



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:39 PM UTC

PDB ID : 2MHA / pdb_00002mha
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

<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

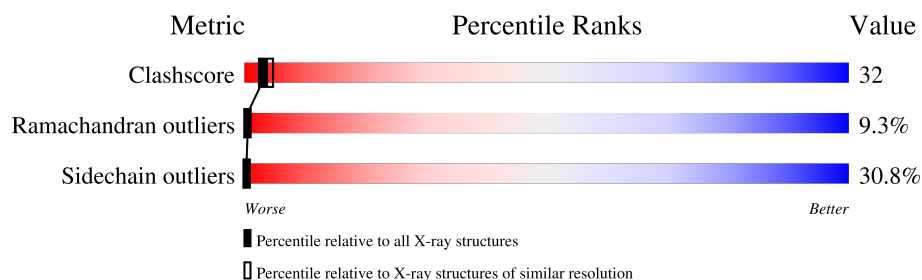
1 Overall quality at a glance

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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	270	27% 40% 26% 7%
1	C	270	23% 49% 23% 6%
2	B	99	26% 53% 19% .
2	D	99	21% 48% 27% .
3	E	8	25% 50% 12% 12%
3	F	8	12% 12% 50% 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.

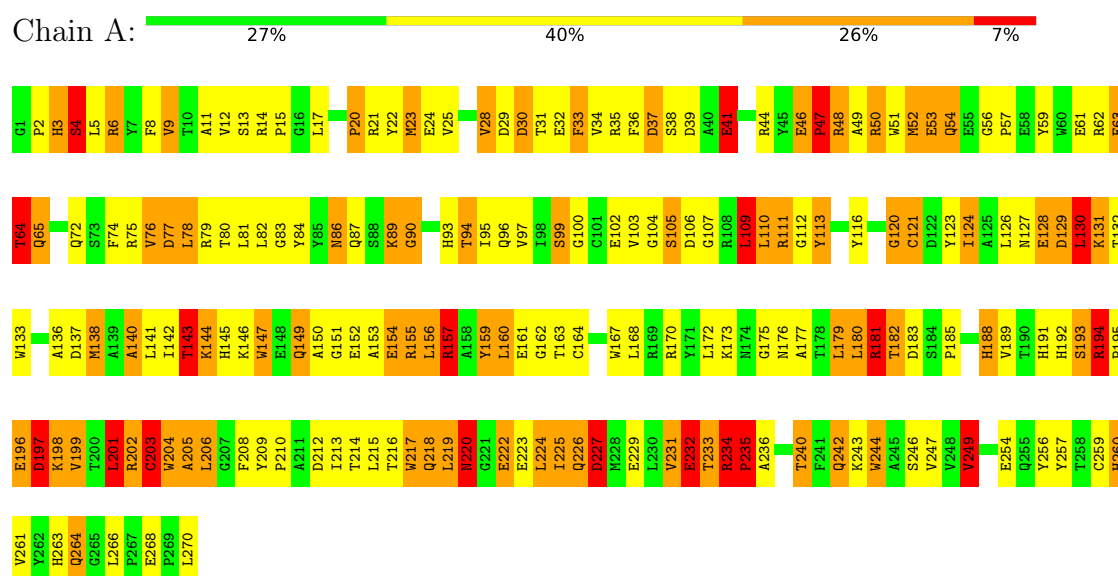
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	0	0	0
			68	44	12	12			
3	F	8	Total	C	N	O	0	0	0
			68	44	12	12			

3 Residue-property plots

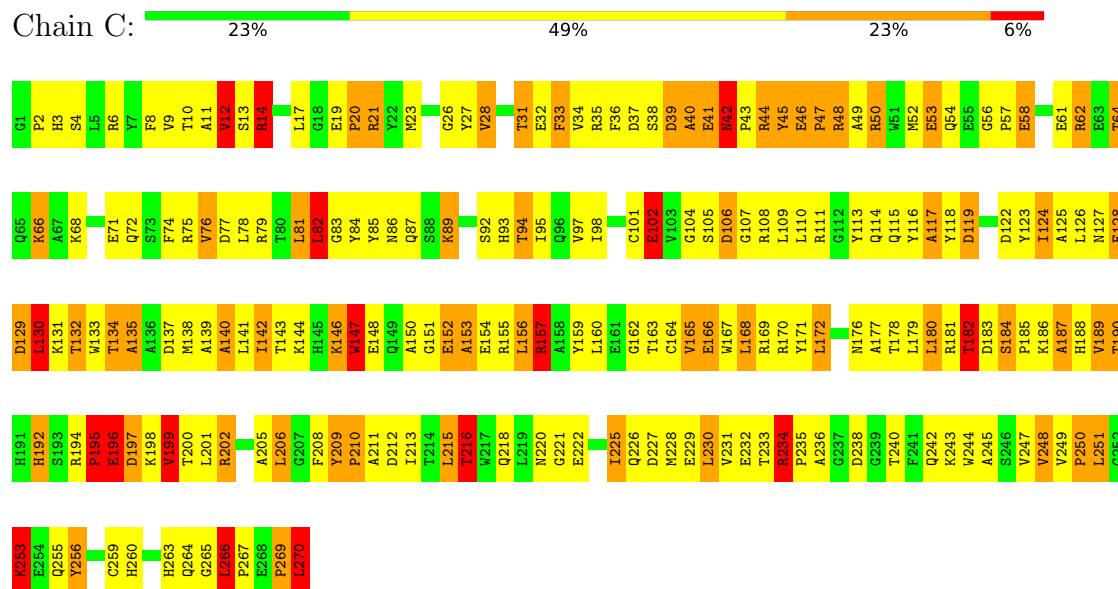
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

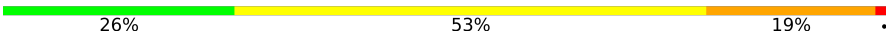
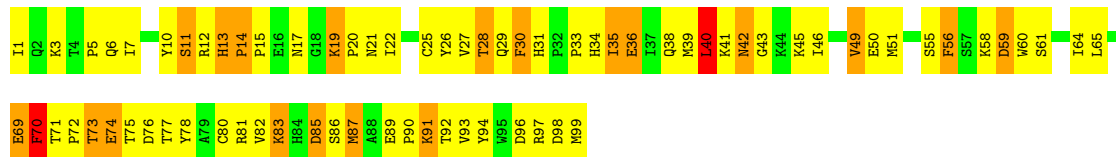
• Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (H-2KB) (ALPHA CHAIN)



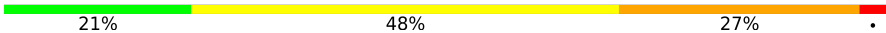
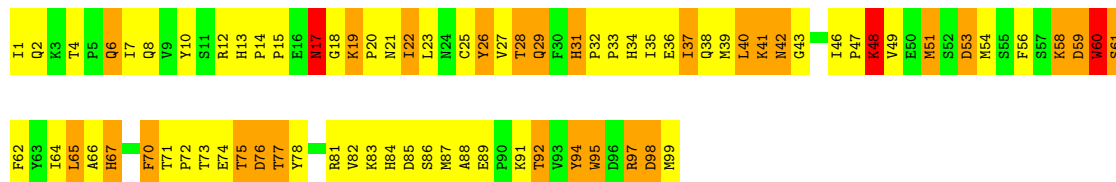
• Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (H-2KB) (ALPHA CHAIN)



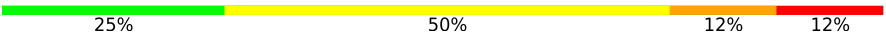
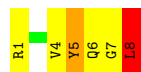
● Molecule 2: BETA 2-MICROGLOBULIN

Chain B:  26% 53% 19%

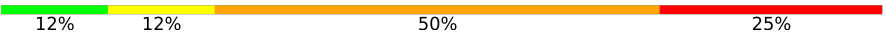
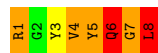
● Molecule 2: BETA 2-MICROGLOBULIN

Chain D:  21% 48% 27%

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

Chain E:  25% 50% 12% 12%

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

Chain F:  12% 12% 50% 25%

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	1.62	22/2250 (1.0%)	1.99	74/3055 (2.4%)
1	C	1.47	15/2250 (0.7%)	1.92	65/3055 (2.1%)
2	B	1.43	2/847 (0.2%)	1.79	15/1148 (1.3%)
2	D	1.54	16/847 (1.9%)	1.83	23/1148 (2.0%)
3	E	1.17	0/69	1.72	1/90 (1.1%)
3	F	3.13	9/69 (13.0%)	2.25	5/90 (5.6%)
All	All	1.55	64/6332 (1.0%)	1.92	183/8586 (2.1%)

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

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	GLU	CA-CB	26.43	1.94	1.53
3	F	7	GLY	N-CA	-13.22	1.30	1.45
2	D	49	VAL	CA-C	-8.98	1.45	1.53
3	F	6	GLN	CA-C	-8.61	1.41	1.52
2	D	49	VAL	N-CA	-7.63	1.38	1.46
1	C	270	LEU	CA-C	7.60	1.69	1.52
3	F	7	GLY	C-N	-7.36	1.23	1.33
3	F	6	GLN	N-CA	-6.89	1.38	1.46
1	A	4	SER	N-CA	6.77	1.54	1.45
2	B	61	SER	CA-C	-6.72	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	HIS	C-N	6.70	1.42	1.33
1	A	259	CYS	N-CA	-6.65	1.37	1.46
3	F	4	VAL	CA-C	6.37	1.60	1.52
3	F	8	LEU	N-CA	-6.17	1.34	1.46
1	C	86	ASN	CA-C	-6.15	1.44	1.52
2	D	67	HIS	CA-C	6.14	1.60	1.52
1	C	45	TYR	CA-C	-5.98	1.45	1.52
1	A	204	TRP	N-CA	-5.96	1.39	1.46
1	A	205	ALA	N-CA	-5.95	1.38	1.46
1	C	218	GLN	CA-C	-5.95	1.45	1.52
1	C	106	ASP	CA-CB	5.83	1.61	1.52
1	A	112	GLY	C-N	5.83	1.41	1.33
1	A	259	CYS	CA-CB	-5.69	1.45	1.53
1	A	111	ARG	N-CA	5.65	1.53	1.45
2	D	48	LYS	C-N	-5.61	1.26	1.33
3	F	6	GLN	C-N	-5.59	1.25	1.33
1	A	94	THR	N-CA	-5.56	1.39	1.46
1	A	218	GLN	N-CA	-5.55	1.39	1.46
1	A	214	THR	CA-C	-5.55	1.46	1.52
1	C	197	ASP	N-CA	-5.53	1.39	1.46
1	C	269	PRO	C-N	5.52	1.41	1.33
1	A	268	GLU	C-N	5.50	1.40	1.33
2	D	18	GLY	N-CA	-5.49	1.37	1.45
3	F	7	GLY	CA-C	-5.49	1.44	1.52
2	D	26	TYR	N-CA	-5.46	1.39	1.46
1	A	113	TYR	N-CA	5.41	1.52	1.45
2	D	66	ALA	C-N	5.35	1.40	1.33
2	B	40	LEU	CA-C	5.34	1.59	1.53
1	C	46	GLU	CA-C	5.34	1.58	1.52
1	C	221	GLY	CA-C	5.34	1.56	1.51
2	D	92	THR	CA-C	-5.30	1.46	1.52
2	D	25	CYS	N-CA	-5.30	1.39	1.46
1	A	142	ILE	N-CA	-5.30	1.40	1.46
1	A	107	GLY	C-N	-5.30	1.28	1.33
1	C	197	ASP	CA-C	-5.30	1.47	1.52
2	D	35	ILE	CA-C	5.26	1.59	1.52
1	A	181	ARG	CA-C	-5.25	1.45	1.52
1	A	233	THR	N-CA	5.24	1.52	1.46
1	C	102	GLU	CA-CB	5.24	1.61	1.53
2	D	25	CYS	C-N	-5.23	1.26	1.33
1	A	113	TYR	CA-C	5.22	1.59	1.52
3	F	3	TYR	C-N	5.20	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	36	GLU	CA-CB	5.19	1.60	1.53
1	C	190	THR	CA-C	-5.18	1.46	1.52
2	D	22	ILE	CA-C	-5.18	1.46	1.52
1	A	232	GLU	CA-C	-5.16	1.46	1.52
2	D	25	CYS	CA-C	-5.13	1.46	1.52
1	C	196	GLU	C-N	-5.13	1.27	1.33
1	A	41	GLU	CA-CB	5.11	1.62	1.53
2	D	17	ASN	C-N	-5.10	1.26	1.33
1	C	129	ASP	CA-CB	5.10	1.59	1.52
1	A	219	LEU	CA-C	-5.09	1.46	1.52
1	C	117	ALA	CA-C	-5.05	1.46	1.52
2	D	94	TYR	CA-C	5.03	1.58	1.52

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	VAL	CA-C-N	-16.12	94.50	122.07
1	A	231	VAL	C-N-CA	-16.12	94.50	122.07
1	C	194	ARG	CA-C-N	12.05	134.90	119.84
1	C	194	ARG	C-N-CA	12.05	134.90	119.84
1	C	150	ALA	CA-C-N	-11.83	103.49	122.30
1	C	150	ALA	C-N-CA	-11.83	103.49	122.30
1	A	232	GLU	CA-CB-CG	11.33	136.76	114.10
1	A	249	VAL	N-CA-C	10.20	117.41	108.63
1	C	197	ASP	N-CA-C	-10.05	99.56	112.93
1	A	197	ASP	N-CA-C	-9.80	99.89	112.93
1	C	194	ARG	N-CA-C	9.51	116.78	108.22
1	A	113	TYR	N-CA-C	9.45	124.16	109.52
1	C	42	ASN	CA-CB-CG	9.28	121.88	112.60
1	A	220	ASN	CA-CB-CG	9.21	121.81	112.60
1	C	106	ASP	CA-CB-CG	9.04	121.64	112.60
2	B	76	ASP	CA-CB-CG	8.84	121.44	112.60
1	A	259	CYS	CA-CB-SG	-8.83	94.10	114.40
2	B	96	ASP	CA-CB-CG	8.64	121.24	112.60
1	A	232	GLU	N-CA-CB	-8.51	96.55	110.41
2	D	94	TYR	N-CA-C	8.34	122.15	109.23
2	D	59	ASP	CA-CB-CG	8.32	120.92	112.60
1	A	268	GLU	CA-C-N	8.26	128.21	120.03
1	A	268	GLU	C-N-CA	8.26	128.21	120.03
1	A	150	ALA	N-CA-C	8.12	121.68	111.69
1	A	249	VAL	N-CA-CB	-7.90	101.78	110.23
1	A	37	ASP	CA-CB-CG	7.85	120.45	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	CA-C-N	7.84	127.60	119.76
1	A	234	ARG	C-N-CA	7.84	127.60	119.76
2	D	17	ASN	N-CA-CB	7.77	121.79	109.51
1	C	227	ASP	CA-CB-CG	7.72	120.32	112.60
2	D	53	ASP	CA-CB-CG	7.71	120.31	112.60
2	B	56	PHE	CA-CB-CG	7.55	121.35	113.80
2	B	35	ILE	N-CA-C	7.45	118.79	107.77
2	B	14	PRO	N-CA-C	7.44	119.78	110.70
1	A	143	THR	N-CA-CB	7.40	121.83	110.14
1	A	232	GLU	N-CA-C	7.40	122.08	110.32
2	B	59	ASP	CA-CB-CG	7.37	119.97	112.60
1	C	195	PRO	CA-C-N	7.34	135.23	123.93
1	C	195	PRO	C-N-CA	7.34	135.23	123.93
2	D	60	TRP	N-CA-CB	7.25	122.75	110.49
1	C	216	THR	CA-CB-OG1	7.20	120.41	109.60
1	A	8	PHE	CA-CB-CG	7.12	120.92	113.80
1	A	227	ASP	CA-CB-CG	7.04	119.64	112.60
1	C	84	TYR	N-CA-CB	7.03	120.17	109.91
1	A	235	PRO	CB-CA-C	-7.00	101.91	111.21
1	A	47	PRO	N-CA-C	6.94	126.76	112.47
1	A	162	GLY	CA-C-N	6.92	131.20	120.82
1	A	162	GLY	C-N-CA	6.92	131.20	120.82
1	A	14	ARG	CA-C-N	6.81	127.88	119.98
1	A	14	ARG	C-N-CA	6.81	127.88	119.98
1	C	267	PRO	CB-CA-C	-6.63	104.20	112.89
1	A	208	PHE	N-CA-C	6.60	119.75	109.52
2	B	98	ASP	N-CA-C	-6.56	102.92	111.71
1	A	201	LEU	N-CA-CB	6.54	121.30	110.63
1	A	100	GLY	N-CA-C	6.54	119.46	110.56
1	C	216	THR	N-CA-CB	6.50	122.52	111.66
2	B	49	VAL	N-CA-C	6.48	117.62	108.36
2	B	59	ASP	N-CA-CB	6.47	121.72	110.39
1	C	195	PRO	CA-N-CD	-6.47	102.94	112.00
1	C	192	HIS	CA-C-N	6.41	130.22	121.05
1	C	192	HIS	C-N-CA	6.41	130.22	121.05
1	C	140	ALA	CA-C-N	6.41	129.16	120.38
1	C	140	ALA	C-N-CA	6.41	129.16	120.38
2	B	50	GLU	N-CA-C	6.25	118.98	107.99
1	A	240	THR	N-CA-C	-6.24	101.54	110.59
1	C	147	TRP	CA-C-O	6.22	127.31	119.78
1	C	66	LYS	CA-C-N	6.22	128.52	120.44
1	C	66	LYS	C-N-CA	6.22	128.52	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ARG	CA-C-N	6.18	127.57	119.84
1	A	194	ARG	C-N-CA	6.18	127.57	119.84
1	A	77	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	30	ASP	CA-CB-CG	6.05	118.65	112.60
2	D	19	LYS	CA-C-N	6.01	127.36	119.84
2	D	19	LYS	C-N-CA	6.01	127.36	119.84
1	C	150	ALA	O-C-N	-6.01	114.64	122.39
1	C	140	ALA	N-CA-C	-6.01	105.21	112.54
1	A	86	ASN	CA-CB-CG	5.99	118.59	112.60
1	A	192	HIS	CA-CB-CG	5.98	119.78	113.80
2	B	40	LEU	N-CA-C	5.97	120.18	107.70
1	C	14	ARG	NE-CZ-NH2	5.97	124.58	119.20
1	C	153	ALA	CA-C-N	5.96	130.67	120.71
1	C	153	ALA	C-N-CA	5.96	130.67	120.71
1	A	47	PRO	CA-C-N	5.96	132.93	121.54
1	A	47	PRO	C-N-CA	5.96	132.93	121.54
1	C	187	ALA	N-CA-C	5.95	118.26	109.69
1	A	231	VAL	N-CA-C	5.93	116.35	107.51
2	D	4	THR	N-CA-C	5.93	117.54	110.07
1	A	181	ARG	N-CA-CB	5.93	120.50	110.49
1	A	232	GLU	O-C-N	-5.92	116.43	123.06
1	C	208	PHE	N-CA-C	5.90	118.82	109.50
3	F	6	GLN	O-C-N	5.86	129.97	123.52
1	A	217	TRP	N-CA-CB	5.86	119.75	110.55
1	A	109	LEU	N-CA-C	5.85	118.63	107.75
1	C	266	LEU	CB-CA-C	5.84	117.96	109.20
1	C	28	VAL	N-CA-CB	5.83	119.22	111.64
1	C	195	PRO	N-CA-C	5.83	124.48	112.47
1	C	3	HIS	CA-CB-CG	-5.83	107.97	113.80
1	C	46	GLU	CB-CA-C	5.81	118.67	109.55
2	D	75	THR	CA-C-N	5.79	132.61	121.54
2	D	75	THR	C-N-CA	5.79	132.61	121.54
1	A	33	PHE	N-CA-C	5.79	121.91	114.56
1	A	20	PRO	CA-N-CD	-5.77	103.92	112.00
1	C	220	ASN	CA-CB-CG	5.73	118.33	112.60
2	D	97	ARG	N-CA-C	5.71	117.18	111.07
1	C	41	GLU	N-CA-C	5.67	122.88	110.80
1	A	56	GLY	CA-C-N	5.66	126.91	119.84
1	A	56	GLY	C-N-CA	5.66	126.91	119.84
1	A	57	PRO	N-CA-C	5.62	124.06	112.47
1	A	259	CYS	CA-C-N	-5.62	114.87	122.86
1	A	259	CYS	C-N-CA	-5.62	114.87	122.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	7	GLY	O-C-N	5.62	128.50	122.60
2	B	42	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	4	SER	CB-CA-C	-5.58	98.83	109.66
2	D	40	LEU	N-CA-C	5.58	117.79	108.02
1	C	33	PHE	CA-CB-CG	5.58	119.38	113.80
1	C	46	GLU	CB-CG-CD	5.57	122.08	112.60
1	C	132	THR	N-CA-C	5.57	117.82	108.23
1	A	140	ALA	N-CA-C	-5.57	106.33	113.23
1	A	157	ARG	CA-C-N	5.55	128.03	120.54
1	A	157	ARG	C-N-CA	5.55	128.03	120.54
1	A	30	ASP	N-CA-CB	5.51	118.49	110.88
1	A	185	PRO	CA-C-N	5.50	130.74	122.99
1	A	185	PRO	C-N-CA	5.50	130.74	122.99
1	C	12	VAL	CB-CA-C	-5.48	104.11	110.91
1	A	229	GLU	CB-CG-CD	5.47	121.91	112.60
1	A	136	ALA	CA-C-N	-5.46	113.22	122.67
1	A	136	ALA	C-N-CA	-5.46	113.22	122.67
2	B	30	PHE	N-CA-C	5.46	118.88	110.42
2	D	77	THR	N-CA-CB	5.45	120.93	111.39
1	C	197	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	260	HIS	N-CA-C	5.44	117.70	108.02
3	F	4	VAL	CA-C-N	5.44	128.96	120.75
3	F	4	VAL	C-N-CA	5.44	128.96	120.75
2	D	59	ASP	CA-C-N	5.43	131.91	121.54
2	D	59	ASP	C-N-CA	5.43	131.91	121.54
1	A	32	GLU	CB-CG-CD	5.43	121.82	112.60
1	A	159	TYR	N-CA-CB	5.43	118.03	109.94
1	A	203	CYS	CA-CB-SG	-5.42	101.94	114.40
2	D	76	ASP	N-CA-C	5.42	122.34	110.80
2	B	28	THR	N-CA-CB	-5.40	101.54	111.37
2	D	67	HIS	N-CA-C	5.37	117.93	108.75
2	D	19	LYS	CB-CA-C	5.36	120.73	110.17
1	A	64	THR	N-CA-C	-5.36	105.00	112.45
1	A	47	PRO	CA-N-CD	-5.36	104.50	112.00
3	F	3	TYR	N-CA-C	5.36	118.44	110.14
1	A	76	VAL	N-CA-C	-5.34	107.21	111.81
2	B	70	PHE	CA-CB-CG	5.34	119.14	113.80
1	C	40	ALA	CA-C-N	5.34	131.75	121.54
1	C	40	ALA	C-N-CA	5.34	131.75	121.54
1	C	146	LYS	CG-CD-CE	-5.34	99.03	111.30
1	C	135	ALA	N-CA-C	5.33	122.15	110.80
2	D	6	GLN	CB-CG-CD	5.33	121.66	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	THR	CA-CB-OG1	5.32	117.58	109.60
1	A	6	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	D	18	GLY	N-CA-C	-5.29	100.63	113.18
1	C	240	THR	N-CA-CB	5.29	118.64	110.60
1	C	84	TYR	CB-CA-C	-5.28	102.82	110.96
1	C	151	GLY	N-CA-C	5.28	122.39	114.95
2	D	6	GLN	N-CA-C	-5.27	102.66	110.46
2	D	42	ASN	CA-CB-CG	5.22	117.82	112.60
1	C	50	ARG	CA-CB-CG	-5.21	103.68	114.10
1	C	256	TYR	CB-CA-C	-5.21	103.90	111.14
1	A	61	GLU	N-CA-C	5.20	117.35	111.11
1	C	82	LEU	N-CA-CB	-5.19	101.72	110.49
1	C	182	THR	N-CA-C	5.18	116.72	108.79
1	C	66	LYS	O-C-N	5.14	127.38	122.03
1	C	238	ASP	CA-CB-CG	5.13	117.73	112.60
2	D	22	ILE	CB-CA-C	-5.13	102.18	110.28
1	C	102	GLU	CB-CG-CD	5.12	121.31	112.60
1	C	46	GLU	CA-C-N	5.11	126.22	119.84
1	C	46	GLU	C-N-CA	5.11	126.22	119.84
3	E	8	LEU	N-CA-CB	5.07	119.12	110.50
1	A	144	LYS	N-CA-CB	5.05	117.50	109.82
1	C	157	ARG	CD-NE-CZ	5.02	131.43	124.40
1	C	234	ARG	CA-C-N	5.02	126.12	119.84
1	C	234	ARG	C-N-CA	5.02	126.12	119.84
1	C	186	LYS	CA-C-N	-5.01	113.90	123.32
1	C	186	LYS	C-N-CA	-5.01	113.90	123.32
1	A	65	GLN	CA-C-N	5.01	127.24	120.38
1	A	65	GLN	C-N-CA	5.01	127.24	120.38
1	A	30	ASP	N-CA-C	-5.01	107.16	114.12
1	C	14	ARG	CG-CD-NE	5.01	123.01	112.00
1	C	129	ASP	CA-CB-CG	5.00	117.60	112.60

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	4	SER	Mainchain
2	B	56	PHE	Sidechain
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	152	0
1	C	2191	0	2086	152	0
2	B	821	0	798	36	0
2	D	821	0	798	56	0
3	E	68	0	67	7	0
3	F	68	0	67	7	0
All	All	6160	0	5902	391	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 32.

All (391) 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:CB	1:A:232:GLU:CA	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:116:TYR:HB2	1:A:124:ILE:HG22	1.54	0.88
1:A:182:THR:HG23	1:A:210:PRO:HD2	1.52	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:3:HIS:HB2	1:A:103:VAL:CG2	2.11	0.79
1:A:168:LEU:O	1:A:172:LEU:HD13	1.82	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
1:A:206:LEU:HB2	1:A:242:GLN:HB3	1.66	0.78
2:D:19:LYS:CB	2:D:20:PRO:HD3	2.12	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:A:133:TRP:HE1	1:A:153:ALA:HB2	1.53	0.73
1:C:101:CYS:SG	1:C:164:CYS:HB3	2.28	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:CB	1:A:232:GLU:N	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:HD2	2:B:91:LYS:N	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ASP:O	1:C:131:LYS:N	2.24	0.71
1:A:170:ARG:HH11	1:A:170:ARG:HB3	1.56	0.71
1:A:175:GLY:O	1:A:179:LEU:HG	1.91	0.71
1:C:68:LYS:O	1:C:71:GLU:HB3	1.90	0.71
1:C:263:HIS:HB3	1:C:266:LEU:HD22	1.71	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:52:MET:HE1	1:C:171:TYR:CE1	2.29	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
1:A:52:MET:HA	1:A:52:MET:HE3	1.78	0.66
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
1:C:75:ARG:O	1:C:79:ARG:HG3	1.98	0.64
3:E:5:TYR:H	3:E:5:TYR:HD1	1.45	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: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:C:210:PRO:HD2	1:C:263:HIS:HE1	1.64	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLU:O	1:C:62:ARG:HD2	2.01	0.61
2:B:25:CYS:HB2	2:B:39:MET:HE3	1.81	0.61
2:B:3:LYS:HB3	2:B:29:GLN:O	2.01	0.61
1:C:205:ALA:CB	1:C:215:LEU:HD11	2.31	0.61
1:A:15:PRO:HG2	1:A:90:GLY:O	2.01	0.60
1:C:234:ARG:NH1	1:C:242:GLN:HE21	1.99	0.60
1:C:27:TYR:HA	1:C:31:THR:O	2.01	0.60
1:A:180:LEU:C	1:A:180:LEU:HD23	2.27	0.59
1:A:181:ARG:NH1	1:A:181:ARG:HB2	2.17	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:C:167:TRP:CZ3	1:C:170:ARG:HD3	2.37	0.59
1:C:269:PRO:O	1:C:270:LEU:HB2	2.01	0.59
1:A:72:GLN:O	1:A:76:VAL:HG23	2.03	0.59
2:D:17:ASN:HD22	2:D:17:ASN:C	2.10	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:23:MET:HA	1:C:36:PHE:O	2.03	0.58
1:C:44:ARG:HG3	1:C:44:ARG:HH11	1.68	0.58
1:C:182:THR:HG23	1:C:183:ASP:N	2.18	0.58
2:D:17:ASN:HB3	2:D:97:ARG:HH22	1.68	0.58
1:C:225:ILE:HD13	1:C:225:ILE:O	2.02	0.58
2:D:19:LYS:HB3	2:D:20:PRO:CD	2.23	0.58
1:A:25:VAL:HA	1:A:34:VAL:O	2.04	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:C:225:ILE:HD13	1:C:225:ILE:C	2.28	0.58
2:D:82:VAL:HG23	2:D:87:MET:HE1	1.85	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
1:C:253:LYS:O	1:C:256:TYR:HB2	2.04	0.57
2:D:27:VAL:HG11	2:D:37:ILE:HG21	1.86	0.57
2:D:32:PRO:HD2	2:D:84:HIS:CE1	2.39	0.57
1:A:225:ILE:O	1:A:227:ASP:N	2.37	0.57
2:D:48:LYS:O	2:D:48:LYS:HG3	2.04	0.57
1:A:128:GLU:O	1:A:130:LEU:N	2.34	0.57
1:C:117:ALA:CB	2:D:60:TRP:CE2	2.87	0.57
1:C:167:TRP:O	1:C:170:ARG:N	2.38	0.57
1:A:5:LEU:HB2	1:A:168:LEU:HD13	1.86	0.57
1:C:13:SER:O	1:C:92:SER:HA	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LYS:C	1:C:146:LYS:H	2.13	0.57
1:A:74:PHE:C	1:A:76:VAL:H	2.12	0.56
1:A:128:GLU:C	1:A:130:LEU:N	2.63	0.56
1:A:131:LYS:NZ	1:A:154:GLU:OE2	2.29	0.56
1:C:180:LEU:HG	1:C:209:TYR:CZ	2.40	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
2:B:36:GLU:CD	2:B:38:GLN:HE21	2.15	0.55
1:C:14:ARG:NH1	1:C:19:GLU:O	2.40	0.55
1:C:216:THR:O	1:C:260:HIS:N	2.38	0.55
3:F:5:TYR:CD1	3:F:5:TYR:N	2.70	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:79:ARG:O	1:C:82:LEU:HB3	2.07	0.55
1:C:106:ASP:HB2	1:C:108:ARG:NH2	2.22	0.55
2:B:17:ASN:HA	2:B:72:PRO:O	2.07	0.54
2:B:25:CYS:SG	2:B:26:TYR:N	2.79	0.54
1:C:263:HIS:CD2	1:C:265:GLY:H	2.25	0.54
2:D:78:TYR:O	2:D:94:TYR:HB2	2.07	0.54
1:A:170:ARG:HB3	1:A:170:ARG:NH1	2.20	0.54
1:C:19:GLU:HG2	1:C:20:PRO:CD	2.36	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
1:A:109:LEU:HD13	1:A:161:GLU:HA	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
2:D:19:LYS:HA	2:D:71:THR:HG23	1.89	0.54
2:D:23:LEU:HD23	2:D:39:MET:HE3	1.90	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:124:ILE:HG12	1:C:140:ALA:HB1	1.90	0.53
1:C:125:ALA:O	1:C:133:TRP:HE3	1.91	0.53
1:A:143:THR:O	1:A:147:TRP:HB2	2.07	0.53
1:A:191:HIS:HB2	1:A:201:LEU:HD13	1.91	0.53
1:C:82:LEU:HD23	1:C:83:GLY:N	2.22	0.53
2:D:13:HIS:HB2	2:D:21:ASN:OD1	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:ASN:HB3	2:D:72:PRO:HB2	1.91	0.53
2:D:23:LEU:HB2	2:D:70:PHE:CD1	2.43	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:A:74:PHE:C	1:A:76:VAL:N	2.67	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
1:A:182:THR:CG2	1:A:210:PRO:HD2	2.32	0.52
1:C:81:LEU:O	1:C:85:TYR:HD2	1.92	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:C:176:ASN:CG	1:C:177:ALA:H	2.18	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:51:MET:HG3	2:D:64:ILE:HD11	1.92	0.51
1:C:146:LYS:O	1:C:146:LYS:HG2	2.10	0.51
1:A:177:ALA:C	1:A:181:ARG:HH12	2.18	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
2:D:82:VAL:HG23	2:D:87:MET:CE	2.41	0.51
1:A:168:LEU:HD12	1:A:172:LEU:HD13	1.92	0.51
1:C:44:ARG:HG3	1:C:44:ARG:NH1	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:156:LEU:HD23	1:C:159:TYR:HD2	1.76	0.51
1:C:234:ARG:HD3	1:C:242:GLN:HB2	1.92	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
1:A:24:GLU:O	1:A:35:ARG:HA	2.12	0.50
1:A:217:TRP:O	1:A:224:LEU:HB2	2.10	0.50
1:A:233:THR:OG1	1:A:243:LYS:HD2	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ILE:HG23	2:B:35:ILE:O	2.12	0.50
1:C:201:LEU:HD12	1:C:249:VAL:HG11	1.92	0.50
2:D:19:LYS:CB	2:D:20:PRO:CD	2.86	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: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
2:B:7:ILE:HD12	2:B:93:VAL:HG23	1.93	0.49
1:C:126:LEU:HD12	1:C:133:TRP:CZ3	2.47	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:C:114:GLN:CD	1:C:156:LEU:HD11	2.38	0.48
1:C:187:ALA:O	1:C:188:HIS:HB3	2.12	0.48
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:177:ALA:HB1	1:A:181:ARG:CZ	2.43	0.48
1:A:189:VAL:HA	1:A:202:ARG:O	2.12	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:180:LEU:O	1:A:181:ARG:HB2	2.13	0.48
1:A:232:GLU:CB	1:A:232:GLU:C	2.78	0.48
1:A:47:PRO:CB	1:A:53:GLU:HG3	2.44	0.48
1:C:116:TYR:HD2	3:F:8:LEU:HD11	1.77	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:A:227:ASP:HB3	1:A:247:VAL:HG23	1.96	0.47
1:C:14:ARG:NH2	1:C:39:ASP:OD2	2.47	0.47
1:A:2:PRO:O	1:A:3:HIS:HD2	1.97	0.47
1:C:180:LEU:HA	1:C:209:TYR:HE2	1.80	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
1:A:50:ARG:HD2	1:A:50:ARG:HA	1.63	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:6:GLN:CG	3:E:7:GLY:H	2.23	0.47
2:D:78:TYR:HB2	2:D:95:TRP:HB3	1.97	0.47
1:C:95:ILE:HG12	1:C:118:TYR:HD1	1.80	0.47
1:C:192:HIS:NE2	2:D:98:ASP:HB2	2.29	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
1:C:2:PRO:HB3	1:C:104:GLY:HA3	1.96	0.46
2:D:17:ASN:HB3	2:D:97:ARG:NH2	2.29	0.46
1:A:44:ARG:NH2	1:A:64:THR:HG21	2.31	0.46
2:D:23:LEU:HD23	2:D:39:MET:CE	2.45	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:B:87:MET:HE3	2:B:87:MET:HB2	1.86	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:O	1:C:38:SER:OG	2.30	0.46
2:D:26:TYR:CE2	2:D:28:THR:CG2	2.99	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:C:33:PHE:O	1:C:48:ARG:N	2.49	0.46
1:C:47:PRO:C	1:C:49:ALA:H	2.24	0.46
1:A:21:ARG:NH1	1:A:23:MET:HG3	2.31	0.46
1:A:205:ALA:CB	1:A:215:LEU:HD11	2.45	0.46
1:C:199:VAL:O	1:C:249:VAL:HG22	2.16	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:A:62:ARG:HD2	1:A:62:ARG:HA	1.72	0.45
1:C:74:PHE:CA	1:C:77:ASP:HB2	2.41	0.45
1:A:138:MET:SD	1:C:61:GLU:OE1	2.74	0.45
1:C:11:ALA:HA	1:C:21:ARG:O	2.16	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
1:A:74:PHE:O	1:A:77:ASP:HB2	2.17	0.45
1:A:123:TYR:CE1	1:A:140:ALA:HA	2.51	0.45
1:A:205:ALA:HB2	1:A:215:LEU:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:LYS:HD3	2:B:83:LYS:C	2.42	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:133:TRP:HB2	1:A:144:LYS:HZ3	1.82	0.44
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
1:A:159:TYR:O	1:A:164:CYS:HB2	2.17	0.44
1:C:172:LEU:HG	1:C:179:LEU:HD13	1.99	0.44
3:F:8:LEU:HA	3:F:8:LEU:HD23	1.46	0.44
1:C:104:GLY:HA3	1:C:110:LEU:HD11	1.99	0.44
1:C:192:HIS:CE1	2:D:98:ASP:HB2	2.52	0.44
1:C:8:PHE:HD2	2:D:56:PHE:CZ	2.35	0.44
1:C:31:THR:HG23	1:C:32:GLU:N	2.33	0.44
1:C:206:LEU:HB2	1:C:242:GLN:HG2	1.99	0.44
1:A:202:ARG:HB2	1:A:246:SER:CB	2.48	0.44
1:C:181:ARG:HB3	1:C:182:THR:H	1.62	0.44
1:C:264:GLN:O	1:C:264:GLN:HG2	2.18	0.44
1:C:152:GLU:HG3	1:C:155:ARG:HB3	1.99	0.44
2:D:17:ASN:OD1	2:D:97:ARG:NH2	2.49	0.44
1:A:104:GLY:C	1:A:106:ASP:H	2.26	0.44
1:A:256:TYR:HD1	1:A:256:TYR:H	1.65	0.44
1:C:213:ILE:HG13	1:C:263:HIS:HB2	1.99	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
1:C:56:GLY:C	1:C:58:GLU:H	2.27	0.43
1:C:196:GLU:HG2	1:C:251:LEU:HD12	1.99	0.43
2:D:17:ASN:CG	2:D:97:ARG:HH22	2.27	0.43
2:D:19:LYS:HA	2:D:71:THR:CG2	2.49	0.43
2:D:82:VAL:CG2	2:D:87:MET:HE1	2.48	0.43
1:A:203:CYS:O	1:A:244:TRP:CB	2.66	0.43
1:A:82:LEU:C	1:A:82:LEU:HD23	2.44	0.43
1:C:93:HIS:HA	1:C:119:ASP:OD1	2.19	0.43
1:C:114:GLN:HB2	1:C:156:LEU:HD11	2.00	0.43
1:C:210:PRO:O	1:C:212:ASP:N	2.51	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
1:A:50:ARG:O	1:A:53:GLU:HB2	2.19	0.43
1:A:120:GLY:O	1:A:121:CYS:SG	2.76	0.43
2:B:5:PRO:HG3	2:B:30:PHE:HB3	2.01	0.43
2:B:28:THR:O	2:B:29:GLN:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:ASP:OD1	2:B:85:ASP:N	2.52	0.43
1:C:74:PHE:C	1:C:77:ASP:H	2.27	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
1:A:37:ASP:C	1:A:39:ASP:H	2.27	0.43
1:C:14:ARG:HD2	1:C:19:GLU:O	2.19	0.43
2:D:7:ILE:HG22	2:D:8:GLN:N	2.34	0.43
3:E:6:GLN:HG2	3:E:7:GLY:N	2.21	0.43
1:A:89:LYS:CD	1:A:89:LYS:H	2.32	0.42
1:A:263:HIS:O	1:A:266:LEU:HB2	2.19	0.42
1:C:44:ARG:HG2	1:C:64:THR:HG21	2.01	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:D:17:ASN:C	2:D:17:ASN:ND2	2.77	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:2:PRO:O	1:A:3:HIS:CD2	2.72	0.41
1:A:2:PRO:C	1:A:3:HIS:CD2	2.98	0.41
1:A:191:HIS:NE2	1:A:199:VAL:HG11	2.35	0.41
2:D:15:PRO:CB	2:D:95:TRP:HZ2	2.33	0.41
1:A:194:ARG:NH2	1:A:202:ARG:HH12	2.17	0.41
1:A:222:GLU:CD	1:A:222:GLU:H	2.29	0.41
1:C:184:SER:HB3	1:C:266:LEU:HD13	2.01	0.41
2:D:58:LYS:O	2:D:58:LYS:HG3	2.19	0.41
1:C:201:LEU:HD12	1:C:249:VAL:CG1	2.50	0.41
1:A:103:VAL:O	1:A:103:VAL:HG23	2.20	0.41
1:C:81:LEU:HD13	1:C:85:TYR:HE2	1.86	0.41
1:C:189:VAL:CG1	1:C:190:THR:N	2.80	0.41
2:B:41:LYS:HA	2:B:77:THR:O	2.20	0.41
2:B:80:CYS:SG	2:B:81:ARG:N	2.93	0.41
1:C:229:GLU:O	1:C:245:ALA:HA	2.21	0.41
1:A:54:GLN:O	1:A:54:GLN:NE2	2.54	0.41
1:A:146:LYS:HA	1:A:149:GLN:HB2	2.02	0.41
1:A:216:THR:O	1:A:260:HIS:N	2.52	0.41
1:C:52:MET:C	1:C:54:GLN:N	2.78	0.41
1:C:97:VAL:HG11	3:F:5:TYR:CE2	2.56	0.41
1:C:234:ARG:HA	1:C:235:PRO:HD3	1.99	0.41
1:A:21:ARG:NH2	1:A:39:ASP:HB2	2.36	0.41
1:A:54:GLN:HE21	1:A:54:GLN:C	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:THR:O	2:B:71:THR:HG22	2.21	0.41
1:C:106:ASP:O	1:C:108:ARG:N	2.50	0.41
1:C:146:LYS:HG2	1:C:146:LYS:HZ3	1.70	0.41
1:C:209:TYR:HD1	1:C:210:PRO:HA	1.76	0.41
2:B:19:LYS:HA	2:B:20:PRO:HD3	1.63	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
1:A:81:LEU:HD13	1:A:84:TYR:HD2	1.85	0.40
1:A:225:ILE:HG13	1:A:226:GLN:N	2.36	0.40
1:C:176:ASN:CG	1:C:177:ALA:N	2.80	0.40
1:C:192:HIS:HE2	2:D:98:ASP:HB2	1.85	0.40
1:C:95:ILE:HD13	1:C:95:ILE:HG21	1.77	0.40
1:C:116:TYR:HB3	1:C:123:TYR:HD2	1.87	0.40
2:D:85:ASP:C	2:D:87:MET:N	2.79	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%)	0	0
2	B	97/99 (98%)	75 (77%)	17 (18%)	5 (5%)	1	1
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%)	0	0

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	157 (69%)	71 (31%)	0	0
1	C	228/228 (100%)	159 (70%)	69 (30%)	0	0
2	B	94/94 (100%)	65 (69%)	29 (31%)	0	0
2	D	94/94 (100%)	70 (74%)	24 (26%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	454 (69%)	202 (31%)	0	0

All (202) 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	28	VAL
1	A	30	ASP
1	A	31	THR
1	A	41	GLU
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	63	GLU
1	A	64	THR
1	A	65	GLN
1	A	78	LEU
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	110	LEU
1	A	113	TYR
1	A	124	ILE
1	A	127	ASN
1	A	130	LEU
1	A	131	LYS
1	A	132	THR
1	A	137	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	141	LEU
1	A	143	THR
1	A	147	TRP
1	A	149	GLN
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	194	ARG
1	A	198	LYS
1	A	199	VAL
1	A	201	LEU
1	A	202	ARG
1	A	206	LEU
1	A	212	ASP
1	A	220	ASN
1	A	222	GLU
1	A	224	LEU
1	A	227	ASP
1	A	231	VAL
1	A	234	ARG
1	A	240	THR
1	A	242	GLN
1	A	244	TRP
1	A	249	VAL
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	64	ILE
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	99	MET
1	C	4	SER
1	C	6	ARG
1	C	10	THR
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	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	76	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	81	LEU
1	C	87	GLN
1	C	89	LYS
1	C	94	THR
1	C	98	ILE
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	156	LEU
1	C	157	ARG
1	C	163	THR
1	C	165	VAL
1	C	166	GLU
1	C	168	LEU
1	C	172	LEU
1	C	182	THR
1	C	184	SER
1	C	189	VAL
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	222	GLU
1	C	225	ILE
1	C	228	MET
1	C	230	LEU
1	C	231	VAL
1	C	232	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	234	ARG
1	C	247	VAL
1	C	248	VAL
1	C	250	PRO
1	C	251	LEU
1	C	253	LYS
1	C	255	GLN
1	C	266	LEU
1	C	270	LEU
2	D	1	ILE
2	D	2	GLN
2	D	6	GLN
2	D	17	ASN
2	D	28	THR
2	D	34	HIS
2	D	37	ILE
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	54	MET
2	D	65	LEU
2	D	67	HIS
2	D	73	THR
2	D	75	THR
2	D	77	THR
2	D	83	LYS
2	D	89	GLU
2	D	91	LYS
2	D	98	ASP
2	D	99	MET
3	E	1	ARG
3	E	4	VAL
3	E	5	TYR
3	E	8	LEU
3	F	1	ARG
3	F	4	VAL
3	F	5	TYR
3	F	6	GLN
3	F	8	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	86	ASN
1	A	242	GLN
1	A	255	GLN
1	C	3	HIS
1	C	72	GLN
1	C	115	GLN
1	C	218	GLN
1	C	242	GLN
1	C	255	GLN
1	C	263	HIS
2	D	38	GLN
3	F	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.