Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:21 AM GMT

PDB ID	:	2MHA
Title	:	CRYSTAL STRUCTURE OF THE MAJOR HISTOCOMPATIBILITY COMPLEX CLASS I H-2KB MOLECULE CONTAINING A SINGLE VIRAL PEPTIDE: IMPLICATIONS FOR PEPTIDE BINDING AND T-CELL RECEPTOR RECOGNITION
Authors	:	Zhang, W.; Young, A.C.M.; Imarai, M.; Nathenson, S.G.; Sacchettini, J.C.
Deposited on	:	1993-07-21
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 ⓘ symbol.

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

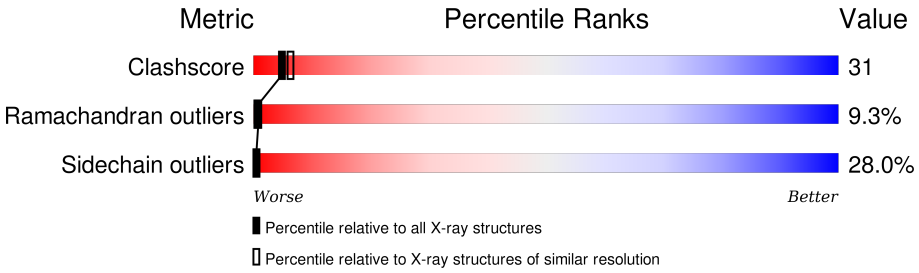
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	270	30% 42% 22% 6%
1	C	270	26% 48% 20% 7%
2	B	99	28% 56% 11% 5%
2	D	99	27% 51% 19% .
3	E	8	25% 38% 38%
3	F	8	25% 13% 38% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6160 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 (H-2KB) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2191	1381	385	416	9			
1	C	270	Total	C	N	O	S	0	0	0
			2191	1381	385	416	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	D	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 3 is a protein called VIRAL OCTAPEPTIDE ARG-GLY-TYR-VAL-TYR-GLN-GLY-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	0	0	0
			68	44	12	12			
3	F	8	Total	C	N	O	0	0	0
			68	44	12	12			

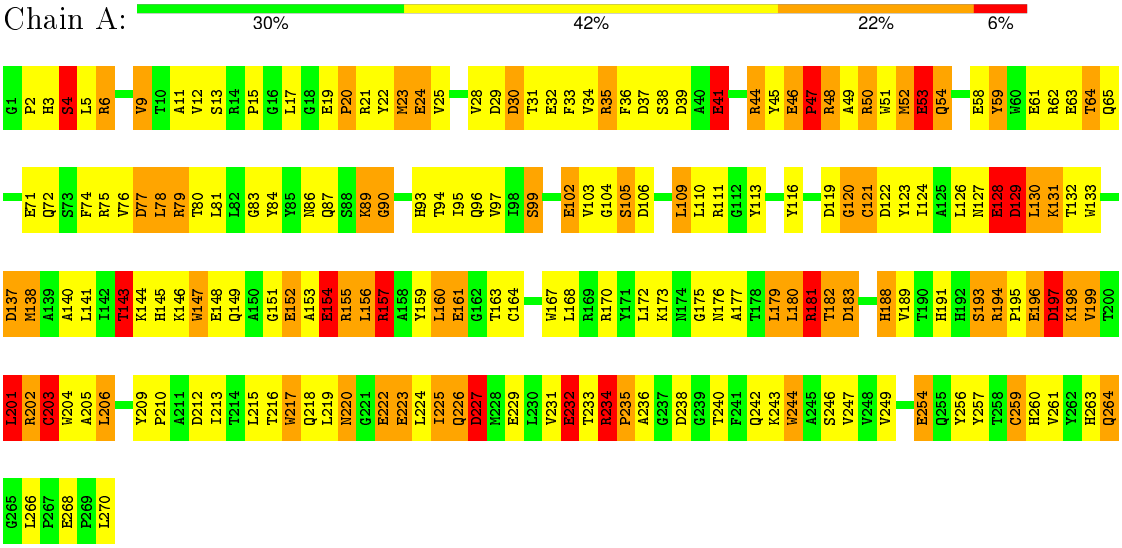
3 Residue-property plots (i)

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.

Note EDS was not executed.

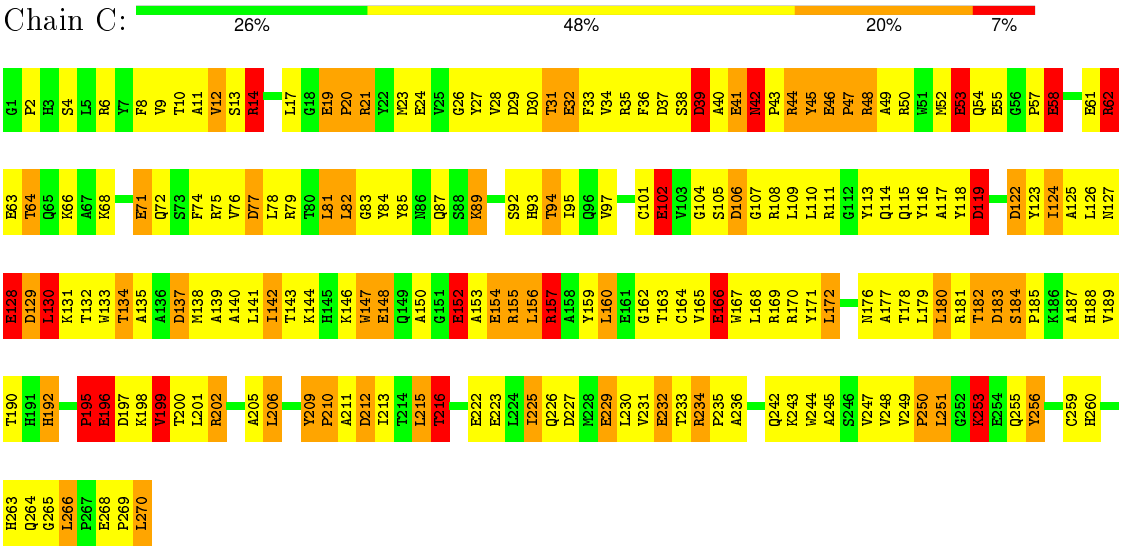
- Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (H-2KB) (ALPHA CHAIN)

Chain A:



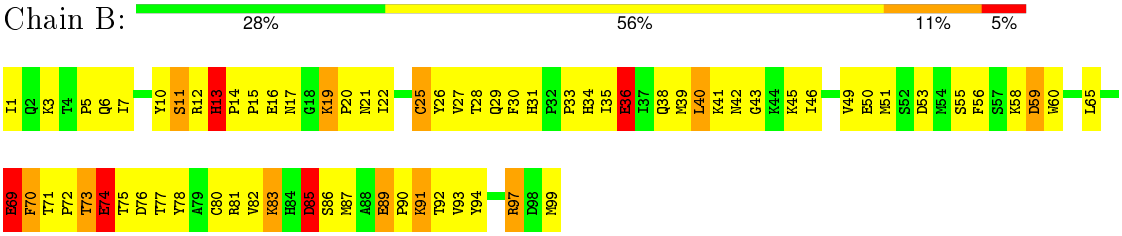
- Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (H-2KB) (ALPHA CHAIN)

Chain C:



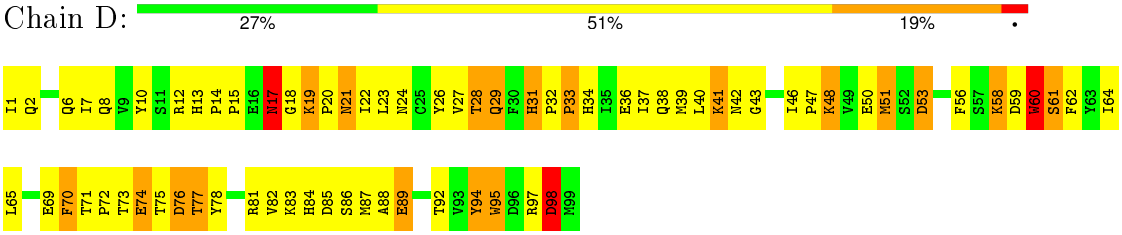
• Molecule 2: BETA 2-MICROGLOBULIN

Chain B:



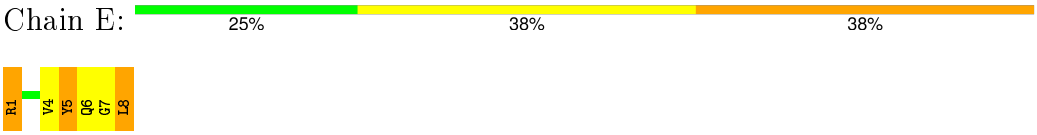
• Molecule 2: BETA 2-MICROGLOBULIN

Chain D:



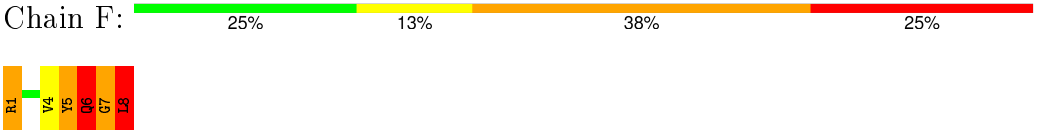
• Molecule 3: VIRAL OCTAPEPTIDE ARG-GLY-TYR-VAL-TYR-GLN-GLY-LEU

Chain E:



• Molecule 3: VIRAL OCTAPEPTIDE ARG-GLY-TYR-VAL-TYR-GLN-GLY-LEU

Chain F:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.90Å 92.20Å 67.50Å 90.00° 111.24° 90.00°	Depositor
Resolution (Å)	54.20 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (54.20-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6160	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

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	1.33	22/2250 (1.0%)	1.61	40/3055 (1.3%)
1	C	1.23	23/2250 (1.0%)	1.58	36/3055 (1.2%)
2	B	1.11	6/847 (0.7%)	1.44	10/1148 (0.9%)
2	D	1.17	6/847 (0.7%)	1.53	13/1148 (1.1%)
3	E	1.01	0/69	1.81	1/90 (1.1%)
3	F	2.29	2/69 (2.9%)	1.89	2/90 (2.2%)
All	All	1.26	59/6332 (0.9%)	1.57	102/8586 (1.2%)

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	9
1	C	0	8
2	B	0	1
2	D	0	2
All	All	0	20

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	GLU	CA-CB	18.38	1.94	1.53
3	F	7	GLY	N-CA	-10.43	1.30	1.46
1	C	53	GLU	CD-OE1	6.90	1.33	1.25
1	A	222	GLU	CD-OE2	6.86	1.33	1.25
1	C	19	GLU	CD-OE2	6.66	1.32	1.25
1	A	259	CYS	CB-SG	-6.49	1.71	1.82
2	B	69	GLU	CD-OE2	6.43	1.32	1.25
1	C	55	GLU	CD-OE1	6.43	1.32	1.25
1	C	58	GLU	CD-OE1	6.37	1.32	1.25
1	A	41	GLU	CD-OE1	6.32	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	GLU	CD-OE1	6.31	1.32	1.25
1	A	254	GLU	CD-OE1	6.29	1.32	1.25
1	C	102	GLU	CD-OE2	6.25	1.32	1.25
1	A	32	GLU	CD-OE1	6.21	1.32	1.25
2	B	36	GLU	CD-OE2	6.19	1.32	1.25
1	C	46	GLU	CD-OE2	6.17	1.32	1.25
1	C	270	LEU	CA-C	6.14	1.69	1.52
2	D	50	GLU	CD-OE2	6.13	1.32	1.25
1	C	232	GLU	CD-OE1	6.02	1.32	1.25
1	C	128	GLU	CD-OE1	6.00	1.32	1.25
1	A	58	GLU	CD-OE1	5.99	1.32	1.25
2	D	89	GLU	CD-OE2	5.95	1.32	1.25
3	F	8	LEU	N-CA	-5.91	1.34	1.46
2	D	69	GLU	CD-OE1	5.89	1.32	1.25
1	A	19	GLU	CD-OE1	5.88	1.32	1.25
1	A	152	GLU	CD-OE2	5.87	1.32	1.25
1	A	223	GLU	CD-OE1	5.86	1.32	1.25
1	C	166	GLU	CD-OE1	5.86	1.32	1.25
1	A	102	GLU	CD-OE1	5.77	1.31	1.25
2	D	36	GLU	CD-OE1	5.76	1.31	1.25
2	D	18	GLY	N-CA	-5.76	1.37	1.46
1	C	148	GLU	CD-OE1	5.74	1.31	1.25
1	A	268	GLU	CD-OE1	5.74	1.31	1.25
2	B	50	GLU	CD-OE1	5.73	1.31	1.25
1	A	154	GLU	CD-OE1	5.71	1.31	1.25
1	A	53	GLU	CD-OE1	5.68	1.31	1.25
1	C	223	GLU	CD-OE1	5.67	1.31	1.25
1	C	229	GLU	CD-OE2	5.62	1.31	1.25
1	C	24	GLU	CD-OE1	5.61	1.31	1.25
1	A	128	GLU	CD-OE2	5.57	1.31	1.25
1	C	32	GLU	CD-OE1	5.54	1.31	1.25
2	D	74	GLU	CD-OE2	5.51	1.31	1.25
1	C	154	GLU	CD-OE1	5.46	1.31	1.25
2	B	89	GLU	CD-OE2	5.40	1.31	1.25
1	C	196	GLU	CD-OE2	5.36	1.31	1.25
1	A	148	GLU	CD-OE1	5.35	1.31	1.25
1	A	232	GLU	CD-OE1	5.34	1.31	1.25
1	C	268	GLU	CD-OE2	5.31	1.31	1.25
1	A	71	GLU	CD-OE2	5.30	1.31	1.25
1	C	71	GLU	CD-OE1	5.30	1.31	1.25
1	C	63	GLU	CD-OE1	5.25	1.31	1.25
1	A	24	GLU	CD-OE1	5.17	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	41	GLU	CD-OE2	5.16	1.31	1.25
2	B	16	GLU	CD-OE2	5.10	1.31	1.25
1	A	61	GLU	CD-OE1	5.08	1.31	1.25
1	C	222	GLU	CD-OE2	5.05	1.31	1.25
1	A	161	GLU	CD-OE1	5.04	1.31	1.25
2	B	74	GLU	CD-OE2	5.02	1.31	1.25
1	C	152	GLU	CD-OE2	5.02	1.31	1.25

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	259	CYS	CA-CB-SG	-11.05	94.10	114.00
1	A	231	VAL	C-N-CA	-10.88	94.50	121.70
1	A	232	GLU	CA-CB-CG	10.62	136.76	113.40
2	D	94	TYR	CB-CG-CD2	-9.21	115.47	121.00
1	C	150	ALA	C-N-CA	-8.96	103.49	122.30
1	A	157	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	C	14	ARG	NE-CZ-NH2	8.55	124.58	120.30
1	C	137	ASP	CB-CG-OD1	8.13	125.62	118.30
1	C	137	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	A	232	GLU	N-CA-CB	-7.81	96.55	110.60
1	C	119	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	C	183	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	A	137	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	C	122	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	A	6	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	C	62	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	238	ASP	CB-CG-OD2	-7.14	111.87	118.30
2	B	59	ASP	CB-CG-OD2	7.14	124.73	118.30
2	D	85	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	C	119	ASP	CB-CG-OD1	7.04	124.64	118.30
2	B	13	HIS	C-N-CD	-6.97	105.27	120.60
3	F	6	GLN	CA-C-N	-6.95	102.30	116.20
2	D	60	TRP	N-CA-CB	6.75	122.75	110.60
2	B	59	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	A	203	CYS	CA-CB-SG	-6.70	101.94	114.00
2	D	94	TYR	CB-CG-CD1	6.53	124.92	121.00
1	C	122	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	157	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	C	183	ASP	CB-CG-OD1	6.47	124.13	118.30
1	A	106	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	C	216	THR	N-CA-CB	6.43	122.52	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	129	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	122	ASP	CB-CG-OD2	-6.36	112.58	118.30
2	B	53	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	C	45	TYR	CB-CG-CD2	-6.29	117.22	121.00
1	A	238	ASP	CB-CG-OD1	6.29	123.96	118.30
2	D	17	ASN	N-CA-CB	6.22	121.79	110.60
2	B	59	ASP	N-CA-CB	6.18	121.72	110.60
1	C	62	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	C	195	PRO	CA-N-CD	-6.11	102.94	111.50
3	E	1	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	106	ASP	CB-CG-OD1	6.07	123.77	118.30
1	A	143	THR	N-CA-CB	6.07	121.83	110.30
1	C	29	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	4	SER	CB-CA-C	-5.93	98.83	110.10
1	A	59	TYR	CB-CG-CD1	5.91	124.55	121.00
2	B	53	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	4	SER	N-CA-CB	5.86	119.30	110.50
1	A	122	ASP	CB-CG-OD1	5.78	123.50	118.30
2	B	85	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	77	ASP	CB-CG-OD1	5.76	123.48	118.30
1	C	39	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	C	77	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	A	47	PRO	N-CA-C	5.64	126.76	112.10
1	A	119	ASP	CB-CG-OD2	-5.63	113.23	118.30
2	D	85	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	129	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	C	157	ARG	CD-NE-CZ	5.59	131.43	123.60
2	D	77	THR	N-CA-CB	5.59	120.93	110.30
3	F	7	GLY	CA-C-N	-5.58	104.92	117.20
2	D	98	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	137	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	106	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	181	ARG	N-CA-CB	5.50	120.50	110.60
1	C	212	ASP	CB-CG-OD2	-5.50	113.35	118.30
2	B	85	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	201	LEU	N-CA-CB	5.45	121.30	110.40
1	A	59	TYR	CB-CG-CD2	-5.45	117.73	121.00
2	B	76	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	216	THR	CA-CB-OG1	5.43	120.41	109.00
1	C	256	TYR	CB-CG-CD1	5.43	124.26	121.00
2	D	98	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	A	20	PRO	CA-N-CD	-5.41	103.92	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	183	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	C	195	PRO	C-N-CA	5.41	135.23	121.70
1	C	30	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	77	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	234	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	A	30	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	231	VAL	CA-CB-CG2	-5.37	102.85	110.90
1	A	77	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	C	14	ARG	CG-CD-NE	5.34	123.01	111.80
1	C	84	TYR	N-CA-CB	5.32	120.17	110.60
2	D	53	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	227	ASP	CB-CG-OD2	5.32	123.08	118.30
2	D	53	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	A	232	GLU	CA-C-N	-5.26	105.63	117.20
1	C	212	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	30	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	C	30	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	197	ASP	CB-CG-OD2	5.22	122.99	118.30
2	B	25	CYS	CA-CB-SG	-5.19	104.67	114.00
1	C	29	ASP	CB-CG-OD1	-5.17	113.64	118.30
2	D	19	LYS	CB-CA-C	5.17	120.73	110.40
2	D	24	ASN	CB-CA-C	-5.13	100.13	110.40
1	A	217	TRP	N-CA-CB	5.08	119.75	110.60
1	C	227	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	129	ASP	CB-CG-OD1	-5.06	113.74	118.30
1	A	227	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	C	160	LEU	CA-CB-CG	-5.04	103.71	115.30
1	C	150	ALA	O-C-N	-5.04	114.64	123.20
1	A	44	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	ARG	Sidechain
1	A	194	ARG	Mainchain,Peptide
1	A	197	ASP	Mainchain
1	A	203	CYS	Mainchain
1	A	232	GLU	Mainchain,Peptide
1	A	235	PRO	Mainchain
1	A	4	SER	Mainchain
2	B	56	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	C	102	GLU	Mainchain
1	C	195	PRO	Mainchain,Peptide
1	C	197	ASP	Mainchain
1	C	209	TYR	Mainchain,Peptide
1	C	42	ASN	Mainchain
1	C	82	LEU	Mainchain
2	D	31	HIS	Mainchain,Peptide

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	2191	0	2086	149	0
1	C	2191	0	2086	149	0
2	B	821	0	798	34	0
2	D	821	0	798	51	0
3	E	68	0	67	7	0
3	F	68	0	66	7	0
All	All	6160	0	5901	378	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 31.

All (378) 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:232:GLU:CA	1:A:232:GLU:CB	1.94	1.45
1:C:185:PRO:HG3	1:C:213:ILE:HD11	1.24	1.15
2:B:36:GLU:HB3	2:B:83:LYS:HB3	1.32	1.10
2:D:19:LYS:HB3	2:D:20:PRO:HD3	1.36	1.08
1:A:35:ARG:NH1	1:A:46:GLU:H	1.55	1.04
1:A:193:SER:HA	1:A:199:VAL:HG12	1.41	0.99
1:A:234:ARG:NH1	1:A:242:GLN:HE21	1.60	0.98
1:A:9:VAL:HG13	1:A:97:VAL:HB	1.46	0.96
1:C:185:PRO:HG3	1:C:213:ILE:CD1	1.96	0.95
1:C:210:PRO:HD2	1:C:263:HIS:CE1	2.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLU:HB2	1:A:111:ARG:HB2	1.49	0.94
2:B:15:PRO:HG2	2:B:97:ARG:HB2	1.54	0.88
1:A:182:THR:HG23	1:A:210:PRO:HD2	1.52	0.88
1:A:116:TYR:HB2	1:A:124:ILE:HG22	1.54	0.88
1:C:13:SER:HB3	1:C:78:LEU:HD13	1.54	0.88
1:A:104:GLY:HA3	1:A:110:LEU:HD23	1.56	0.87
1:C:130:LEU:HD12	1:C:130:LEU:H	1.40	0.86
1:A:234:ARG:HH11	1:A:242:GLN:HE21	1.22	0.83
1:A:5:LEU:HD22	1:A:168:LEU:HB2	1.60	0.83
3:E:6:GLN:HG2	3:E:7:GLY:H	1.45	0.82
1:C:126:LEU:HB2	1:C:133:TRP:CZ3	2.14	0.82
1:A:78:LEU:HD22	1:A:95:ILE:HD12	1.62	0.81
1:C:209:TYR:CD1	1:C:210:PRO:HA	2.15	0.80
1:A:156:LEU:HD22	1:A:160:LEU:HD21	1.64	0.80
1:A:234:ARG:NH1	1:A:242:GLN:NE2	2.29	0.80
1:A:168:LEU:O	1:A:172:LEU:HD13	1.82	0.79
1:A:3:HIS:HB2	1:A:103:VAL:CG2	2.11	0.79
1:C:126:LEU:HB2	1:C:133:TRP:HZ3	1.47	0.79
1:C:19:GLU:HG2	1:C:20:PRO:N	1.98	0.79
2:B:27:VAL:HG11	2:B:82:VAL:HG21	1.64	0.78
2:D:19:LYS:CB	2:D:20:PRO:HD3	2.12	0.78
1:A:206:LEU:HB2	1:A:242:GLN:HB3	1.66	0.78
1:C:74:PHE:HA	1:C:77:ASP:HB2	1.66	0.76
1:A:3:HIS:HB2	1:A:103:VAL:HG22	1.68	0.74
1:C:162:GLY:O	1:C:166:GLU:HB2	1.88	0.74
2:D:29:GLN:HA	2:D:61:SER:OG	1.88	0.74
1:C:101:CYS:SG	1:C:164:CYS:HB3	2.28	0.73
1:A:133:TRP:HE1	1:A:153:ALA:HB2	1.53	0.73
1:A:129:ASP:O	1:A:131:LYS:N	2.22	0.73
1:C:35:ARG:HH11	1:C:37:ASP:H	1.34	0.73
1:A:232:GLU:N	1:A:232:GLU:CB	2.52	0.72
1:A:156:LEU:CD2	1:A:160:LEU:HD21	2.19	0.72
1:C:12:VAL:HG13	1:C:94:THR:HG23	1.70	0.72
2:B:91:LYS:N	2:B:91:LYS:HD2	2.02	0.72
1:A:151:GLY:O	1:A:155:ARG:HB2	1.90	0.72
1:A:35:ARG:HH12	1:A:46:GLU:H	1.37	0.71
1:C:106:ASP:HB2	1:C:108:ARG:HH21	1.54	0.71
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.26	0.71
1:C:117:ALA:HB2	2:D:60:TRP:CZ2	2.24	0.71
1:C:129:ASP:O	1:C:131:LYS:N	2.24	0.71
1:A:170:ARG:HB3	1:A:170:ARG:HH11	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLY:O	1:A:179:LEU:HG	1.91	0.71
1:C:263:HIS:HB3	1:C:266:LEU:HD22	1.71	0.71
1:C:68:LYS:O	1:C:71:GLU:HB3	1.90	0.71
1:C:200:THR:OG1	1:C:248:VAL:HG12	1.91	0.70
1:A:218:GLN:HG3	1:A:223:GLU:HG2	1.73	0.69
1:A:197:ASP:HB3	1:A:198:LYS:HD3	1.74	0.69
2:D:12:ARG:HH11	2:D:22:ILE:HG13	1.55	0.69
1:A:202:ARG:HG2	1:A:204:TRP:HE1	1.56	0.69
1:C:160:LEU:HD23	1:C:164:CYS:SG	2.33	0.69
1:A:5:LEU:CD2	1:A:168:LEU:HB2	2.21	0.68
1:A:167:TRP:CZ3	1:A:170:ARG:HD3	2.29	0.68
1:C:168:LEU:HD23	1:C:168:LEU:O	1.94	0.68
1:A:232:GLU:HA	1:A:243:LYS:HZ2	1.59	0.67
1:A:74:PHE:O	1:A:77:ASP:N	2.27	0.67
1:C:198:LYS:O	1:C:199:VAL:HG13	1.94	0.67
1:A:22:TYR:HD2	1:A:36:PHE:CE1	2.13	0.67
1:C:116:TYR:O	1:C:123:TYR:HB3	1.95	0.67
2:B:22:ILE:HD13	2:B:69:GLU:HA	1.78	0.65
2:D:81:ARG:HG2	2:D:92:THR:OG1	1.96	0.65
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.32	0.65
1:C:50:ARG:O	1:C:53:GLU:HB2	1.97	0.64
1:C:205:ALA:HB2	1:C:215:LEU:HD11	1.79	0.64
1:C:38:SER:HA	1:C:43:PRO:HB3	1.80	0.64
3:E:5:TYR:H	3:E:5:TYR:HD1	1.45	0.64
1:C:75:ARG:O	1:C:79:ARG:HG3	1.98	0.64
1:A:59:TYR:O	1:A:63:GLU:HB2	1.99	0.63
1:C:236:ALA:HB2	1:C:242:GLN:HG3	1.80	0.63
2:B:39:MET:O	2:B:46:ILE:HG22	1.99	0.63
1:C:210:PRO:HD2	1:C:263:HIS:HE1	1.64	0.62
1:A:156:LEU:HD22	1:A:160:LEU:CD2	2.29	0.62
1:C:202:ARG:HD3	1:C:244:TRP:CE3	2.33	0.62
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.34	0.62
1:C:196:GLU:O	1:C:196:GLU:HG2	1.99	0.62
1:C:230:LEU:HA	1:C:244:TRP:O	2.00	0.62
2:D:37:ILE:HG22	2:D:82:VAL:HG12	1.82	0.62
1:C:26:GLY:HA3	1:C:34:VAL:HG22	1.81	0.61
1:C:76:VAL:HA	1:C:79:ARG:HD3	1.81	0.61
1:C:58:GLU:O	1:C:62:ARG:HD2	2.01	0.61
1:C:205:ALA:CB	1:C:215:LEU:HD11	2.31	0.61
2:B:3:LYS:HB3	2:B:29:GLN:O	2.01	0.61
1:C:234:ARG:NH1	1:C:242:GLN:HE21	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PRO:HG2	1:A:90:GLY:O	2.01	0.60
1:C:27:TYR:HA	1:C:31:THR:O	2.01	0.60
1:C:269:PRO:O	1:C:270:LEU:HB2	2.01	0.59
1:A:196:GLU:HG2	1:A:196:GLU:O	2.02	0.59
2:D:23:LEU:HB2	2:D:70:PHE:CE1	2.37	0.59
1:A:181:ARG:HB2	1:A:181:ARG:NH1	2.17	0.59
1:C:167:TRP:CZ3	1:C:170:ARG:HD3	2.37	0.59
1:A:72:GLN:O	1:A:76:VAL:HG23	2.03	0.59
1:A:163:THR:O	1:A:167:TRP:HB2	2.03	0.58
1:C:124:ILE:HG21	1:C:147:TRP:CZ3	2.39	0.58
1:C:182:THR:HG23	1:C:183:ASP:N	2.18	0.58
1:C:23:MET:HA	1:C:36:PHE:O	2.03	0.58
1:C:44:ARG:HH11	1:C:44:ARG:HG3	1.68	0.58
2:D:17:ASN:HB3	2:D:97:ARG:HH22	1.68	0.58
2:D:19:LYS:HB3	2:D:20:PRO:CD	2.23	0.58
1:C:225:ILE:O	1:C:225:ILE:HD13	2.02	0.58
1:A:234:ARG:HH12	1:A:242:GLN:NE2	2.02	0.58
1:C:26:GLY:HA3	1:C:34:VAL:CG2	2.34	0.58
1:A:25:VAL:HA	1:A:34:VAL:O	2.04	0.58
1:A:9:VAL:O	1:A:96:GLN:HA	2.04	0.58
1:A:181:ARG:HB2	1:A:181:ARG:HH11	1.69	0.57
1:A:193:SER:HA	1:A:199:VAL:CG1	2.26	0.57
2:D:27:VAL:HG11	2:D:37:ILE:HG21	1.86	0.57
1:C:253:LYS:O	1:C:256:TYR:HB2	2.04	0.57
2:D:32:PRO:HD2	2:D:84:HIS:CE1	2.39	0.57
2:D:48:LYS:HG3	2:D:48:LYS:O	2.04	0.57
1:A:225:ILE:O	1:A:227:ASP:N	2.37	0.57
1:C:117:ALA:CB	2:D:60:TRP:CE2	2.87	0.57
1:A:128:GLU:O	1:A:130:LEU:N	2.34	0.57
1:A:203:CYS:HG	1:A:259:CYS:HG	1.38	0.57
1:C:167:TRP:O	1:C:170:ARG:N	2.38	0.57
1:C:13:SER:O	1:C:92:SER:HA	2.03	0.57
1:A:5:LEU:HB2	1:A:168:LEU:HD13	1.86	0.57
1:C:180:LEU:HG	1:C:209:TYR:CZ	2.40	0.56
1:A:131:LYS:NZ	1:A:154:GLU:OE2	2.29	0.56
1:A:126:LEU:HB2	1:A:133:TRP:CZ3	2.41	0.56
1:A:133:TRP:NE1	1:A:153:ALA:HB2	2.19	0.56
1:C:160:LEU:O	1:C:164:CYS:HB2	2.05	0.56
2:B:40:LEU:HD11	2:B:81:ARG:HE	1.72	0.55
1:C:47:PRO:O	1:C:49:ALA:N	2.38	0.55
1:C:14:ARG:NH1	1:C:19:GLU:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:5:TYR:N	3:F:5:TYR:CD1	2.70	0.55
1:C:216:THR:O	1:C:260:HIS:N	2.38	0.55
1:C:210:PRO:HD2	1:C:263:HIS:NE2	2.22	0.55
1:A:103:VAL:HG13	1:A:168:LEU:HD21	1.89	0.55
1:A:156:LEU:O	1:A:160:LEU:HG	2.06	0.55
1:C:106:ASP:HB2	1:C:108:ARG:NH2	2.22	0.55
1:C:79:ARG:O	1:C:82:LEU:HB3	2.07	0.55
1:A:180:LEU:C	1:A:180:LEU:HD23	2.27	0.55
1:C:263:HIS:CD2	1:C:265:GLY:H	2.25	0.54
2:B:17:ASN:HA	2:B:72:PRO:O	2.07	0.54
2:D:78:TYR:O	2:D:94:TYR:HB2	2.07	0.54
2:B:25:CYS:SG	2:B:26:TYR:N	2.79	0.54
1:C:19:GLU:HG2	1:C:20:PRO:CD	2.36	0.54
1:A:170:ARG:HB3	1:A:170:ARG:NH1	2.20	0.54
2:B:39:MET:HB2	2:B:49:VAL:HG11	1.90	0.54
1:C:233:THR:OG1	1:C:243:LYS:HD2	2.07	0.54
2:D:17:ASN:HD22	2:D:17:ASN:C	2.10	0.54
1:A:109:LEU:HD13	1:A:161:GLU:HA	1.89	0.54
2:D:19:LYS:HA	2:D:71:THR:HG23	1.89	0.54
1:A:201:LEU:O	1:A:246:SER:HB2	2.08	0.54
1:A:206:LEU:CB	1:A:242:GLN:HB3	2.35	0.54
1:A:24:GLU:HG3	1:A:36:PHE:HB3	1.90	0.54
2:B:69:GLU:O	2:B:70:PHE:HB3	2.07	0.54
1:A:35:ARG:NH1	1:A:46:GLU:N	2.40	0.53
1:C:125:ALA:O	1:C:133:TRP:HE3	1.91	0.53
1:C:124:ILE:HG12	1:C:140:ALA:HB1	1.90	0.53
1:A:191:HIS:HB2	1:A:201:LEU:HD13	1.91	0.53
1:A:143:THR:O	1:A:147:TRP:HB2	2.07	0.53
1:C:82:LEU:HD23	1:C:83:GLY:N	2.22	0.53
2:D:23:LEU:HB2	2:D:70:PHE:CD1	2.43	0.53
2:D:17:ASN:HB3	2:D:72:PRO:HB2	1.91	0.53
1:C:225:ILE:C	1:C:225:ILE:HD13	2.28	0.53
2:D:13:HIS:HB2	2:D:21:ASN:OD1	2.08	0.53
1:A:203:CYS:O	1:A:244:TRP:HB2	2.08	0.53
1:A:194:ARG:HH22	1:A:202:ARG:HH12	1.56	0.53
1:C:143:THR:O	1:C:147:TRP:HB2	2.09	0.53
1:C:124:ILE:HG21	1:C:147:TRP:HZ3	1.74	0.53
1:C:102:GLU:HB3	1:C:111:ARG:HB2	1.91	0.53
1:C:116:TYR:HE2	3:F:8:LEU:HG	1.74	0.52
2:D:65:LEU:HD13	2:D:65:LEU:O	2.09	0.52
1:A:87:GLN:OE1	1:A:93:HIS:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LYS:C	1:C:146:LYS:H	2.13	0.52
1:A:182:THR:CG2	1:A:210:PRO:HD2	2.32	0.52
1:A:128:GLU:C	1:A:130:LEU:N	2.63	0.52
1:C:81:LEU:O	1:C:85:TYR:HD2	1.92	0.52
1:A:74:PHE:C	1:A:76:VAL:H	2.12	0.52
1:A:22:TYR:O	1:A:37:ASP:HA	2.09	0.52
1:A:234:ARG:HH11	1:A:242:GLN:NE2	2.00	0.52
1:A:11:ALA:HA	1:A:21:ARG:O	2.10	0.52
1:A:74:PHE:O	1:A:76:VAL:N	2.43	0.52
1:A:202:ARG:CG	1:A:204:TRP:HE1	2.19	0.51
2:D:82:VAL:HG23	2:D:87:MET:CE	2.41	0.51
2:D:51:MET:HG3	2:D:64:ILE:HD11	1.92	0.51
1:C:146:LYS:HG2	1:C:146:LYS:O	2.10	0.51
1:A:233:THR:OG1	1:A:243:LYS:NZ	2.30	0.51
1:A:147:TRP:HE1	3:E:7:GLY:HA3	1.75	0.51
1:C:183:ASP:HB2	1:C:209:TYR:H	1.75	0.51
1:A:168:LEU:HD12	1:A:172:LEU:HD13	1.92	0.51
1:C:44:ARG:NH1	1:C:44:ARG:HG3	2.23	0.51
1:C:165:VAL:HG12	1:C:169:ARG:NH2	2.26	0.51
1:A:156:LEU:HD22	1:A:160:LEU:CG	2.40	0.51
1:C:234:ARG:HD3	1:C:242:GLN:HB2	1.92	0.51
1:C:156:LEU:HD23	1:C:159:TYR:HD2	1.76	0.51
1:A:28:VAL:O	1:A:29:ASP:HB2	2.09	0.51
1:C:216:THR:O	1:C:259:CYS:SG	2.66	0.50
1:A:160:LEU:O	1:A:164:CYS:HB3	2.12	0.50
1:A:203:CYS:O	1:A:244:TRP:HA	2.12	0.50
1:C:153:ALA:O	1:C:157:ARG:HB2	2.10	0.50
1:C:128:GLU:O	1:C:130:LEU:HD12	2.12	0.50
2:B:36:GLU:CD	2:B:38:GLN:HE21	2.15	0.50
1:C:187:ALA:O	1:C:188:HIS:HB3	2.12	0.50
1:C:52:MET:HE1	1:C:171:TYR:CE1	2.46	0.50
1:A:233:THR:OG1	1:A:243:LYS:HD2	2.10	0.50
2:D:19:LYS:CB	2:D:20:PRO:CD	2.86	0.50
1:A:24:GLU:O	1:A:35:ARG:HA	2.12	0.50
1:C:201:LEU:HD12	1:C:249:VAL:HG11	1.92	0.50
1:A:217:TRP:O	1:A:224:LEU:HB2	2.10	0.50
2:B:35:ILE:HG23	2:B:35:ILE:O	2.12	0.50
1:C:192:HIS:HB2	1:C:200:THR:O	2.12	0.50
1:A:51:TRP:CZ2	1:A:179:LEU:HD21	2.47	0.50
1:C:117:ALA:CB	2:D:60:TRP:CZ2	2.94	0.49
1:A:52:MET:HE2	1:A:52:MET:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ILE:HG23	1:A:226:GLN:H	1.77	0.49
1:C:9:VAL:HB	1:C:97:VAL:HB	1.93	0.49
1:C:126:LEU:HD12	1:C:133:TRP:CZ3	2.47	0.49
2:B:7:ILE:HD12	2:B:93:VAL:HG23	1.93	0.49
2:D:10:TYR:N	2:D:10:TYR:CD1	2.81	0.49
1:C:167:TRP:CE3	1:C:170:ARG:HD3	2.48	0.49
1:C:225:ILE:HD12	1:C:226:GLN:HG3	1.94	0.49
1:C:8:PHE:HD2	2:D:56:PHE:CE2	2.30	0.49
3:E:5:TYR:CD1	3:E:5:TYR:N	2.81	0.49
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.49	0.48
2:D:31:HIS:CD2	2:D:62:PHE:HE1	2.31	0.48
1:A:133:TRP:CZ2	1:A:153:ALA:HA	2.48	0.48
2:D:33:PRO:HB3	2:D:62:PHE:CZ	2.48	0.48
2:B:28:THR:HG22	2:B:29:GLN:HG3	1.95	0.48
1:A:189:VAL:HA	1:A:202:ARG:O	2.12	0.48
1:A:177:ALA:HB1	1:A:181:ARG:CZ	2.43	0.48
1:C:139:ALA:O	1:C:142:ILE:HG22	2.13	0.48
2:B:36:GLU:CB	2:B:83:LYS:HB3	2.24	0.48
1:C:40:ALA:O	1:C:42:ASN:N	2.46	0.48
1:A:74:PHE:C	1:A:76:VAL:N	2.67	0.48
1:A:180:LEU:O	1:A:181:ARG:HB2	2.13	0.48
1:C:116:TYR:HD2	3:F:8:LEU:HD11	1.77	0.48
1:A:47:PRO:CB	1:A:53:GLU:HG3	2.44	0.48
1:C:196:GLU:CG	1:C:251:LEU:HD12	2.44	0.47
1:A:188:HIS:ND1	1:A:204:TRP:HB2	2.29	0.47
1:C:14:ARG:NH2	1:C:39:ASP:OD2	2.47	0.47
1:A:227:ASP:HB3	1:A:247:VAL:HG23	1.96	0.47
1:C:180:LEU:HA	1:C:209:TYR:HE2	1.80	0.47
1:A:2:PRO:O	1:A:3:HIS:HD2	1.97	0.47
1:A:37:ASP:O	1:A:39:ASP:N	2.47	0.47
1:C:52:MET:O	1:C:54:GLN:N	2.47	0.47
2:D:13:HIS:HB3	2:D:14:PRO:HD2	1.96	0.47
3:E:6:GLN:CG	3:E:7:GLY:H	2.23	0.47
1:A:50:ARG:HD2	1:A:50:ARG:HA	1.63	0.47
1:C:176:ASN:CG	1:C:177:ALA:H	2.18	0.47
2:D:78:TYR:HB2	2:D:95:TRP:HB3	1.97	0.47
1:C:192:HIS:NE2	2:D:98:ASP:HB2	2.29	0.47
2:D:23:LEU:HD23	2:D:39:MET:CE	2.45	0.47
1:C:95:ILE:HG12	1:C:118:TYR:HD1	1.80	0.47
1:A:218:GLN:HG3	1:A:223:GLU:CG	2.43	0.46
2:B:70:PHE:HD2	2:B:78:TYR:CE2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ALA:C	1:A:181:ARG:HH12	2.18	0.46
2:D:17:ASN:HB3	2:D:97:ARG:NH2	2.29	0.46
1:C:2:PRO:HB3	1:C:104:GLY:HA3	1.96	0.46
1:A:44:ARG:NH2	1:A:64:THR:HG21	2.31	0.46
2:D:26:TYR:CE2	2:D:28:THR:HG21	2.50	0.46
2:B:83:LYS:HG2	2:B:90:PRO:HG3	1.96	0.46
2:D:17:ASN:CB	2:D:97:ARG:HH22	2.28	0.46
1:C:180:LEU:HG	1:C:209:TYR:OH	2.15	0.46
1:A:23:MET:HA	1:A:36:PHE:O	2.15	0.46
1:A:202:ARG:HB2	1:A:246:SER:HB3	1.97	0.46
1:A:219:LEU:HD12	1:A:256:TYR:O	2.15	0.46
1:C:38:SER:OG	1:C:38:SER:O	2.30	0.46
2:D:26:TYR:CE2	2:D:28:THR:CG2	2.99	0.46
1:A:146:LYS:HG2	1:A:146:LYS:O	2.13	0.46
1:C:33:PHE:O	1:C:48:ARG:N	2.49	0.46
1:A:81:LEU:HD13	1:A:84:TYR:CD2	2.50	0.46
2:B:11:SER:HB2	2:B:13:HIS:O	2.16	0.46
1:A:21:ARG:NH1	1:A:23:MET:HG3	2.31	0.46
1:C:199:VAL:O	1:C:249:VAL:HG22	2.16	0.46
1:A:205:ALA:CB	1:A:215:LEU:HD11	2.45	0.46
1:A:234:ARG:HG3	2:B:10:TYR:CZ	2.52	0.45
1:A:236:ALA:O	2:B:12:ARG:HD2	2.16	0.45
2:D:41:LYS:O	2:D:43:GLY:N	2.49	0.45
1:C:8:PHE:HB3	2:D:56:PHE:CE1	2.50	0.45
3:F:6:GLN:HG3	3:F:7:GLY:N	2.31	0.45
1:C:74:PHE:CA	1:C:77:ASP:HB2	2.41	0.45
1:A:62:ARG:HA	1:A:62:ARG:HD2	1.72	0.45
1:C:11:ALA:HA	1:C:21:ARG:O	2.16	0.45
1:A:138:MET:SD	1:C:61:GLU:OE1	2.74	0.45
1:A:168:LEU:HD12	1:A:172:LEU:CD1	2.46	0.45
1:C:82:LEU:HD11	1:C:89:LYS:HG3	1.99	0.45
2:D:82:VAL:HG23	2:D:87:MET:HE1	1.98	0.45
1:A:74:PHE:O	1:A:77:ASP:HB2	2.17	0.45
1:C:33:PHE:CE2	1:C:52:MET:HE1	2.51	0.45
1:A:205:ALA:HB2	1:A:215:LEU:HD11	1.99	0.45
1:A:123:TYR:CE1	1:A:140:ALA:HA	2.51	0.45
1:C:127:ASN:HB2	1:C:134:THR:OG1	2.15	0.45
1:A:164:CYS:O	1:A:168:LEU:HB3	2.17	0.45
1:A:6:ARG:HA	1:A:99:SER:O	2.17	0.45
1:A:143:THR:HG21	3:E:8:LEU:HD23	1.99	0.44
2:D:59:ASP:OD2	2:D:61:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:VAL:CG1	1:C:190:THR:N	2.80	0.44
1:A:159:TYR:O	1:A:164:CYS:HB2	2.17	0.44
3:F:8:LEU:HA	3:F:8:LEU:HD23	1.46	0.44
1:C:172:LEU:HG	1:C:179:LEU:HD13	1.99	0.44
1:C:192:HIS:CE1	2:D:98:ASP:HB2	2.52	0.44
1:C:104:GLY:HA3	1:C:110:LEU:HD11	1.99	0.44
1:A:133:TRP:HB2	1:A:144:LYS:HZ3	1.82	0.44
1:C:206:LEU:HB2	1:C:242:GLN:HG2	1.99	0.44
1:C:31:THR:HG23	1:C:32:GLU:N	2.33	0.44
1:C:114:GLN:CD	1:C:156:LEU:HD11	2.38	0.44
1:C:8:PHE:HD2	2:D:56:PHE:CZ	2.35	0.44
1:C:181:ARG:HB3	1:C:182:THR:H	1.62	0.44
1:A:202:ARG:HB2	1:A:246:SER:CB	2.48	0.44
1:C:264:GLN:HG2	1:C:264:GLN:O	2.18	0.44
2:D:17:ASN:OD1	2:D:97:ARG:NH2	2.49	0.44
1:C:152:GLU:HG3	1:C:155:ARG:HB3	1.99	0.44
1:C:213:ILE:HG13	1:C:263:HIS:HB2	1.99	0.44
1:A:256:TYR:H	1:A:256:TYR:HD1	1.65	0.44
1:A:235:PRO:HG2	2:B:26:TYR:CE1	2.52	0.43
1:A:83:GLY:O	1:A:86:ASN:N	2.49	0.43
2:D:19:LYS:HA	2:D:71:THR:CG2	2.49	0.43
1:C:196:GLU:HG2	1:C:251:LEU:HD12	1.99	0.43
1:A:203:CYS:O	1:A:244:TRP:CB	2.66	0.43
1:C:210:PRO:O	1:C:212:ASP:N	2.51	0.43
1:C:114:GLN:HB2	1:C:156:LEU:HD11	2.00	0.43
1:C:93:HIS:HA	1:C:119:ASP:OD1	2.19	0.43
1:A:232:GLU:C	1:A:232:GLU:CB	2.78	0.43
2:B:73:THR:HG22	2:B:74:GLU:OE2	2.19	0.43
1:C:89:LYS:HB2	1:C:89:LYS:HE2	1.92	0.43
2:B:28:THR:O	2:B:29:GLN:HB2	2.19	0.43
1:A:50:ARG:O	1:A:53:GLU:HB2	2.19	0.43
2:B:5:PRO:HG3	2:B:30:PHE:HB3	2.01	0.43
1:A:120:GLY:O	1:A:121:CYS:SG	2.76	0.43
2:B:85:ASP:OD1	2:B:85:ASP:N	2.52	0.43
1:A:133:TRP:HB2	1:A:144:LYS:NZ	2.32	0.43
1:A:22:TYR:HD2	1:A:36:PHE:HE1	1.63	0.43
3:E:6:GLN:HG2	3:E:7:GLY:N	2.21	0.43
1:C:14:ARG:HD2	1:C:19:GLU:O	2.19	0.43
2:D:58:LYS:O	2:D:58:LYS:HG3	2.19	0.43
2:D:7:ILE:HG22	2:D:8:GLN:N	2.34	0.43
1:C:44:ARG:HG2	1:C:64:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:H	1:A:89:LYS:CD	2.32	0.42
1:A:263:HIS:O	1:A:266:LEU:HB2	2.19	0.42
1:A:76:VAL:O	1:A:79:ARG:HG2	2.18	0.42
1:C:33:PHE:CD2	1:C:34:VAL:HG13	2.55	0.42
1:C:250:PRO:HB2	1:C:253:LYS:HB2	2.01	0.42
1:C:19:GLU:HG2	1:C:20:PRO:HD2	2.02	0.42
2:B:14:PRO:HA	2:B:15:PRO:HD3	1.82	0.42
2:D:12:ARG:NH1	2:D:22:ILE:HG13	2.30	0.42
1:A:191:HIS:NE2	1:A:199:VAL:HG11	2.35	0.41
1:A:2:PRO:O	1:A:3:HIS:CD2	2.72	0.41
2:D:15:PRO:CB	2:D:95:TRP:HZ2	2.33	0.41
1:C:184:SER:HB3	1:C:266:LEU:HD13	2.01	0.41
1:A:194:ARG:NH2	1:A:202:ARG:HH12	2.17	0.41
1:C:201:LEU:HD12	1:C:249:VAL:CG1	2.50	0.41
1:A:103:VAL:HG23	1:A:103:VAL:O	2.20	0.41
1:C:81:LEU:HD13	1:C:85:TYR:HE2	1.86	0.41
2:B:80:CYS:SG	2:B:81:ARG:N	2.93	0.41
2:B:41:LYS:HA	2:B:77:THR:O	2.20	0.41
1:C:229:GLU:O	1:C:245:ALA:HA	2.21	0.41
1:A:216:THR:O	1:A:260:HIS:N	2.52	0.41
1:C:47:PRO:C	1:C:49:ALA:H	2.24	0.41
1:A:146:LYS:HA	1:A:149:GLN:HB2	2.02	0.41
1:A:54:GLN:O	1:A:54:GLN:NE2	2.54	0.41
1:C:234:ARG:HA	1:C:235:PRO:HD3	1.99	0.41
1:A:259:CYS:SG	1:A:260:HIS:N	2.91	0.41
1:C:97:VAL:HG11	3:F:5:TYR:CE2	2.56	0.41
1:C:209:TYR:HD1	1:C:210:PRO:HA	1.76	0.41
1:A:21:ARG:NH2	1:A:39:ASP:HB2	2.36	0.41
1:C:106:ASP:O	1:C:108:ARG:N	2.50	0.41
2:B:71:THR:HG22	2:B:71:THR:O	2.21	0.41
2:B:92:THR:HG22	2:B:93:VAL:N	2.35	0.41
3:F:1:ARG:HH11	3:F:1:ARG:HD2	1.69	0.41
2:B:19:LYS:HA	2:B:20:PRO:HD3	1.63	0.41
1:C:33:PHE:HE2	1:C:52:MET:HE1	1.86	0.40
1:A:225:ILE:HG13	1:A:226:GLN:N	2.36	0.40
1:A:81:LEU:HD13	1:A:84:TYR:HD2	1.85	0.40
2:B:83:LYS:C	2:B:83:LYS:HD3	2.42	0.40
1:C:192:HIS:HE2	2:D:98:ASP:HB2	1.85	0.40
1:C:116:TYR:HB3	1:C:123:TYR:HD2	1.87	0.40
1:C:95:ILE:HG21	1:C:95:ILE:HD13	1.77	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	268/270 (99%)	188 (70%)	51 (19%)	29 (11%)	0 0
1	C	268/270 (99%)	201 (75%)	45 (17%)	22 (8%)	1 1
2	B	97/99 (98%)	75 (77%)	17 (18%)	5 (5%)	2 2
2	D	97/99 (98%)	71 (73%)	13 (13%)	13 (13%)	0 0
3	E	6/8 (75%)	5 (83%)	1 (17%)	0	100 100
3	F	6/8 (75%)	4 (67%)	2 (33%)	0	100 100
All	All	742/754 (98%)	544 (73%)	129 (17%)	69 (9%)	1 1

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	PRO
1	A	121	CYS
1	A	128	GLU
1	A	130	LEU
1	A	181	ARG
1	A	195	PRO
1	A	226	GLN
1	A	227	ASP
1	A	264	GLN
1	C	41	GLU
1	C	48	ARG
1	C	53	GLU
1	C	107	GLY
1	C	122	ASP
1	C	130	LEU
1	C	195	PRO
1	C	211	ALA
2	D	53	ASP
2	D	70	PHE
2	D	74	GLU

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Mol	Chain	Res	Type
2	D	76	ASP
2	D	88	ALA
1	A	38	SER
1	A	48	ARG
1	A	49	ALA
1	A	75	ARG
1	A	90	GLY
1	A	120	GLY
1	A	138	MET
1	A	173	LYS
1	A	179	LEU
1	C	39	ASP
1	C	105	SER
1	C	138	MET
1	C	180	LEU
1	C	253	LYS
2	D	42	ASN
2	D	86	SER
1	A	105	SER
1	A	129	ASP
1	A	176	ASN
2	B	45	LYS
2	B	60	TRP
1	C	57	PRO
1	C	113	TYR
1	C	135	ALA
1	C	137	ASP
1	C	210	PRO
2	D	29	GLN
2	D	58	LYS
2	D	61	SER
1	A	41	GLU
1	A	145	HIS
1	A	196	GLU
2	D	95	TRP
1	A	53	GLU
1	A	220	ASN
1	A	225	ILE
2	B	13	HIS
2	B	33	PRO
1	C	178	THR
2	D	47	PRO

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Mol	Chain	Res	Type
2	D	60	TRP
1	C	199	VAL
1	A	20	PRO
2	B	43	GLY
1	C	20	PRO
1	A	213	ILE
1	C	47	PRO

5.3.2 Protein sidechains

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	228/228 (100%)	165 (72%)	63 (28%)	0	0
1	C	228/228 (100%)	166 (73%)	62 (27%)	0	0
2	B	94/94 (100%)	65 (69%)	29 (31%)	0	0
2	D	94/94 (100%)	73 (78%)	21 (22%)	1	2
3	E	6/6 (100%)	2 (33%)	4 (67%)	0	0
3	F	6/6 (100%)	1 (17%)	5 (83%)	0	0
All	All	656/656 (100%)	472 (72%)	184 (28%)	0	0

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	9	VAL
1	A	12	VAL
1	A	13	SER
1	A	17	LEU
1	A	23	MET
1	A	30	ASP
1	A	31	THR
1	A	35	ARG
1	A	41	GLU
1	A	45	TYR

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Mol	Chain	Res	Type
1	A	46	GLU
1	A	47	PRO
1	A	48	ARG
1	A	50	ARG
1	A	52	MET
1	A	54	GLN
1	A	64	THR
1	A	65	GLN
1	A	78	LEU
1	A	79	ARG
1	A	80	THR
1	A	89	LYS
1	A	94	THR
1	A	99	SER
1	A	105	SER
1	A	109	LEU
1	A	113	TYR
1	A	127	ASN
1	A	131	LYS
1	A	132	THR
1	A	137	ASP
1	A	141	LEU
1	A	143	THR
1	A	147	TRP
1	A	152	GLU
1	A	154	GLU
1	A	155	ARG
1	A	156	LEU
1	A	157	ARG
1	A	160	LEU
1	A	180	LEU
1	A	181	ARG
1	A	182	THR
1	A	183	ASP
1	A	188	HIS
1	A	193	SER
1	A	198	LYS
1	A	199	VAL
1	A	201	LEU
1	A	202	ARG
1	A	206	LEU
1	A	212	ASP

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Mol	Chain	Res	Type
1	A	220	ASN
1	A	222	GLU
1	A	227	ASP
1	A	234	ARG
1	A	240	THR
1	A	244	TRP
1	A	254	GLU
1	A	261	VAL
1	A	264	GLN
1	A	270	LEU
2	B	1	ILE
2	B	6	GLN
2	B	11	SER
2	B	19	LYS
2	B	21	ASN
2	B	31	HIS
2	B	34	HIS
2	B	36	GLU
2	B	40	LEU
2	B	42	ASN
2	B	51	MET
2	B	55	SER
2	B	58	LYS
2	B	59	ASP
2	B	65	LEU
2	B	69	GLU
2	B	70	PHE
2	B	73	THR
2	B	74	GLU
2	B	75	THR
2	B	83	LYS
2	B	85	ASP
2	B	86	SER
2	B	87	MET
2	B	89	GLU
2	B	91	LYS
2	B	94	TYR
2	B	97	ARG
2	B	99	MET
1	C	4	SER
1	C	6	ARG
1	C	10	THR

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Mol	Chain	Res	Type
1	C	12	VAL
1	C	14	ARG
1	C	17	LEU
1	C	21	ARG
1	C	28	VAL
1	C	31	THR
1	C	42	ASN
1	C	44	ARG
1	C	45	TYR
1	C	46	GLU
1	C	58	GLU
1	C	62	ARG
1	C	64	THR
1	C	66	LYS
1	C	72	GLN
1	C	81	LEU
1	C	87	GLN
1	C	89	LYS
1	C	94	THR
1	C	109	LEU
1	C	115	GLN
1	C	119	ASP
1	C	124	ILE
1	C	128	GLU
1	C	130	LEU
1	C	132	THR
1	C	134	THR
1	C	141	LEU
1	C	142	ILE
1	C	147	TRP
1	C	148	GLU
1	C	152	GLU
1	C	154	GLU
1	C	155	ARG
1	C	156	LEU
1	C	157	ARG
1	C	163	THR
1	C	166	GLU
1	C	172	LEU
1	C	182	THR
1	C	184	SER
1	C	192	HIS

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Mol	Chain	Res	Type
1	C	195	PRO
1	C	196	GLU
1	C	199	VAL
1	C	202	ARG
1	C	206	LEU
1	C	215	LEU
1	C	216	THR
1	C	225	ILE
1	C	231	VAL
1	C	232	GLU
1	C	234	ARG
1	C	247	VAL
1	C	250	PRO
1	C	251	LEU
1	C	253	LYS
1	C	255	GLN
1	C	266	LEU
2	D	1	ILE
2	D	2	GLN
2	D	6	GLN
2	D	17	ASN
2	D	21	ASN
2	D	28	THR
2	D	33	PRO
2	D	34	HIS
2	D	38	GLN
2	D	40	LEU
2	D	41	LYS
2	D	46	ILE
2	D	48	LYS
2	D	51	MET
2	D	73	THR
2	D	75	THR
2	D	76	ASP
2	D	77	THR
2	D	83	LYS
2	D	89	GLU
2	D	98	ASP
3	E	1	ARG
3	E	4	VAL
3	E	5	TYR
3	E	8	LEU

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Mol	Chain	Res	Type
3	F	1	ARG
3	F	4	VAL
3	F	5	TYR
3	F	6	GLN
3	F	8	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	242	GLN
1	C	218	GLN
1	C	242	GLN
3	F	6	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.