



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:22 PM UTC

PDB ID : 2JCC / pdb_00002jcc
Title : AH3 recognition of mutant HLA-A2 W167A
Authors : Miller, P.; Benhar, Y.P.; Biddison, W.; Collins, E.J.
Deposited on : 2006-12-21
Resolution : 2.50 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

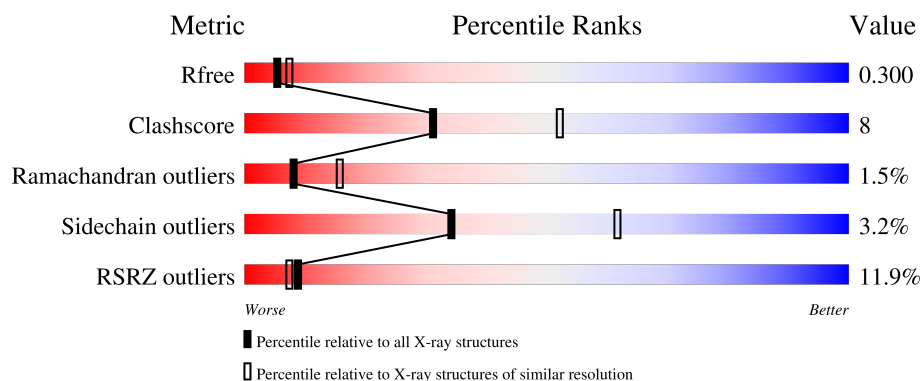
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	13% 83% 15% ..
1	H	275	8% 85% 14% .
2	B	100	6% 91% 9%
2	I	100	12% 89% 11%
3	C	9	11% 89% 11%

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Mol	Chain	Length	Quality of chain
3	J	9	33% 89% 11%
4	E	194	16% 66% 26% 6%
4	L	194	11% 71% 22%
5	F	238	17% 74% 18% 5%
5	M	238	7% 84% 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13180 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	4	0	0
			2238	1395	408	426	9			
1	H	275	Total	C	N	O	S	3	0	0
			2238	1395	408	426	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	ALA	TRP	engineered mutation	UNP P01892
H	167	ALA	TRP	engineered mutation	UNP P01892

- Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

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

- Molecule 3 is a protein called 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 TCR ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	194	Total	C	N	O	S	86	0	0
			1521	965	245	302	9			
4	L	194	Total	C	N	O	S	87	0	0
			1521	965	245	302	9			

- Molecule 5 is a protein called TCR BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	237	Total	C	N	O	S	0	0	0
			1891	1194	331	361	5			
5	M	237	Total	C	N	O	S	3	0	0
			1891	1194	331	361	5			

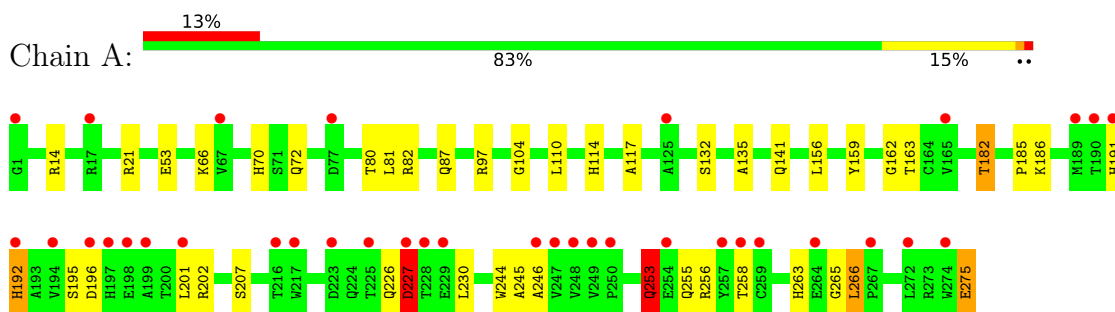
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	1	Total	O	0	0
			1	1		
6	E	10	Total	O	0	0
			10	10		
6	F	5	Total	O	0	0
			5	5		
6	H	9	Total	O	0	0
			9	9		
6	I	6	Total	O	0	0
			6	6		
6	L	9	Total	O	0	0
			9	9		
6	M	5	Total	O	0	0
			5	5		

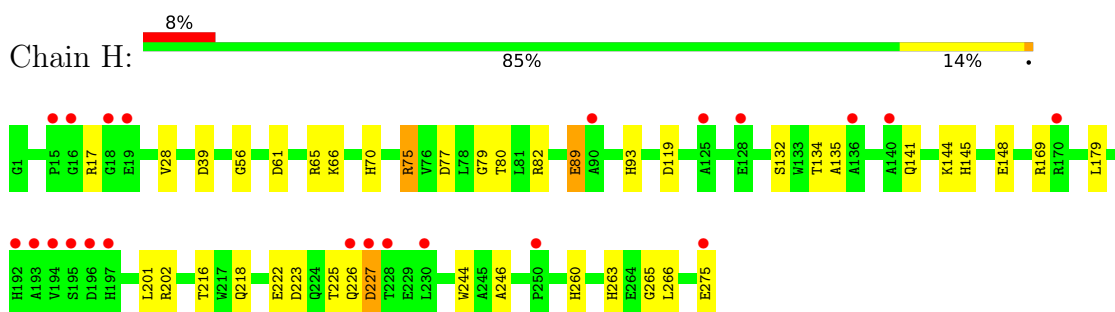
3 Residue-property plots [i](#)

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.

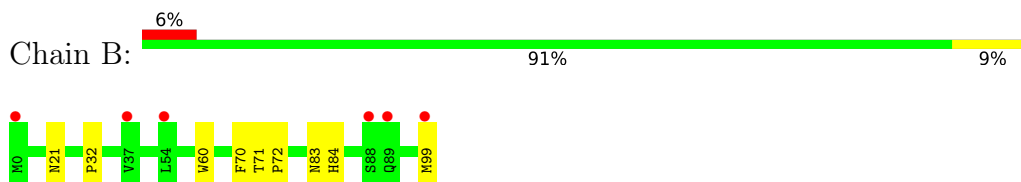
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN



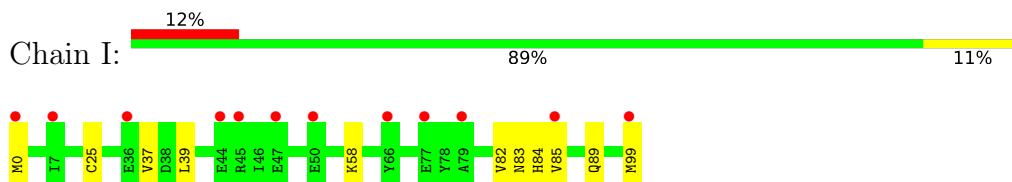
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN



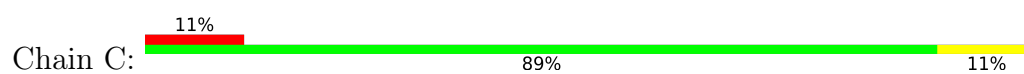
- Molecule 2: BETA-2-MICROGLOBULIN



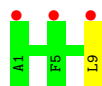
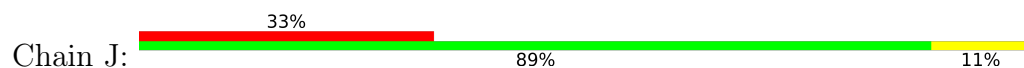
- Molecule 2: BETA-2-MICROGLOBULIN



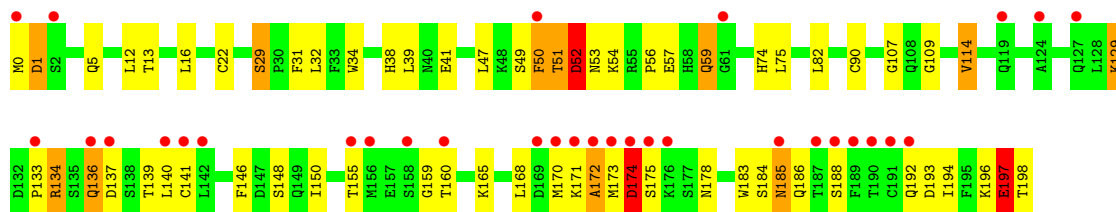
- Molecule 3: P1049



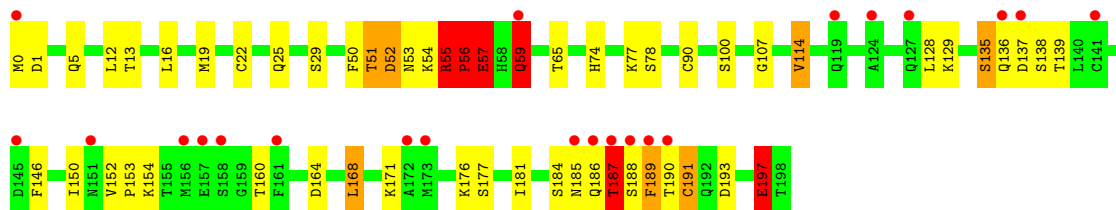
• Molecule 3: P1049



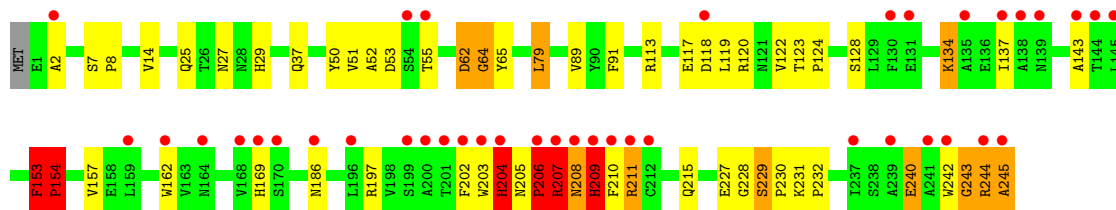
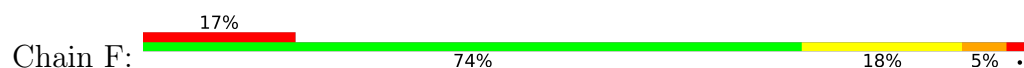
• Molecule 4: TCR ALPHA



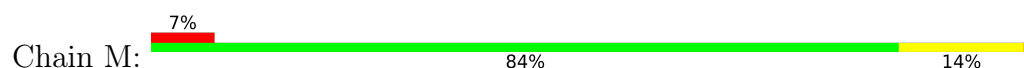
• Molecule 4: TCR ALPHA

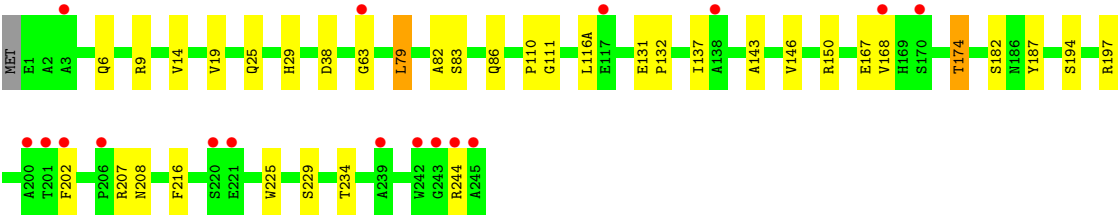


• Molecule 5: TCR BETA



• Molecule 5: TCR BETA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.28Å 84.35Å 122.47Å 90.00° 92.53° 90.00°	Depositor
Resolution (Å)	122.17 – 2.50 122.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.5 (122.17-2.50) 92.6 (122.17-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.292 0.270 , 0.300	Depositor DCC
R_{free} test set	3099 reflections (2.42%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 23.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13180	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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 42.51 % 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 2.0198e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.14	14/2301 (0.6%)	0.94	5/3121 (0.2%)
1	H	0.92	5/2301 (0.2%)	0.91	5/3121 (0.2%)
2	B	0.76	1/860 (0.1%)	0.88	1/1162 (0.1%)
2	I	0.88	4/860 (0.5%)	0.94	3/1162 (0.3%)
3	C	0.88	0/80	0.85	0/108
3	J	0.81	0/80	0.79	0/108
4	E	1.68	31/1555 (2.0%)	1.28	20/2106 (0.9%)
4	L	1.63	17/1557 (1.1%)	1.94	38/2112 (1.8%)
5	F	1.97	40/1947 (2.1%)	1.38	19/2649 (0.7%)
5	M	0.80	3/1947 (0.2%)	0.80	2/2649 (0.1%)
All	All	1.32	115/13488 (0.9%)	1.18	93/18298 (0.5%)

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	1
4	E	0	2
4	L	0	4
5	F	0	4
All	All	0	11

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	209	HIS	CE1-NE2	34.35	1.66	1.32
4	L	52	ASP	C-N	26.45	1.70	1.33
5	F	62	ASP	C-N	25.58	1.73	1.33
5	F	208	ASN	C-N	25.51	1.68	1.33
1	A	275	GLU	C-O	24.46	1.72	1.23
5	F	209	HIS	CG-ND1	22.48	1.62	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	56	PRO	N-CD	21.88	1.78	1.47
4	E	59	GLN	C-N	-20.22	1.06	1.33
4	L	59	GLN	C-N	20.14	1.62	1.33
5	F	64	GLY	N-CA	19.64	1.75	1.45
1	H	145	HIS	CE1-NE2	18.61	1.51	1.32
4	L	57	GLU	N-CA	18.30	1.69	1.46
5	F	204	HIS	CE1-NE2	18.25	1.50	1.32
4	E	197	GLU	C-O	17.69	1.46	1.24
1	A	253	GLN	CD-NE2	17.32	1.69	1.33
4	L	57	GLU	CA-C	16.82	1.75	1.52
5	F	242	TRP	C-O	16.53	1.45	1.23
4	L	56	PRO	CA-C	16.42	1.75	1.52
5	M	182	SER	C-N	15.94	1.55	1.33
4	L	59	GLN	C-O	15.39	1.43	1.24
4	E	188	SER	C-N	14.86	1.52	1.33
5	F	154	PRO	N-CD	14.81	1.68	1.47
4	L	56	PRO	C-N	14.42	1.53	1.33
5	F	207	ARG	NE-CZ	-13.59	1.18	1.33
4	L	56	PRO	N-CA	12.88	1.63	1.47
4	E	174	ASP	CG-OD1	12.86	1.49	1.25
5	F	210	PHE	C-N	12.54	1.49	1.33
1	A	275	GLU	C-OXT	12.46	1.48	1.23
4	E	186	GLN	CD-NE2	12.11	1.58	1.33
5	F	244	ARG	CZ-NH2	12.11	1.49	1.33
5	F	243	GLY	C-O	12.03	1.40	1.23
5	F	117	GLU	CD-OE1	11.86	1.47	1.25
1	H	145	HIS	CG-ND1	11.71	1.51	1.38
4	E	136	GLN	C-O	-11.48	1.09	1.24
5	F	242	TRP	C-N	11.10	1.49	1.33
1	H	145	HIS	CG-CD2	10.81	1.47	1.35
4	E	134	ARG	NE-CZ	10.26	1.44	1.33
4	E	188	SER	C-O	10.25	1.35	1.23
5	F	204	HIS	CG-ND1	10.15	1.49	1.38
5	F	209	HIS	CD2-NE2	-9.61	1.27	1.37
4	L	197	GLU	C-N	9.49	1.46	1.33
1	A	253	GLN	CD-OE1	9.48	1.41	1.23
4	E	52	ASP	N-CA	-9.37	1.34	1.46
4	E	136	GLN	C-N	8.80	1.46	1.33
4	E	51	THR	N-CA	-8.61	1.35	1.46
4	E	50	PHE	C-N	-8.50	1.21	1.33
4	E	186	GLN	CD-OE1	-8.44	1.07	1.23
5	F	204	HIS	CG-CD2	8.37	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	227	ASP	CG-OD2	8.27	1.41	1.25
1	A	196	ASP	CG-OD2	-8.22	1.09	1.25
4	E	51	THR	CA-C	-8.21	1.41	1.52
4	E	197	GLU	C-N	7.95	1.44	1.33
5	F	244	ARG	CZ-NH1	7.95	1.43	1.32
1	H	223	ASP	CB-CG	-7.85	1.32	1.52
4	L	136	GLN	CD-OE1	7.83	1.38	1.23
5	F	207	ARG	CZ-NH2	-7.79	1.23	1.33
4	L	136	GLN	CD-NE2	7.68	1.49	1.33
5	F	169	HIS	CE1-NE2	7.65	1.40	1.32
4	E	174	ASP	CG-OD2	-7.61	1.10	1.25
2	B	32	PRO	N-CD	7.60	1.58	1.47
1	A	192	HIS	CE1-NE2	7.54	1.40	1.32
1	A	195	SER	CB-OG	7.51	1.57	1.42
5	F	209	HIS	C-N	7.42	1.43	1.33
4	E	197	GLU	CD-OE2	7.37	1.39	1.25
4	E	193	ASP	CG-OD1	7.30	1.39	1.25
1	A	255	GLN	CD-OE1	7.21	1.37	1.23
2	I	58	LYS	CD-CE	7.11	1.73	1.52
4	E	53	ASN	N-CA	-7.02	1.37	1.46
2	I	89	GLN	CD-OE1	6.96	1.36	1.23
5	F	134	LYS	CE-NZ	6.96	1.70	1.49
5	F	240	GLU	CD-OE2	6.85	1.38	1.25
5	F	211	ARG	CZ-NH1	6.85	1.42	1.32
4	E	52	ASP	CA-C	-6.81	1.43	1.52
5	F	209	HIS	CG-CD2	6.75	1.43	1.35
5	F	245	ALA	C-OXT	6.61	1.36	1.23
4	E	52	ASP	C-N	-6.59	1.24	1.33
4	E	197	GLU	CD-OE1	6.53	1.37	1.25
1	A	227	ASP	CG-OD1	6.45	1.37	1.25
4	L	197	GLU	C-O	6.42	1.32	1.24
4	L	51	THR	C-N	6.42	1.42	1.33
4	E	137	ASP	CB-CG	6.40	1.68	1.52
5	F	206	PRO	C-N	6.34	1.43	1.33
2	I	89	GLN	CD-NE2	6.27	1.46	1.33
4	E	185	ASN	CG-OD1	6.26	1.35	1.23
5	F	240	GLU	CD-OE1	6.26	1.37	1.25
4	E	129	LYS	C-O	6.25	1.31	1.24
1	A	256	ARG	CZ-NH1	6.24	1.41	1.32
5	F	206	PRO	CA-C	6.22	1.61	1.52
5	M	187	TYR	C-N	6.20	1.41	1.33
4	L	187	THR	CB-OG1	-6.19	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	63	GLY	C-O	6.18	1.33	1.24
5	F	117	GLU	CD-OE2	-6.17	1.13	1.25
5	F	243	GLY	CA-C	-6.10	1.45	1.52
4	L	176	LYS	CD-CE	6.02	1.70	1.52
4	E	193	ASP	CB-CG	5.77	1.66	1.52
4	E	192	GLN	CD-OE1	5.74	1.34	1.23
5	F	206	PRO	C-O	-5.74	1.16	1.24
1	A	192	HIS	CG-ND1	5.73	1.44	1.38
4	L	186	GLN	C-O	5.63	1.30	1.24
5	F	204	HIS	C-N	5.57	1.42	1.33
5	F	245	ALA	CA-CB	5.50	1.70	1.52
1	H	275	GLU	C-O	5.45	1.34	1.23
1	A	191	HIS	CE1-NE2	5.44	1.38	1.32
5	F	211	ARG	CZ-NH2	-5.35	1.26	1.33
5	F	227	GLU	CD-OE1	5.30	1.35	1.25
5	F	207	ARG	CD-NE	-5.16	1.39	1.46
5	F	202	PHE	C-O	5.16	1.30	1.24
2	I	0	MET	SD-CE	5.16	1.92	1.79
5	F	204	HIS	ND1-CE1	-5.13	1.27	1.32
4	E	56	PRO	CB-CG	5.13	1.75	1.49
5	F	169	HIS	CG-ND1	5.10	1.43	1.38
4	E	193	ASP	C-O	5.05	1.30	1.24
4	E	188	SER	CA-CB	5.04	1.59	1.52
1	A	191	HIS	CG-ND1	5.04	1.43	1.38
4	L	186	GLN	C-N	5.01	1.40	1.33

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	153	PHE	CA-C-N	27.17	153.81	119.84
5	F	153	PHE	C-N-CA	27.17	153.81	119.84
4	L	59	GLN	CA-C-O	-24.53	85.44	120.51
4	L	52	ASP	CA-C-N	-21.72	80.05	121.54
4	L	52	ASP	C-N-CA	-21.72	80.05	121.54
4	L	197	GLU	O-C-N	-20.88	94.83	122.59
4	L	51	THR	O-C-N	20.44	149.78	122.59
4	L	59	GLN	O-C-N	-19.22	97.02	122.59
4	L	57	GLU	N-CA-C	17.07	147.16	110.80
4	L	57	GLU	CB-CA-C	-15.88	78.83	110.42
4	L	56	PRO	N-CA-C	15.31	144.00	112.47
4	L	57	GLU	CA-C-O	-14.30	100.06	120.51
4	E	59	GLN	CA-C-N	14.26	141.65	121.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	59	GLN	C-N-CA	14.26	141.65	121.96
4	L	55	ARG	CA-C-N	14.15	137.53	119.84
4	L	55	ARG	C-N-CA	14.15	137.53	119.84
4	L	51	THR	CA-C-N	13.36	147.05	121.54
4	L	51	THR	C-N-CA	13.36	147.05	121.54
5	F	62	ASP	CA-C-N	-13.06	101.44	122.20
5	F	62	ASP	C-N-CA	-13.06	101.44	122.20
2	I	99	MET	CA-C-O	12.51	158.52	121.00
1	H	275	GLU	CA-C-O	12.39	158.18	121.00
4	E	197	GLU	O-C-N	-11.09	107.84	122.59
4	L	56	PRO	CB-CA-C	-10.89	93.60	111.56
4	L	59	GLN	CB-CA-C	10.86	132.02	110.42
1	A	255	GLN	CG-CD-NE2	10.70	132.45	116.40
4	L	57	GLU	CA-C-N	-10.65	107.53	122.87
4	L	57	GLU	C-N-CA	-10.65	107.53	122.87
5	F	244	ARG	NE-CZ-NH1	10.51	132.00	121.50
5	F	210	PHE	CA-C-O	-10.49	109.18	121.46
1	A	253	GLN	OE1-CD-NE2	10.18	132.78	122.60
4	E	59	GLN	OE1-CD-NE2	-10.10	112.50	122.60
4	L	137	ASP	CA-CB-CG	10.09	122.69	112.60
4	L	59	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	A	255	GLN	OE1-CD-NE2	-9.79	112.81	122.60
4	L	52	ASP	O-C-N	-9.52	109.92	122.59
4	L	197	GLU	CA-C-N	9.44	138.69	121.70
4	L	197	GLU	C-N-CA	9.44	138.69	121.70
5	F	207	ARG	NE-CZ-NH2	-9.39	110.75	119.20
4	E	136	GLN	CA-C-O	9.08	130.51	119.79
4	E	134	ARG	NE-CZ-NH1	8.32	129.82	121.50
4	L	59	GLN	N-CA-C	-8.19	93.36	110.80
4	L	56	PRO	CA-C-N	-8.06	106.14	121.54
4	L	56	PRO	C-N-CA	-8.06	106.14	121.54
4	L	56	PRO	N-CA-CB	-7.80	95.06	103.25
4	E	174	ASP	OD1-CG-OD2	7.74	141.47	122.90
4	E	51	THR	O-C-N	7.56	132.65	122.59
4	E	134	ARG	NE-CZ-NH2	-7.46	112.48	119.20
5	F	244	ARG	NE-CZ-NH2	-7.29	112.64	119.20
1	H	145	HIS	ND1-CG-CD2	7.18	113.28	106.10
4	E	59	GLN	CG-CD-NE2	6.84	126.67	116.40
4	E	47	LEU	N-CA-C	6.76	119.34	109.07
5	F	206	PRO	O-C-N	-6.75	113.53	122.64
5	F	153	PHE	C-N-CD	-6.73	97.40	125.00
4	L	59	GLN	CG-CD-NE2	6.66	126.39	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	50	PHE	O-C-N	-6.65	113.44	122.36
5	F	245	ALA	CB-CA-C	-6.61	100.58	110.50
5	F	64	GLY	N-CA-C	-6.59	106.65	115.21
4	E	50	PHE	O-C-N	6.52	130.85	122.89
4	E	136	GLN	O-C-N	-6.43	113.71	122.33
4	E	174	ASP	CB-CG-OD1	-6.33	103.84	118.40
1	H	145	HIS	CG-CD2-NE2	-6.29	100.91	107.20
5	F	154	PRO	CA-N-CD	-6.27	103.22	112.00
4	E	51	THR	CA-C-O	6.26	129.46	120.51
4	L	52	ASP	N-CA-C	6.24	124.10	110.80
1	H	56	GLY	CA-C-N	6.24	125.80	119.19
1	H	56	GLY	C-N-CA	6.24	125.80	119.19
5	F	210	PHE	O-C-N	6.15	131.36	123.11
2	I	58	LYS	CG-CD-CE	-6.14	97.18	111.30
4	L	56	PRO	CA-C-O	-6.05	109.59	120.60
5	M	182	SER	CA-C-N	-5.97	111.05	120.60
5	M	182	SER	C-N-CA	-5.97	111.05	120.60
4	E	29	SER	CA-C-N	5.96	127.57	120.23
4	E	29	SER	C-N-CA	5.96	127.57	120.23
4	L	136	GLN	CG-CD-NE2	5.96	125.33	116.40
2	B	32	PRO	N-CD-CG	-5.84	96.79	103.80
4	L	50	PHE	CA-C-N	5.81	132.64	121.54
4	L	50	PHE	C-N-CA	5.81	132.64	121.54
2	I	89	GLN	OE1-CD-NE2	5.72	128.32	122.60
1	A	275	GLU	CA-C-O	-5.63	104.09	121.00
4	L	50	PHE	N-CA-C	5.57	117.10	110.19
4	L	57	GLU	N-CA-CB	-5.56	101.09	110.49
5	F	117	GLU	OE1-CD-OE2	5.51	136.12	122.90
5	F	243	GLY	CA-C-N	-5.51	112.97	123.32
5	F	243	GLY	C-N-CA	-5.51	112.97	123.32
4	E	53	ASN	CA-C-N	-5.44	113.78	121.83
4	E	53	ASN	C-N-CA	-5.44	113.78	121.83
4	L	56	PRO	O-C-N	-5.41	115.33	122.64
5	F	208	ASN	N-CA-C	5.36	117.88	108.56
5	F	207	ARG	NH1-CZ-NH2	5.29	126.18	119.30
4	E	56	PRO	N-CD-CG	-5.26	95.31	103.20
1	A	253	GLN	CG-CD-OE1	-5.09	110.62	120.80
4	L	193	ASP	N-CA-C	5.04	117.51	111.71

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	253	GLN	Sidechain
4	E	197	GLU	Sidechain,Mainchain
5	F	153	PHE	Peptide
5	F	204	HIS	Mainchain
5	F	206	PRO	Mainchain
5	F	209	HIS	Sidechain
4	L	197	GLU	Mainchain
4	L	55	ARG	Mainchain
4	L	56	PRO	Peptide
4	L	59	GLN	Mainchain

5.2 Too-close contacts [i](#)

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	2238	0	2091	36	0
1	H	2238	0	2091	25	1
2	B	837	0	803	8	0
2	I	837	0	803	6	0
3	C	76	0	76	2	0
3	J	76	0	76	2	0
4	E	1521	0	1472	32	1
4	L	1521	0	1476	36	0
5	F	1891	0	1793	59	0
5	M	1891	0	1794	21	0
6	A	9	0	0	0	0
6	B	1	0	0	0	0
6	E	10	0	0	0	0
6	F	5	0	0	0	0
6	H	9	0	0	0	0
6	I	6	0	0	0	0
6	L	9	0	0	1	0
6	M	5	0	0	0	0
All	All	13180	0	12475	205	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (205) 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:F:134:LYS:CE	5:F:134:LYS:NZ	1.70	1.51
1:A:253:GLN:CD	1:A:253:GLN:NE2	1.69	1.47
5:F:64:GLY:N	5:F:64:GLY:CA	1.75	1.47
5:F:208:ASN:C	5:F:209:HIS:N	1.68	1.46
5:F:154:PRO:CD	5:F:154:PRO:N	1.68	1.46
5:F:62:ASP:C	5:F:64:GLY:N	1.73	1.43
1:A:275:GLU:O	1:A:275:GLU:C	1.72	1.32
4:L:129:LYS:HD2	4:L:139:THR:HG22	1.30	1.11
4:L:184:SER:HB3	4:L:189:PHE:CE1	1.87	1.08
4:L:184:SER:HB3	4:L:189:PHE:HE1	1.04	1.08
5:F:153:PHE:C	5:F:154:PRO:CD	2.28	1.07
4:L:190:THR:HG22	4:L:191:CYS:H	1.18	1.04
4:L:129:LYS:CD	4:L:139:THR:HG22	1.91	0.99
4:E:31:PHE:CD2	4:E:50:PHE:HE1	1.81	0.98
2:I:83:ASN:HD22	2:I:84:HIS:H	0.98	0.97
1:A:72:GLN:HG3	5:F:51:VAL:HG11	1.52	0.89
2:I:83:ASN:HD22	2:I:84:HIS:N	1.70	0.88
2:B:83:ASN:HD22	2:B:84:HIS:H	1.20	0.86
1:A:97:ARG:HH21	1:A:114:HIS:HE1	1.24	0.85
4:L:184:SER:CB	4:L:189:PHE:HE1	1.88	0.85
1:H:66:LYS:O	1:H:70:HIS:HD2	1.60	0.83
4:E:134:ARG:NH2	5:F:128:SER:HA	1.93	0.83
4:L:22:CYS:H	4:L:74:HIS:HD2	1.26	0.83
1:H:263:HIS:CD2	1:H:265:GLY:H	1.96	0.82
2:B:83:ASN:HD22	2:B:84:HIS:N	1.78	0.81
1:H:263:HIS:HD2	1:H:265:GLY:H	1.28	0.80
4:E:5:GLN:HE21	4:E:107:GLY:HA3	1.48	0.79
4:L:190:THR:HG22	4:L:191:CYS:N	1.98	0.79
1:H:75:ARG:HH11	1:H:75:ARG:CG	1.96	0.78
4:E:38:HIS:HB2	4:E:41:GLU:OE1	1.83	0.78
1:A:66:LYS:O	1:A:70:HIS:HD2	1.66	0.77
1:A:14:ARG:HH11	1:A:21:ARG:HB2	1.50	0.76
4:E:31:PHE:CD2	4:E:50:PHE:CE1	2.72	0.76
4:E:196:LYS:O	4:E:197:GLU:HG2	1.85	0.75
1:A:263:HIS:CD2	1:A:265:GLY:H	2.05	0.73
5:F:208:ASN:CA	5:F:209:HIS:N	2.52	0.72
4:L:190:THR:CG2	4:L:191:CYS:H	2.01	0.71
4:L:129:LYS:CD	4:L:139:THR:CG2	2.67	0.71
1:A:97:ARG:HH21	1:A:114:HIS:CE1	2.09	0.69
4:L:160:THR:HG23	4:L:184:SER:HB2	1.75	0.68
5:F:208:ASN:C	5:F:209:HIS:CA	2.67	0.67
1:A:72:GLN:CG	5:F:51:VAL:HG11	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:75:ARG:HH11	1:H:75:ARG:HG2	1.60	0.66
5:F:62:ASP:C	5:F:64:GLY:CA	2.69	0.66
4:E:136:GLN:H	4:E:136:GLN:CD	2.04	0.66
5:F:162:TRP:HB2	5:F:211:ARG:CG	2.27	0.65
5:F:162:TRP:HB2	5:F:211:ARG:HG3	1.80	0.64
4:L:129:LYS:HD2	4:L:139:THR:CG2	2.17	0.64
1:A:263:HIS:HD2	1:A:265:GLY:H	1.46	0.64
5:F:162:TRP:CE3	5:F:211:ARG:NH2	2.66	0.64
5:F:186:ASN:CB	4:L:171:LYS:O	2.46	0.63
4:L:0:MET:HE2	6:L:2001:HOH:O	1.96	0.63
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.80	0.63
5:M:207:ARG:HD3	5:M:207:ARG:C	2.24	0.63
5:F:203:TRP:CZ3	5:F:243:GLY:HA2	2.34	0.62
4:L:185:ASN:HD21	5:M:150:ARG:HH22	1.45	0.62
5:M:83:SER:H	5:M:86:GLN:HE21	1.47	0.62
4:E:31:PHE:HD2	4:E:50:PHE:HE1	1.41	0.62
2:I:83:ASN:ND2	2:I:84:HIS:H	1.83	0.61
4:L:129:LYS:HD3	4:L:139:THR:HG22	1.81	0.61
5:F:143:ALA:O	5:F:197:ARG:HA	2.01	0.61
5:M:25:GLN:NE2	5:M:29:HIS:H	1.98	0.61
5:F:25:GLN:HE22	5:F:29:HIS:H	1.48	0.60
4:E:22:CYS:H	4:E:74:HIS:HD2	1.47	0.60
1:A:97:ARG:NH2	1:A:114:HIS:HE1	1.96	0.60
1:H:66:LYS:O	1:H:70:HIS:CD2	2.50	0.59
5:F:229:SER:HB2	5:F:230:PRO:CD	2.33	0.58
5:F:153:PHE:CD2	5:F:154:PRO:HD3	2.38	0.58
1:A:66:LYS:O	1:A:70:HIS:CD2	2.55	0.58
1:H:226:GLN:O	1:H:227:ASP:CB	2.52	0.58
4:L:5:GLN:HE21	4:L:107:GLY:HA3	1.70	0.57
5:F:186:ASN:HB2	4:L:171:LYS:O	2.05	0.56
1:A:104:GLY:HA2	1:A:110:LEU:HD11	1.88	0.56
4:E:82:LEU:HA	4:E:114:VAL:HG13	1.88	0.55
5:F:137:ILE:HD11	5:F:143:ALA:HB2	1.89	0.55
5:F:64:GLY:N	5:F:64:GLY:C	2.62	0.55
5:F:153:PHE:C	5:F:154:PRO:HD2	2.30	0.55
4:E:129:LYS:HG2	4:E:139:THR:HG22	1.88	0.55
5:F:118:ASP:OD2	5:F:120:ARG:NE	2.40	0.55
1:H:135:ALA:HB3	1:H:141:GLN:NE2	2.22	0.55
4:L:188:SER:O	4:L:189:PHE:HB2	2.07	0.55
1:H:226:GLN:O	1:H:227:ASP:HB2	2.08	0.54
4:L:129:LYS:HD3	4:L:139:THR:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:50:TYR:HD1	5:F:51:VAL:HG13	1.73	0.54
1:A:80:THR:HG21	3:C:9:LEU:O	2.07	0.54
5:F:37:GLN:OE1	5:F:91:PHE:HE1	1.90	0.54
5:M:25:GLN:HE22	5:M:29:HIS:H	1.56	0.53
4:E:159:GLY:O	4:E:184:SER:HA	2.08	0.53
4:L:135:SER:HB3	4:L:138:SER:HB3	1.91	0.53
5:M:216:PHE:O	5:M:234:THR:HA	2.09	0.53
4:E:31:PHE:HD2	4:E:50:PHE:CE1	2.19	0.52
1:A:253:GLN:NE2	1:A:253:GLN:CG	2.68	0.52
4:L:12:LEU:O	4:L:114:VAL:HA	2.10	0.52
5:F:52:ALA:O	5:F:53:ASP:HB2	2.09	0.52
1:A:135:ALA:HB3	1:A:141:GLN:HE21	1.75	0.52
4:E:13:THR:HB	4:E:16:LEU:HD12	1.91	0.52
1:H:93:HIS:HD2	1:H:119:ASP:OD2	1.92	0.52
4:E:32:LEU:O	4:E:49:SER:HB3	2.11	0.51
1:H:263:HIS:HD2	1:H:265:GLY:N	2.03	0.51
4:L:168:LEU:HB3	4:L:177:SER:HB2	1.92	0.51
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.46	0.51
5:F:25:GLN:HE21	5:F:27:ASN:H	1.58	0.51
5:F:153:PHE:O	5:F:154:PRO:CD	2.59	0.51
5:F:203:TRP:O	5:F:243:GLY:HA3	2.11	0.51
1:A:226:GLN:O	1:A:227:ASP:CB	2.58	0.50
4:L:184:SER:CB	4:L:189:PHE:CE1	2.74	0.50
1:A:14:ARG:NH1	1:A:21:ARG:HB2	2.23	0.50
4:E:172:ALA:O	4:E:173:MET:HG2	2.10	0.50
5:F:118:ASP:OD1	5:F:119:LEU:N	2.45	0.50
5:F:120:ARG:NH1	5:M:168:VAL:HG12	2.26	0.50
4:E:134:ARG:HH21	5:F:128:SER:HA	1.75	0.50
1:H:28:VAL:HG11	1:H:179:LEU:HD13	1.93	0.50
5:M:6:GLN:HG3	5:M:110:PRO:HD2	1.93	0.50
4:E:171:LYS:O	4:E:172:ALA:C	2.54	0.50
1:A:53:GLU:OE1	1:H:134:THR:HG23	2.12	0.50
1:A:202:ARG:HD3	1:A:244:TRP:CD2	2.46	0.50
1:H:77:ASP:HB3	3:J:9:LEU:HD12	1.94	0.50
1:A:275:GLU:O	1:A:275:GLU:CA	2.57	0.50
5:M:82:ALA:HA	5:M:86:GLN:NE2	2.27	0.49
5:F:186:ASN:HB3	4:L:171:LYS:O	2.11	0.49
2:B:83:ASN:ND2	2:B:84:HIS:N	2.55	0.49
4:L:13:THR:HB	4:L:16:LEU:HD12	1.94	0.49
2:I:83:ASN:ND2	2:I:84:HIS:N	2.52	0.49
1:H:144:LYS:O	1:H:148:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:THR:CG2	1:A:265:GLY:HA2	2.43	0.48
1:H:79:GLY:HA2	1:H:82:ARG:NH1	2.29	0.48
1:H:82:ARG:HD3	1:H:89:GLU:HB3	1.95	0.48
1:A:192:HIS:HE1	2:B:99:MET:OXT	1.96	0.48
1:H:75:ARG:HH11	1:H:75:ARG:HG3	1.77	0.48
5:M:143:ALA:O	5:M:197:ARG:HA	2.14	0.48
1:H:225:THR:HG22	1:H:225:THR:O	2.15	0.47
4:E:0:MET:O	4:E:1:ASP:HB2	2.14	0.47
4:E:170:MET:HB2	4:E:175:SER:HB2	1.97	0.47
5:F:25:GLN:NE2	5:F:29:HIS:H	2.12	0.47
5:F:122:VAL:HG12	5:F:232:PRO:HB2	1.97	0.47
5:M:19:VAL:HB	5:M:79:LEU:HG	1.97	0.47
4:L:146:PHE:CD2	4:L:150:ILE:HD11	2.50	0.47
5:F:204:HIS:HA	5:F:244:ARG:O	2.15	0.46
1:A:201:LEU:O	1:A:246:ALA:HA	2.14	0.46
4:E:134:ARG:HH22	5:F:128:SER:HA	1.78	0.46
4:L:154:LYS:NZ	4:L:164:ASP:OD1	2.48	0.46
1:A:72:GLN:HG3	5:F:51:VAL:CG1	2.36	0.46
4:E:141:CYS:HB2	4:E:194:ILE:HD11	1.98	0.46
4:L:129:LYS:NZ	4:L:139:THR:HG23	2.31	0.46
5:M:79:LEU:N	5:M:79:LEU:HD23	2.31	0.46
1:A:81:LEU:HD11	3:C:9:LEU:HD12	1.98	0.45
4:E:173:MET:O	4:E:174:ASP:C	2.60	0.45
1:A:186:LYS:HE2	1:A:207:SER:CB	2.45	0.45
1:H:216:THR:HG23	1:H:260:HIS:HB2	1.98	0.45
2:B:71:THR:HA	2:B:72:PRO:HD2	1.80	0.45
2:I:25:CYS:HB2	2:I:39:LEU:HD21	1.99	0.45
5:M:14:VAL:HA	5:M:116(A):LEU:O	2.17	0.45
1:A:230:LEU:HD12	1:A:245:ALA:HB2	1.98	0.45
4:E:160:THR:HG23	4:E:184:SER:HB2	1.99	0.45
5:F:79:LEU:HD23	5:F:79:LEU:N	2.32	0.45
5:F:209:HIS:NE2	5:F:240:GLU:OE1	2.45	0.45
5:M:174:THR:HB	5:M:194:SER:HB2	1.98	0.45
5:F:204:HIS:ND1	5:F:245:ALA:OXT	2.50	0.45
4:E:140:LEU:HD12	4:E:183:TRP:HB3	1.99	0.44
1:H:80:THR:HG21	3:J:9:LEU:O	2.18	0.44
4:L:187:THR:HG22	4:L:188:SER:N	2.31	0.44
2:I:37:VAL:HG22	2:I:82:VAL:HG22	1.99	0.44
5:F:157:VAL:HA	5:F:215:GLN:O	2.18	0.44
5:M:225:TRP:HE1	5:M:229:SER:HB3	1.82	0.44
5:F:123:THR:HA	5:F:124:PRO:HD3	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:HA	1:A:87:GLN:HE21	1.82	0.44
5:F:153:PHE:O	5:F:154:PRO:HD2	2.18	0.43
5:F:203:TRP:CE3	5:F:243:GLY:HA2	2.53	0.43
5:F:229:SER:HB2	5:F:230:PRO:HD2	1.98	0.43
4:E:148:SER:O	4:E:165:LYS:NZ	2.51	0.43
1:A:104:GLY:CA	1:A:110:LEU:HD11	2.48	0.43
5:M:202:PHE:O	5:M:208:ASN:ND2	2.42	0.43
4:L:1:ASP:HA	4:L:25:GLN:O	2.19	0.43
4:L:128:LEU:HD22	5:M:131:GLU:O	2.18	0.43
4:L:5:GLN:NE2	4:L:90:CYS:H	2.16	0.43
4:E:5:GLN:NE2	4:E:109:GLY:H	2.17	0.43
5:F:120:ARG:NH2	5:M:167:GLU:O	2.46	0.42
5:F:231:LYS:HA	5:F:232:PRO:HD3	1.88	0.42
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.54	0.42
1:A:117:ALA:HB2	2:B:60:TRP:CD2	2.54	0.42
4:E:34:TRP:CE2	4:E:75:LEU:HB2	2.54	0.42
5:F:7:SER:HA	5:F:8:PRO:C	2.45	0.42
5:F:50:TYR:CE1	5:F:51:VAL:HG22	2.54	0.42
5:F:134:LYS:NZ	5:F:134:LYS:CD	2.69	0.42
4:E:12:LEU:O	4:E:114:VAL:HA	2.20	0.42
5:F:64:GLY:N	5:F:65:TYR:N	2.67	0.42
4:E:146:PHE:CE2	4:E:178:ASN:HB3	2.54	0.42
5:F:205:ASN:HA	5:F:206:PRO:HD3	1.91	0.42
1:H:218:GLN:HG2	1:H:222:GLU:O	2.20	0.42
5:F:2:ALA:HA	5:F:27:ASN:CG	2.45	0.41
4:E:5:GLN:NE2	4:E:90:CYS:H	2.18	0.41
5:F:89:VAL:HG22	5:F:113:ARG:HG2	2.02	0.41
4:L:152:VAL:HA	4:L:153:PRO:HD3	1.94	0.41
1:H:61:ASP:HB3	1:H:65:ARG:NH2	2.36	0.41
4:L:22:CYS:H	4:L:74:HIS:CD2	2.18	0.41
1:H:202:ARG:HD3	1:H:244:TRP:CD2	2.56	0.41
5:M:132:PRO:HB2	5:M:137:ILE:HD11	2.03	0.41
1:A:186:LYS:HE2	1:A:207:SER:HB3	2.02	0.41
5:F:205:ASN:C	5:F:207:ARG:H	2.29	0.41
1:H:202:ARG:HG3	1:H:246:ALA:HB2	2.03	0.41
1:A:159:TYR:CD1	1:A:163:THR:HB	2.57	0.40
4:E:129:LYS:O	4:E:133:PRO:HD3	2.21	0.40
1:A:14:ARG:HH11	1:A:21:ARG:CB	2.26	0.40
4:L:177:SER:OG	5:M:197:ARG:NH2	2.53	0.40
5:M:9:ARG:NH1	5:M:111:GLY:O	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:198:THR:O	1:H:169:ARG:NH2[2_645]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	273/275 (99%)	268 (98%)	3 (1%)	2 (1%)	18	34
1	H	273/275 (99%)	262 (96%)	9 (3%)	2 (1%)	18	34
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	I	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	J	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	E	189/194 (97%)	165 (87%)	17 (9%)	7 (4%)	2	3
4	L	192/194 (99%)	164 (85%)	17 (9%)	11 (6%)	1	1
5	F	235/238 (99%)	219 (93%)	14 (6%)	2 (1%)	14	27
5	M	235/238 (99%)	227 (97%)	8 (3%)	0	100	100
All	All	1607/1632 (98%)	1509 (94%)	74 (5%)	24 (2%)	8	16

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	51	THR
4	E	52	ASP
4	E	174	ASP
5	F	154	PRO
4	L	51	THR
4	L	53	ASN
4	L	55	ARG
4	L	57	GLU

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Mol	Chain	Res	Type
4	L	59	GLN
1	A	227	ASP
4	E	59	GLN
1	H	227	ASP
4	L	56	PRO
4	E	1	ASP
4	E	172	ALA
4	E	197	GLU
1	H	17	ARG
4	L	52	ASP
4	L	54	LYS
4	L	187	THR
4	L	189	PHE
4	L	197	GLU
5	F	228	GLY
1	A	162	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/230 (100%)	225 (98%)	5 (2%)	45	73
1	H	230/230 (100%)	224 (97%)	6 (3%)	40	68
2	B	95/95 (100%)	95 (100%)	0	100	100
2	I	95/95 (100%)	94 (99%)	1 (1%)	65	84
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%)	167 (94%)	10 (6%)	19	39
4	L	177/177 (100%)	164 (93%)	13 (7%)	13	27
5	F	205/206 (100%)	199 (97%)	6 (3%)	37	65
5	M	205/206 (100%)	200 (98%)	5 (2%)	43	70
All	All	1428/1430 (100%)	1382 (97%)	46 (3%)	34	62

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	A	156	LEU
1	A	182	THR
1	A	258	THR
1	A	266	LEU
4	E	29	SER
4	E	39	LEU
4	E	52	ASP
4	E	54	LYS
4	E	57	GLU
4	E	114	VAL
4	E	150	ILE
4	E	155	THR
4	E	168	LEU
4	E	185	ASN
5	F	14	VAL
5	F	55	THR
5	F	79	LEU
5	F	154	PRO
5	F	207	ARG
5	F	229	SER
1	H	39	ASP
1	H	75	ARG
1	H	89	GLU
1	H	132	SER
1	H	201	LEU
1	H	266	LEU
2	I	85	VAL
4	L	19	MET
4	L	29	SER
4	L	57	GLU
4	L	65	THR
4	L	77	LYS
4	L	78	SER
4	L	100	SER
4	L	114	VAL
4	L	135	SER
4	L	168	LEU
4	L	181	ILE
4	L	191	CYS
4	L	197	GLU
5	M	38	ASP

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Mol	Chain	Res	Type
5	M	79	LEU
5	M	146	VAL
5	M	174	THR
5	M	244	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	87	GLN
1	A	96	GLN
1	A	114	HIS
1	A	141	GLN
1	A	145	HIS
1	A	180	GLN
1	A	192	HIS
1	A	263	HIS
2	B	2	GLN
2	B	83	ASN
4	E	5	GLN
4	E	40	ASN
4	E	74	HIS
4	E	81	GLN
5	F	24	HIS
5	F	25	GLN
5	F	28	ASN
5	F	74	ASN
5	F	139	ASN
5	F	186	ASN
5	F	213	GLN
1	H	70	HIS
1	H	86	ASN
1	H	93	HIS
1	H	141	GLN
1	H	263	HIS
2	I	13	HIS
2	I	83	ASN
4	L	5	GLN
4	L	38	HIS
4	L	40	ASN
4	L	63	HIS
4	L	74	HIS

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Mol	Chain	Res	Type
4	L	108	GLN
4	L	185	ASN
4	L	186	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	M	204	HIS
5	M	215	GLN

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	E	3

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Mol	Chain	Number of breaks
5	F	2
4	L	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	56:PRO	C	57:GLU	N	4.37
1	E	57:GLU	C	58:HIS	N	3.72
1	F	62:ASP	C	64:GLY	N	1.73
1	L	52:ASP	C	53:ASN	N	1.70
1	F	208:ASN	C	209:HIS	N	1.68
1	L	59:GLN	C	61:GLY	N	1.62
1	E	59:GLN	C	61:GLY	N	1.06

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%)	1.09	36 (13%) 7 6	26, 50, 58, 67	1 (0%)
1	H	275/275 (100%)	0.98	22 (8%) 18 16	38, 50, 59, 74	1 (0%)
2	B	100/100 (100%)	0.88	6 (6%) 27 24	42, 49, 59, 73	0
2	I	100/100 (100%)	0.97	12 (12%) 9 7	43, 51, 60, 76	0
3	C	9/9 (100%)	1.18	1 (11%) 10 8	44, 45, 51, 54	0
3	J	9/9 (100%)	1.57	3 (33%) 1 1	48, 50, 54, 57	0
4	E	184/194 (94%)	1.06	32 (17%) 4 3	37, 49, 66, 75	0
4	L	185/194 (95%)	1.07	22 (11%) 9 7	12, 49, 67, 73	2 (1%)
5	F	237/238 (99%)	1.06	40 (16%) 4 3	35, 50, 63, 69	0
5	M	237/238 (99%)	0.82	17 (7%) 21 19	31, 49, 58, 66	1 (0%)
All	All	1611/1632 (98%)	1.00	191 (11%) 9 7	12, 50, 62, 76	5 (0%)

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	172	ALA	6.2
1	H	16	GLY	5.8
4	E	173	MET	5.3
1	A	196	ASP	5.1
1	A	197	HIS	5.1
4	E	189	PHE	5.0
1	H	136	ALA	5.0
1	A	199	ALA	4.7
1	A	259	CYS	4.6
1	H	18	GLY	4.4
5	F	245	ALA	4.3
4	E	187	THR	4.2
5	F	200	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
4	E	190	THR	4.2
5	M	245	ALA	4.1
5	F	145	LEU	4.1
1	A	227	ASP	4.0
5	F	210	PHE	4.0
1	A	272	LEU	4.0
4	L	189	PHE	3.8
1	A	248	VAL	3.8
1	A	246	ALA	3.7
4	L	190	THR	3.7
5	F	170	SER	3.7
5	F	201	THR	3.7
4	E	175	SER	3.7
4	L	59	GLN	3.6
4	L	173	MET	3.6
2	I	99	MET	3.6
4	E	171	LYS	3.5
4	E	136	GLN	3.5
4	E	156	MET	3.5
4	L	156	MET	3.5
1	A	274	TRP	3.5
4	E	176	LYS	3.4
1	H	128	GLU	3.4
1	A	192	HIS	3.3
4	L	188	SER	3.3
1	H	90	ALA	3.3
4	L	0	MET	3.2
5	F	138	ALA	3.2
5	F	211	ARG	3.2
1	H	275	GLU	3.2
5	M	243	GLY	3.2
5	F	241	ALA	3.2
1	A	250	PRO	3.2
5	F	2	ALA	3.1
1	H	197	HIS	3.1
1	A	228	THR	3.1
5	M	201	THR	3.1
5	M	239	ALA	3.1
5	M	242	TRP	3.1
4	L	124	ALA	3.1
5	F	244	ARG	3.1
4	E	191	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
5	F	207	ARG	3.1
1	A	247	VAL	3.1
5	F	196	LEU	3.0
1	A	229	GLU	3.0
1	H	230	LEU	3.0
5	F	212	CYS	3.0
4	L	187	THR	2.9
5	F	162	TRP	2.9
5	F	169	HIS	2.9
5	M	244	ARG	2.9
4	E	137	ASP	2.9
1	A	225	THR	2.9
1	H	193	ALA	2.9
4	E	192	GLN	2.9
4	E	158	SER	2.9
4	L	185	ASN	2.9
1	H	19	GLU	2.9
4	L	119	GLN	2.8
5	M	138	ALA	2.8
2	B	89	GLN	2.8
5	F	131	GLU	2.8
5	F	203	TRP	2.7
3	J	9	LEU	2.7
5	F	55	THR	2.7
5	F	143	ALA	2.7
1	A	216	THR	2.7
5	F	135	ALA	2.7
1	A	194	VAL	2.7
4	E	188	SER	2.7
1	A	189	MET	2.7
1	A	17	ARG	2.7
1	H	140	ALA	2.7
4	L	137	ASP	2.7
3	C	1	ALA	2.7
4	E	124	ALA	2.7
4	L	172	ALA	2.7
4	L	127	GLN	2.7
5	F	209	HIS	2.7
1	H	226	GLN	2.6
2	I	45	ARG	2.6
5	F	242	TRP	2.6
1	A	267	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	196	ASP	2.6
1	A	217	TRP	2.5
5	F	137	ILE	2.5
1	A	201	LEU	2.5
5	M	3	ALA	2.5
1	A	198	GLU	2.5
4	E	141	CYS	2.5
4	E	0	MET	2.5
5	F	186	ASN	2.5
1	H	170	ARG	2.5
2	I	7	ILE	2.5
3	J	1	ALA	2.5
4	L	141	CYS	2.4
4	E	169	ASP	2.4
5	F	202	PHE	2.4
2	B	99	MET	2.4
5	F	199	SER	2.4
5	F	118	ASP	2.4
5	M	168	VAL	2.4
1	A	258	THR	2.4
4	E	119	GLN	2.4
4	E	142	LEU	2.4
2	I	0	MET	2.4
4	E	185	ASN	2.4
1	A	254	GLU	2.4
5	F	206	PRO	2.4
1	A	77	ASP	2.3
4	L	157	GLU	2.3
4	L	136	GLN	2.3
5	F	168	VAL	2.3
1	A	190	THR	2.3
5	F	54	SER	2.3
1	A	191	HIS	2.3
5	F	237	ILE	2.3
4	E	174	ASP	2.3
4	E	155	THR	2.3
1	A	1	GLY	2.3
4	L	186	GLN	2.3
5	M	170	SER	2.3
2	B	0	MET	2.3
4	E	170	MET	2.3
2	I	47	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
5	M	202	PHE	2.3
1	H	125	ALA	2.2
4	L	161	PHE	2.2
2	I	85	VAL	2.2
5	F	204	HIS	2.2
5	M	63	GLY	2.2
1	A	249	VAL	2.2
1	H	15	PRO	2.2
4	E	160	THR	2.2
2	B	88	SER	2.2
2	B	37	VAL	2.2
4	E	127	GLN	2.2
4	E	133	PRO	2.2
1	H	192	HIS	2.1
2	I	79	ALA	2.1
5	M	200	ALA	2.1
5	F	144	THR	2.1
1	A	223	ASP	2.1
1	H	250	PRO	2.1
1	H	194	VAL	2.1
1	A	125	ALA	2.1
5	F	164	ASN	2.1
1	H	228	THR	2.1
1	A	264	GLU	2.1
1	H	227	ASP	2.1
4	L	145	ASP	2.1
4	L	158	SER	2.1
5	M	206	PRO	2.1
5	F	130	PHE	2.1
2	I	44	GLU	2.1
5	M	117	GLU	2.1
5	M	220	SER	2.1
3	J	5	PHE	2.1
4	E	50	PHE	2.1
4	E	140	LEU	2.1
4	L	151	ASN	2.1
5	F	208	ASN	2.1
2	I	50	GLU	2.1
1	A	257	TYR	2.1
2	I	66	TYR	2.1
1	H	195	SER	2.1
1	A	67	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
5	F	239	ALA	2.0
5	F	159	LEU	2.0
2	I	77	GLU	2.0
1	A	165	VAL	2.0
2	B	54	LEU	2.0
2	I	36	GLU	2.0
5	M	221	GLU	2.0
4	E	61	GLY	2.0
5	F	139	ASN	2.0
4	E	2	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.