Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2023 – 03:11 PM EDT

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 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:

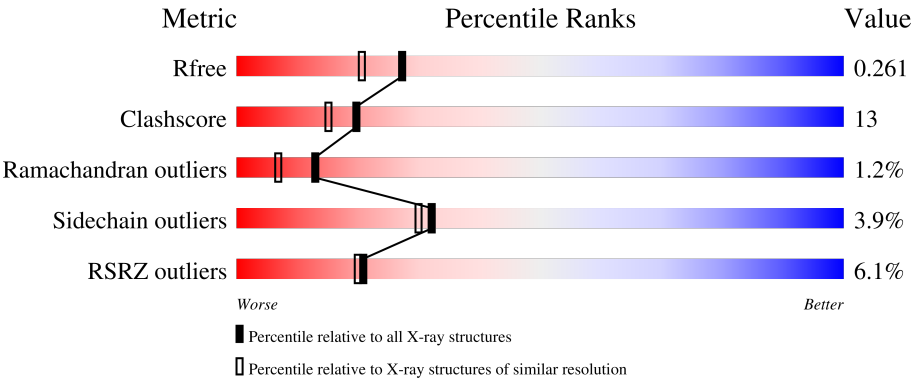
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	3% 81% 13%
1	H	275	5% 80% 16%
2	B	100	3% 85% 12%
2	I	100	4% 80% 16%
3	C	9	89% 11%

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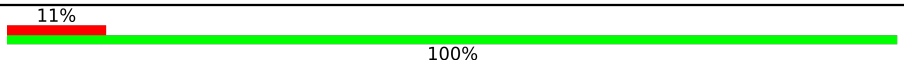
Mol	Chain	Length	Quality of chain
3	J	9	
4	E	194	
4	L	194	
5	F	238	
5	M	238	

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			

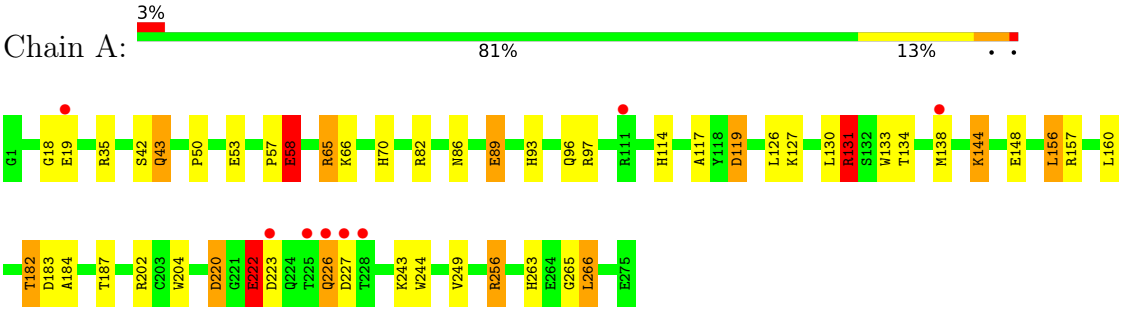
- Molecule 6 is water.

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		

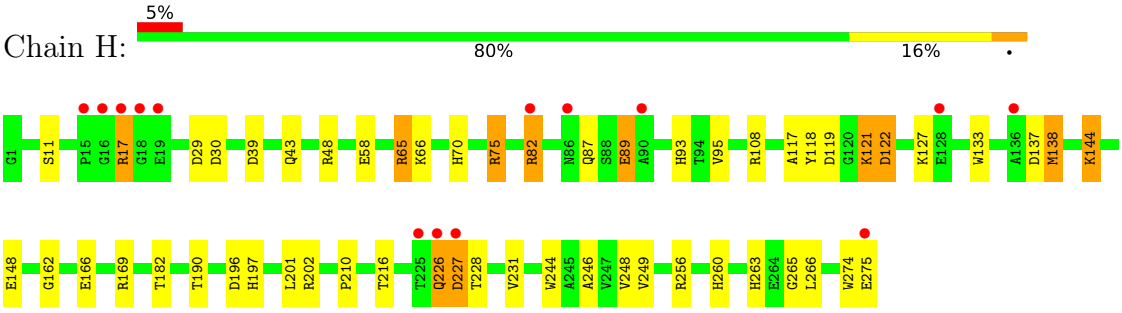
3 Residue-property plots (i)

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.

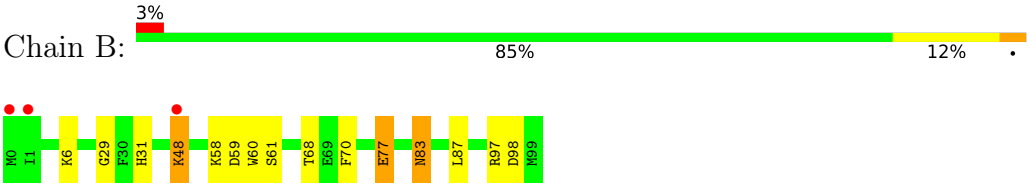
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



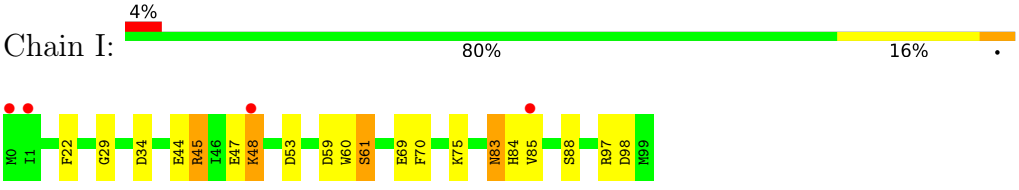
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin

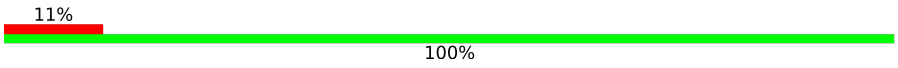


• Molecule 3: self-peptide P1049

Chain C:

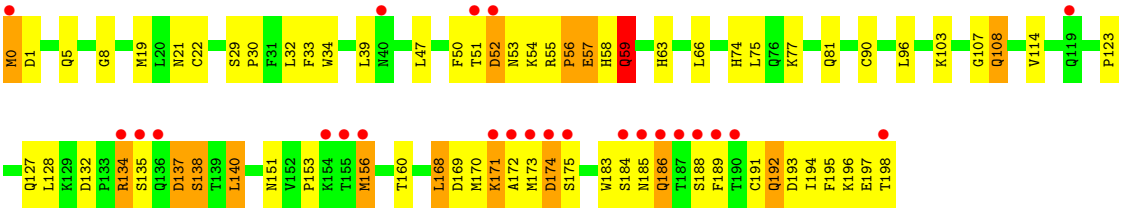
• Molecule 3: self-peptide P1049

Chain J:



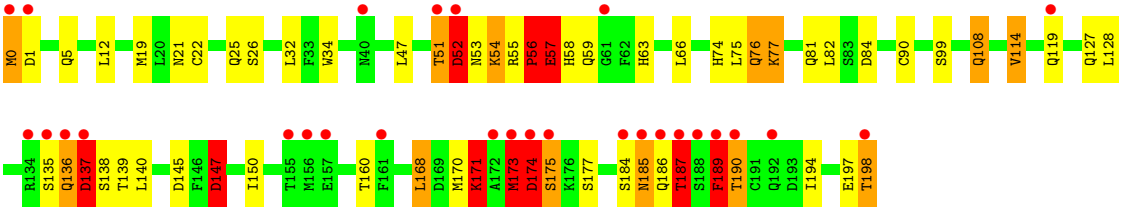
• Molecule 4: T-cell Receptor alpha chain

Chain E:



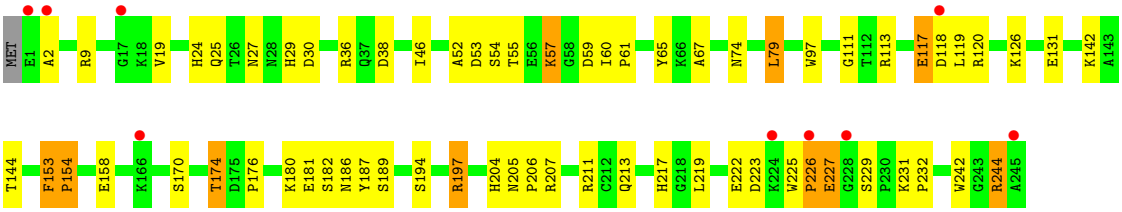
• Molecule 4: T-cell Receptor alpha chain

Chain L:



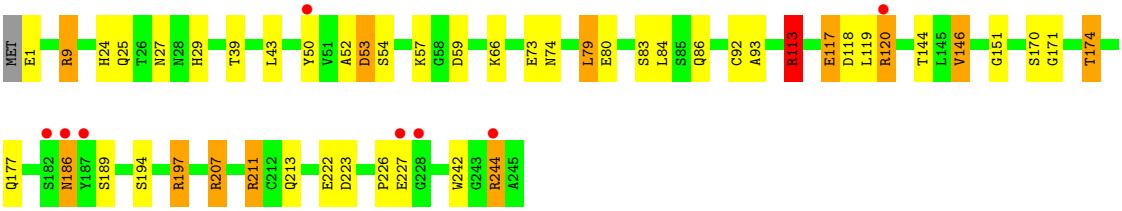
• Molecule 5: T-cell Receptor beta chain

Chain F:



• Molecule 5: T-cell Receptor beta chain

Chain M:


MET E1 R9 H24 Q25 T26 N27 N28 H29 T39 L43 Y50 V51 A52 D53 S54 K57 G58 D59 K66 E73 N74 L79 E80 S83 L84 S85 Q86 C92 A93 R113 E117 D118 L119 R120 T144 L145 V146 G151 S170 G171 T174
Q177 S182 N186 Y187 S189 S194 R197 R207 R211 C212 Q213 E222 D223 P226 E227 G228 W242 G243 R244 A245

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.36 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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 $< |L| >$, $< L^2 >$ 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	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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	Peptide,Mainchain
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 (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	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
4	L	1521	0	1475	63	0
5	F	1887	0	1790	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 (316) 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
4:L:0:MET:HE2	4:L:1:ASP:H	1.17	1.08
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
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	Interatomic distance (Å)	Clash overlap (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:CA	4:L:171:LYS:CD	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:174:THR:HB	5:M:194:SER:HB2	1.66	0.75
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: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
4:L:0:MET:HE1	4:L:25:GLN:C	2.10	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:HA	1:H:43:GLN:NE2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:58:GLU:CD	1:A:58:GLU:HB3	2.20	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
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:HE3	4:L:0:MET:CA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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:CE	4:L:0:MET:CA	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: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
4:L:0:MET:HE1	4:L:26:SER:N	2.24	0.52
5:M:52:ALA:O	5:M:53:ASP:HB2	2.09	0.52
4:E:127:GLN:C	4:E:128:LEU:HD23	2.29	0.52
4:L:22:CYS:H	4:L:74:HIS:CD2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	4:E:168:LEU:C	2.31	0.51
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:HE3	4:L:1:ASP:N	2.13	0.51
4:E:0:MET:HA	4:E:0:MET:HE2	1.93	0.51
1:A:42:SER:CB	1:H:138:MET:CE	2.87	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
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
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:O	4:E:197:GLU:CG	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
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:19:MET:HE2	4:E:21:ASN:OD1	2.19	0.43
4:E:34:TRP:HD1	4:E:47:LEU:HD11	1.81	0.43
4:L:186:GLN:OE1	4:L:189:PHE:HD1	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:E:171:LYS:O	4:E:172:ALA:C	2.57	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
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:47:LEU:HD12	4:E:47:LEU:C	2.39	0.42
4:E:170:MET:SD	5:F:142:LYS:HE2	2.60	0.42
1:H:43:GLN:HE21	1:H:43:GLN:CA	2.26	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
1:A:222:GLU:CD	1:A:222:GLU:CB	2.88	0.42
1:A:58:GLU:CD	1:A:58:GLU:CB	2.87	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
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
5:F:60:ILE:N	5:F:61:PRO:HD2	2.35	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
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
5:F:181:GLU:HG2	5:F:189:SER:O	2.21	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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%)	266 (97%)	6 (2%)	1 (0%)	34 30
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%)	5 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	L	192/194 (99%)	172 (90%)	9 (5%)	11 (6%)	1 0
5	F	235/238 (99%)	223 (95%)	10 (4%)	2 (1%)	17 11
5	M	235/238 (99%)	225 (96%)	9 (4%)	1 (0%)	34 30
All	All	1610/1632 (99%)	1533 (95%)	57 (4%)	20 (1%)	13 7

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
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 (i)

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%)	52 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	231/231 (100%)	227 (98%)	4 (2%)	60 65
2	B	95/95 (100%)	93 (98%)	2 (2%)	53 57
2	I	95/95 (100%)	92 (97%)	3 (3%)	39 38
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%)	14 9
4	L	177/177 (100%)	161 (91%)	16 (9%)	9 6
5	F	204/206 (99%)	199 (98%)	5 (2%)	47 49
5	M	204/206 (99%)	197 (97%)	7 (3%)	37 36
All	All	1428/1432 (100%)	1373 (96%)	55 (4%)	32 30

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

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Mol	Chain	Res	Type
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
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

Sometimes 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

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Mol	Chain	Res	Type
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
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 (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 monosaccharides 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	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, 95^{th} 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%)	0.16	8 (2%) 51 50	9, 15, 20, 24	8 (2%)
1	H	275/275 (100%)	0.15	14 (5%) 28 27	11, 15, 20, 26	11 (4%)
2	B	100/100 (100%)	-0.05	3 (3%) 50 49	11, 15, 22, 25	6 (6%)
2	I	100/100 (100%)	-0.05	4 (4%) 38 37	11, 15, 20, 25	3 (3%)
3	C	9/9 (100%)	1.10	0 100 100	13, 13, 14, 15	0
3	J	9/9 (100%)	1.27	1 (11%) 5 4	13, 14, 15, 16	0
4	E	187/194 (96%)	0.66	24 (12%) 3 3	10, 15, 21, 29	19 (10%)
4	L	187/194 (96%)	0.71	28 (14%) 2 2	10, 15, 21, 31	22 (11%)
5	F	237/238 (99%)	0.21	9 (3%) 40 39	11, 15, 19, 23	11 (4%)
5	M	237/238 (99%)	0.04	8 (3%) 45 44	11, 15, 19, 24	13 (5%)
All	All	1616/1632 (99%)	0.25	99 (6%) 21 20	9, 15, 20, 31	93 (5%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	52	ASP	8.6
4	E	187	THR	8.5
4	L	188	SER	8.4
4	E	190	THR	8.0
4	E	188	SER	7.9
4	L	156	MET	7.7
4	E	189	PHE	7.4
4	L	189	PHE	7.0
4	L	186	GLN	6.8
4	L	187	THR	6.6
4	L	198	THR	6.6
4	L	0	MET	6.4
1	A	225	THR	6.0

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Mol	Chain	Res	Type	RSRZ
1	H	16	GLY	5.9
2	B	0	MET	5.8
4	E	198	THR	5.8
4	E	52	ASP	5.8
4	E	0	MET	5.6
4	E	172	ALA	5.4
4	E	156	MET	5.4
2	I	0	MET	5.3
1	H	226	GLN	5.2
5	M	227	GLU	5.0
5	M	228	GLY	5.0
4	L	173	MET	5.0
4	L	174	ASP	4.8
4	E	51	THR	4.8
4	E	174	ASP	4.8
5	F	2	ALA	4.5
4	L	192	GLN	4.4
5	F	228	GLY	4.4
4	E	184	SER	4.3
4	L	190	THR	4.2
4	L	136	GLN	4.1
4	E	186	GLN	4.0
5	F	224	LYS	3.9
4	E	136	GLN	3.9
1	H	18	GLY	3.8
4	E	155	THR	3.7
4	L	51	THR	3.5
1	A	227	ASP	3.3
5	F	226	PRO	3.3
4	E	185	ASN	3.3
2	I	1	ILE	3.2
4	E	154	LYS	3.2
1	H	136	ALA	3.2
1	H	275	GLU	3.1
2	B	1	ILE	3.0
4	L	185	ASN	3.0
1	A	226	GLN	3.0
5	F	245	ALA	2.9
5	F	1	GLU	2.9
1	H	225	THR	2.9
4	E	119	GLN	2.8
1	H	19	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	86	ASN	2.8
4	L	184	SER	2.8
4	L	175	SER	2.7
1	A	228	THR	2.7
1	A	111	ARG	2.7
1	H	227	ASP	2.7
2	I	85	VAL	2.7
4	L	172	ALA	2.6
1	A	223	ASP	2.5
4	L	134	ARG	2.5
4	L	119	GLN	2.5
4	L	40	ASN	2.5
4	L	137	ASP	2.5
4	L	155	THR	2.4
4	L	135	SER	2.4
4	E	135	SER	2.4
5	F	118	ASP	2.4
4	E	173	MET	2.4
4	E	134	ARG	2.4
1	H	82	ARG	2.4
4	L	161	PHE	2.3
5	M	186	ASN	2.3
4	E	171	LYS	2.3
5	F	17	GLY	2.3
3	J	3	TRP	2.3
1	H	15	PRO	2.3
4	L	1	ASP	2.3
5	M	120	ARG	2.3
1	A	19	GLU	2.3
4	E	175	SER	2.3
4	L	157	GLU	2.3
5	M	182	SER	2.2
4	L	61	GLY	2.2
1	H	17	ARG	2.2
5	F	166	LYS	2.2
5	M	187	TYR	2.2
4	E	40	ASN	2.1
1	H	128	GLU	2.1
1	A	138	MET	2.1
1	H	90	ALA	2.1
2	B	48	LYS	2.1
2	I	48	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
5	M	50	TYR	2.0
5	M	244	ARG	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 monosaccharides 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.