Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:58 AM GMT

PDB ID	:	2JCC
Title	:	AH3 RECOGNITION OF MUTANT HLA-A2 W167A
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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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

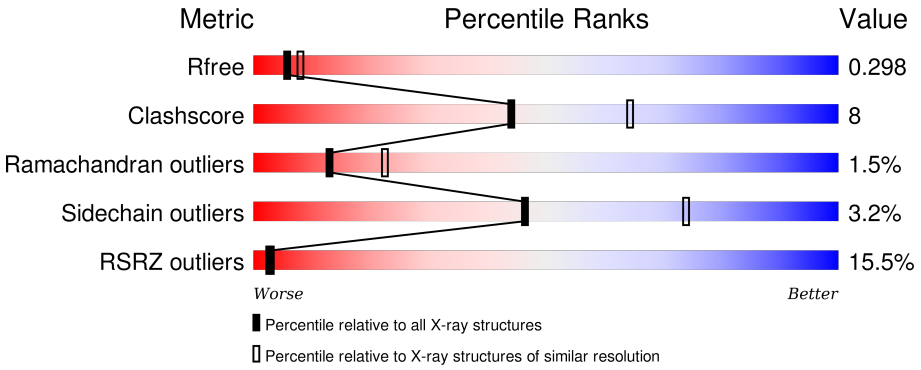
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	20% 83% 16%
1	H	275	12% 85% 14%
2	B	100	11% 88% 10%
2	I	100	11% 89% 10%
3	C	9	67% 89% 11%

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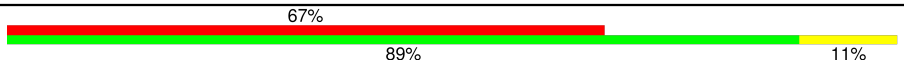
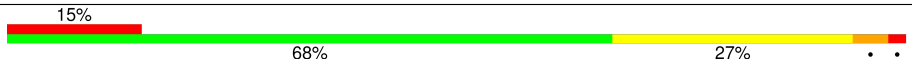
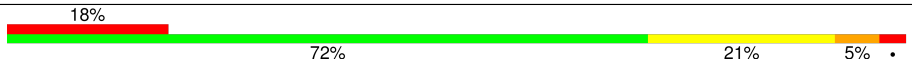
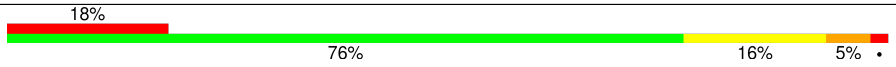
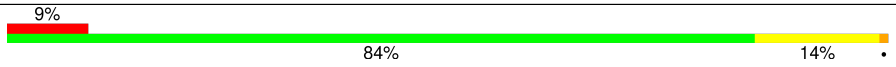
Mol	Chain	Length	Quality of chain
3	J	9	
4	E	194	
4	L	194	
5	F	238	
5	M	238	

2 Entry composition

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.

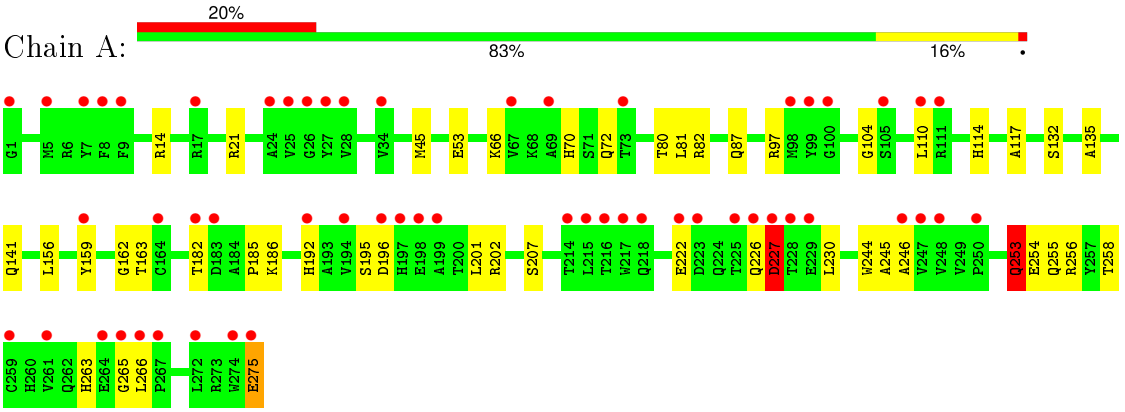
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	1	Total	O	0	0
			1	1		
6	E	10	Total	O	0	0
			10	10		
6	F	5	Total	O	0	0
			5	5		
6	H	9	Total	O	0	0
			9	9		
6	I	6	Total	O	0	0
			6	6		
6	L	9	Total	O	0	0
			9	9		
6	M	5	Total	O	0	0
			5	5		

3 Residue-property plots (i)

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

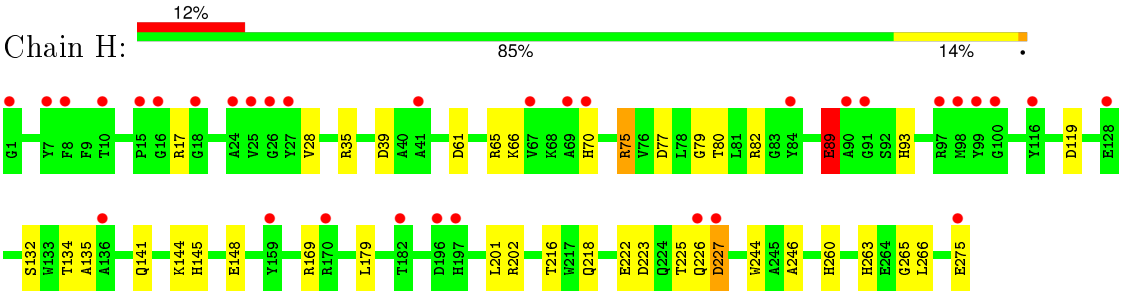
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN

Chain A:



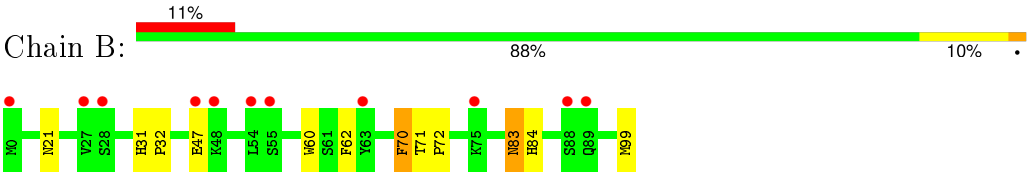
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN

Chain H:



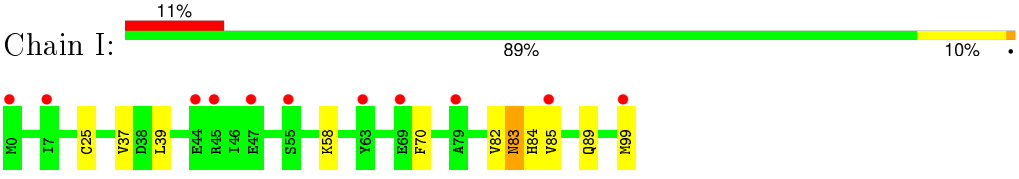
- Molecule 2: BETA-2-MICROGLOBULIN

Chain B:



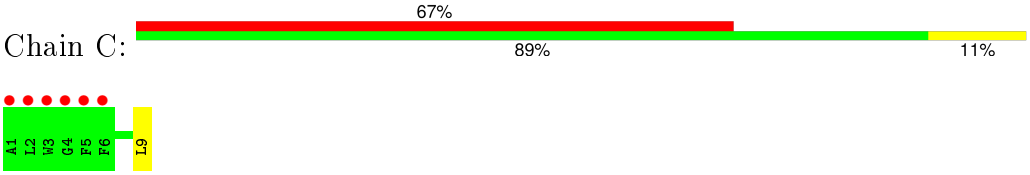
- Molecule 2: BETA-2-MICROGLOBULIN

Chain I:



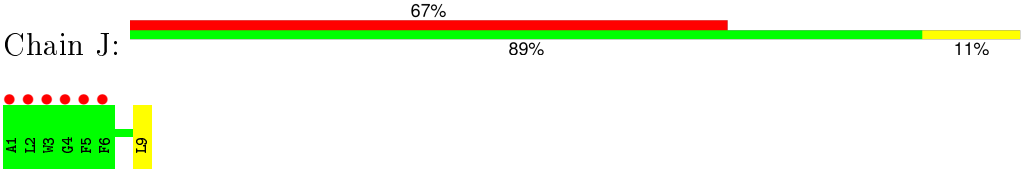
• Molecule 3: P1049

Chain C:



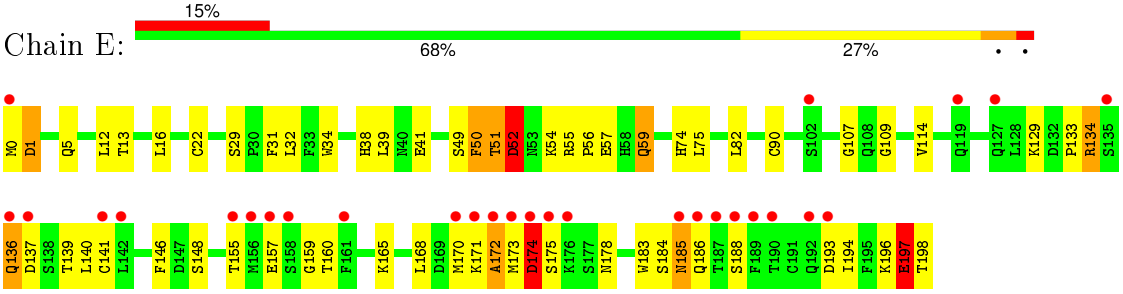
• Molecule 3: P1049

Chain J:



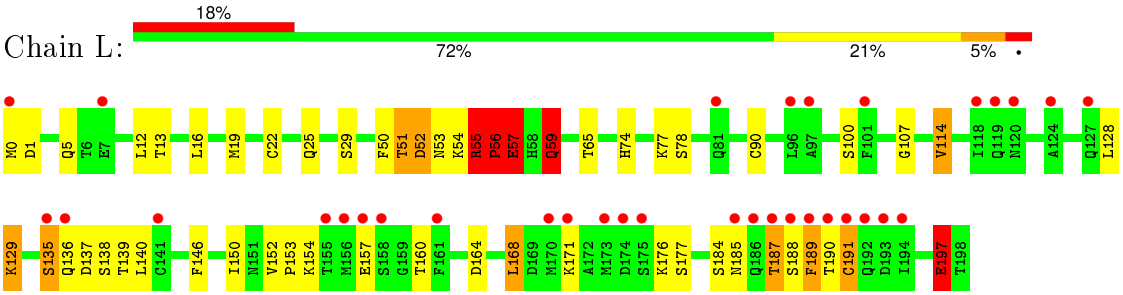
• Molecule 4: TCR ALPHA

Chain E:



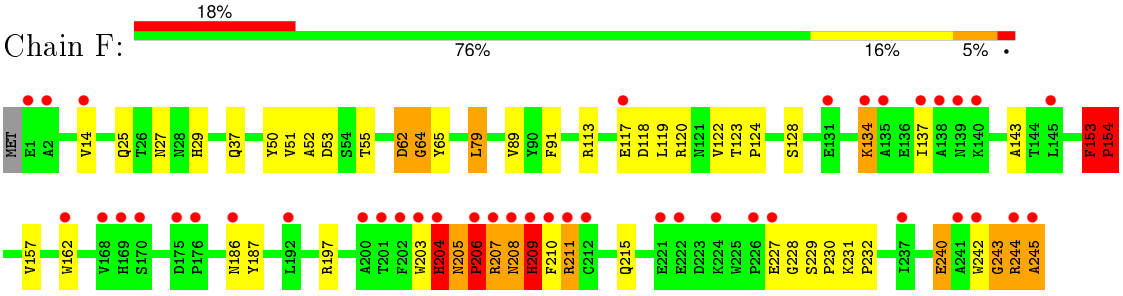
• Molecule 4: TCR ALPHA

Chain L:



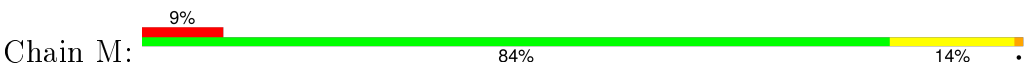
• Molecule 5: TCR BETA

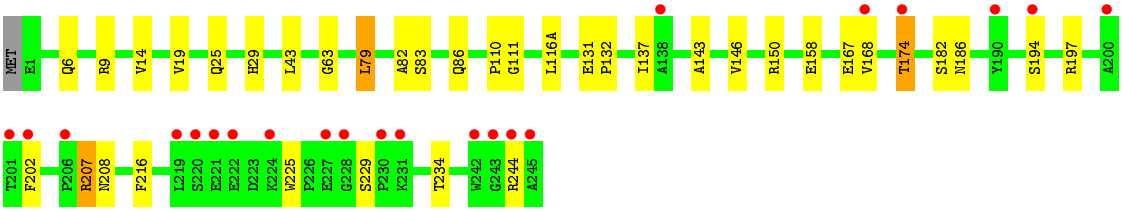
Chain F:



• Molecule 5: TCR BETA

Chain M:




MET
E1
Q6
R9
V14
V19
Q25
H29
L43
G63
L79
A82
S83
Q86
P110
G111
L116A
E131
P132
I137
A138
A143
V146
R150
E158
E167
V168
T174
S182
N186
Y190
S194
R197
A200
T201
F202
P206
R207
N208
F216
L219
S220
E221
E222
D223
K224
W225
P226
E227
G228
S229
P230
K231
T234
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	94.28Å 84.35Å 122.47Å 90.00° 92.53° 90.00°	Depositor
Resolution (Å)	122.17 – 2.50 40.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.5 (122.17-2.50) 92.5 (40.78-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.292 0.268 , 0.298	Depositor DCC
R_{free} test set	3091 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	47.7	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 32.0	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 61770 reflections (0.003%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.07	14/2301 (0.6%)	0.72	7/3121 (0.2%)
1	H	0.76	7/2301 (0.3%)	0.72	1/3121 (0.0%)
2	B	0.73	2/860 (0.2%)	0.65	0/1162
2	I	0.82	3/860 (0.3%)	0.85	1/1162 (0.1%)
3	C	0.81	0/80	0.62	0/108
3	J	0.76	0/80	0.62	0/108
4	E	1.40	24/1555 (1.5%)	1.12	12/2106 (0.6%)
4	L	1.22	14/1557 (0.9%)	1.54	31/2112 (1.5%)
5	F	1.60	29/1947 (1.5%)	1.13	18/2649 (0.7%)
5	M	0.68	3/1947 (0.2%)	0.59	1/2649 (0.0%)
All	All	1.10	96/13488 (0.7%)	0.95	71/18298 (0.4%)

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 (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	GLU	C-O	25.85	1.72	1.23
5	F	62	ASP	C-N	22.68	1.73	1.33
4	E	56	PRO	N-CD	21.81	1.78	1.47
5	F	117	GLU	CD-OE1	20.21	1.47	1.25
5	F	64	GLY	N-CA	19.33	1.75	1.46
4	L	59	GLN	C-N	16.59	1.62	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	52	ASP	C-N	15.94	1.70	1.34
5	F	208	ASN	C-N	14.96	1.68	1.34
5	F	209	HIS	CE1-NE2	14.89	1.66	1.32
5	F	154	PRO	N-CD	14.74	1.68	1.47
1	A	253	GLN	CD-NE2	14.71	1.69	1.32
4	E	59	GLN	C-N	-14.52	1.06	1.33
1	A	275	GLU	C-OXT	13.22	1.48	1.23
4	E	197	GLU	CD-OE2	12.46	1.39	1.25
5	F	244	ARG	CZ-NH2	12.41	1.49	1.33
4	E	197	GLU	C-O	12.06	1.46	1.23
4	L	57	GLU	N-CA	11.72	1.69	1.46
5	F	240	GLU	CD-OE2	11.57	1.38	1.25
5	F	242	TRP	C-O	11.53	1.45	1.23
5	F	207	ARG	NE-CZ	-11.50	1.18	1.33
1	A	195	SER	CB-OG	11.48	1.57	1.42
4	L	56	PRO	CA-C	11.43	1.75	1.52
5	F	209	HIS	CG-ND1	11.01	1.62	1.38
4	E	197	GLU	CD-OE1	11.01	1.37	1.25
5	F	117	GLU	CD-OE2	-10.93	1.13	1.25
4	E	174	ASP	CG-OD1	10.62	1.49	1.25
4	L	59	GLN	C-O	10.54	1.43	1.23
5	F	240	GLU	CD-OE1	10.53	1.37	1.25
4	E	186	GLN	CD-NE2	10.33	1.58	1.32
5	F	243	GLY	C-O	10.27	1.40	1.23
4	L	56	PRO	N-CA	9.74	1.63	1.47
5	M	182	SER	C-N	9.31	1.55	1.34
5	F	242	TRP	C-N	9.31	1.49	1.33
1	H	223	ASP	CB-CG	-9.20	1.32	1.51
2	I	58	LYS	CD-CE	9.01	1.73	1.51
5	F	227	GLU	CD-OE1	8.88	1.35	1.25
4	E	134	ARG	NE-CZ	8.69	1.44	1.33
5	F	245	ALA	CA-CB	8.69	1.70	1.52
4	L	56	PRO	C-N	8.62	1.53	1.34
4	L	57	GLU	CA-C	8.60	1.75	1.52
5	F	134	LYS	CE-NZ	8.47	1.70	1.49
5	F	244	ARG	CZ-NH1	8.33	1.43	1.33
1	H	145	HIS	CE1-NE2	8.05	1.51	1.32
1	A	253	GLN	CD-OE1	8.00	1.41	1.24
5	F	227	GLU	CD-OE2	7.98	1.34	1.25
4	E	188	SER	C-N	7.95	1.52	1.34
5	F	204	HIS	CE1-NE2	7.89	1.50	1.32
4	E	137	ASP	CB-CG	7.76	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	176	LYS	CD-CE	7.70	1.70	1.51
2	B	32	PRO	N-CD	7.60	1.58	1.47
5	F	207	ARG	CZ-NH2	-7.48	1.23	1.33
4	E	186	GLN	CD-OE1	-7.47	1.07	1.24
1	A	275	GLU	CD-OE1	7.46	1.33	1.25
4	E	136	GLN	C-O	-7.42	1.09	1.23
5	F	211	ARG	CZ-NH1	7.14	1.42	1.33
4	L	157	GLU	CD-OE1	7.11	1.33	1.25
5	M	158	GLU	CG-CD	-7.07	1.41	1.51
5	F	245	ALA	C-OXT	7.06	1.36	1.23
1	H	145	HIS	CG-CD2	7.06	1.47	1.35
4	E	193	ASP	CB-CG	7.02	1.66	1.51
1	A	222	GLU	CD-OE1	6.90	1.33	1.25
1	A	227	ASP	CG-OD2	6.83	1.41	1.25
1	A	196	ASP	CG-OD2	-6.79	1.09	1.25
4	L	136	GLN	CD-NE2	6.61	1.49	1.32
4	L	136	GLN	CD-OE1	6.58	1.38	1.24
5	F	210	PHE	C-N	6.49	1.49	1.34
1	A	256	ARG	CZ-NH1	6.48	1.41	1.33
1	H	275	GLU	CD-OE1	6.48	1.32	1.25
2	B	47	GLU	CG-CD	6.42	1.61	1.51
4	E	174	ASP	CG-OD2	-6.28	1.10	1.25
4	E	188	SER	C-O	6.25	1.35	1.23
4	E	52	ASP	N-CA	-6.13	1.34	1.46
4	E	157	GLU	CD-OE1	6.10	1.32	1.25
1	A	255	GLN	CD-OE1	6.05	1.37	1.24
4	E	193	ASP	CG-OD1	6.03	1.39	1.25
5	M	63	GLY	C-O	5.86	1.33	1.23
1	H	275	GLU	C-O	5.84	1.34	1.23
2	I	89	GLN	CD-OE1	5.83	1.36	1.24
5	F	187	TYR	CE1-CZ	5.74	1.46	1.38
4	E	51	THR	N-CA	-5.63	1.35	1.46
1	H	145	HIS	CG-ND1	5.63	1.51	1.38
1	A	222	GLU	CD-OE2	5.54	1.31	1.25
5	F	204	HIS	CG-CD2	5.47	1.45	1.35
4	L	197	GLU	C-N	5.47	1.46	1.34
2	I	89	GLN	CD-NE2	5.43	1.46	1.32
4	E	50	PHE	C-N	-5.33	1.21	1.34
1	A	227	ASP	CG-OD1	5.33	1.37	1.25
5	F	205	ASN	CB-CG	5.23	1.63	1.51
4	E	185	ASN	CG-OD1	5.23	1.35	1.24
1	A	254	GLU	CD-OE1	5.22	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	136	GLN	C-N	5.20	1.46	1.34
1	H	89	GLU	CB-CG	5.14	1.61	1.52
4	E	56	PRO	CB-CG	5.07	1.75	1.50
4	E	56	PRO	C-O	5.06	1.33	1.23
4	L	129	LYS	CE-NZ	5.05	1.61	1.49
5	F	211	ARG	CZ-NH2	-5.04	1.26	1.33

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	244	ARG	NE-CZ-NH1	23.41	132.00	120.30
4	L	52	ASP	CA-C-N	-21.03	70.94	117.20
5	F	207	ARG	NE-CZ-NH2	-19.11	110.75	120.30
4	E	134	ARG	NE-CZ-NH1	19.05	129.82	120.30
2	I	99	MET	CA-C-O	18.29	158.52	120.10
1	H	275	GLU	CA-C-O	18.13	158.18	120.10
4	L	197	GLU	O-C-N	-17.42	94.83	122.70
4	L	51	THR	O-C-N	16.93	149.78	122.70
4	L	52	ASP	C-N-CA	-16.66	80.05	121.70
4	L	59	GLN	CA-C-O	-16.51	85.44	120.10
4	L	51	THR	CA-C-N	-16.34	81.26	117.20
4	E	174	ASP	CB-CG-OD1	-16.07	103.84	118.30
4	L	57	GLU	CB-CA-C	-15.79	78.83	110.40
4	E	134	ARG	NE-CZ-NH2	-15.64	112.48	120.30
4	L	59	GLN	O-C-N	-15.40	97.02	123.20
5	F	244	ARG	NE-CZ-NH2	-15.32	112.64	120.30
4	L	57	GLU	N-CA-C	13.39	147.16	111.00
4	L	56	PRO	N-CA-C	12.27	144.00	112.10
4	L	59	GLN	CB-CA-C	10.81	132.02	110.40
5	F	117	GLU	OE1-CD-OE2	10.68	136.12	123.30
5	F	153	PHE	C-N-CD	-10.54	97.40	120.60
4	L	51	THR	C-N-CA	10.14	147.05	121.70
5	F	62	ASP	C-N-CA	-9.94	101.44	122.30
4	E	174	ASP	OD1-CG-OD2	9.56	141.47	123.30
4	L	57	GLU	CA-C-O	-9.54	100.06	120.10
4	E	197	GLU	O-C-N	-9.29	107.84	122.70
4	E	59	GLN	C-N-CA	9.21	141.65	122.30
4	L	137	ASP	CB-CG-OD2	9.16	126.55	118.30
4	E	51	THR	CA-C-N	-8.78	97.89	117.20
4	L	197	GLU	CA-C-N	8.62	136.16	117.20
5	F	211	ARG	NE-CZ-NH2	-8.41	116.09	120.30
4	L	137	ASP	CB-CG-OD1	-8.32	110.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	56	PRO	CA-C-N	8.10	135.01	117.20
4	L	52	ASP	O-C-N	-7.99	109.92	122.70
1	A	275	GLU	CA-C-O	-7.62	104.09	120.10
5	F	153	PHE	C-N-CA	7.57	153.81	122.00
1	A	256	ARG	NE-CZ-NH2	-7.55	116.53	120.30
4	L	56	PRO	CB-CA-C	-7.36	93.60	112.00
4	L	57	GLU	CA-C-N	7.35	133.38	117.20
4	L	59	GLN	CA-C-N	-7.30	101.60	116.20
5	F	210	PHE	CB-CG-CD2	7.18	125.83	120.80
4	L	56	PRO	N-CA-CB	-6.86	95.06	102.60
4	L	197	GLU	C-N-CA	6.80	138.69	121.70
5	F	208	ASN	CA-C-N	-6.79	102.27	117.20
1	A	255	GLN	CG-CD-NE2	6.56	132.45	116.70
4	L	59	GLN	N-CA-C	-6.53	93.36	111.00
5	F	245	ALA	CB-CA-C	-6.35	100.58	110.10
4	L	56	PRO	C-N-CA	-6.22	106.14	121.70
4	E	51	THR	O-C-N	6.22	132.65	122.70
1	A	227	ASP	CB-CG-OD1	-6.20	112.72	118.30
5	F	207	ARG	NH1-CZ-NH2	6.17	126.18	119.40
5	F	154	PRO	CA-N-CD	-5.92	103.22	111.50
4	L	50	PHE	O-C-N	-5.79	113.44	122.70
4	L	55	ARG	C-N-CD	-5.77	107.90	120.60
5	F	206	PRO	O-C-N	-5.73	113.53	122.70
4	E	55	ARG	C-N-CD	-5.67	108.13	120.60
4	L	57	GLU	C-N-CA	-5.67	107.53	121.70
4	E	136	GLN	O-C-N	-5.62	113.71	122.70
5	F	207	ARG	NE-CZ-NH1	5.53	123.07	120.30
5	F	243	GLY	CA-C-N	-5.52	105.06	117.20
1	A	253	GLN	CG-CD-OE1	-5.49	110.62	121.60
5	F	210	PHE	O-C-N	5.41	131.36	122.70
4	L	168	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	227	ASP	CB-CG-OD2	-5.31	113.52	118.30
4	L	57	GLU	N-CA-CB	-5.28	101.09	110.60
4	L	140	LEU	CA-CB-CG	5.28	127.43	115.30
4	E	56	PRO	N-CD-CG	-5.26	95.31	103.20
5	F	210	PHE	CA-C-O	-5.20	109.18	120.10
1	A	227	ASP	OD1-CG-OD2	5.16	133.11	123.30
4	E	50	PHE	O-C-N	5.09	130.85	122.70
5	M	43	LEU	CA-CB-CG	5.08	126.97	115.30

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	9	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	55	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	202	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 (202) 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
5:F:64:GLY:CA	5:F:64:GLY:N	1.75	1.47
5:F:154:PRO:N	5:F:154:PRO:CD	1.68	1.46
1:A:253:GLN:CD	1:A:253:GLN:NE2	1.69	1.43
5:F:62:ASP:C	5:F:64:GLY:N	1.73	1.41
5:F:208:ASN:C	5:F:209:HIS:N	1.68	1.41
1:A:275:GLU:C	1:A:275:GLU:O	1.72	1.27
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
4:L:190:THR:HG22	4:L:191:CYS:H	1.18	1.04
5:F:153:PHE:C	5:F:154:PRO:CD	2.28	1.02
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
4:L:184:SER:CB	4:L:189:PHE:HE1	1.88	0.85
1:A:97:ARG:HH21	1:A:114:HIS:HE1	1.24	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:CG	1:H:75:ARG:HH11	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
1:A:72:GLN:CG	5:F:51:VAL:HG11	2.24	0.67
1:H:75:ARG:HG2	1:H:75:ARG:HH11	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:L:185:ASN:HD21	5:M:150:ARG:HH22	1.45	0.62
5:F:203:TRP:CZ3	5:F:243:GLY:HA2	2.34	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:M:25:GLN:NE2	5:M:29:HIS:H	1.98	0.61
5:F:143:ALA:O	5:F:197:ARG:HA	2.01	0.61
5:F:62:ASP:C	5:F:64:GLY:CA	2.69	0.61
4:E:136:GLN:H	4:E:136:GLN:CD	2.04	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
5:F:208:ASN:C	5:F:209:HIS:CA	2.67	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
5:M:207:ARG:C	5:M:207:ARG:HD3	2.24	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
4:L:188:SER:O	4:L:189:PHE:HB2	2.07	0.55
1:H:135:ALA:HB3	1:H:141:GLN:NE2	2.22	0.55
5:F:118:ASP:OD2	5:F:120:ARG:NE	2.40	0.55
4:E:129:LYS:HG2	4:E:139:THR:HG22	1.88	0.55
4:L:129:LYS:HD3	4:L:139:THR:CG2	2.38	0.54
1:H:226:GLN:O	1:H:227:ASP:HB2	2.08	0.54
2:B:31:HIS:HD1	2:B:62:PHE:HE2	1.54	0.54
5:F:50:TYR:HD1	5:F:51:VAL:HG13	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:263:HIS:HD2	1:H:265:GLY:N	2.03	0.51
4:E:32:LEU:O	4:E:49:SER:HB3	2.11	0.51
4:L:168:LEU:HB3	4:L:177:SER:HB2	1.92	0.51
5:F:25:GLN:HE21	5:F:27:ASN:H	1.58	0.51
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.46	0.51
5:F:153:PHE:O	5:F:154:PRO:CD	2.59	0.51
1:A:275:GLU:CA	1:A:275:GLU:O	2.57	0.51
5:F:203:TRP:O	5:F:243:GLY:HA3	2.11	0.51
4:L:184:SER:CB	4:L:189:PHE:CE1	2.74	0.50
1:A:226:GLN:O	1:A:227:ASP:CB	2.58	0.50
1:A:14:ARG:NH1	1:A:21:ARG:HB2	2.23	0.50
5:F:118:ASP:OD1	5:F:119:LEU:N	2.45	0.50
4:E:172:ALA:O	4:E:173:MET:HG2	2.10	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
1:A:53:GLU:OE1	1:H:134:THR:HG23	2.12	0.50
1:H:77:ASP:HB3	3:J:9:LEU:HD12	1.94	0.50
1:A:202:ARG:HD3	1:A:244:TRP:CD2	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:ARG:HD3	1:H:89:GLU:HB3	1.95	0.48
1:H:75:ARG:HG3	1:H:75:ARG:HH11	1.77	0.48
5:M:143:ALA:O	5:M:197:ARG:HA	2.14	0.48
1:A:192:HIS:HE1	2:B:99:MET:OXT	1.96	0.48
1:H:225:THR:HG22	1:H:225:THR:O	2.15	0.47
4:E:170:MET:HB2	4:E:175:SER:HB2	1.97	0.47
4:E:0:MET:O	4:E:1:ASP:HB2	2.14	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:171:LYS:O	4:E:172:ALA:C	2.54	0.45
4:L:187:THR:HG22	4:L:188:SER:N	2.31	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
5:F:209:HIS:NE2	5:F:240:GLU:OE1	2.45	0.45
4:E:160:THR:HG23	4:E:184:SER:HB2	1.99	0.45
5:F:79:LEU:N	5:F:79:LEU:HD23	2.32	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
1:H:80:THR:HG21	3:J:9:LEU:O	2.18	0.44
4:E:140:LEU:HD12	4:E:183:TRP:HB3	1.99	0.44
2:I:37:VAL:HG22	2:I:82:VAL:HG22	1.99	0.44
5:M:225:TRP:HE1	5:M:229:SER:HB3	1.82	0.44
5:F:157:VAL:HA	5:F:215:GLN:O	2.18	0.44
5:F:123:THR:HA	5:F:124:PRO:HD3	1.88	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:134:LYS:CD	5:F:134:LYS:NZ	2.69	0.42
5:F:50:TYR:CE1	5:F:51:VAL:HG22	2.54	0.42
5:F:64:GLY:N	5:F:65:TYR:N	2.67	0.42
4:E:12:LEU:O	4:E:114:VAL:HA	2.20	0.42
1:H:218:GLN:HG2	1:H:222:GLU:O	2.20	0.42
5:F:205:ASN:HA	5:F:206:PRO:HD3	1.91	0.42
4:E:146:PHE:CE2	4:E:178:ASN:HB3	2.54	0.42
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
4:L:22:CYS:H	4:L:74:HIS:CD2	2.18	0.41
1:H:61:ASP:HB3	1:H:65:ARG:NH2	2.36	0.41
5:M:132:PRO:HB2	5:M:137:ILE:HD11	2.03	0.41
1:H:202:ARG:HD3	1:H:244:TRP:CD2	2.56	0.41
1:A:186:LYS:HE2	1:A:207:SER:HB3	2.02	0.41
1:H:202:ARG:HG3	1:H:246:ALA:HB2	2.03	0.41
4:E:173:MET:O	4:E:174:ASP:C	2.60	0.41
4:E:129:LYS:O	4:E:133:PRO:HD3	2.21	0.40
1:A:159:TYR:CD1	1:A:163:THR:HB	2.57	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:F:153:PHE:C	5:F:154:PRO:HD2	2.30	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 symmetry 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%)	26 46
1	H	273/275 (99%)	262 (96%)	9 (3%)	2 (1%)	26 46
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%)	4 5
4	L	192/194 (99%)	164 (85%)	17 (9%)	11 (6%)	2 2
5	F	235/238 (99%)	219 (93%)	14 (6%)	2 (1%)	21 37
5	M	235/238 (99%)	227 (97%)	8 (3%)	0	100 100
All	All	1607/1632 (98%)	1509 (94%)	74 (5%)	24 (2%)	13 22

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
4	L	59	GLN

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Mol	Chain	Res	Type
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 (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	230/230 (100%)	226 (98%)	4 (2%)	68 89
1	H	230/230 (100%)	223 (97%)	7 (3%)	48 76
2	B	95/95 (100%)	93 (98%)	2 (2%)	61 85
2	I	95/95 (100%)	92 (97%)	3 (3%)	46 74
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%)	169 (96%)	8 (4%)	34 59
4	L	177/177 (100%)	166 (94%)	11 (6%)	23 41
5	F	205/206 (100%)	200 (98%)	5 (2%)	57 82
5	M	205/206 (100%)	199 (97%)	6 (3%)	50 77
All	All	1428/1430 (100%)	1382 (97%)	46 (3%)	46 74

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

Mol	Chain	Res	Type
1	A	45	MET
1	A	132	SER
1	A	156	LEU
1	A	258	THR
2	B	70	PHE
2	B	83	ASN
4	E	29	SER
4	E	39	LEU
4	E	52	ASP
4	E	54	LYS
4	E	57	GLU
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
1	H	35	ARG
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	70	PHE
2	I	83	ASN
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	191	CYS
4	L	197	GLU
5	M	79	LEU
5	M	146	VAL
5	M	174	THR

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Mol	Chain	Res	Type
5	M	186	ASN
5	M	207	ARG
5	M	244	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	87	GLN
1	A	114	HIS
1	A	141	GLN
1	A	192	HIS
1	A	263	HIS
2	B	2	GLN
2	B	83	ASN
4	E	5	GLN
4	E	74	HIS
4	E	81	GLN
5	F	24	HIS
5	F	25	GLN
5	F	28	ASN
5	F	139	ASN
1	H	70	HIS
1	H	87	GLN
1	H	93	HIS
1	H	141	GLN
1	H	263	HIS
2	I	83	ASN
4	L	5	GLN
4	L	38	HIS
4	L	74	HIS
4	L	185	ASN
5	M	24	HIS
5	M	25	GLN
5	M	74	ASN
5	M	86	GLN
5	M	186	ASN
5	M	215	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.18	56 (20%) 1 1	40, 50, 58, 67	1 (0%)
1	H	275/275 (100%)	0.98	33 (12%) 6 6	38, 50, 59, 74	1 (0%)
2	B	100/100 (100%)	0.81	11 (11%) 7 7	42, 49, 59, 73	0
2	I	100/100 (100%)	0.90	11 (11%) 7 7	43, 51, 60, 76	0
3	C	9/9 (100%)	2.13	6 (66%) 0 0	44, 45, 51, 54	0
3	J	9/9 (100%)	2.37	6 (66%) 0 0	48, 50, 54, 57	0
4	E	184/194 (94%)	1.20	29 (15%) 3 2	37, 49, 66, 75	0
4	L	185/194 (95%)	1.17	34 (18%) 2 2	36, 49, 67, 73	2 (1%)
5	F	237/238 (99%)	1.09	42 (17%) 2 2	35, 50, 63, 69	0
5	M	237/238 (99%)	0.80	22 (9%) 11 11	37, 49, 58, 66	1 (0%)
All	All	1611/1632 (98%)	1.05	250 (15%) 3 3	35, 50, 62, 76	5 (0%)

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	189	PHE	9.6
5	M	245	ALA	9.0
4	E	173	MET	8.6
5	F	245	ALA	8.1
4	L	156	MET	7.7
4	E	187	THR	7.5
5	F	201	THR	7.4
1	A	197	HIS	7.0
4	E	136	GLN	6.5
4	L	187	THR	6.4
4	L	188	SER	6.2
1	A	196	ASP	6.0
4	L	119	GLN	6.0

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Mol	Chain	Res	Type	RSRZ
4	E	156	MET	6.0
5	F	244	ARG	6.0
4	L	173	MET	5.8
4	L	190	THR	5.7
4	L	186	GLN	5.6
4	E	190	THR	5.5
1	A	227	ASP	5.4
4	E	158	SER	5.3
1	A	228	THR	5.3
1	H	128	GLU	5.3
4	L	0	MET	5.2
4	E	175	SER	5.2
4	L	189	PHE	5.2
1	A	259	CYS	5.2
5	F	200	ALA	5.1
5	F	138	ALA	5.0
4	E	137	ASP	5.0
1	H	136	ALA	4.9
4	E	188	SER	4.8
5	F	135	ALA	4.8
4	L	185	ASN	4.6
4	E	192	GLN	4.6
1	H	1	GLY	4.5
4	E	0	MET	4.5
4	L	136	GLN	4.4
5	M	138	ALA	4.4
1	A	223	ASP	4.4
5	F	145	LEU	4.4
5	F	210	PHE	4.3
4	E	172	ALA	4.3
4	E	186	GLN	4.3
1	A	225	THR	4.3
1	A	1	GLY	4.2
1	H	16	GLY	4.2
2	B	0	MET	4.1
1	A	248	VAL	4.1
2	I	0	MET	4.1
5	M	222	GLU	4.0
5	F	227	GLU	4.0
4	E	171	LYS	4.0
4	E	119	GLN	4.0
1	A	229	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
3	J	4	GLY	3.9
4	L	161	PHE	3.9
5	F	207	ARG	3.8
4	L	158	SER	3.8
5	M	228	GLY	3.8
1	A	199	ALA	3.7
4	L	157	GLU	3.7
1	A	266	LEU	3.7
1	A	246	ALA	3.6
5	M	244	ARG	3.6
1	H	226	GLN	3.5
5	F	2	ALA	3.5
5	M	224	LYS	3.5
5	F	186	ASN	3.4
5	F	170	SER	3.4
1	H	18	GLY	3.4
1	A	250	PRO	3.4
5	F	222	GLU	3.4
1	A	217	TRP	3.4
2	I	99	MET	3.4
5	M	221	GLU	3.3
3	J	3	TRP	3.3
4	E	193	ASP	3.3
1	A	267	PRO	3.3
1	H	99	TYR	3.3
4	E	174	ASP	3.3
1	H	84	TYR	3.2
1	A	265	GLY	3.2
1	H	275	GLU	3.2
1	A	222	GLU	3.2
1	A	192	HIS	3.2
1	H	70	HIS	3.2
3	J	2	LEU	3.2
4	E	141	CYS	3.2
4	L	155	THR	3.2
4	E	157	GLU	3.1
1	A	25	VAL	3.1
5	F	204	HIS	3.1
4	E	170	MET	3.1
1	A	8	PHE	3.1
3	C	3	TRP	3.0
4	L	191	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	26	GLY	3.0
1	A	99	TYR	3.0
1	A	272	LEU	3.0
4	L	192	GLN	3.0
3	C	1	ALA	2.9
1	H	67	VAL	2.9
4	L	127	GLN	2.9
5	M	201	THR	2.9
5	F	134	LYS	2.9
1	H	8	PHE	2.9
1	A	216	THR	2.9
1	A	226	GLN	2.9
1	H	25	VAL	2.9
5	F	242	TRP	2.8
1	A	26	GLY	2.8
5	M	219	LEU	2.8
4	E	155	THR	2.8
5	F	202	PHE	2.8
1	A	264	GLU	2.8
3	J	1	ALA	2.8
1	A	5	MET	2.7
5	F	137	ILE	2.7
5	M	231	LYS	2.7
5	M	227	GLU	2.7
3	C	2	LEU	2.7
4	L	135	SER	2.7
4	L	171	LYS	2.7
4	L	120	ASN	2.7
5	F	131	GLU	2.7
1	A	183	ASP	2.7
4	E	127	GLN	2.7
5	F	140	LYS	2.7
5	F	169	HIS	2.7
4	L	175	SER	2.6
1	A	24	ALA	2.6
1	A	67	VAL	2.6
1	A	274	TRP	2.6
4	L	141	CYS	2.6
5	F	221	GLU	2.6
5	F	211	ARG	2.6
2	I	55	SER	2.6
5	F	162	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
5	M	242	TRP	2.6
1	A	34	VAL	2.6
1	A	198	GLU	2.6
5	F	237	ILE	2.6
1	H	15	PRO	2.5
1	H	182	THR	2.5
2	B	48	LYS	2.5
2	I	45	ARG	2.5
1	H	197	HIS	2.5
1	A	215	LEU	2.5
4	L	194	ILE	2.5
3	J	6	PHE	2.5
5	F	14	VAL	2.5
5	F	241	ALA	2.5
5	M	220	SER	2.5
2	I	63	TYR	2.5
4	L	124	ALA	2.5
3	C	5	PHE	2.5
1	A	73	THR	2.5
1	H	159	TYR	2.5
1	H	24	ALA	2.5
2	I	85	VAL	2.4
1	A	275	GLU	2.4
1	H	7	TYR	2.4
1	A	9	PHE	2.4
5	M	230	PRO	2.4
1	A	247	VAL	2.4
1	H	100	GLY	2.4
2	I	79	ALA	2.4
3	J	5	PHE	2.4
5	M	200	ALA	2.4
5	M	174	THR	2.4
4	L	101	PHE	2.4
2	I	47	GLU	2.4
4	L	170	MET	2.4
5	F	208	ASN	2.3
1	A	164	CYS	2.3
1	H	116	TYR	2.3
4	E	142	LEU	2.3
5	F	209	HIS	2.3
2	B	75	LYS	2.3
4	L	193	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	182	THR	2.3
1	H	41	ALA	2.3
4	L	118	ILE	2.3
2	B	63	TYR	2.3
1	H	196	ASP	2.3
1	A	7	TYR	2.3
1	A	159	TYR	2.3
4	L	7	GLU	2.3
3	C	4	GLY	2.3
1	H	98	MET	2.3
5	F	203	TRP	2.3
1	H	90	ALA	2.3
3	C	6	PHE	2.3
1	H	27	TYR	2.3
2	I	7	ILE	2.2
1	A	100	GLY	2.2
5	M	243	GLY	2.2
5	M	168	VAL	2.2
4	E	176	LYS	2.2
4	L	174	ASP	2.2
2	B	88	SER	2.2
5	F	192	LEU	2.2
1	A	27	TYR	2.2
1	H	69	ALA	2.2
5	F	175	ASP	2.2
2	B	89	GLN	2.2
5	M	202	PHE	2.2
4	L	96	LEU	2.2
1	A	69	ALA	2.2
1	A	105	SER	2.2
4	E	135	SER	2.2
1	H	227	ASP	2.2
1	H	91	GLY	2.1
4	L	97	ALA	2.1
5	F	212	CYS	2.1
4	E	185	ASN	2.1
1	A	218	GLN	2.1
1	A	17	ARG	2.1
1	H	170	ARG	2.1
2	B	47	GLU	2.1
1	A	214	THR	2.1
4	E	102	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	27	VAL	2.1
2	I	44	GLU	2.1
5	F	139	ASN	2.1
4	L	81	GLN	2.1
2	B	28	SER	2.1
1	A	28	VAL	2.1
1	A	261	VAL	2.1
1	A	98	MET	2.1
5	F	176	PRO	2.1
5	F	206	PRO	2.1
1	H	10	THR	2.1
2	I	69	GLU	2.1
5	F	168	VAL	2.1
1	A	111	ARG	2.1
5	F	1	GLU	2.1
5	F	117	GLU	2.1
5	M	190	TYR	2.1
5	F	224	LYS	2.1
5	F	226	PRO	2.1
5	M	206	PRO	2.1
5	M	194	SER	2.1
1	A	194	VAL	2.0
1	A	110	LEU	2.0
2	B	55	SER	2.0
2	B	54	LEU	2.0
4	E	161	PHE	2.0
1	H	97	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 carbohydrates 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.