	GLN	O-C-N	-16.95	104.16	122.12
5	F	222	GLU	CA-CB-CG	16.93	147.96	114.10
4	E	56	PRO	N-CA-CB	-16.79	85.62	103.25
5	F	2	ALA	CA-C-O	16.71	139.18	120.96
4	L	171	LYS	CA-CB-CG	16.51	147.13	114.10
5	M	207	ARG	CG-CD-NE	16.47	148.24	112.00
1	H	121	LYS	CG-CD-CE	16.36	148.94	111.30
2	B	77	GLU	OE1-CD-OE2	-16.25	83.90	122.90
5	F	113	ARG	NE-CZ-NH1	16.19	137.69	121.50
4	E	59	GLN	N-CA-CB	16.15	135.94	111.23
4	L	56	PRO	N-CA-C	15.35	144.09	112.47
2	I	48	LYS	CG-CD-CE	-15.23	76.27	111.30
1	H	256	ARG	NE-CZ-NH2	15.03	132.73	119.20
5	F	222	GLU	CB-CG-CD	15.00	138.09	112.60
4	E	57	GLU	N-CA-C	14.74	142.19	110.80
4	E	192	GLN	CA-CB-CG	-14.59	84.93	114.10
4	L	119	GLN	CG-CD-NE2	14.57	138.26	116.40
5	F	153	PHE	C-N-CD	-14.11	67.16	125.00
1	H	121	LYS	CD-CE-NZ	13.71	155.77	111.90
5	F	2	ALA	O-C-N	-13.70	106.62	123.06
4	E	192	GLN	CG-CD-OE1	13.20	147.20	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	59	GLN	CB-CA-C	-12.57	93.37	111.85
5	F	227	GLU	OE1-CD-OE2	-12.16	93.71	122.90
1	H	58	GLU	OE1-CD-OE2	-12.12	93.82	122.90
4	E	59	GLN	CA-C-N	11.79	142.92	121.70
4	E	59	GLN	C-N-CA	11.79	142.92	121.70
4	E	58	HIS	N-CA-C	11.63	135.57	110.80
4	L	174	ASP	CB-CG-OD2	-11.50	91.94	118.40
1	H	58	GLU	CG-CD-OE2	11.43	144.69	118.40
4	L	66	LEU	CD1-CG-CD2	-11.35	85.84	110.80
5	M	113	ARG	NE-CZ-NH2	-11.19	109.13	119.20
5	F	227	GLU	N-CA-CB	-11.15	93.04	110.44
1	A	131	ARG	NE-CZ-NH1	-11.06	110.44	121.50
4	E	192	GLN	CA-C-O	11.00	132.21	120.55
5	M	117	GLU	CG-CD-OE2	-10.92	93.28	118.40
4	E	53	ASN	CA-C-N	-10.63	104.21	123.34
4	E	53	ASN	C-N-CA	-10.63	104.21	123.34
5	M	117	GLU	CA-CB-CG	-10.61	92.89	114.10
5	F	222	GLU	CG-CD-OE1	-10.42	94.42	118.40
4	L	137	ASP	CB-CG-OD1	-10.30	94.72	118.40
4	E	55	ARG	N-CA-C	10.10	125.92	108.75
4	E	140	LEU	CD1-CG-CD2	-9.92	88.97	110.80
5	F	222	GLU	CG-CD-OE2	-9.92	95.58	118.40
4	L	127	GLN	OE1-CD-NE2	-9.83	112.77	122.60
4	E	127	GLN	OE1-CD-NE2	-9.79	112.81	122.60
4	L	59	GLN	OE1-CD-NE2	-9.79	112.81	122.60
2	B	58	LYS	CB-CG-CD	-9.75	88.88	111.30
4	L	58	HIS	O-C-N	-9.70	109.68	122.59
5	F	126	LYS	CG-CD-CE	-9.64	89.13	111.30
1	H	256	ARG	NH1-CZ-NH2	-9.54	106.91	119.30
1	A	226	GLN	CA-CB-CG	9.38	132.86	114.10
4	L	56	PRO	CA-C-O	-9.36	103.57	120.60
4	L	137	ASP	N-CA-CB	-9.24	95.74	110.98
5	F	120	ARG	CB-CG-CD	-9.12	90.33	111.30
4	L	57	GLU	N-CA-C	9.05	130.07	110.80
4	L	187	THR	OG1-CB-CG2	-8.94	91.43	109.30
1	A	249	VAL	CA-CB-CG1	8.89	125.51	110.40
4	E	57	GLU	N-CA-CB	-8.87	95.51	110.49
5	M	106	GLN	OE1-CD-NE2	-8.86	113.74	122.60
4	L	190	THR	OG1-CB-CG2	8.81	126.92	109.30
4	L	171	LYS	N-CA-CB	-8.81	96.22	110.14
4	L	185	ASN	OD1-CG-ND2	8.79	131.38	122.60
4	L	108	GLN	OE1-CD-NE2	-8.52	114.08	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	GLN	CB-CG-CD	8.41	126.90	112.60
4	E	56	PRO	N-CA-C	8.33	129.63	112.47
1	A	222	GLU	CG-CD-OE2	-8.29	99.34	118.40
5	F	207	ARG	NE-CZ-NH2	-8.22	111.80	119.20
4	L	137	ASP	CB-CG-OD2	8.04	136.90	118.40
2	B	89	GLN	OE1-CD-NE2	-7.95	114.65	122.60
5	M	227	GLU	CB-CG-CD	7.87	125.98	112.60
4	E	192	GLN	CG-CD-NE2	-7.81	104.68	116.40
5	M	50	TYR	CG-CD1-CE1	7.78	132.88	121.20
1	H	226	GLN	CB-CG-CD	7.69	125.67	112.60
1	A	65	ARG	NH1-CZ-NH2	-7.68	109.32	119.30
4	E	56	PRO	N-CD-CG	7.60	114.61	103.20
4	L	56	PRO	CB-CA-C	-7.58	99.06	111.56
5	F	57	LYS	CD-CE-NZ	7.54	136.03	111.90
4	E	190	THR	N-CA-C	7.51	121.78	110.14
5	F	153	PHE	CA-C-N	7.44	129.13	119.84
5	F	153	PHE	C-N-CA	7.44	129.13	119.84
1	A	58	GLU	OE1-CD-OE2	-7.21	105.58	122.90
1	H	182	THR	OG1-CB-CG2	-7.13	95.04	109.30
4	L	52	ASP	CA-C-N	-7.06	108.06	121.54
4	L	52	ASP	C-N-CA	-7.06	108.06	121.54
4	E	134	ARG	NE-CZ-NH2	-7.03	112.87	119.20
4	L	194	ILE	CB-CG1-CD1	-7.00	99.11	113.80
1	H	89	GLU	CG-CD-OE1	-6.99	102.32	118.40
2	B	6	LYS	CD-CE-NZ	6.86	133.85	111.90
5	F	227	GLU	N-CA-C	-6.85	104.74	113.23
4	E	127	GLN	CG-CD-NE2	6.70	126.44	116.40
4	L	127	GLN	CG-CD-NE2	6.69	126.44	116.40
4	L	59	GLN	CG-CD-NE2	6.65	126.38	116.40
4	L	138	SER	CA-CB-OG	6.54	124.17	111.10
5	M	227	GLU	CA-CB-CG	6.52	127.14	114.10
5	M	207	ARG	CB-CG-CD	6.51	126.27	111.30
4	L	57	GLU	O-C-N	-6.49	113.96	122.59
1	H	138	MET	CB-CA-C	6.48	121.87	110.85
5	F	57	LYS	CG-CD-CE	6.43	126.10	111.30
4	E	55	ARG	CA-C-N	6.42	127.86	119.84
4	E	55	ARG	C-N-CA	6.42	127.86	119.84
4	L	61	GLY	N-CA-C	-6.38	104.51	115.61
4	L	174	ASP	N-CA-C	6.35	120.00	111.24
5	M	106	GLN	CG-CD-NE2	6.35	125.92	116.40
1	H	144	LYS	CD-CE-NZ	-6.34	91.61	111.90
1	H	249	VAL	CA-CB-CG1	6.34	121.17	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	55	ARG	CB-CA-C	-6.33	101.97	111.27
2	B	48	LYS	CD-CE-NZ	-6.26	91.88	111.90
4	L	189	PHE	CB-CG-CD2	-6.25	110.08	120.70
4	E	156	MET	CG-SD-CE	-6.24	87.17	100.90
4	E	108	GLN	CG-CD-OE1	-6.07	108.66	120.80
5	M	227	GLU	N-CA-C	6.06	118.73	110.55
4	E	56	PRO	CA-C-N	6.05	133.10	121.54
4	E	56	PRO	C-N-CA	6.05	133.10	121.54
5	F	126	LYS	CD-CE-NZ	6.04	131.24	111.90
1	H	89	GLU	OE1-CD-OE2	5.96	137.22	122.90
4	L	190	THR	CA-CB-CG2	5.89	120.52	110.50
4	E	194	ILE	N-CA-C	5.82	117.26	110.62
1	H	75	ARG	NE-CZ-NH1	5.81	127.31	121.50
4	L	171	LYS	CB-CG-CD	-5.78	98.01	111.30
4	E	59	GLN	N-CA-C	5.72	117.93	108.49
4	E	137	ASP	CA-C-O	5.68	126.29	119.59
5	F	227	GLU	CA-CB-CG	-5.68	102.75	114.10
4	L	108	GLN	CG-CD-NE2	-5.66	107.92	116.40
4	L	57	GLU	CA-C-O	-5.64	112.44	120.51
4	E	57	GLU	CA-CB-CG	5.60	125.30	114.10
1	A	89	GLU	OE1-CD-OE2	5.53	136.17	122.90
5	F	154	PRO	N-CD-CG	5.51	111.46	103.20
4	E	57	GLU	CB-CA-C	5.43	121.23	110.42
2	I	45	ARG	NH1-CZ-NH2	-5.41	112.27	119.30
2	B	89	GLN	CG-CD-NE2	5.37	124.45	116.40
5	M	113	ARG	NE-CZ-NH1	-5.36	116.14	121.50
4	E	134	ARG	NH1-CZ-NH2	5.35	126.26	119.30
4	L	32	LEU	CB-CG-CD1	5.35	126.75	110.70
5	M	50	TYR	CE1-CZ-CE2	-5.30	109.70	120.30
5	F	62	ASP	N-CA-C	5.22	118.36	110.64
4	E	52	ASP	CA-CB-CG	5.17	117.77	112.60
4	E	189	PHE	N-CA-C	-5.17	100.66	108.46
4	E	57	GLU	CA-C-N	5.16	131.39	121.54
4	E	57	GLU	C-N-CA	5.16	131.39	121.54
4	E	136	GLN	N-CA-C	5.15	116.71	111.14
1	A	249	VAL	CG1-CB-CG2	5.15	122.13	110.80
4	L	58	HIS	CA-CB-CG	-5.15	108.65	113.80
4	L	59	GLN	O-C-N	-5.12	115.78	122.59
2	I	45	ARG	NE-CZ-NH1	5.10	126.60	121.50
4	E	52	ASP	O-C-N	5.08	129.35	122.59
4	L	189	PHE	CD1-CG-CD2	5.08	126.22	118.60
4	E	54	LYS	CB-CA-C	5.07	123.34	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	140	LEU	CB-CG-CD2	-5.07	95.48	110.70
5	M	50	TYR	CB-CG-CD1	5.03	128.34	120.80

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 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	2247	0	2096	49	0
1	H	2247	0	2096	37	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	67	4
4	L	1521	0	1475	65	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	322	5

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 13.

All (322) 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)
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
1:A:43:GLN:HA	1:A:43:GLN:HE21	1.12	1.07
5:M:242:TRP:O	6:M:306:HOH:O	1.71	1.07
1:A:86:ASN:ND2	6:A:342:HOH:O	1.88	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:0:MET:HE3	4:L:0:MET:HA	1.41	1.03
4:L:0:MET:HE3	4:L:1:ASP:H	1.22	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
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:L:0:MET:CE	4:L:1:ASP:N	2.30	0.94
4:E:0:MET:HG3	4:E:1:ASP:H	1.33	0.94
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:CA	4:L:171:LYS:CD	2.48	0.90
4:L:0:MET:HE3	4:L:1:ASP:N	1.86	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:HE2	4:L:1:ASP:H	1.38	0.87
4:L:171:LYS:HD2	4:L:171:LYS:HA	1.57	0.87
5:F:244:ARG:HH11	5:F:244:ARG:CG	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
4:L:0:MET:HE3	4:L:0:MET:CA	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:77:LYS:HZ3	4:E:81:GLN:HE21	1.29	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:L:0:MET:HE1	4:L:25:GLN:C	2.07	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:42:SER:CB	1:H:138:MET:HE2	2.13	0.78
1:A:43:GLN:HE21	1:A:43:GLN:CA	1.92	0.78
1:A:97:ARG:HH21	1:A:114:HIS:HE1	1.32	0.78
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
4:L:0:MET:HE2	4:L:1:ASP:N	1.97	0.75
4:L:174:ASP:CG	4:L:174:ASP:O	2.28	0.75
5:M:174:THR:HG21	6:M:265:HOH:O	1.85	0.75
1:A:42:SER:HB2	1:H:138:MET:HE2	1.67	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:H:138:MET:SD	1:H:138:MET:CA	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
4:E:103:LYS:NZ	5:F:59:ASP:OD1	2.24	0.71
5:F:244:ARG:NH1	5:F:244:ARG:HG2	1.99	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: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:HA	1:H:43:GLN:NE2	2.07	0.68
4:L:186:GLN:O	4:L:187:THR:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:25:GLN:HE21	5:F:27:ASN:N	1.92	0.67
1:A:58:GLU:CD	1:A:58:GLU:HB3	2.20	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
2:I:69:GLU:CD	6:I:121:HOH:O	2.37	0.66
4:E:0:MET:HG3	4:E:1:ASP:N	2.10	0.66
1:H:138:MET:SD	1:H:138:MET:HA	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
4:L:127:GLN:C	4:L:128:LEU:HD23	2.23	0.64
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.80	0.64
6:A:284:HOH:O	1:H:144:LYS:HE3	1.97	0.63
5:F:60:ILE:N	5:F:61:PRO:CD	2.61	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
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:HA	1:H:43:GLN:HE21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ASN:ND2	6:B:115:HOH:O	2.31	0.60
4:L:47:LEU:HD12	4:L:47:LEU:C	2.26	0.60
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
2:I:83:ASN:ND2	6:I:117:HOH:O	2.35	0.57
4:E:0:MET:HE2	4:E:25:GLN:HB3	1.87	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:E:127:GLN:C	4:E:128:LEU:HD23	2.29	0.57
4:L:34:TRP:HD1	4:L:47:LEU:HD11	1.69	0.56
5:F:9:ARG:NH1	5:F:111:GLY:O	2.38	0.56
5:F:118:ASP:O	6:F:283:HOH:O	2.18	0.56
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
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.88	0.56
4:E:151:ASN:ND2	4:E:198:THR:HG22	2.13	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
4:E:168:LEU:HD12	4:E:168:LEU:C	2.31	0.56
5:F:65:TYR:CD1	5:F:79:LEU:HD22	2.41	0.56
4:L:198:THR:O	4:L:198:THR:OG1	2.22	0.56
5:M:118:ASP:OD1	5:M:120:ARG:HG3	2.05	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
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
4:L:77:LYS:NZ	4:L:81:GLN:HE21	2.06	0.54
5:M:244:ARG:NE	6:M:306:HOH:O	2.39	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
5:F:174:THR:HB	5:F:194:SER:HB2	1.89	0.54
4:L:135:SER:HB3	4:L:138:SER:HB3	1.89	0.54
1:H:66:LYS:O	1:H:70:HIS:HD2	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	4:L:0:MET:C	2.32	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:E:77:LYS:HZ1	4:E:81:GLN:HE21	1.56	0.53
4:E:128:LEU:HD23	4:E:128:LEU:N	2.24	0.52
5:M:52:ALA:O	5:M:53:ASP:HB2	2.09	0.52
5:M:73:GLU:CD	5:M:73:GLU:H	2.18	0.52
4:L:22:CYS:H	4:L:74:HIS:CD2	2.22	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
2:I:59:ASP:O	2:I:60:TRP:HB2	2.09	0.51
2:B:48:LYS:HG3	2:B:68:THR:HG1	1.76	0.51
4:L:0:MET:CE	4:L:0:MET:CA	2.85	0.51
4:E:63:HIS:HE1	6:E:244:HOH:O	1.94	0.51
5:M:24:HIS:CD2	5:M:74:ASN:ND2	2.69	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:CD	2:I:48:LYS:CB	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
4:E:19:MET:HE1	4:E:74:HIS:HB3	1.93	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:32:LEU:C	4:E:33:PHE:CD1	2.91	0.49
4:E:170:MET:SD	5:F:197:ARG:HG2	2.52	0.49
1:A:182:THR:HG23	1:A:265:GLY:CA	2.42	0.49
5:F:55:THR:HG21	5:F:67:ALA:HB3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:E:171:LYS:O	4:E:172:ALA:C	2.57	0.47
4:L:171:LYS:HG2	5:M:170:SER:CB	2.44	0.47
4:E:77:LYS:HZ3	4:E:81:GLN:NE2	2.04	0.47
5:F:59:ASP:C	5:F:61:PRO:HD2	2.40	0.47
5:F:65:TYR:HD1	5:F:79:LEU:HD22	1.78	0.47
5:M:25:GLN:HE21	5:M:27:ASN:HB2	1.79	0.47
5:M:174:THR:CG2	6:M:265:HOH:O	2.55	0.47
4:E:194:ILE:HG13	4:E:195:PHE:CD1	2.50	0.47
1:H:274:TRP:O	1:H:275:GLU:O	2.32	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
4:E:47:LEU:HD12	4:E:47:LEU:C	2.39	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
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:58:GLU:CD	1:A:58:GLU:CB	2.87	0.46
1:A:133:TRP:HB2	1:A:144:LYS:HE3	1.98	0.46
1:A:222:GLU:CD	1:A:222:GLU:CB	2.88	0.46
2:B:48:LYS:O	2:B:48:LYS:CG	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
1:A:148:GLU:OE1	6:A:330:HOH:O	2.21	0.45
4:E:0:MET:CG	4:E:1:ASP:N	2.75	0.45
4:E:77:LYS:NZ	4:E:81:GLN:NE2	2.55	0.45
4:E:188:SER:O	4:E:189:PHE:CG	2.69	0.45
1:H:121:LYS:HG3	1:H:122:ASP:N	2.29	0.45
5:M:83:SER:H	5:M:86:GLN:NE2	2.11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:E:186:GLN:O	4:E:187:THR:C	2.61	0.44
5:M:186:ASN:HD22	5:M:186:ASN:HA	1.63	0.44
4:E:197:GLU:O	4:E:197:GLU:CG	2.65	0.44
4:L:34:TRP:CE2	4:L:75:LEU:HB2	2.53	0.44
1:A:82:ARG:HG2	1:A:82:ARG:HH11	1.83	0.44
4:E:34:TRP:CE2	4:E:75:LEU:HB2	2.52	0.44
5:M:244:ARG:HG3	6:M:306:HOH:O	1.84	0.44
4:E:29:SER:HA	4:E:30:PRO:HD3	1.84	0.43
5:F:187:TYR:CE1	4:L:171:LYS:CG	3.00	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:E:34:TRP:HD1	4:E:47:LEU:HD11	1.81	0.43
4:E:159:GLY:O	4:E:184:SER:OG	2.32	0.43
4:L:186:GLN:OE1	4:L:189:PHE:HD1	1.98	0.43
1:A:182:THR:CG2	1:A:265:GLY:HA3	2.48	0.43
1:A:220:ASP:OD2	1:A:256:ARG:NH2	2.50	0.43
4:L:51:THR:CA	6:L:251:HOH:O	2.48	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:19:MET:CE	4:E:21:ASN:OD1	2.67	0.43
1:A:157:ARG:HB2	1:A:157:ARG:CZ	2.49	0.42
1:H:190:THR:OG1	1:H:202:ARG:HB3	2.18	0.42
5:F:153:PHE:C	5:F:154:PRO:O	2.61	0.42
1:H:162:GLY:O	1:H:166:GLU:HG3	2.18	0.42
4:L:0:MET:HE1	4:L:26:SER:N	2.32	0.42
5:M:92:CYS:SG	5:M:93:ALA:N	2.92	0.42
4:E:170:MET:SD	5:F:142:LYS:HE2	2.60	0.42
4:E:19:MET:HE1	4:E:74:HIS:CB	2.50	0.42
1:H:43:GLN:HE21	1:H:43:GLN:CA	2.26	0.42
1:A:130:LEU:C	1:A:157:ARG:HH12	2.25	0.42
3:C:7:PRO:HA	5:F:97:TRP:CE3	2.53	0.42
4:L:171:LYS:CG	4:L:171:LYS:N	2.80	0.42
2:I:22:PHE:CZ	2:I:69:GLU:HG2	2.55	0.42
4:E:135:SER:HB2	4:E:138:SER:HB2	2.01	0.42
4:L:21:ASN:HA	4:L:74:HIS:CD2	2.55	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
4:E:132:ASP:O	4:E:135:SER:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:L:140:LEU:C	4:L:140:LEU:HD23	2.45	0.41
5:M:144:THR:HG1	5:M:197:ARG:HD3	1.81	0.41
5:F:60:ILE:N	5:F:61:PRO:HD2	2.35	0.41
5:F:205:ASN:HA	5:F:206:PRO:HD3	1.92	0.41
1:H:210:PRO:O	1:H:263:HIS:HE1	2.03	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
4:E:173:MET:O	4:E:174:ASP:C	2.63	0.41
5:F:181:GLU:HG2	5:F:189:SER:O	2.21	0.41
4:L:32:LEU:C	4:L:33:PHE:CD1	2.99	0.41
1:A:42:SER:CB	1:H:138:MET:CE	2.87	0.40
4:E:123:PRO:HG3	6:E:205:HOH:O	2.20	0.40
5:F:79:LEU:N	5:F:79:LEU:HD23	2.36	0.40
1:A:187:THR:HA	1:A:204:TRP:O	2.20	0.40
4:E:50:PHE:O	4:E:51:THR:CG2	2.69	0.40
5:F:231:LYS:HA	5:F:232:PRO:HD3	1.81	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: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	Interatomic distance (Å)	Clash overlap (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%)	30	27
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%)	4	1
4	L	192/194 (99%)	172 (90%)	9 (5%)	11 (6%)	1	0
5	F	235/238 (99%)	223 (95%)	10 (4%)	2 (1%)	14	9
5	M	235/238 (99%)	225 (96%)	9 (4%)	1 (0%)	30	27
All	All	1610/1632 (99%)	1533 (95%)	57 (4%)	20 (1%)	10	6

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
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

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Mol	Chain	Res	Type
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%)	224 (97%)	7 (3%)	36	38
1	H	231/231 (100%)	228 (99%)	3 (1%)	61	68
2	B	95/95 (100%)	95 (100%)	0	100	100
2	I	95/95 (100%)	94 (99%)	1 (1%)	65	73
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%)	163 (92%)	14 (8%)	11	8
4	L	177/177 (100%)	160 (90%)	17 (10%)	8	5
5	F	204/206 (99%)	197 (97%)	7 (3%)	32	33
5	M	204/206 (99%)	196 (96%)	8 (4%)	28	28
All	All	1428/1432 (100%)	1371 (96%)	57 (4%)	28	27

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	43	GLN
1	A	156	LEU
1	A	178	THR
1	A	182	THR
1	A	249	VAL
1	A	266	LEU

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Mol	Chain	Res	Type
4	E	0	MET
4	E	52	ASP
4	E	57	GLU
4	E	114	VAL
4	E	128	LEU
4	E	134	ARG
4	E	137	ASP
4	E	138	SER
4	E	156	MET
4	E	168	LEU
4	E	173	MET
4	E	174	ASP
4	E	175	SER
4	E	185	ASN
5	F	61	PRO
5	F	79	LEU
5	F	158	GLU
5	F	174	THR
5	F	197	ARG
5	F	229	SER
5	F	244	ARG
1	H	75	ARG
1	H	201	LEU
1	H	266	LEU
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	128	LEU
4	L	140	LEU
4	L	147	ASP
4	L	168	LEU
4	L	171	LYS
4	L	173	MET
4	L	175	SER
4	L	185	ASN
4	L	187	THR
4	L	190	THR
4	L	198	THR

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Mol	Chain	Res	Type
5	M	9	ARG
5	M	54	SER
5	M	73	GLU
5	M	79	LEU
5	M	146	VAL
5	M	174	THR
5	M	186	ASN
5	M	244	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) 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	188	HIS
1	A	263	HIS
2	B	2	GLN
2	B	13	HIS
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	76	GLN
4	E	81	GLN
4	E	151	ASN
5	F	24	HIS
5	F	25	GLN
5	F	37	GLN
5	F	74	ASN
5	F	186	ASN
5	F	235	GLN
1	H	43	GLN
1	H	70	HIS
1	H	74	HIS
1	H	87	GLN
1	H	93	HIS

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Mol	Chain	Res	Type
1	H	141	GLN
1	H	263	HIS
2	I	2	GLN
2	I	83	ASN
4	L	5	GLN
4	L	21	ASN
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	37	GLN
5	M	74	ASN
5	M	86	GLN
5	M	186	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	59:GLN	C	61:GLY	N	0.94

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%)	0.03	4 (1%) 72 71	9, 15, 20, 24	8 (2%)
1	H	275/275 (100%)	0.18	10 (3%) 46 45	10, 15, 20, 25	11 (4%)
2	B	100/100 (100%)	0.78	8 (8%) 18 17	9, 15, 21, 25	6 (6%)
2	I	100/100 (100%)	0.34	5 (5%) 34 33	11, 15, 20, 25	3 (3%)
3	C	9/9 (100%)	-0.54	0 100 100	13, 13, 14, 15	0
3	J	9/9 (100%)	-0.31	0 100 100	13, 14, 15, 16	0
4	E	187/194 (96%)	0.49	16 (8%) 16 15	9, 14, 20, 29	19 (10%)
4	L	187/194 (96%)	0.52	20 (10%) 11 10	9, 14, 20, 31	22 (11%)
5	F	237/238 (99%)	0.24	10 (4%) 40 39	7, 15, 19, 22	11 (4%)
5	M	237/238 (99%)	0.04	5 (2%) 63 63	11, 15, 19, 24	13 (5%)
All	All	1616/1632 (99%)	0.26	78 (4%) 35 34	7, 15, 20, 31	93 (5%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	173	MET	6.5
2	B	0	MET	6.0
4	E	190	THR	5.9
4	L	198	THR	5.5
4	E	198	THR	5.4
4	L	52	ASP	5.2
4	E	52	ASP	5.1
1	H	16	GLY	5.0
2	I	0	MET	5.0
4	E	187	THR	4.9
4	L	187	THR	4.9
4	L	186	GLN	4.7
4	L	189	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	H	136	ALA	4.5
2	I	85	VAL	4.5
4	L	172	ALA	4.4
4	L	51	THR	4.3
5	M	227	GLU	4.2
4	L	190	THR	4.1
4	E	156	MET	4.1
4	L	61	GLY	4.0
4	L	188	SER	3.9
4	E	189	PHE	3.8
4	L	156	MET	3.6
1	H	226	GLN	3.6
4	E	188	SER	3.6
5	F	245	ALA	3.4
4	L	0	MET	3.4
4	L	192	GLN	3.4
2	B	1	ILE	3.3
4	E	51	THR	3.3
4	L	197	GLU	3.2
4	E	186	GLN	3.2
1	A	19	GLU	3.2
2	B	48	LYS	3.2
2	I	1	ILE	3.1
1	H	227	ASP	3.1
1	A	225	THR	3.0
5	M	228	GLY	2.9
4	L	137	ASP	2.9
4	E	155	THR	2.9
2	I	48	LYS	2.8
5	M	244	ARG	2.8
4	E	174	ASP	2.8
2	B	89	GLN	2.7
1	H	275	GLU	2.7
2	I	18	GLY	2.6
2	B	2	GLN	2.6
4	L	174	ASP	2.6
2	B	88	SER	2.6
1	H	19	GLU	2.5
5	F	228	GLY	2.4
4	E	0	MET	2.4
5	M	182	SER	2.4
4	L	1	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
5	F	182	SER	2.4
4	E	191	CYS	2.4
1	A	227	ASP	2.3
5	F	118	ASP	2.3
5	M	207	ARG	2.3
4	E	170	MET	2.3
1	H	17	ARG	2.3
1	H	145	HIS	2.2
4	L	175	SER	2.2
5	F	229	SER	2.2
2	B	20	SER	2.2
2	B	22	PHE	2.2
1	H	225	THR	2.2
4	E	184	SER	2.1
4	E	39	LEU	2.1
1	A	16	GLY	2.1
4	L	161	PHE	2.1
5	F	1	GLU	2.0
5	F	61	PRO	2.0
1	H	18	GLY	2.0
5	F	241	ALA	2.0
5	F	226	PRO	2.0
5	F	179	TYR	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.