



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:06 AM UTC

PDB ID : 1I1F / pdb_00001i1f
Title : Crystal structure of human class i mhc (hla-a2.1) complexed with beta 2-microglobulin and hiv-rt variant peptide ily
Authors : Kirksey, T.J.; Pogue-Caley, R.R.; Frelinger, J.A.; Collins, E.J.
Deposited on : 1999-04-16
Resolution : 2.80 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:

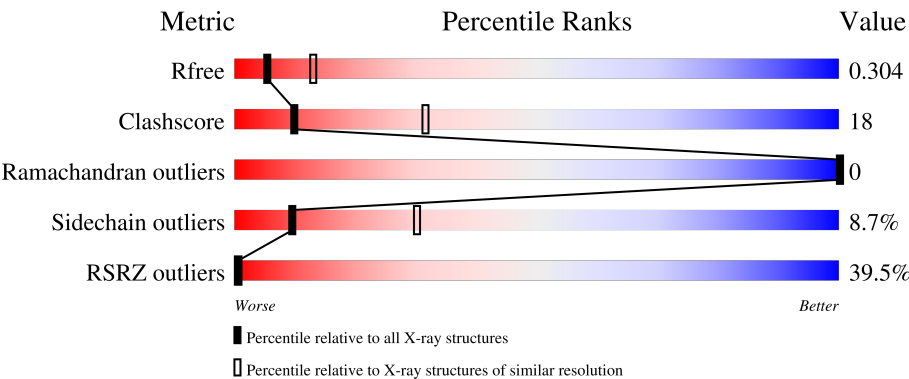
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	
1	D	275	
2	B	100	
2	E	100	
3	C	9	

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Mol	Chain	Length	Quality of chain
3	F	9	22% 56% 44%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6311 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 PROTEIN (CLASS I HISTOCOMPATIBILITY ANTIGEN, GOGO-A0201 ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			
1	D	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			

- Molecule 2 is a protein called PROTEIN (BETA 2-MICROGLOBULIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	E	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

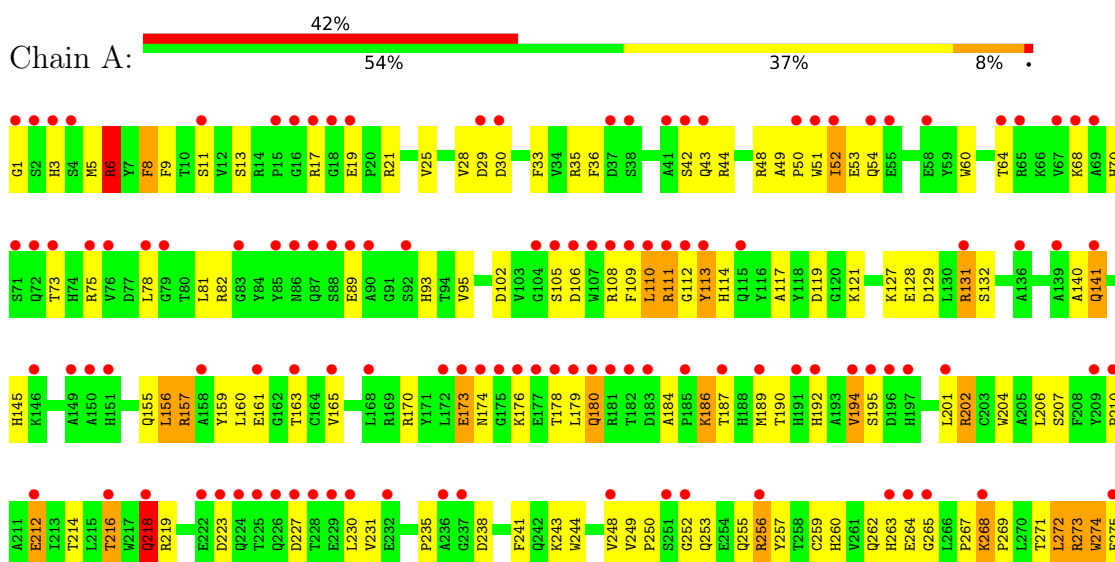
- Molecule 3 is a protein called PROTEIN (HIV-RT VARIANT PEPTIDE I1F (FLKEPVHGV)).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			73	49	12	12			
3	F	9	Total	C	N	O	0	0	0
			73	49	12	12			

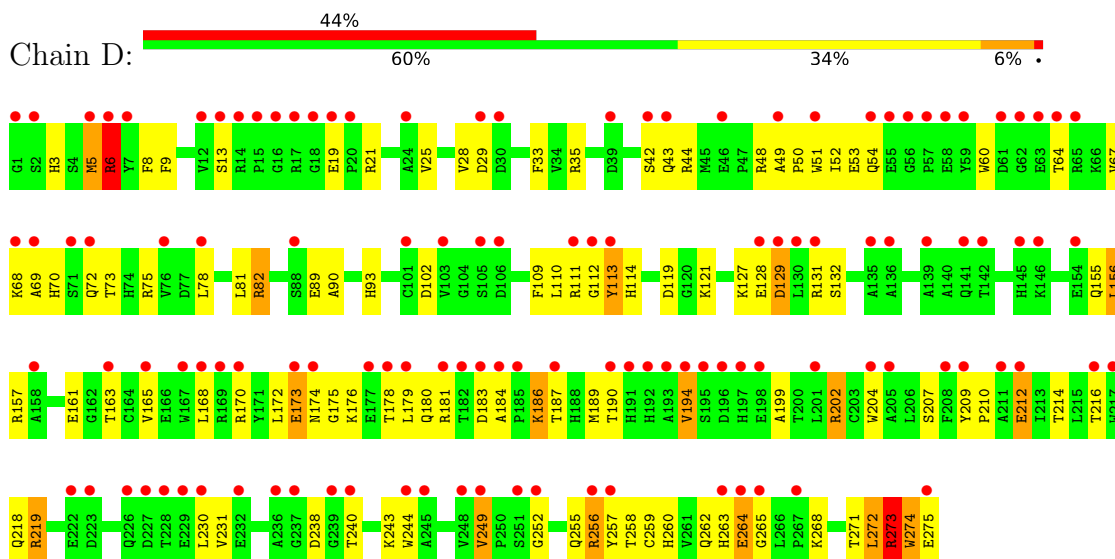
3 Residue-property plots [i](#)

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.

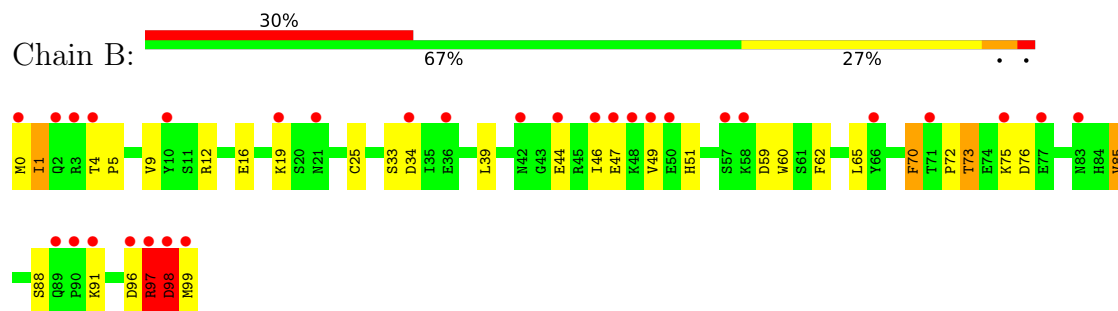
- Molecule 1: PROTEIN (CLASS I HISTOCOMPATIBILITY ANTIGEN, GOGO-A0201 ALPHA CHAIN)



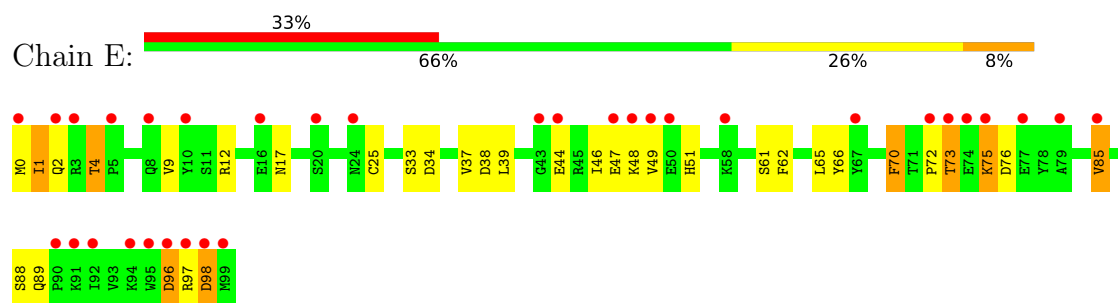
- Molecule 1: PROTEIN (CLASS I HISTOCOMPATIBILITY ANTIGEN, GOGO-A0201 ALPHA CHAIN)



- Molecule 2: PROTEIN (BETA 2-MICROGLOBULIN)



- Molecule 2: PROTEIN (BETA 2-MICROGLOBULIN)



- Molecule 3: PROTEIN (HIV-RT VARIANT PEPTIDE I1F (FLKEPVHGV))



- Molecule 3: PROTEIN (HIV-RT VARIANT PEPTIDE I1F (FLKEPVHGV))



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.57Å 62.97Å 74.56Å 82.09° 76.47° 77.78°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (15.00-2.80) 98.1 (15.00-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.16Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.260 , 0.315 0.296 , 0.304	Depositor DCC
R_{free} test set	3615 reflections (8.20%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	6311	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.66	0/2312	1.75	38/3137 (1.2%)
1	D	0.66	0/2311	1.69	27/3137 (0.9%)
2	B	0.68	0/859	1.79	15/1162 (1.3%)
2	E	0.63	0/859	1.77	17/1162 (1.5%)
3	C	0.72	0/75	1.46	0/99
3	F	0.77	0/75	1.33	0/99
All	All	0.66	0/6491	1.73	97/8796 (1.1%)

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	2
1	D	0	1
2	B	1	0
All	All	1	3

There are no bond length outliers.

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ARG	NE-CZ-NH2	13.92	131.72	119.20
1	D	256	ARG	NE-CZ-NH2	13.03	130.92	119.20
1	A	256	ARG	CG-CD-NE	12.27	139.00	112.00
2	B	44	GLU	OE1-CD-OE2	-11.27	95.86	122.90
2	E	44	GLU	OE1-CD-OE2	-10.69	97.23	122.90
1	A	256	ARG	NH1-CZ-NH2	-9.92	106.40	119.30
2	B	34	ASP	CA-CB-CG	9.49	122.09	112.60
2	E	44	GLU	CG-CD-OE2	9.49	140.22	118.40
2	B	44	GLU	CG-CD-OE1	9.44	140.11	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	85	VAL	CB-CA-C	-9.26	99.91	112.04
2	E	2	GLN	OE1-CD-NE2	-9.21	113.39	122.60
2	B	75	LYS	N-CA-C	8.41	120.22	111.14
2	B	85	VAL	CB-CA-C	-8.31	101.15	112.04
1	D	6	ARG	NE-CZ-NH1	-8.21	113.29	121.50
1	A	111	ARG	CA-C-N	8.19	127.22	121.65
1	A	111	ARG	C-N-CA	8.19	127.22	121.65
1	D	5	MET	CA-C-O	-8.02	111.69	120.36
1	A	6	ARG	NE-CZ-NH1	-7.99	113.51	121.50
2	E	34	ASP	CA-CB-CG	7.93	120.53	112.60
2	B	98	ASP	CA-CB-CG	7.71	120.31	112.60
2	E	85	VAL	N-CA-CB	7.48	119.82	110.47
1	D	256	ARG	NH1-CZ-NH2	-7.47	109.59	119.30
2	B	98	ASP	CA-C-O	-7.44	111.42	119.97
2	E	75	LYS	N-CA-C	7.32	119.05	111.14
2	E	47	GLU	N-CA-C	7.21	118.79	111.07
1	A	5	MET	CA-C-O	-7.19	112.61	120.30
2	B	85	VAL	N-CA-CB	7.11	119.36	110.47
2	E	38	ASP	CA-CB-CG	6.98	119.58	112.60
1	A	157	ARG	CA-C-O	6.74	127.69	120.55
1	A	131	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	D	219	ARG	CD-NE-CZ	6.66	133.72	124.40
1	A	192	HIS	CA-C-O	-6.61	113.23	120.30
1	A	173	GLU	OE1-CD-OE2	-6.58	107.10	122.90
1	A	180	GLN	OE1-CD-NE2	6.57	129.17	122.60
1	D	129	ASP	CA-CB-CG	6.56	119.16	112.60
1	D	256	ARG	CG-CD-NE	6.32	125.89	112.00
1	A	274	TRP	CA-C-O	-6.27	113.46	120.54
1	A	129	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	173	GLU	CG-CD-OE2	6.22	132.72	118.40
2	B	47	GLU	N-CA-C	6.22	117.73	111.07
1	A	252	GLY	N-CA-C	-6.17	106.57	115.27
1	A	140	ALA	CA-C-O	6.17	127.06	119.97
1	A	173	GLU	CB-CG-CD	6.15	123.06	112.60
1	A	202	ARG	CD-NE-CZ	6.12	132.97	124.40
1	D	173	GLU	CG-CD-OE2	6.08	132.40	118.40
1	D	6	ARG	CD-NE-CZ	-5.99	116.01	124.40
2	E	4	THR	CA-C-O	5.95	125.19	120.19
1	D	181	ARG	NE-CZ-NH2	5.94	124.54	119.20
1	D	249	VAL	N-CA-C	5.82	114.54	107.61
2	E	98	ASP	CA-C-O	-5.80	114.40	120.55
1	A	273	ARG	CA-C-O	-5.80	114.49	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	21	ARG	CD-NE-CZ	5.79	132.50	124.40
1	A	206	LEU	CA-C-N	5.77	131.02	122.82
1	A	206	LEU	C-N-CA	5.77	131.02	122.82
1	A	52	ILE	CA-C-O	5.75	123.96	118.90
1	D	173	GLU	OE1-CD-OE2	-5.74	109.14	122.90
1	D	172	LEU	CA-C-O	-5.71	114.79	120.90
1	D	274	TRP	CA-C-O	-5.71	114.18	120.69
1	A	6	ARG	CD-NE-CZ	-5.62	116.53	124.40
1	D	69	ALA	N-CA-C	-5.57	104.90	110.97
1	A	8	PHE	CA-CB-CG	-5.57	108.23	113.80
2	E	98	ASP	O-C-N	5.49	127.93	122.12
2	B	97	ARG	NH1-CZ-NH2	5.47	126.41	119.30
2	E	48	LYS	CA-C-O	-5.40	115.88	122.41
1	A	235	PRO	CA-C-O	5.38	127.77	121.31
1	D	244	TRP	CA-C-O	5.38	127.48	121.40
2	B	97	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	D	82	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	D	6	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	235	PRO	O-C-N	-5.30	116.74	123.10
1	A	21	ARG	CD-NE-CZ	5.29	131.81	124.40
1	D	202	ARG	CD-NE-CZ	5.26	131.77	124.40
1	A	6	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	244	TRP	CA-C-O	5.22	126.97	121.33
1	D	90	ALA	CA-C-O	-5.21	113.64	119.79
2	E	2	GLN	CA-C-O	5.21	127.50	120.47
1	A	145	HIS	CA-CB-CG	-5.20	108.60	113.80
1	D	264	GLU	CA-C-N	5.17	130.00	120.79
1	D	264	GLU	C-N-CA	5.17	130.00	120.79
1	D	273	ARG	CA-C-O	-5.17	115.20	120.99
1	A	267	PRO	N-CA-C	-5.15	106.83	113.57
1	A	114	HIS	CA-CB-CG	-5.13	108.67	113.80
1	D	249	VAL	N-CA-CB	-5.12	106.94	112.37
1	A	17	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	A	218	GLN	CA-CB-CG	5.10	124.29	114.10
1	A	248	VAL	N-CA-CB	5.08	116.79	111.00
2	E	2	GLN	CG-CD-NE2	5.07	124.01	116.40
2	E	96	ASP	CA-CB-CG	5.07	117.67	112.60
1	D	168	LEU	N-CA-C	-5.06	105.67	111.14
1	D	252	GLY	N-CA-C	-5.06	108.14	115.27
2	B	91	LYS	CA-CB-CG	5.05	124.21	114.10
2	B	97	ARG	CD-NE-CZ	-5.05	117.33	124.40
2	E	61	SER	CB-CA-C	5.05	118.75	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	PHE	N-CA-CB	5.04	119.27	110.81
2	B	1	ILE	CA-CB-CG2	5.03	119.06	110.50
2	B	5	PRO	CB-CA-C	-5.02	105.38	111.46
1	A	141	GLN	CG-CD-NE2	-5.02	108.87	116.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	ILE	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	GLY	Mainchain
1	A	218	GLN	Mainchain
1	D	112	GLY	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	2247	0	2096	92	0
1	D	2246	0	2096	91	0
2	B	836	0	803	24	0
2	E	836	0	803	26	0
3	C	73	0	76	10	0
3	F	73	0	76	13	0
All	All	6311	0	5950	215	0

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 18.

All (215) 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)
1:D:93:HIS:CD2	2:E:0:MET:HE1	1.96	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:HIS:CD2	2:E:0:MET:CE	2.46	0.97
1:D:6:ARG:HH12	1:D:113:TYR:HE1	1.15	0.94
1:D:35:ARG:HH12	1:D:48:ARG:NH1	1.67	0.93
1:D:263:HIS:HD2	1:D:265:GLY:H	1.15	0.91
1:A:219:ARG:HD2	1:A:256:ARG:HH11	1.35	0.90
1:A:35:ARG:HH12	1:A:48:ARG:NH1	1.69	0.90
1:A:6:ARG:HH12	1:A:113:TYR:HE1	1.18	0.89
1:D:93:HIS:NE2	2:E:0:MET:HE1	1.88	0.87
1:A:93:HIS:CD2	2:B:0:MET:CE	2.57	0.87
1:A:263:HIS:HD2	1:A:265:GLY:H	1.23	0.83
1:D:263:HIS:CD2	1:D:265:GLY:H	1.96	0.82
1:A:238:ASP:HB3	2:B:12:ARG:HD3	1.63	0.81
1:A:93:HIS:CD2	2:B:0:MET:HE2	2.14	0.80
1:A:204:TRP:HZ2	2:B:98:ASP:O	1.63	0.80
1:D:204:TRP:HZ2	2:E:98:ASP:O	1.63	0.80
1:A:263:HIS:CD2	1:A:265:GLY:H	2.00	0.80
1:D:259:CYS:HB3	1:D:272:LEU:HD12	1.65	0.77
1:D:93:HIS:NE2	2:E:0:MET:CE	2.48	0.77
1:D:93:HIS:CD2	2:E:0:MET:HE2	2.19	0.76
2:B:73:THR:HG22	2:B:76:ASP:H	1.49	0.76
1:D:35:ARG:NH1	1:D:48:ARG:NH1	2.34	0.75
1:A:93:HIS:NE2	2:B:0:MET:HE1	2.03	0.73
1:A:35:ARG:NH1	1:A:48:ARG:NH1	2.36	0.73
1:A:259:CYS:HB3	1:A:272:LEU:HD12	1.70	0.73
1:D:249:VAL:HG22	1:D:257:TYR:CE2	2.24	0.73
1:A:6:ARG:NH1	1:A:113:TYR:HE1	1.88	0.72
2:E:73:THR:HG22	2:E:76:ASP:H	1.55	0.72
1:A:93:HIS:CD2	2:B:0:MET:HE1	2.25	0.71
1:D:6:ARG:NH1	1:D:113:TYR:HE1	1.88	0.71
1:A:6:ARG:NH1	1:A:113:TYR:CE1	2.58	0.70
2:E:73:THR:CG2	2:E:76:ASP:H	2.05	0.69
1:D:6:ARG:NH1	1:D:113:TYR:CE1	2.58	0.68
1:D:156:LEU:HD13	3:F:3:LYS:HZ2	1.59	0.68
2:B:73:THR:CG2	2:B:76:ASP:H	2.06	0.68
1:D:238:ASP:HB3	2:E:12:ARG:HD3	1.78	0.66
1:D:93:HIS:HD2	2:E:0:MET:HE2	1.61	0.66
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.77	0.65
1:A:73:THR:HG21	3:C:6:VAL:HG12	1.79	0.65
1:A:93:HIS:HD2	2:B:0:MET:HE2	1.59	0.65
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.79	0.65
1:D:73:THR:HG21	3:F:6:VAL:HG12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:HD2	1:A:256:ARG:NH1	2.10	0.64
1:A:70:HIS:CE1	3:C:6:VAL:HG21	2.32	0.64
2:B:96:ASP:CG	2:B:99:MET:HG2	2.22	0.64
1:D:93:HIS:HD2	1:D:119:ASP:OD2	1.82	0.62
1:D:156:LEU:HD13	3:F:3:LYS:NZ	2.14	0.62
1:A:42:SER:O	1:A:43:GLN:HB2	1.98	0.62
1:A:110:LEU:HG	1:A:111:ARG:HH21	1.64	0.62
1:A:6:ARG:HH11	1:A:6:ARG:CG	2.13	0.61
1:D:131:ARG:NH1	1:D:157:ARG:HH12	1.96	0.61
1:D:19:GLU:OE1	1:D:75:ARG:NE	2.34	0.61
1:D:70:HIS:CE1	3:F:6:VAL:HG21	2.35	0.61
1:A:19:GLU:OE1	1:A:75:ARG:NE	2.34	0.61
1:D:218:GLN:NE2	1:D:260:HIS:NE2	2.47	0.61
1:D:121:LYS:HG3	2:E:1:ILE:HD12	1.81	0.61
1:D:155:GLN:NE2	3:F:5:PRO:HD2	2.17	0.59
1:A:250:PRO:O	1:A:253:GLN:HB2	2.02	0.59
1:D:54:GLN:HE22	1:D:174:ASN:HB3	1.67	0.59
1:A:230:LEU:HD11	1:A:243:LYS:HE2	1.85	0.59
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.38	0.59
1:A:64:THR:O	1:A:68:LYS:HG2	2.03	0.59
1:D:119:ASP:OD2	2:E:0:MET:HE2	2.03	0.59
2:B:70:PHE:CZ	2:B:72:PRO:HG3	2.39	0.58
1:D:6:ARG:HH11	1:D:6:ARG:CG	2.15	0.58
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.87	0.58
1:A:93:HIS:NE2	2:B:0:MET:CE	2.65	0.58
1:A:218:GLN:NE2	1:A:260:HIS:NE2	2.52	0.58
1:D:42:SER:O	1:D:43:GLN:HB2	2.04	0.57
3:F:3:LYS:CG	3:F:4:GLU:N	2.67	0.57
1:A:268:LYS:HG2	1:A:269:PRO:HD2	1.86	0.57
1:A:170:ARG:HG2	1:A:174:ASN:ND2	2.20	0.56
2:E:46:ILE:O	2:E:49:VAL:HG23	2.05	0.56
1:D:64:THR:O	1:D:68:LYS:HG2	2.05	0.56
1:A:249:VAL:HG22	1:A:257:TYR:CE2	2.40	0.56
1:A:274:TRP:O	1:A:275:GLU:HB3	2.06	0.56
2:B:46:ILE:O	2:B:49:VAL:HG23	2.06	0.56
1:D:13:SER:HB3	1:D:78:LEU:HD13	1.88	0.56
1:D:51:TRP:CZ2	1:D:179:LEU:HD11	2.40	0.56
1:A:170:ARG:HG2	1:A:174:ASN:HD22	1.70	0.55
2:E:73:THR:HG23	2:E:75:LYS:H	1.71	0.55
2:E:70:PHE:CZ	2:E:72:PRO:HG3	2.41	0.55
1:A:131:ARG:NH1	1:A:157:ARG:HH12	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ARG:NH2	1:A:113:TYR:OH	2.39	0.54
1:A:184:ALA:HB2	1:A:265:GLY:O	2.08	0.54
1:D:184:ALA:HB2	1:D:265:GLY:O	2.08	0.54
1:D:263:HIS:HD2	1:D:265:GLY:N	1.96	0.53
3:C:3:LYS:CG	3:C:4:GLU:N	2.71	0.53
1:A:260:HIS:CE1	1:A:271:THR:HG23	2.44	0.53
1:A:54:GLN:HE22	1:A:174:ASN:HB3	1.73	0.53
2:E:51:HIS:HA	2:E:65:LEU:O	2.09	0.53
1:A:156:LEU:HD13	3:C:3:LYS:NZ	2.25	0.52
2:B:51:HIS:HA	2:B:65:LEU:O	2.10	0.52
1:D:259:CYS:HB3	1:D:272:LEU:CD1	2.37	0.52
1:D:6:ARG:NH1	1:D:6:ARG:CG	2.72	0.52
1:D:157:ARG:O	1:D:161:GLU:HB2	2.10	0.52
1:D:219:ARG:HD3	1:D:257:TYR:CZ	2.45	0.51
1:A:156:LEU:HD13	3:C:3:LYS:HZ2	1.74	0.51
1:D:6:ARG:NH2	1:D:113:TYR:OH	2.41	0.51
1:A:102:ASP:OD1	1:A:113:TYR:OH	2.28	0.51
1:A:119:ASP:OD2	2:B:0:MET:HE2	2.10	0.51
1:A:127:LYS:HG2	1:A:132:SER:O	2.11	0.51
1:A:9:PHE:CE2	1:A:70:HIS:HD2	2.28	0.51
1:A:6:ARG:NH1	1:A:6:ARG:CG	2.72	0.51
1:D:110:LEU:HG	1:D:111:ARG:HH21	1.76	0.51
1:D:170:ARG:HG2	1:D:174:ASN:HD22	1.76	0.51
1:D:35:ARG:NH1	1:D:48:ARG:HH11	2.09	0.50
1:D:156:LEU:HA	3:F:3:LYS:HZ2	1.76	0.50
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.47	0.50
1:A:109:PHE:CD1	1:A:161:GLU:HA	2.47	0.50
1:D:189:MET:HA	1:D:202:ARG:O	2.11	0.50
1:D:204:TRP:CZ2	2:E:98:ASP:O	2.55	0.50
3:F:3:LYS:HG3	3:F:4:GLU:N	2.26	0.49
1:D:109:PHE:CD1	1:D:161:GLU:HA	2.47	0.49
1:A:3:HIS:ND1	1:A:29:ASP:OD2	2.38	0.49
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.95	0.49
1:A:28:VAL:HG23	1:A:33:PHE:CD2	2.47	0.49
1:A:70:HIS:HE1	3:C:3:LYS:O	1.95	0.49
1:D:183:ASP:N	1:D:209:TYR:O	2.45	0.49
2:E:73:THR:O	2:E:97:ARG:NH2	2.46	0.49
2:E:33:SER:HB3	2:E:62:PHE:CE2	2.48	0.49
1:D:28:VAL:HG23	1:D:33:PHE:CD1	2.48	0.48
1:D:8:PHE:HB2	1:D:25:VAL:HG22	1.96	0.48
1:A:6:ARG:NH1	1:A:6:ARG:HG2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ARG:HA	1:D:64:THR:HG23	1.94	0.48
1:D:129:ASP:HB2	1:D:131:ARG:HH21	1.79	0.48
1:A:35:ARG:HH12	1:A:48:ARG:HH11	1.54	0.48
1:A:187:THR:HA	1:A:204:TRP:O	2.13	0.48
1:A:263:HIS:HD2	1:A:265:GLY:N	2.02	0.48
1:D:9:PHE:CE1	1:D:70:HIS:HD2	2.31	0.48
1:D:6:ARG:NH1	1:D:6:ARG:HG2	2.29	0.48
1:A:189:MET:HA	1:A:202:ARG:O	2.13	0.47
1:D:70:HIS:CE1	3:F:6:VAL:CG2	2.97	0.47
1:D:102:ASP:OD1	1:D:113:TYR:OH	2.32	0.47
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.14	0.47
1:D:274:TRP:O	1:D:275:GLU:CB	2.61	0.47
1:A:106:ASP:OD1	1:A:108:ARG:HB2	2.15	0.47
1:D:3:HIS:ND1	1:D:29:ASP:OD2	2.40	0.47
1:D:70:HIS:ND1	3:F:6:VAL:HG21	2.30	0.47
1:D:170:ARG:HG2	1:D:174:ASN:ND2	2.30	0.47
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.49	0.47
2:E:17:ASN:HD21	2:E:97:ARG:HH12	1.62	0.47
1:A:35:ARG:NH1	1:A:48:ARG:HH11	2.08	0.47
1:A:214:THR:HB	1:A:262:GLN:HB2	1.96	0.47
1:D:35:ARG:HH12	1:D:48:ARG:HH11	1.56	0.47
1:D:258:THR:HG22	1:D:273:ARG:HG3	1.96	0.46
1:A:44:ARG:HH21	1:A:60:TRP:HB3	1.80	0.46
1:D:187:THR:HA	1:D:204:TRP:O	2.14	0.46
1:A:157:ARG:O	1:A:161:GLU:HB2	2.15	0.46
1:A:70:HIS:ND1	3:C:6:VAL:HG21	2.31	0.46
1:D:72:GLN:OE1	1:D:75:ARG:NH1	2.48	0.46
1:D:214:THR:HB	1:D:262:GLN:HB2	1.97	0.46
2:E:96:ASP:O	2:E:97:ARG:C	2.59	0.45
1:A:155:GLN:NE2	3:C:5:PRO:HD2	2.31	0.45
1:D:190:THR:OG1	1:D:202:ARG:HB3	2.17	0.44
1:A:121:LYS:HG3	2:B:1:ILE:CD1	2.46	0.44
1:D:64:THR:HA	1:D:67:VAL:HG12	1.99	0.44
2:E:73:THR:HG23	2:E:75:LYS:N	2.31	0.44
1:A:82:ARG:NH2	1:A:89:GLU:OE1	2.50	0.44
3:C:3:LYS:HG3	3:C:4:GLU:N	2.33	0.43
1:D:82:ARG:NH2	1:D:89:GLU:OE1	2.50	0.43
1:A:176:LYS:HA	1:A:180:GLN:HE21	1.84	0.43
2:B:96:ASP:O	2:B:99:MET:N	2.51	0.43
1:A:50:PRO:HA	1:A:53:GLU:OE1	2.19	0.43
1:D:49:ALA:O	1:D:52:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ARG:HH11	1:D:170:ARG:HD2	1.67	0.43
1:A:231:VAL:O	1:A:243:LYS:HE3	2.19	0.43
1:A:186:LYS:HD3	1:A:207:SER:OG	2.19	0.43
1:A:259:CYS:HB3	1:A:272:LEU:CD1	2.43	0.43
1:D:186:LYS:HD3	1:D:207:SER:OG	2.19	0.43
1:A:9:PHE:CE2	1:A:70:HIS:CD2	3.06	0.42
1:D:231:VAL:O	1:D:243:LYS:HE3	2.19	0.42
1:D:54:GLN:NE2	1:D:174:ASN:HB3	2.34	0.42
1:D:78:LEU:HD23	1:D:78:LEU:HA	1.95	0.42
1:D:176:LYS:HA	1:D:180:GLN:HE21	1.85	0.42
2:B:16:GLU:OE1	2:B:19:LYS:HD2	2.19	0.42
1:A:119:ASP:HB3	2:B:0:MET:HG2	2.01	0.42
1:A:156:LEU:HA	3:C:3:LYS:HZ2	1.85	0.42
1:A:189:MET:CE	1:A:272:LEU:HB2	2.49	0.42
1:D:44:ARG:HH21	1:D:60:TRP:HB3	1.85	0.42
1:D:50:PRO:HA	1:D:53:GLU:OE1	2.20	0.42
1:D:212:GLU:OE1	1:D:212:GLU:HA	2.18	0.42
2:B:73:THR:O	2:B:97:ARG:NH2	2.52	0.42
1:D:210:PRO:O	1:D:263:HIS:HE1	2.02	0.42
2:E:37:VAL:HB	2:E:66:TYR:CZ	2.55	0.42
1:A:216:THR:HG23	1:A:223:ASP:OD1	2.20	0.42
1:D:230:LEU:HD11	1:D:243:LYS:HE2	2.02	0.42
1:A:28:VAL:HG23	1:A:33:PHE:CE2	2.55	0.42
1:A:8:PHE:HB2	1:A:25:VAL:HG22	2.02	0.41
1:D:114:HIS:CD2	1:D:156:LEU:HD21	2.54	0.41
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.55	0.41
1:A:159:TYR:CD2	1:A:160:LEU:HD23	2.55	0.41
1:D:127:LYS:HG2	1:D:132:SER:O	2.21	0.41
3:F:3:LYS:HG3	3:F:4:GLU:H	1.85	0.41
1:A:44:ARG:HA	1:A:64:THR:HG23	2.01	0.41
2:E:73:THR:HG22	2:E:76:ASP:N	2.28	0.41
1:A:30:ASP:HB3	1:A:241:PHE:CZ	2.56	0.41
1:D:155:GLN:HE21	3:F:5:PRO:HD2	1.85	0.41
1:A:54:GLN:NE2	1:A:174:ASN:HB3	2.34	0.41
1:A:210:PRO:O	1:A:263:HIS:HE1	2.02	0.41
1:A:212:GLU:OE1	1:A:212:GLU:HA	2.21	0.41
1:D:260:HIS:CE1	1:D:271:THR:HG23	2.56	0.41
1:D:70:HIS:HE1	3:F:3:LYS:O	2.03	0.41
2:E:89:GLN:HE21	2:E:89:GLN:HB3	1.53	0.41
1:A:1:GLY:O	1:A:105:SER:HA	2.21	0.40
1:A:78:LEU:CD2	1:A:95:VAL:HG23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:PHE:CE1	1:D:70:HIS:CD2	3.09	0.40
1:D:194:VAL:HG13	1:D:199:ALA:HA	2.03	0.40
1:A:194:VAL:CG2	1:A:195:SER:N	2.85	0.40
1:A:219:ARG:HD3	1:A:257:TYR:CZ	2.57	0.40
1:D:175:GLY:O	1:D:176:LYS:C	2.64	0.40
1:A:28:VAL:O	1:A:29:ASP:HB2	2.21	0.40
1:A:49:ALA:O	1:A:52:ILE:HG22	2.21	0.40
2:B:59:ASP:O	2:B:60:TRP:HB2	2.21	0.40
1:D:238:ASP:OD1	1:D:240:THR:OG1	2.35	0.40

There are no symmetry-related clashes.

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%)	262 (96%)	11 (4%)	0	100	100
1	D	273/275 (99%)	261 (96%)	12 (4%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	E	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	756/768 (98%)	727 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	208 (90%)	23 (10%)	7	24
1	D	231/231 (100%)	211 (91%)	20 (9%)	9	30
2	B	95/95 (100%)	87 (92%)	8 (8%)	10	32
2	E	95/95 (100%)	88 (93%)	7 (7%)	13	37
3	C	8/8 (100%)	8 (100%)	0	100	100
3	F	8/8 (100%)	8 (100%)	0	100	100
All	All	668/668 (100%)	610 (91%)	58 (9%)	9	30

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	11	SER
1	A	81	LEU
1	A	110	LEU
1	A	113	TYR
1	A	128	GLU
1	A	141	GLN
1	A	156	LEU
1	A	163	THR
1	A	165	VAL
1	A	173	GLU
1	A	178	THR
1	A	186	LYS
1	A	194	VAL
1	A	201	LEU
1	A	212	GLU
1	A	216	THR
1	A	227	ASP
1	A	255	GLN
1	A	264	GLU
1	A	268	LYS
1	A	272	LEU
1	A	273	ARG
2	B	4	THR
2	B	9	VAL
2	B	70	PHE
2	B	73	THR

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Mol	Chain	Res	Type
2	B	85	VAL
2	B	88	SER
2	B	97	ARG
2	B	98	ASP
1	D	5	MET
1	D	6	ARG
1	D	81	LEU
1	D	113	TYR
1	D	128	GLU
1	D	156	LEU
1	D	163	THR
1	D	165	VAL
1	D	173	GLU
1	D	178	THR
1	D	186	LYS
1	D	194	VAL
1	D	212	GLU
1	D	216	THR
1	D	255	GLN
1	D	256	ARG
1	D	264	GLU
1	D	268	LYS
1	D	272	LEU
1	D	273	ARG
2	E	1	ILE
2	E	4	THR
2	E	9	VAL
2	E	70	PHE
2	E	73	THR
2	E	85	VAL
2	E	88	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	70	HIS
1	A	93	HIS
1	A	174	ASN
1	A	180	GLN
1	A	218	GLN
1	A	262	GLN

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Mol	Chain	Res	Type
1	A	263	HIS
2	B	2	GLN
2	B	89	GLN
1	D	54	GLN
1	D	93	HIS
1	D	155	GLN
1	D	174	ASN
1	D	180	GLN
1	D	192	HIS
1	D	218	GLN
1	D	262	GLN
1	D	263	HIS
2	E	13	HIS
2	E	89	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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	275/275 (100%)	2.01	115 (41%) 0 0	29, 43, 45, 49	0
1	D	275/275 (100%)	1.98	121 (44%) 0 0	29, 43, 45, 51	0
2	B	100/100 (100%)	1.75	30 (30%) 1 1	31, 43, 45, 50	0
2	E	100/100 (100%)	1.84	33 (33%) 1 1	31, 43, 45, 54	0
3	C	9/9 (100%)	1.37	2 (22%) 2 1	35, 43, 44, 44	0
3	F	9/9 (100%)	1.80	2 (22%) 2 1	35, 43, 44, 44	0
All	All	768/768 (100%)	1.93	303 (39%) 1 0	29, 43, 45, 54	0

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	58	GLU	7.8
1	A	105	SER	7.6
1	D	196	ASP	6.5
2	E	99	MET	6.4
1	A	106	ASP	6.3
1	D	183	ASP	6.1
1	A	104	GLY	5.8
1	A	183	ASP	5.4
2	B	99	MET	5.4
1	A	54	GLN	5.4
1	A	223	ASP	5.4
1	A	58	GLU	5.3
1	D	69	ALA	5.1
1	A	113	TYR	5.0
1	D	193	ALA	5.0
1	A	251	SER	4.9
1	A	182	THR	4.9
1	A	1	GLY	4.8
1	A	136	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	184	ALA	4.7
2	E	47	GLU	4.7
1	D	18	GLY	4.6
1	A	51	TRP	4.6
1	D	182	THR	4.5
1	A	17	ARG	4.5
1	A	222	GLU	4.5
1	D	54	GLN	4.4
1	A	192	HIS	4.4
1	A	173	GLU	4.3
1	A	16	GLY	4.2
1	D	223	ASP	4.2
1	D	17	ARG	4.1
1	D	192	HIS	4.1
1	A	237	GLY	4.1
1	D	72	GLN	4.0
1	D	88	SER	4.0
2	B	48	LYS	3.9
1	A	18	GLY	3.9
1	D	195	SER	3.9
1	D	275	GLU	3.8
1	A	150	ALA	3.8
2	B	98	ASP	3.8
1	D	248	VAL	3.8
1	D	251	SER	3.7
1	A	225	THR	3.7
1	A	212	GLU	3.7
2	B	96	ASP	3.7
2	E	77	GLU	3.7
2	E	20	SER	3.6
1	A	29	ASP	3.6
1	A	69	ALA	3.5
1	A	131	ARG	3.5
1	D	1	GLY	3.5
2	E	98	ASP	3.5
1	D	15	PRO	3.5
1	A	174	ASN	3.5
1	D	128	GLU	3.5
1	D	141	GLN	3.5
1	D	226	GLN	3.5
2	E	44	GLU	3.5
1	A	50	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	178	THR	3.5
2	B	89	GLN	3.4
1	A	108	ARG	3.4
1	A	196	ASP	3.4
3	F	1	PHE	3.4
1	D	239	GLY	3.4
1	D	191	HIS	3.4
1	D	56	GLY	3.4
1	A	264	GLU	3.4
2	B	34	ASP	3.4
1	A	111	ARG	3.3
1	A	224	GLN	3.3
1	A	79	GLY	3.3
2	B	97	ARG	3.3
1	A	88	SER	3.3
1	A	107	TRP	3.3
1	D	65	ARG	3.3
1	D	59	TYR	3.3
1	A	15	PRO	3.3
1	D	185	PRO	3.3
1	D	174	ASN	3.3
2	B	0	MET	3.2
1	D	14	ARG	3.2
1	A	252	GLY	3.2
1	A	185	PRO	3.2
2	E	2	GLN	3.2
1	A	175	GLY	3.2
1	D	55	GLU	3.1
1	A	141	GLN	3.1
2	B	44	GLU	3.1
1	A	41	ALA	3.1
1	D	263	HIS	3.1
1	D	194	VAL	3.1
2	E	91	LYS	3.1
1	D	113	TYR	3.1
1	A	265	GLY	3.1
1	D	265	GLY	3.1
1	A	90	ALA	3.0
2	B	83	ASN	3.0
1	D	158	ALA	3.0
1	A	226	GLN	3.0
1	D	30	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	47	GLU	3.0
1	A	68	LYS	3.0
1	A	172	LEU	2.9
2	B	42	ASN	2.9
1	A	2	SER	2.9
1	D	39	ASP	2.9
1	D	245	ALA	2.9
1	A	109	PHE	2.9
1	A	65	ARG	2.9
1	D	131	ARG	2.9
1	D	19	GLU	2.9
2	E	96	ASP	2.9
1	D	190	THR	2.9
2	E	97	ARG	2.9
1	D	229	GLU	2.9
1	A	3	HIS	2.9
1	A	275	GLU	2.8
2	B	77	GLU	2.8
1	D	216	THR	2.8
1	A	72	GLN	2.8
2	B	75	LYS	2.8
1	D	177	GLU	2.8
1	D	249	VAL	2.8
1	D	64	THR	2.8
1	A	165	VAL	2.8
1	D	169	ARG	2.8
1	A	71	SER	2.8
1	A	75	ARG	2.8
1	D	236	ALA	2.8
2	E	58	LYS	2.8
1	A	161	GLU	2.7
1	A	86	ASN	2.7
1	D	252	GLY	2.7
2	E	16	GLU	2.7
1	D	197	HIS	2.7
1	A	176	LYS	2.7
2	E	75	LYS	2.7
1	A	194	VAL	2.7
1	D	49	ALA	2.7
1	D	167	TRP	2.7
2	E	95	TRP	2.7
2	E	3	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	37	ASP	2.7
1	A	232	GLU	2.7
2	E	8	GLN	2.7
1	D	165	VAL	2.7
1	A	268	LYS	2.7
1	A	216	THR	2.7
2	E	43	GLY	2.7
1	A	110	LEU	2.7
1	D	68	LYS	2.6
1	D	7	TYR	2.6
1	D	101	CYS	2.6
1	D	181	ARG	2.6
1	D	57	PRO	2.6
2	B	58	LYS	2.6
1	A	230	LEU	2.6
1	A	112	GLY	2.6
1	D	163	THR	2.6
1	D	187	THR	2.6
1	D	146	LYS	2.6
1	A	78	LEU	2.6
1	D	228	THR	2.6
1	A	11	SER	2.5
1	D	42	SER	2.5
1	D	20	PRO	2.5
1	A	89	GLU	2.5
1	D	205	ALA	2.5
1	D	111	ARG	2.5
1	D	51	TRP	2.5
1	D	237	GLY	2.5
2	E	10	TYR	2.5
1	A	228	THR	2.5
1	D	211	ALA	2.5
1	A	197	HIS	2.5
1	D	267	PRO	2.5
2	E	73	THR	2.5
2	E	79	ALA	2.5
1	D	16	GLY	2.5
1	A	229	GLU	2.5
1	A	64	THR	2.5
1	A	146	LYS	2.5
1	D	61	ASP	2.4
1	D	106	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	195	SER	2.4
1	D	170	ARG	2.4
1	D	264	GLU	2.4
1	D	136	ALA	2.4
1	A	263	HIS	2.4
1	D	78	LEU	2.4
1	D	179	LEU	2.4
2	E	0	MET	2.4
1	A	227	ASP	2.4
1	A	236	ALA	2.4
2	B	4	THR	2.4
1	A	151	HIS	2.4
1	A	189	MET	2.4
1	A	256	ARG	2.4
1	A	4	SER	2.4
1	A	19	GLU	2.4
2	B	57	SER	2.4
2	E	74	GLU	2.4
3	C	1	PHE	2.4
1	D	24	ALA	2.4
1	D	204	TRP	2.4
1	D	244	TRP	2.4
1	A	179	LEU	2.4
2	E	5	PRO	2.4
2	B	49	VAL	2.4
2	E	49	VAL	2.4
1	D	222	GLU	2.4
1	A	191	HIS	2.4
1	D	145	HIS	2.4
1	A	30	ASP	2.3
1	A	201	LEU	2.3
1	A	209	TYR	2.3
1	A	76	VAL	2.3
2	B	3	ARG	2.3
1	D	208	PHE	2.3
1	D	29	ASP	2.3
1	D	13	SER	2.3
1	D	230	LEU	2.3
2	B	91	LYS	2.3
2	E	48	LYS	2.3
1	A	248	VAL	2.3
1	D	135	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	139	ALA	2.3
1	D	71	SER	2.3
1	D	105	SER	2.3
2	B	19	LYS	2.3
1	D	142	THR	2.3
2	B	90	PRO	2.3
3	C	5	PRO	2.3
1	A	83	GLY	2.3
1	D	173	GLU	2.3
2	B	46	ILE	2.3
1	D	217	TRP	2.3
1	D	2	SER	2.3
2	B	71	THR	2.3
1	D	103	VAL	2.3
1	D	154	GLU	2.2
1	D	232	GLU	2.2
1	A	218	GLN	2.2
1	A	178	THR	2.2
2	E	85	VAL	2.2
1	D	257	TYR	2.2
2	B	66	TYR	2.2
1	D	63	GLU	2.2
1	A	181	ARG	2.2
1	A	38	SER	2.2
1	A	139	ALA	2.2
1	A	168	LEU	2.2
1	D	201	LEU	2.2
1	A	43	GLN	2.2
1	D	227	ASP	2.2
1	A	73	THR	2.2
1	D	112	GLY	2.2
1	D	130	LEU	2.2
1	A	52	ILE	2.2
1	D	6	ARG	2.2
1	A	115	GLN	2.2
1	A	67	VAL	2.2
2	E	90	PRO	2.2
2	B	50	GLU	2.2
1	A	180	GLN	2.1
2	B	2	GLN	2.1
2	B	21	ASN	2.1
2	E	72	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	129	ASP	2.1
1	D	240	THR	2.1
2	E	92	ILE	2.1
1	D	43	GLN	2.1
3	F	6	VAL	2.1
1	D	209	TYR	2.1
2	E	94	LYS	2.1
1	D	62	GLY	2.1
2	B	10	TYR	2.1
1	A	210	PRO	2.1
1	D	168	LEU	2.1
1	D	256	ARG	2.1
1	A	158	ALA	2.1
1	D	46	GLU	2.1
1	A	42	SER	2.0
1	A	87	GLN	2.0
1	D	5	MET	2.0
1	D	76	VAL	2.0
1	A	149	ALA	2.0
1	A	177	GLU	2.0
1	D	198	GLU	2.0
1	D	212	GLU	2.0
2	B	36	GLU	2.0
2	E	67	TYR	2.0
1	A	92	SER	2.0
2	E	24	ASN	2.0
1	A	163	THR	2.0
1	A	187	THR	2.0
1	A	55	GLU	2.0
2	E	50	GLU	2.0
1	A	85	TYR	2.0
1	D	12	VAL	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.