Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 05:58 AM EDT

PDB ID	:	1I1F
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.; 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 (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:

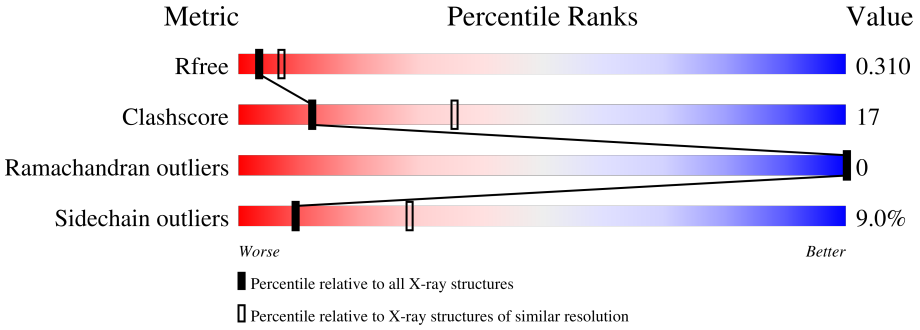
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 <=5%

Mol	Chain	Length	Quality of chain
1	A	275	57% 35% 6% •
1	D	275	60% 35% • •
2	B	100	71% 20% 7% •
2	E	100	68% 27% 5%
3	C	9	56% 44%
3	F	9	56% 44%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	275	2247	1403	409	426	9	0	0	0
1	D	275	2246	1403	409	425	9	0	0	0

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

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

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

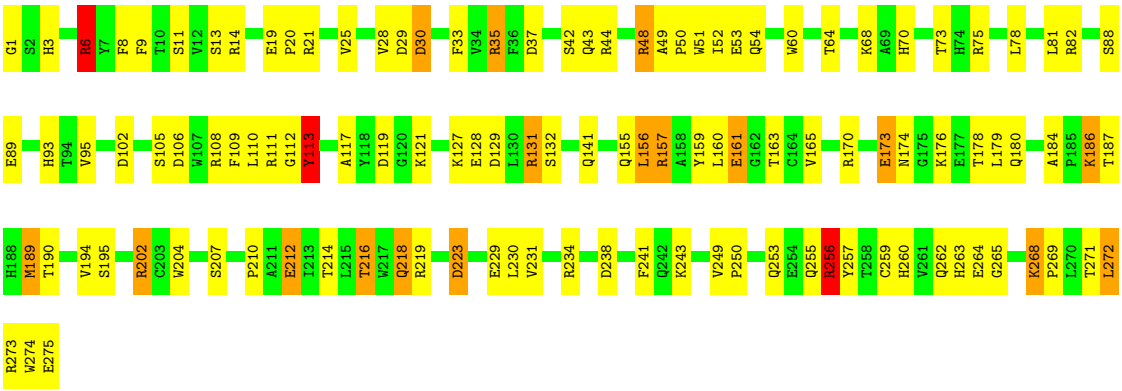
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	73	49	12	12	0	0	0
3	F	9	73	49	12	12	0	0	0

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. 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. 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.

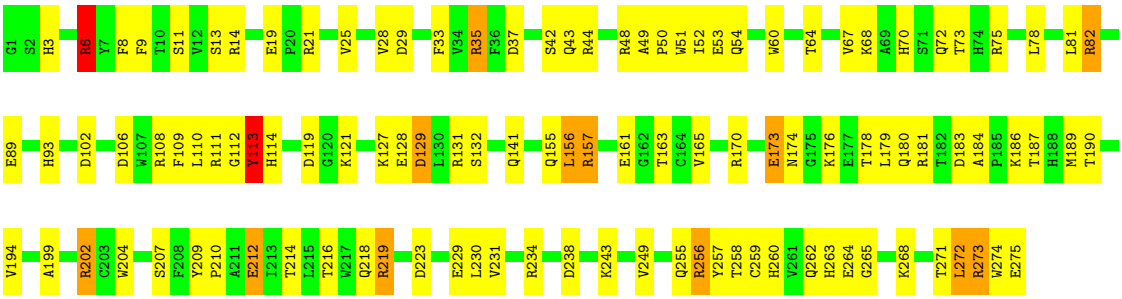
• Molecule 1: PROTEIN (CLASS I HISTOCOMPATIBILITY ANTIGEN, GOGO-A0201 ALPHA CHAIN)

Chain A: 57% 35% 6%



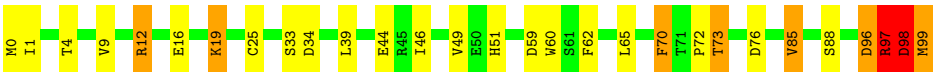
• Molecule 1: PROTEIN (CLASS I HISTOCOMPATIBILITY ANTIGEN, GOGO-A0201 ALPHA CHAIN)

Chain D: 60% 35%



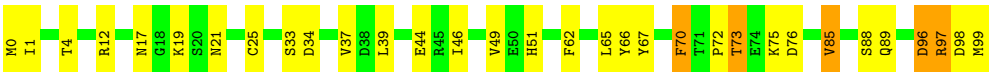
• Molecule 2: PROTEIN (BETA 2-MICROGLOBULIN)

Chain B: 71% 20% 7%



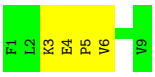
• Molecule 2: PROTEIN (BETA 2-MICROGLOBULIN)

Chain E:



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

Chain C:



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

Chain F:

4 Data and refinement statistics (i)

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 29.19 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (15.00-2.80) 95.4 (29.19-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.16Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.260 , 0.315 0.302 , 0.310	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)	0.34 , 39.3	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	0.80	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.*

[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	0.52	0/2312	1.55	28/3137 (0.9%)
1	D	0.52	0/2311	1.49	29/3137 (0.9%)
2	B	0.57	0/859	1.59	12/1162 (1.0%)
2	E	0.53	0/859	1.50	8/1162 (0.7%)
3	C	0.82	0/75	1.15	0/99
3	F	0.84	0/75	1.11	0/99
All	All	0.54	0/6491	1.52	77/8796 (0.9%)

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 (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	44	GLU	OE1-CD-OE2	-22.86	95.86	123.30
1	A	256	ARG	NE-CZ-NH2	22.85	131.72	120.30
2	E	44	GLU	OE1-CD-OE2	-21.72	97.23	123.30
1	D	256	ARG	NE-CZ-NH2	21.25	130.92	120.30
1	D	6	ARG	NE-CZ-NH1	-14.03	113.29	120.30
1	A	6	ARG	NE-CZ-NH1	-13.59	113.51	120.30
1	A	173	GLU	OE1-CD-OE2	-13.50	107.10	123.30
1	A	256	ARG	CG-CD-NE	12.95	139.00	111.80
1	A	256	ARG	NH1-CZ-NH2	-11.82	106.40	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	173	GLU	OE1-CD-OE2	-11.80	109.14	123.30
2	E	44	GLU	CG-CD-OE2	10.96	140.22	118.30
2	B	44	GLU	CG-CD-OE1	10.91	140.11	118.30
1	A	131	ARG	NE-CZ-NH2	9.90	125.25	120.30
2	B	34	ASP	CB-CG-OD1	9.81	127.13	118.30
1	D	21	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	D	256	ARG	NH1-CZ-NH2	-8.91	109.59	119.40
1	A	157	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	D	181	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	A	21	ARG	NE-CZ-NH2	-8.40	116.10	120.30
2	E	96	ASP	CB-CG-OD1	8.29	125.76	118.30
2	B	97	ARG	NE-CZ-NH1	-8.27	116.17	120.30
1	A	129	ASP	CB-CG-OD1	8.23	125.71	118.30
1	D	129	ASP	CB-CG-OD1	7.77	125.30	118.30
1	A	37	ASP	CB-CG-OD1	7.76	125.29	118.30
1	D	219	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	D	82	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	D	6	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	6	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	D	219	ARG	CD-NE-CZ	7.23	133.72	123.60
1	A	173	GLU	CG-CD-OE2	7.21	132.72	118.30
1	D	37	ASP	CB-CG-OD1	7.07	124.66	118.30
2	E	97	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	D	173	GLU	CG-CD-OE2	7.05	132.40	118.30
1	D	14	ARG	NE-CZ-NH1	-7.01	116.80	120.30
1	A	229	GLU	OE1-CD-OE2	6.97	131.67	123.30
1	A	14	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	D	256	ARG	CG-CD-NE	6.71	125.89	111.80
1	A	48	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	202	ARG	CD-NE-CZ	6.69	132.97	123.60
1	D	108	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	30	ASP	CB-CG-OD1	6.58	124.22	118.30
1	D	157	ARG	NE-CZ-NH1	6.49	123.55	120.30
2	B	97	ARG	NH1-CZ-NH2	6.38	126.41	119.40
1	D	21	ARG	CD-NE-CZ	6.36	132.50	123.60
2	B	98	ASP	CB-CG-OD1	6.20	123.88	118.30
2	E	99	MET	CG-SD-CE	6.14	110.03	100.20
1	A	273	ARG	NE-CZ-NH2	6.05	123.32	120.30
2	E	85	VAL	CB-CA-C	-6.05	99.91	111.40
1	D	113	TYR	CG-CD1-CE1	-6.03	116.47	121.30
1	D	229	GLU	OE1-CD-OE2	6.02	130.52	123.30
2	B	12	ARG	NE-CZ-NH2	5.98	123.29	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	99	MET	CG-SD-CE	5.96	109.74	100.20
1	A	234	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	21	ARG	CD-NE-CZ	5.86	131.81	123.60
1	D	202	ARG	CD-NE-CZ	5.84	131.77	123.60
2	B	97	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	D	157	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	113	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	A	189	MET	CA-CB-CG	5.62	122.84	113.30
1	A	157	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	202	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	113	TYR	CG-CD1-CE1	-5.58	116.84	121.30
2	B	96	ASP	CB-CG-OD1	5.51	123.26	118.30
1	D	106	ASP	CB-CG-OD1	5.47	123.23	118.30
2	E	34	ASP	CB-CG-OD1	5.47	123.22	118.30
1	D	6	ARG	CD-NE-CZ	-5.42	116.01	123.60
1	A	131	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
2	B	85	VAL	CB-CA-C	-5.39	101.15	111.40
1	D	113	TYR	CD1-CE1-CZ	5.37	124.64	119.80
2	B	34	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	D	234	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	202	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	D	82	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	A	161	GLU	OE1-CD-OE2	-5.08	117.21	123.30
1	A	6	ARG	CD-NE-CZ	-5.05	116.53	123.60
1	A	157	ARG	CD-NE-CZ	5.04	130.66	123.60
2	E	67	TYR	CB-CG-CD1	-5.02	117.99	121.00

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	88	0
1	D	2246	0	2096	90	0
2	B	836	0	803	20	0
2	E	836	0	803	26	0
3	C	73	0	76	9	0
3	F	73	0	76	14	0
All	All	6311	0	5950	210	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 17.

All (210) 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	1.69	1.28
1:A:93:HIS:CD2	2:B:0:MET:HE1	1.85	1.10
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: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: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
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:35:ARG:NH1	1:A:48:ARG:NH1	2.36	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:93:HIS:NE2	2:E:0:MET:HE1	2.02	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: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
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
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
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
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
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
2:B:96:ASP:CG	2:B:99:MET:HG2	2.22	0.59
1:D:156:LEU:HA	3:F:3:LYS:HZ2	1.68	0.59
1:A:93:HIS:NE2	2:B:0:MET:CE	2.65	0.58
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:218:GLN:NE2	1:A:260:HIS:NE2	2.52	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:93:HIS:HD2	2:E:0:MET:HE1	1.60	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: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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:TRP:CZ2	2:E:98:ASP:O	2.55	0.50
1:D:93:HIS:NE2	2:E:0:MET:HE3	2.28	0.49
1:D:156:LEU:HD13	3:F:3:LYS:HZ3	1.77	0.49
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:102:ASP:OD1	1:D:113:TYR:OH	2.32	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:156:LEU:CA	3:F:3:LYS:HZ2	2.30	0.45
1:A:156:LEU:HA	3:C:3:LYS:HZ2	1.82	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
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:D:93:HIS:HD2	2:E:0:MET:CE	2.22	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
1:A:189:MET:HE3	1:A:272:LEU:HB2	2.01	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:96:ASP:O	2:E:97:ARG:C	2.59	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
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: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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	22
1	D	231/231 (100%)	210 (91%)	21 (9%)	9	27
2	B	95/95 (100%)	86 (90%)	9 (10%)	8	25
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%)	608 (91%)	60 (9%)	9	28

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	11	SER
1	A	20	PRO
1	A	35	ARG
1	A	81	LEU
1	A	88	SER
1	A	113	TYR
1	A	128	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	212	GLU
1	A	216	THR
1	A	223	ASP
1	A	255	GLN
1	A	256	ARG
1	A	264	GLU
1	A	268	LYS
1	A	272	LEU
2	B	4	THR
2	B	9	VAL
2	B	19	LYS
2	B	70	PHE
2	B	73	THR
2	B	85	VAL
2	B	88	SER
2	B	97	ARG
2	B	98	ASP
1	D	6	ARG
1	D	11	SER
1	D	35	ARG
1	D	81	LEU
1	D	113	TYR
1	D	128	GLU
1	D	141	GLN
1	D	156	LEU
1	D	163	THR
1	D	165	VAL
1	D	173	GLU
1	D	178	THR
1	D	212	GLU
1	D	216	THR
1	D	223	ASP
1	D	255	GLN
1	D	256	ARG
1	D	264	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	268	LYS
1	D	272	LEU
1	D	273	ARG
2	E	4	THR
2	E	19	LYS
2	E	21	ASN
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 (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	93	HIS
1	A	155	GLN
1	A	174	ASN
1	A	180	GLN
1	A	218	GLN
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	218	GLN
1	D	263	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 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.