Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 02:33 AM EDT

PDB ID	:	1I1Y
Title	:	CRYSTAL STRUCTURE OF HUMAN CLASS I MHC (HLA-A2.1) COMPLEXED WITH BETA 2-MICROGLOBULIN AND HIV-RT VARIANT PEPTIDE I1Y
Authors	:	Kirksey, T.J.; Collins, E.J.
Deposited on	:	1999-04-16
Resolution	:	2.20 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 (i) 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 (1)) were used in the production of this report:

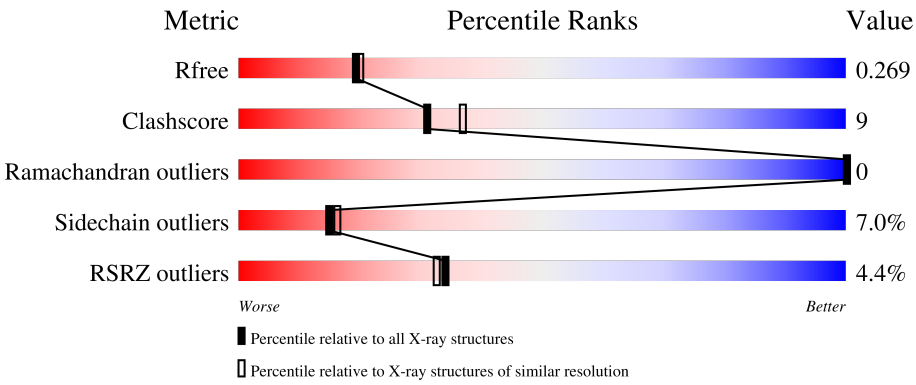
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	7% 78% 17%
1	D	275	5% 73% 23%
2	B	100	2% 73% 24%
2	E	100	% 70% 26%
3	C	9	67% 22% 11%

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Mol	Chain	Length	Quality of chain
3	F	9	67% 22% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6515 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 CLASS I HISTOCOMPATIBILITY ANTIGEN.

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

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

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

- Molecule 3 is a protein called HIV-RT VARIANT PEPTIDE I1Y (YLKEPVHGV).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	74	49	12	13	0	0	0
3	F	9	74	49	12	13	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	64	64	64	0	0
4	B	23	23	23	0	0
4	C	5	5	5	0	0
4	D	67	67	67	0	0

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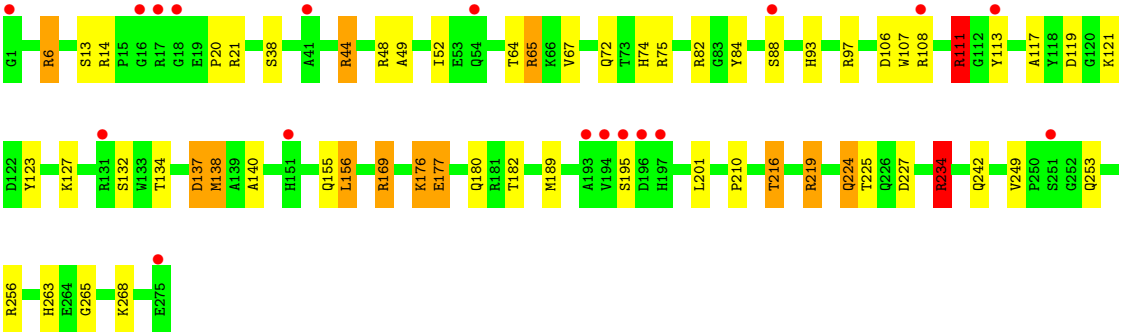
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	37	37	37	0	0
			Total	O		
4	F	3	3	3	0	0

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.

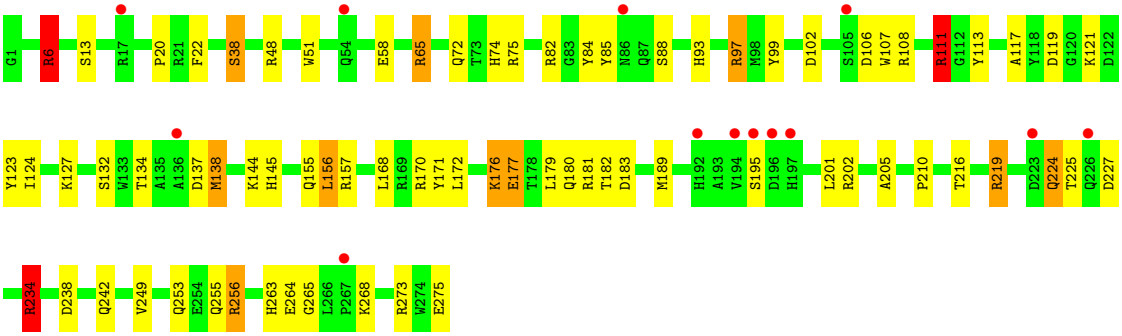
• Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN

Chain A:



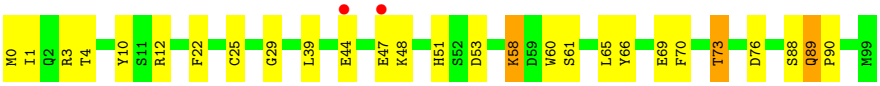
• Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN

Chain D:



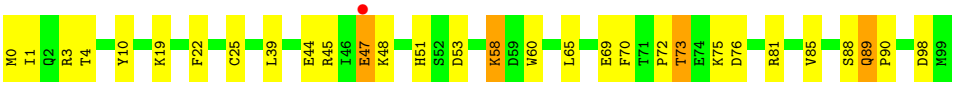
• Molecule 2: BETA 2-MICROGLOBULIN

Chain B:



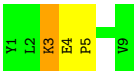
• Molecule 2: BETA 2-MICROGLOBULIN

Chain E:



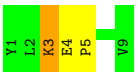
• Molecule 3: HIV-RT VARIANT PEPTIDE I1Y (YLKEPVHGV)

Chain C:



• Molecule 3: HIV-RT VARIANT PEPTIDE I1Y (YLKEPVHGV)

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.61Å 63.59Å 75.33Å 81.93° 75.94° 78.00°	Depositor
Resolution (Å)	15.00 – 2.20 29.51 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-2.20) 97.9 (29.51-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.233 , 0.289 0.231 , 0.269	Depositor DCC
R_{free} test set	3615 reflections (8.20%)	wwPDB-VP
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6515	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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	0.56	0/2312	1.66	33/3137 (1.1%)
1	D	0.62	0/2312	1.71	41/3137 (1.3%)
2	B	0.55	0/860	1.24	5/1162 (0.4%)
2	E	0.58	0/860	1.29	9/1162 (0.8%)
3	C	0.83	0/76	1.25	0/101
3	F	0.89	0/76	1.17	0/101
All	All	0.59	0/6496	1.58	88/8800 (1.0%)

There are no bond length outliers.

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	ARG	CD-NE-CZ	38.96	178.15	123.60
1	D	234	ARG	CD-NE-CZ	34.55	171.97	123.60
1	D	65	ARG	NE-CZ-NH2	20.71	130.66	120.30
1	A	6	ARG	NE-CZ-NH1	19.12	129.86	120.30
1	D	65	ARG	NE-CZ-NH1	-18.36	111.12	120.30
1	A	65	ARG	NE-CZ-NH2	17.78	129.19	120.30
1	A	108	ARG	NE-CZ-NH1	16.73	128.67	120.30
1	A	65	ARG	NE-CZ-NH1	-16.45	112.08	120.30
1	D	6	ARG	NE-CZ-NH1	15.59	128.10	120.30
1	D	219	ARG	NE-CZ-NH1	14.75	127.67	120.30
1	A	234	ARG	NE-CZ-NH2	12.45	126.52	120.30
1	D	6	ARG	NE-CZ-NH2	-10.91	114.84	120.30
1	D	111	ARG	NE-CZ-NH2	-10.89	114.86	120.30
1	D	108	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	A	219	ARG	CD-NE-CZ	10.13	137.79	123.60
1	D	219	ARG	CD-NE-CZ	9.96	137.54	123.60
1	D	6	ARG	CD-NE-CZ	9.20	136.47	123.60
1	D	157	ARG	NE-CZ-NH2	-8.95	115.83	120.30
2	E	3	ARG	NE-CZ-NH2	8.61	124.61	120.30
1	A	224	GLN	CG-CD-OE1	8.57	138.74	121.60
1	D	234	ARG	NE-CZ-NH1	8.26	124.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	82	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	169	ARG	NE-CZ-NH1	-8.05	116.28	120.30
1	D	108	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	6	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	6	ARG	CD-NE-CZ	7.96	134.74	123.60
1	A	224	GLN	OE1-CD-NE2	-7.64	104.33	121.90
1	A	111	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	D	183	ASP	CB-CG-OD2	7.47	125.02	118.30
1	D	227	ASP	CB-CG-OD2	7.33	124.90	118.30
1	D	238	ASP	CB-CG-OD1	7.32	124.89	118.30
1	D	224	GLN	CG-CD-OE1	7.31	136.23	121.60
1	A	219	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	227	ASP	CB-CG-OD2	7.21	124.79	118.30
1	A	14	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	A	138	MET	CG-SD-CE	6.90	111.23	100.20
1	D	275	GLU	OE1-CD-OE2	-6.86	115.07	123.30
1	A	44	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	D	205	ALA	N-CA-CB	6.69	119.47	110.10
1	D	123	TYR	CB-CG-CD1	-6.67	117.00	121.00
1	D	48	ARG	NE-CZ-NH1	6.59	123.60	120.30
2	B	12	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	D	170	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	E	44	GLU	OE1-CD-OE2	-6.54	115.45	123.30
2	E	3	ARG	NH1-CZ-NH2	-6.50	112.25	119.40
1	A	108	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	D	234	ARG	CG-CD-NE	6.49	125.43	111.80
1	D	181	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	106	ASP	CB-CG-OD1	6.37	124.03	118.30
1	D	224	GLN	OE1-CD-NE2	-6.37	107.26	121.90
1	D	138	MET	CG-SD-CE	6.23	110.17	100.20
1	D	189	MET	CA-CB-CG	6.07	123.62	113.30
1	A	21	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	A	82	ARG	NE-CZ-NH1	5.99	123.29	120.30
2	B	3	ARG	NE-CZ-NH2	5.97	123.29	120.30
2	B	44	GLU	OE1-CD-OE2	-5.97	116.13	123.30
1	D	58	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	A	234	ARG	NH1-CZ-NH2	-5.86	112.95	119.40
1	A	189	MET	CA-CB-CG	5.85	123.24	113.30
1	A	119	ASP	CB-CG-OD1	5.84	123.56	118.30
1	D	181	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	82	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	84	TYR	CA-CB-CG	5.74	124.30	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	202	ARG	NE-CZ-NH2	-5.73	117.44	120.30
2	E	3	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	84	TYR	CA-CB-CG	5.66	124.16	113.40
2	E	98	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	171	TYR	CB-CG-CD1	5.61	124.37	121.00
1	D	182	THR	N-CA-CB	5.57	120.88	110.30
1	D	256	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	D	234	ARG	NH1-CZ-NH2	-5.47	113.38	119.40
2	E	3	ARG	CD-NE-CZ	5.42	131.19	123.60
1	A	123	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	D	99	TYR	CA-CB-CG	5.37	123.60	113.40
1	D	219	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	B	66	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	D	82	ARG	CD-NE-CZ	5.24	130.94	123.60
1	A	48	ARG	CD-NE-CZ	5.23	130.93	123.60
1	D	97	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	E	45	ARG	NE-CZ-NH1	-5.22	117.69	120.30
2	B	53	ASP	CB-CG-OD2	5.21	122.99	118.30
2	E	53	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	137	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	182	THR	N-CA-CB	5.12	120.02	110.30
2	E	81	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	65	ARG	CD-NE-CZ	-5.08	116.49	123.60
1	A	6	ARG	NH1-CZ-NH2	-5.07	113.82	119.40
1	D	157	ARG	NH1-CZ-NH2	5.04	124.95	119.40

There are no chirality outliers.

There are no planarity outliers.

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	40	0
1	D	2247	0	2096	47	0
2	B	837	0	803	18	0
2	E	837	0	803	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	74	0	76	8	0
3	F	74	0	76	7	0
4	A	64	0	0	2	0
4	B	23	0	0	0	0
4	C	5	0	0	0	0
4	D	67	0	0	7	0
4	E	37	0	0	3	0
4	F	3	0	0	0	0
All	All	6515	0	5950	111	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 9.

All (111) 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:A:93:HIS:CD2	2:B:0:MET:HE1	1.48	1.45
1:D:93:HIS:CD2	2:E:0:MET:HE1	1.63	1.33
1:D:93:HIS:NE2	2:E:0:MET:HE1	1.55	1.21
1:A:93:HIS:NE2	2:B:0:MET:HE1	1.55	1.19
1:D:93:HIS:CD2	2:E:0:MET:CE	2.34	1.10
1:A:93:HIS:CD2	2:B:0:MET:CE	2.37	1.06
1:D:93:HIS:NE2	2:E:0:MET:CE	2.24	1.00
2:E:47:GLU:HG2	4:E:102:HOH:O	1.60	0.99
1:A:93:HIS:NE2	2:B:0:MET:CE	2.30	0.90
1:D:234:ARG:HD2	1:D:242:GLN:HB2	1.54	0.88
1:A:234:ARG:HD2	1:A:242:GLN:HB2	1.57	0.86
1:A:93:HIS:HD2	2:B:0:MET:HE1	1.40	0.85
1:D:72:GLN:HE22	1:D:75:ARG:HH11	1.27	0.82
1:A:155:GLN:HE21	3:C:3:LYS:NZ	1.83	0.76
1:A:72:GLN:HE22	1:A:75:ARG:HH11	1.32	0.75
2:E:89:GLN:HB2	2:E:90:PRO:HD2	1.70	0.74
2:E:73:THR:HG22	2:E:76:ASP:H	1.56	0.71
3:C:3:LYS:HG3	3:C:4:GLU:N	2.07	0.69
2:B:89:GLN:HB2	2:B:90:PRO:HD2	1.75	0.69
2:B:58:LYS:HD2	2:B:58:LYS:H	1.58	0.68
1:A:155:GLN:HE21	3:C:3:LYS:HZ2	1.39	0.68
1:D:155:GLN:NE2	3:F:5:PRO:HD2	2.09	0.68
1:D:263:HIS:HD2	1:D:265:GLY:H	1.41	0.67
2:E:58:LYS:H	2:E:58:LYS:HD2	1.59	0.67
1:D:93:HIS:CD2	2:E:0:MET:HE2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:LEU:HD22	1:D:249:VAL:HG21	1.75	0.67
2:B:73:THR:HG22	2:B:76:ASP:H	1.59	0.67
1:D:65:ARG:NH1	4:D:303:HOH:O	2.27	0.65
1:D:263:HIS:CD2	1:D:265:GLY:H	2.15	0.65
1:A:65:ARG:NH1	4:A:329:HOH:O	2.29	0.65
2:E:75:LYS:HA	4:E:127:HOH:O	1.97	0.64
1:A:263:HIS:CD2	1:A:265:GLY:H	2.17	0.62
1:D:155:GLN:HE21	3:F:3:LYS:NZ	1.99	0.60
1:D:219:ARG:HB2	1:D:224:GLN:HE21	1.65	0.60
1:D:176:LYS:HG2	1:D:180:GLN:NE2	2.16	0.60
3:F:3:LYS:HG3	3:F:4:GLU:N	2.14	0.60
1:A:155:GLN:NE2	3:C:5:PRO:HD2	2.18	0.58
1:A:176:LYS:HG2	1:A:180:GLN:NE2	2.19	0.58
1:A:263:HIS:HD2	1:A:265:GLY:H	1.50	0.58
1:A:219:ARG:HB3	1:A:224:GLN:HE21	1.70	0.57
1:A:201:LEU:HD22	1:A:249:VAL:HG21	1.88	0.56
2:E:85:VAL:HG13	4:E:100:HOH:O	2.06	0.55
1:A:253:GLN:HE21	1:A:256:ARG:HD3	1.72	0.55
1:D:127:LYS:HE3	1:D:134:THR:OG1	2.06	0.55
1:A:216:THR:HG21	4:A:296:HOH:O	2.07	0.54
1:D:74:HIS:CE1	1:D:97:ARG:HE	2.26	0.54
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.26	0.54
1:D:93:HIS:HD2	2:E:0:MET:CE	2.11	0.54
1:A:219:ARG:CB	1:A:224:GLN:HE21	2.21	0.53
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.42	0.53
1:D:177:GLU:H	1:D:177:GLU:CD	2.12	0.53
1:D:72:GLN:NE2	1:D:75:ARG:HH11	2.02	0.53
1:A:121:LYS:HG3	2:B:1:ILE:HD12	1.89	0.52
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.91	0.52
1:A:93:HIS:HD2	2:B:0:MET:CE	2.03	0.51
1:A:253:GLN:NE2	1:A:256:ARG:HH11	2.09	0.50
2:E:89:GLN:HB2	2:E:90:PRO:CD	2.40	0.50
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.93	0.50
1:D:264:GLU:HB2	4:D:305:HOH:O	2.11	0.50
1:A:107:TRP:O	1:A:169:ARG:NH2	2.44	0.50
1:A:121:LYS:HG3	2:B:1:ILE:CD1	2.42	0.50
1:D:6:ARG:NH2	1:D:102:ASP:OD1	2.45	0.50
3:C:3:LYS:CG	3:C:4:GLU:N	2.74	0.49
1:D:155:GLN:HE21	3:F:3:LYS:HZ3	1.60	0.49
1:D:156:LEU:HD12	3:F:3:LYS:HE3	1.94	0.49
1:D:255:GLN:HG2	4:D:321:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLN:NE2	1:A:75:ARG:HH11	2.05	0.48
1:A:155:GLN:NE2	3:C:3:LYS:NZ	2.58	0.48
1:A:127:LYS:HE3	1:A:134:THR:OG1	2.14	0.47
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.49	0.47
1:D:111:ARG:HG3	1:D:113:TYR:CZ	2.49	0.47
1:D:124:ILE:HG13	1:D:134:THR:O	2.15	0.47
2:E:51:HIS:HA	2:E:65:LEU:O	2.14	0.47
3:F:3:LYS:CG	3:F:4:GLU:N	2.77	0.47
1:A:177:GLU:H	1:A:177:GLU:CD	2.17	0.47
1:D:6:ARG:HD2	4:D:293:HOH:O	2.14	0.47
1:D:144:LYS:HE2	4:D:297:HOH:O	2.14	0.46
2:B:29:GLY:HA2	2:B:61:SER:OG	2.16	0.46
1:D:22:PHE:H	1:D:38:SER:HB2	1.81	0.46
1:A:49:ALA:O	1:A:52:ILE:HG22	2.15	0.46
1:A:210:PRO:O	1:A:263:HIS:HE1	1.99	0.45
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.51	0.45
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.53	0.44
2:E:19:LYS:O	2:E:72:PRO:HD2	2.18	0.44
1:D:253:GLN:NE2	1:D:256:ARG:HH11	2.15	0.44
1:A:65:ARG:HH11	1:A:65:ARG:HD3	1.34	0.44
2:B:51:HIS:HA	2:B:65:LEU:O	2.17	0.44
1:A:111:ARG:HG3	1:A:113:TYR:CZ	2.52	0.44
1:A:137:ASP:H	1:A:140:ALA:HB3	1.83	0.43
1:D:156:LEU:CD1	3:F:3:LYS:HE3	2.47	0.43
2:B:58:LYS:H	2:B:58:LYS:CD	2.29	0.43
1:D:93:HIS:HD2	2:E:0:MET:HE2	1.79	0.43
2:E:22:PHE:CE2	2:E:69:GLU:HG3	2.53	0.43
1:D:253:GLN:HE21	1:D:256:ARG:HD3	1.83	0.43
1:D:65:ARG:HH11	1:D:65:ARG:HD3	1.36	0.43
1:A:44:ARG:HA	1:A:64:THR:HG23	2.00	0.43
1:D:85:TYR:OH	1:D:137:ASP:OD2	2.17	0.42
1:A:156:LEU:HD12	3:C:3:LYS:HE3	2.00	0.42
2:B:22:PHE:CE2	2:B:69:GLU:HG3	2.55	0.42
1:D:13:SER:HA	1:D:20:PRO:HB3	2.02	0.42
1:D:210:PRO:O	1:D:263:HIS:HE1	2.02	0.42
1:D:273:ARG:NH1	4:D:333:HOH:O	2.52	0.42
1:D:51:TRP:CZ2	1:D:179:LEU:HD11	2.55	0.41
1:D:168:LEU:O	1:D:172:LEU:HG	2.20	0.41
1:A:13:SER:HA	1:A:20:PRO:HB3	2.02	0.41
1:A:155:GLN:HE21	3:C:3:LYS:HZ3	1.62	0.41
1:D:93:HIS:HD2	1:D:119:ASP:OD2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:LYS:HG3	2:E:1:ILE:HD12	2.03	0.40
1:D:145:HIS:HD2	4:D:280:HOH:O	2.04	0.40
2:E:73:THR:HG23	2:E:75:LYS:H	1.87	0.40
1:D:106:ASP:O	1:D:107:TRP:HB2	2.22	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%)	265 (97%)	8 (3%)	0	100	100
1	D	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	E	98/100 (98%)	96 (98%)	2 (2%)	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%)	734 (97%)	22 (3%)	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%)	216 (94%)	15 (6%)	17	19
1	D	231/231 (100%)	217 (94%)	14 (6%)	18	21
2	B	95/95 (100%)	87 (92%)	8 (8%)	11	11
2	E	95/95 (100%)	87 (92%)	8 (8%)	11	11
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	4
3	F	8/8 (100%)	7 (88%)	1 (12%)	4	4
All	All	668/668 (100%)	621 (93%)	47 (7%)	15	16

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	38	SER
1	A	67	VAL
1	A	88	SER
1	A	111	ARG
1	A	132	SER
1	A	138	MET
1	A	156	LEU
1	A	176	LYS
1	A	177	GLU
1	A	195	SER
1	A	216	THR
1	A	225	THR
1	A	234	ARG
1	A	268	LYS
2	B	4	THR
2	B	47	GLU
2	B	48	LYS
2	B	58	LYS
2	B	70	PHE
2	B	73	THR
2	B	88	SER
2	B	89	GLN
3	C	3	LYS
1	D	6	ARG
1	D	38	SER
1	D	88	SER
1	D	111	ARG
1	D	132	SER
1	D	138	MET

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Mol	Chain	Res	Type
1	D	156	LEU
1	D	176	LYS
1	D	177	GLU
1	D	195	SER
1	D	216	THR
1	D	225	THR
1	D	234	ARG
1	D	268	LYS
2	E	4	THR
2	E	47	GLU
2	E	48	LYS
2	E	58	LYS
2	E	70	PHE
2	E	73	THR
2	E	88	SER
2	E	89	GLN
3	F	3	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	72	GLN
1	A	74	HIS
1	A	93	HIS
1	A	155	GLN
1	A	180	GLN
1	A	192	HIS
1	A	224	GLN
1	A	253	GLN
1	A	263	HIS
2	B	2	GLN
3	C	7	HIS
1	D	70	HIS
1	D	72	GLN
1	D	74	HIS
1	D	93	HIS
1	D	145	HIS
1	D	155	GLN
1	D	180	GLN
1	D	224	GLN
1	D	253	GLN

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Mol	Chain	Res	Type
1	D	263	HIS
2	E	2	GLN
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 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)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	275/275 (100%)	0.33	18 (6%)	18	17	9, 21, 40, 57	0
1	D	275/275 (100%)	0.27	13 (4%)	31	30	9, 21, 40, 57	0
2	B	100/100 (100%)	-0.01	2 (2%)	65	63	9, 17, 34, 38	0
2	E	100/100 (100%)	-0.12	1 (1%)	82	81	9, 17, 34, 38	0
3	C	9/9 (100%)	0.16	0	100	100	14, 19, 24, 29	0
3	F	9/9 (100%)	-0.18	0	100	100	14, 20, 24, 29	0
All	All	768/768 (100%)	0.20	34 (4%)	34	32	9, 20, 38, 57	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLY	5.1
1	A	196	ASP	4.7
1	D	105	SER	4.3
1	D	196	ASP	3.7
1	A	17	ARG	3.6
1	A	113	TYR	3.5
2	B	44	GLU	3.4
1	D	17	ARG	3.2
1	D	192	HIS	3.1
1	A	193	ALA	3.0
1	A	16	GLY	3.0
1	A	195	SER	3.0
1	A	88	SER	2.8
1	A	41	ALA	2.8
2	B	47	GLU	2.8
1	A	108	ARG	2.8
1	A	151	HIS	2.7
1	A	197	HIS	2.7
1	A	194	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	267	PRO	2.6
1	D	223	ASP	2.6
1	D	195	SER	2.5
1	D	136	ALA	2.5
1	D	86	ASN	2.4
1	A	251	SER	2.4
1	D	194	VAL	2.3
1	D	54	GLN	2.3
1	A	18	GLY	2.3
1	A	54	GLN	2.3
2	E	47	GLU	2.1
1	D	197	HIS	2.1
1	A	275	GLU	2.1
1	D	226	GLN	2.0
1	A	131	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.