



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:03 AM UTC

PDB ID : 1HIM / pdb_00001him
Title : STRUCTURAL EVIDENCE FOR INDUCED FIT AS A MECHANISM FOR
ANTIBODY-ANTIGEN RECOGNITION
Authors : Schulze-Gahmen, U.; Wilson, I.A.
Deposited on : 1992-07-08
Resolution : 2.90 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

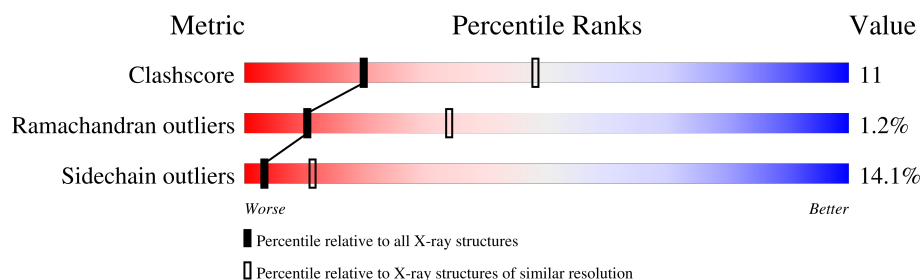
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	H	217	
1	J	217	
2	L	220	
2	M	220	
3	P	9	
4	R	10	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6742 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 IGG2A-KAPPA 17/9 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	217	Total	C	N	O	S	0	0	0
			1680	1047	279	347	7			
1	J	217	Total	C	N	O	S	0	0	0
			1680	1047	279	347	7			

- Molecule 2 is a protein called IGG2A-KAPPA 17/9 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	1
			1621	1024	268	322	7			
2	M	215	Total	C	N	O	S	0	0	1
			1621	1024	268	322	7			

- Molecule 3 is a protein called INFLUENZA HEMAGGLUTININ HA1 (STRAIN X47) (RESIDUES 100-108).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	0	0	1
			66	42	9	15			

- Molecule 4 is a protein called INFLUENZA HEMAGGLUTININ HA1 (STRAIN X47) (RESIDUES 100-108).

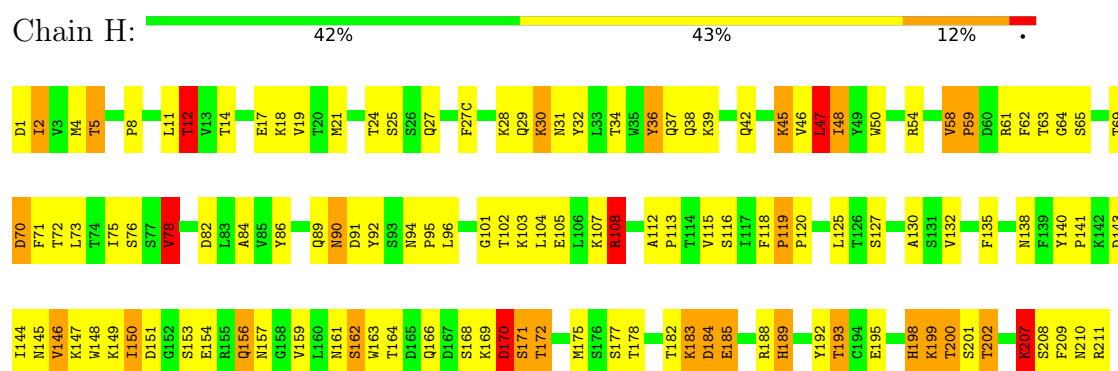
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	R	10	Total	C	N	O	0	0	1
			74	48	10	16			

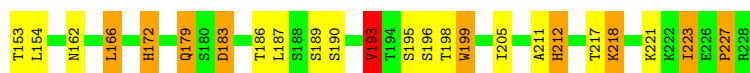
3 Residue-property plots

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.

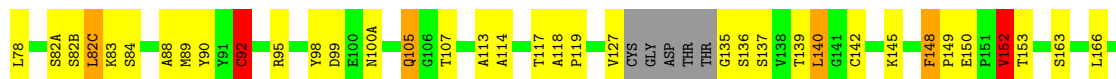
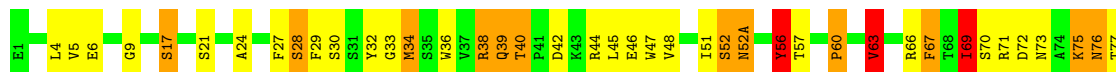
• Molecule 1: IGG2A-KAPPA 17/9 FAB (LIGHT CHAIN)





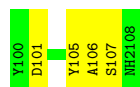
• Molecule 2: IGG2A-KAPPA 17/9 FAB (HEAVY CHAIN)

Chain M: 49% 36% 10%



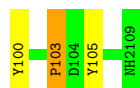
• Molecule 3: INFLUENZA HEMAGGLUTININ HA1 (STRAIN X47) (RESIDUES 100-108)

Chain P: 56% 44%



• Molecule 4: INFLUENZA HEMAGGLUTININ HA1 (STRAIN X47) (RESIDUES 100-108)

Chain R: 70% 20% 10%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.08Å 67.07Å 73.24Å 89.90° 101.80° 96.50°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6742	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

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	H	1.13	4/1718 (0.2%)	2.09	61/2334 (2.6%)
1	J	1.14	3/1718 (0.2%)	2.09	58/2334 (2.5%)
2	L	1.19	7/1661 (0.4%)	2.10	63/2263 (2.8%)
2	M	1.17	8/1661 (0.5%)	2.07	57/2263 (2.5%)
3	P	1.18	0/67	1.95	1/92 (1.1%)
4	R	1.30	0/75	1.95	3/103 (2.9%)
All	All	1.16	22/6900 (0.3%)	2.08	243/9389 (2.6%)

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	H	0	1
1	J	0	1
2	M	0	1
All	All	0	3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	223	ILE	CA-CB	10.83	1.64	1.53
1	H	189	HIS	CD2-NE2	-7.82	1.29	1.37
1	J	189	HIS	CD2-NE2	-7.42	1.29	1.37
1	J	198	HIS	CD2-NE2	-6.97	1.30	1.37
2	L	212	HIS	CD2-NE2	-6.95	1.30	1.37
2	L	227	PRO	C-N	-6.95	1.23	1.33
1	H	198	HIS	CD2-NE2	-6.81	1.30	1.37
2	M	72	ASP	CA-CB	-6.62	1.45	1.53
2	M	227	PRO	C-N	-6.61	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	212	HIS	CD2-NE2	-6.49	1.30	1.37
2	L	63	VAL	CA-CB	5.96	1.63	1.55
2	M	172	HIS	CD2-NE2	-5.92	1.31	1.37
2	L	212	HIS	CG-ND1	-5.82	1.31	1.38
2	M	52	SER	CA-CB	-5.76	1.44	1.53
2	L	172	HIS	CD2-NE2	-5.64	1.31	1.37
2	L	172	HIS	CG-ND1	-5.63	1.32	1.38
2	M	40	THR	CA-C	5.55	1.59	1.52
1	J	53	THR	CA-CB	5.52	1.60	1.53
2	M	46	GLU	CA-CB	-5.51	1.44	1.53
1	H	78	VAL	CA-CB	5.18	1.60	1.54
2	M	60	PRO	CA-CB	-5.06	1.47	1.53
1	H	103	LYS	CA-CB	-5.05	1.46	1.53

All (243) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	170	ASP	CA-CB-CG	14.76	127.36	112.60
2	M	100(A)	ASN	N-CA-C	11.54	127.15	112.03
2	M	152	VAL	N-CA-C	-10.38	93.53	108.48
1	H	184	ASP	CA-CB-CG	10.10	122.70	112.60
1	H	138	ASN	N-CA-C	9.25	124.21	111.17
2	M	69	ILE	CB-CA-C	-9.21	98.92	111.63
1	J	170	ASP	N-CA-C	9.00	124.14	112.26
1	H	113	PRO	N-CA-C	8.97	125.28	111.19
2	L	100(A)	ASN	CB-CG-ND2	-8.67	103.39	116.40
2	L	100(A)	ASN	N-CA-C	8.55	125.29	109.56
2	L	193	VAL	N-CA-CB	-8.49	97.23	111.23
1	J	189	HIS	CB-CG-CD2	-8.39	120.29	131.20
2	L	63	VAL	N-CA-C	-8.38	105.75	113.71
2	L	110	THR	CA-CB-OG1	-8.29	97.16	109.60
2	L	152	VAL	N-CA-C	-8.18	96.23	108.99
1	J	2	ILE	N-CA-C	-8.18	99.03	109.58
2	M	17	SER	N-CA-C	8.16	121.87	109.23
1	H	145	ASN	CA-CB-CG	8.08	120.68	112.60
1	H	208	SER	N-CA-C	8.07	119.27	108.38
2	L	42	ASP	CA-CB-CG	7.97	120.57	112.60
2	L	27	PHE	CA-CB-CG	7.88	121.68	113.80
2	L	221	LYS	N-CA-C	7.71	122.09	107.75
1	J	91	ASP	CA-CB-CG	7.70	120.30	112.60
1	J	58	VAL	N-CA-C	-7.66	99.54	107.89
1	J	198	HIS	CB-CG-CD2	-7.63	121.28	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	150	ILE	N-CA-C	-7.62	97.45	108.11
1	J	31	ASN	OD1-CG-ND2	-7.60	115.00	122.60
2	M	83	LYS	N-CA-C	-7.56	97.52	109.23
2	L	179	GLN	CA-CB-CG	7.44	128.99	114.10
1	J	81	GLU	N-CA-C	-7.43	103.26	111.36
2	M	89	MET	N-CA-C	-7.43	96.40	108.52
2	L	20	LEU	O-C-N	-7.38	114.93	123.27
1	H	94	ASN	CB-CG-ND2	7.33	127.40	116.40
1	J	172	THR	N-CA-CB	-7.31	99.36	111.20
1	J	76	SER	N-CA-C	7.20	119.75	111.11
1	J	210	ASN	CA-CB-CG	7.17	119.77	112.60
2	M	148	PHE	CA-CB-CG	-7.15	106.65	113.80
1	J	138	ASN	N-CA-C	7.14	121.24	111.39
2	L	112	SER	CA-C-O	7.11	128.71	120.75
1	H	157	ASN	OD1-CG-ND2	-7.09	115.51	122.60
1	J	90	ASN	CA-CB-CG	7.08	119.68	112.60
1	H	189	HIS	CB-CG-CD2	-7.03	122.06	131.20
2	M	36	TRP	CG-CD2-CE3	6.96	140.85	133.90
1	J	110	ASP	CA-CB-CG	6.95	119.55	112.60
2	M	183	ASP	N-CA-C	6.94	121.50	113.38
2	L	38	ARG	CB-CG-CD	-6.94	95.34	111.30
2	M	52(A)	ASN	CA-CB-CG	6.91	119.51	112.60
2	L	48	VAL	N-CA-CB	-6.90	102.44	111.90
1	J	140	TYR	O-C-N	-6.90	116.46	121.84
2	M	114	ALA	N-CA-C	6.84	119.89	110.24
1	H	1	ASP	CA-CB-CG	6.79	119.39	112.60
2	M	42	ASP	CA-CB-CG	6.78	119.38	112.60
1	H	143	ASP	CA-CB-CG	6.77	119.37	112.60
2	M	69	ILE	CB-CG1-CD1	-6.75	99.62	113.80
2	M	45	LEU	O-C-N	-6.74	115.03	123.05
1	J	102	THR	N-CA-C	-6.70	97.98	108.90
1	J	60	ASP	CA-CB-CG	6.67	119.28	112.60
2	M	140	LEU	CD1-CG-CD2	6.66	125.45	110.80
2	L	100	GLU	CB-CG-CD	6.65	123.91	112.60
1	H	182	THR	N-CA-C	-6.63	100.15	110.42
1	J	161	ASN	OD1-CG-ND2	-6.60	116.00	122.60
2	L	99	ASP	N-CA-C	6.55	121.28	113.28
1	H	145	ASN	N-CA-CB	-6.55	100.27	110.55
1	J	30	LYS	CA-CB-CG	6.51	127.11	114.10
3	P	106	ALA	N-CA-CB	-6.50	101.04	110.47
1	J	170	ASP	CA-CB-CG	6.44	119.04	112.60
2	L	73	ASN	OD1-CG-ND2	-6.42	116.18	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	30	LYS	CA-C-O	-6.40	113.64	121.06
2	M	6	GLU	CA-C-O	-6.37	113.77	121.28
2	M	63	VAL	N-CA-CB	-6.32	100.80	111.23
1	J	37	GLN	OE1-CD-NE2	-6.29	116.31	122.60
2	L	76	ASN	OD1-CG-ND2	-6.29	116.31	122.60
2	M	113	ALA	CA-C-N	6.27	129.74	120.90
2	M	113	ALA	C-N-CA	6.27	129.74	120.90
2	L	34	MET	CA-C-O	-6.25	114.15	121.46
1	J	185	GLU	CB-CG-CD	6.25	123.22	112.60
1	J	58	VAL	O-C-N	6.16	126.95	121.41
1	J	119	PRO	CA-C-N	6.16	126.52	119.93
1	J	119	PRO	C-N-CA	6.16	126.52	119.93
1	J	189	HIS	CB-CG-ND1	6.15	131.93	122.70
2	L	5	VAL	N-CA-CB	-6.14	104.24	112.10
1	H	145	ASN	CA-C-O	-6.13	113.58	120.32
1	J	43	PRO	CA-C-O	-6.12	111.69	120.56
2	L	150	GLU	CA-CB-CG	-6.12	101.87	114.10
1	J	42	GLN	CA-C-N	6.12	126.68	120.38
1	J	42	GLN	C-N-CA	6.12	126.68	120.38
1	H	92	TYR	CA-C-O	-6.12	114.01	120.55
1	J	176	SER	O-C-N	-6.11	115.24	123.19
2	L	67	PHE	CA-CB-CG	6.11	119.91	113.80
1	J	198	HIS	O-C-N	-6.10	116.29	123.25
1	H	147	LYS	N-CA-C	6.10	118.39	108.26
2	M	136	SER	N-CA-C	6.08	117.99	111.36
2	L	1	GLU	N-CA-C	-6.07	94.02	111.00
2	M	215	SER	CA-CB-OG	6.06	123.23	111.10
2	M	5	VAL	N-CA-CB	-6.06	103.04	111.41
1	H	72	THR	CA-C-O	-6.06	113.33	120.60
2	L	166	LEU	N-CA-C	-6.03	99.37	108.96
2	M	56	TYR	O-C-N	-6.02	115.61	123.02
1	H	210	ASN	O-C-N	6.02	130.07	123.27
1	J	58	VAL	CA-C-N	5.99	125.90	119.85
1	J	58	VAL	C-N-CA	5.99	125.90	119.85
2	M	107	THR	CA-CB-OG1	-5.99	100.62	109.60
2	L	195	SER	N-CA-C	5.98	119.41	111.75
2	M	67	PHE	CA-CB-CG	5.98	119.78	113.80
1	H	151	ASP	CA-CB-CG	5.97	118.57	112.60
2	M	92	CYS	N-CA-C	-5.96	99.99	109.76
2	M	75	LYS	N-CA-C	-5.95	105.20	112.88
1	H	200	THR	CA-CB-OG1	-5.92	100.71	109.60
1	H	42	GLN	CA-C-O	-5.92	114.53	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	83	LYS	CA-C-N	5.91	128.48	120.38
2	M	83	LYS	C-N-CA	5.91	128.48	120.38
1	J	69	THR	N-CA-CB	-5.91	103.04	110.90
1	H	145	ASN	O-C-N	-5.90	116.31	123.27
2	M	36	TRP	CB-CG-CD1	-5.90	118.05	126.90
2	L	19	LYS	CA-C-O	-5.90	113.99	120.24
2	M	203	GLN	N-CA-C	-5.89	99.59	109.07
4	R	100	TYR	N-CA-C	-5.88	94.53	111.00
1	J	94	ASN	O-C-N	-5.87	115.38	121.60
2	M	187	LEU	O-C-N	-5.87	116.46	123.27
4	R	103	PRO	CB-CA-C	5.87	118.70	110.60
2	L	14	PRO	N-CA-C	-5.86	101.45	110.95
1	H	29	GLN	OE1-CD-NE2	-5.85	116.75	122.60
1	H	96	LEU	N-CA-C	-5.83	101.21	109.96
2	L	100(C)	PHE	O-C-N	5.83	130.04	122.87
1	H	193	THR	CA-CB-OG1	-5.80	100.89	109.60
2	L	199	TRP	CE2-CD2-CG	-5.80	100.24	107.20
1	J	6	GLN	OE1-CD-NE2	-5.79	116.81	122.60
2	L	56	TYR	CA-CB-CG	5.79	124.33	113.90
1	J	182	THR	N-CA-C	-5.77	100.30	109.76
1	J	114	THR	N-CA-C	-5.76	99.13	108.41
1	J	172	THR	CB-CA-C	5.76	120.83	109.66
1	H	162	SER	N-CA-C	-5.71	100.82	109.85
1	H	47	LEU	N-CA-C	-5.71	105.08	112.68
1	H	46	VAL	CB-CA-C	-5.71	102.83	111.33
2	M	145	LYS	CA-CB-CG	-5.68	102.74	114.10
2	M	216	SER	N-CA-CB	-5.68	103.30	111.70
1	J	108	ARG	N-CA-CB	-5.67	101.73	111.21
2	M	223	ILE	CB-CA-C	-5.67	105.79	111.80
2	L	75	LYS	CA-CB-CG	-5.66	102.78	114.10
1	H	156	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	H	198	HIS	CB-CG-CD2	-5.65	123.86	131.20
1	J	89	GLN	O-C-N	5.63	130.00	123.41
2	L	193	VAL	CB-CA-C	5.61	120.49	111.29
1	J	143	ASP	CA-CB-CG	-5.61	106.99	112.60
2	M	214	ALA	N-CA-C	5.61	122.74	110.80
1	H	207	LYS	O-C-N	-5.59	116.70	123.29
1	J	91	ASP	N-CA-C	-5.58	105.79	112.59
1	J	205	ILE	N-CA-C	-5.58	102.33	109.30
1	H	112	ALA	CA-C-N	5.57	125.33	119.76
1	H	112	ALA	C-N-CA	5.57	125.33	119.76
4	R	105	TYR	CA-CB-CG	5.57	123.93	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	48	VAL	CB-CA-C	5.56	116.36	110.91
1	H	192	TYR	O-C-N	-5.56	115.78	123.12
2	L	43	LYS	CA-C-O	5.56	128.15	121.65
1	H	119	PRO	N-CA-C	5.55	117.48	110.70
1	H	163	TRP	CG-CD2-CE3	5.55	139.46	133.90
2	L	37	VAL	O-C-N	-5.55	116.98	122.76
2	M	119	PRO	N-CA-C	5.55	120.00	111.57
2	M	145	LYS	N-CA-C	5.54	118.44	109.40
1	H	113	PRO	O-C-N	-5.51	116.48	123.10
1	H	189	HIS	CB-CG-ND1	5.50	130.95	122.70
1	J	209	PHE	N-CA-C	-5.47	101.00	108.38
2	L	100	GLU	CA-CB-CG	-5.46	103.18	114.10
2	M	105	GLN	OE1-CD-NE2	-5.46	117.14	122.60
2	L	179	GLN	CB-CA-C	-5.44	101.03	113.33
1	H	95	PRO	O-C-N	5.41	131.39	121.10
2	M	172	HIS	CB-CG-CD2	-5.41	124.17	131.20
2	L	107	THR	O-C-N	-5.41	117.08	123.41
1	H	199	LYS	N-CA-C	5.39	117.86	111.33
2	L	94	ARG	CB-CG-CD	-5.39	98.90	111.30
2	M	117	THR	CA-CB-OG1	-5.38	101.53	109.60
2	M	42	ASP	N-CA-C	-5.37	106.57	113.02
1	H	5	THR	CA-C-O	5.37	126.03	120.40
1	H	12	THR	CA-CB-OG1	-5.37	101.55	109.60
1	H	195	GLU	N-CA-CB	-5.36	102.27	110.85
2	L	2	VAL	N-CA-C	-5.34	102.17	109.55
2	L	35	SER	CA-C-N	5.34	130.30	122.77
2	L	35	SER	C-N-CA	5.34	130.30	122.77
2	M	92	CYS	CB-CA-C	5.31	118.41	109.48
2	M	82(C)	LEU	CA-C-O	5.30	126.96	120.92
1	H	202	THR	CA-C-O	5.30	126.06	119.12
2	L	199	TRP	CB-CA-C	5.29	116.01	108.76
2	L	148	PHE	CA-CB-CG	-5.29	108.51	113.80
2	M	34	MET	CA-C-O	-5.29	115.42	121.40
2	M	202	SER	N-CA-C	5.29	116.73	111.07
2	L	83	LYS	CA-CB-CG	-5.28	103.54	114.10
1	H	58	VAL	CA-C-N	5.28	126.43	119.84
1	H	58	VAL	C-N-CA	5.28	126.43	119.84
2	L	100(C)	PHE	CA-CB-CG	5.26	119.06	113.80
2	L	172	HIS	CB-CG-CD2	-5.26	124.36	131.20
2	L	86	ASP	CA-CB-CG	5.26	117.86	112.60
1	H	150	ILE	CA-CB-CG2	-5.25	101.58	110.50
2	L	40	THR	O-C-N	-5.24	116.04	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	171	SER	N-CA-CB	-5.24	104.03	111.84
1	H	46	VAL	N-CA-CB	5.24	116.75	110.31
2	M	56	TYR	CA-CB-CG	5.24	123.33	113.90
2	L	68	THR	N-CA-C	5.24	116.86	107.80
2	L	223	ILE	CB-CA-C	5.24	117.35	111.80
1	H	70	ASP	N-CA-C	5.23	117.17	108.02
2	L	100(A)	ASN	CA-CB-CG	5.23	117.83	112.60
1	H	127	SER	N-CA-C	5.22	119.52	113.20
2	L	44	ARG	CA-CB-CG	5.22	124.53	114.10
2	L	73	ASN	CB-CG-ND2	5.22	124.23	116.40
2	L	110	THR	CA-CB-CG2	5.21	119.36	110.50
1	H	91	ASP	CA-CB-CG	5.20	117.80	112.60
1	J	164	THR	N-CA-C	-5.20	102.37	110.42
1	H	108	ARG	O-C-N	-5.18	117.65	123.04
1	H	144	ILE	CA-C-O	5.17	126.45	120.76
2	L	44	ARG	N-CA-C	-5.17	100.02	108.76
1	H	130	ALA	O-C-N	-5.17	117.28	123.28
1	J	203	SER	O-C-N	-5.17	116.45	121.56
2	M	100(A)	ASN	CA-CB-CG	5.17	117.77	112.60
1	H	71	PHE	CA-CB-CG	5.15	118.95	113.80
2	L	11	LEU	N-CA-C	-5.14	100.92	109.46
1	H	45	LYS	CA-CB-CG	5.14	124.38	114.10
2	M	69	ILE	N-CA-CB	5.14	119.48	110.49
2	M	205	ILE	N-CA-C	-5.13	100.25	107.75
1	J	39	LYS	CA-C-N	5.13	124.89	119.76
1	J	39	LYS	C-N-CA	5.13	124.89	119.76
1	J	198	HIS	CB-CG-ND1	5.12	130.38	122.70
1	J	72	THR	CA-C-O	-5.12	114.64	120.32
1	J	116	SER	O-C-N	-5.11	116.50	123.14
2	M	39	GLN	N-CA-C	-5.11	100.57	108.90
2	L	70	SER	N-CA-CB	-5.10	102.04	111.52
2	L	3	GLN	OE1-CD-NE2	-5.09	117.51	122.60
2	L	179	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	J	28	LYS	CA-CB-CG	-5.08	103.94	114.10
1	J	97	THR	N-CA-C	5.08	117.84	109.72
1	J	32	TYR	CA-C-O	5.07	127.87	121.58
1	J	108	ARG	O-C-N	-5.07	116.99	122.92
2	L	82(B)	SER	N-CA-C	-5.06	104.43	111.52
1	H	116	SER	N-CA-CB	-5.06	101.97	111.13
2	L	107	THR	CA-CB-CG2	5.06	119.10	110.50
2	M	150	GLU	CA-CB-CG	-5.06	103.99	114.10
1	H	70	ASP	CA-CB-CG	-5.05	107.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	116	SER	CA-CB-OG	5.05	121.19	111.10
2	M	33	GLY	N-CA-C	-5.03	104.75	112.85
1	J	191	SER	N-CA-C	5.03	116.94	109.25
2	M	98	TYR	CA-C-O	5.02	126.07	120.80
2	M	76	ASN	OD1-CG-ND2	-5.01	117.59	122.60
2	L	154	LEU	CA-C-O	-5.01	114.81	120.32
2	M	38	ARG	CA-C-N	-5.01	115.93	122.99
2	M	38	ARG	C-N-CA	-5.01	115.93	122.99

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	36	TYR	Sidechain
1	J	192	TYR	Sidechain
2	M	56	TYR	Sidechain

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	H	1680	0	1612	44	0
1	J	1680	0	1612	34	0
2	L	1621	0	1576	40	0
2	M	1621	0	1576	38	0
3	P	66	0	51	3	0
4	R	74	0	62	1	0
All	All	6742	0	6489	152	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 11.

All (152) 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:J:120:PRO:HD3	1:J:132:VAL:HG22	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:51:ILE:HB	2:M:69:ILE:HD12	1.69	0.74
2:L:193:VAL:HG13	2:L:198:THR:HB	1.70	0.71
1:H:149:LYS:HB2	1:H:193:THR:HB	1.78	0.66
1:H:82:ASP:O	1:H:104:LEU:HD12	1.98	0.64
2:L:162:ASN:HD21	2:L:205:ILE:HA	1.62	0.63
2:L:70:SER:HB3	2:L:79:TYR:HB2	1.81	0.63
2:L:39:GLN:HB2	2:L:45:LEU:HD23	1.81	0.61
2:L:61:ASP:HA	2:L:64:LYS:HE3	1.82	0.61
1:J:63:THR:O	1:J:73:LEU:HD12	2.01	0.61
2:M:63:VAL:HG13	2:M:67:PHE:HB2	1.83	0.61
2:M:24:ALA:HB1	2:M:27:PHE:CE1	2.36	0.60
2:L:28:SER:HB3	2:L:31:SER:OG	2.01	0.60
2:M:39:GLN:O	2:M:88:ALA:HB1	2.00	0.60
1:H:27(C):PHE:HA	1:H:31:ASN:HA	1.83	0.59
1:H:14:THR:O	1:H:17:GLU:HG2	2.01	0.59
1:J:48:ILE:HA	1:J:53:THR:O	2.02	0.59
2:L:52:SER:HB3	3:P:101:ASP:OD1	2.02	0.59
1:J:25:SER:O	1:J:69:THR:HG23	2.03	0.58
2:L:11:LEU:HD12	2:L:110:THR:HB	1.86	0.58
1:H:12:THR:HA	1:H:105:GLU:O	2.04	0.57
1:H:37:GLN:HB2	1:H:47:LEU:HD21	1.86	0.57
2:M:179:GLN:HG2	2:M:184:LEU:O	2.05	0.57
1:H:25:SER:O	1:H:69:THR:HG23	2.05	0.56
2:M:39:GLN:HA	2:M:44:ARG:O	2.05	0.56
1:H:125:LEU:O	1:H:183:LYS:HD2	2.06	0.55
1:J:31:ASN:HD21	1:J:68:GLY:H	1.54	0.55
2:L:59:TYR:OH	2:L:68:THR:HA	2.07	0.54
1:H:108:ARG:HD2	1:H:140:TYR:CG	2.42	0.54
1:H:198:HIS:HD2	1:H:200:THR:OG1	1.89	0.54
1:H:159:VAL:HA	1:H:178:THR:O	2.07	0.54
1:H:185:GLU:O	1:H:189:HIS:HD2	1.90	0.54
1:J:27(C):PHE:HA	1:J:31:ASN:HA	1.90	0.54
1:J:13:VAL:HB	1:J:78:VAL:HG11	1.90	0.54
1:H:37:GLN:HG3	1:H:86:TYR:CE1	2.42	0.53
1:H:54:ARG:HG2	1:H:58:VAL:HB	1.89	0.53
1:J:164:THR:HG23	2:M:174:PHE:CD1	2.43	0.53
1:H:2:ILE:HG13	1:H:27:GLN:OE1	2.09	0.53
2:L:58:TYR:CE2	3:P:107:SER:HB2	2.43	0.53
2:M:71:ARG:HB3	2:M:78:LEU:HD12	1.90	0.52
2:L:172:HIS:HB2	2:L:190:SER:OG	2.09	0.52
1:H:166:GLN:HG2	1:H:171:SER:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:ASP:OD1	1:H:172:THR:HB	2.10	0.52
1:J:90:ASN:HB3	1:J:97:THR:H	1.75	0.52
2:L:66:ARG:HG2	2:L:82(B):SER:HB2	1.90	0.52
1:H:39:LYS:HZ3	1:H:84:ALA:HB2	1.75	0.51
1:J:110:ASP:HB3	1:J:200:THR:HG22	1.91	0.51
2:M:152:VAL:HG13	2:M:210:VAL:HG13	1.93	0.51
2:L:89:MET:HE2	2:L:108:LEU:HB2	1.92	0.51
2:M:51:ILE:HG13	2:M:57:THR:HG22	1.93	0.51
1:H:118:PHE:CE1	1:H:135:PHE:HD2	2.29	0.51
1:H:17:GLU:O	1:H:78:VAL:HG12	2.11	0.51
1:J:29:GLN:O	1:J:30:LYS:HE2	2.11	0.51
2:L:39:GLN:O	2:L:88:ALA:HB1	2.11	0.50
2:L:66:ARG:HB3	2:L:82(A):SER:O	2.10	0.50
1:J:28:LYS:O	1:J:29:GLN:HB2	2.11	0.50
1:H:132:VAL:HG12	1:H:148:TRP:CH2	2.47	0.49
2:L:19:LYS:HA	2:L:80:LEU:O	2.12	0.49
1:H:141:PRO:O	1:H:198:HIS:HE1	1.95	0.49
1:H:50:TRP:HZ2	2:L:99:ASP:O	1.95	0.49
1:H:63:THR:O	1:H:73:LEU:HD12	2.13	0.49
1:H:119:PRO:HG3	1:H:209:PHE:CE2	2.48	0.49
2:M:173:THR:HG23	2:M:189:SER:HB2	1.95	0.49
1:H:39:LYS:NZ	1:H:84:ALA:HB2	2.28	0.48
2:M:48:VAL:O	2:M:60:PRO:HD2	2.13	0.48
2:M:139:THR:OG1	2:M:192:THR:HG22	2.13	0.48
2:M:118:ALA:HB1	2:M:217:THR:HG21	1.95	0.48
2:L:39:GLN:HA	2:L:44:ARG:O	2.13	0.48
1:J:191:SER:HA	1:J:210:ASN:HB3	1.96	0.48
1:J:124:GLN:HG2	1:J:129:GLY:O	2.14	0.48
2:L:212:HIS:HB3	2:L:217:THR:HB	1.94	0.48
1:H:62:PHE:CD1	1:H:75:ILE:HG12	2.49	0.48
1:H:199:LYS:HG3	1:H:200:THR:N	2.29	0.48
2:L:162:ASN:ND2	2:L:205:ILE:HA	2.28	0.48
1:J:115:VAL:HG12	1:J:207:LYS:HG3	1.96	0.47
2:M:137:SER:HA	2:M:194:THR:HA	1.97	0.47
2:L:199:TRP:CH2	2:L:227:PRO:HB3	2.49	0.47
1:J:50:TRP:HZ2	2:M:99:ASP:O	1.98	0.46
1:J:61:ARG:O	1:J:75:ILE:HA	2.15	0.46
1:H:184:ASP:O	1:H:188:ARG:HG3	2.15	0.46
1:J:136:LEU:HD21	1:J:146:VAL:HG22	1.97	0.46
1:H:34:THR:HG22	1:H:36:TYR:CE1	2.50	0.46
2:M:27:PHE:HD2	2:M:32:TYR:CD2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:GLN:O	1:H:84:ALA:HB1	2.16	0.45
1:H:89:GLN:HG2	1:H:90:ASN:N	2.31	0.45
1:H:118:PHE:CE1	1:H:135:PHE:CD2	3.04	0.45
2:L:95:ARG:HA	2:L:95:ARG:HD2	1.64	0.45
2:L:19:LYS:HB2	2:L:81:GLN:NE2	2.32	0.45
2:M:135:GLY:O	2:M:195:SER:HB3	2.17	0.45
2:M:24:ALA:HB1	2:M:27:PHE:CZ	2.52	0.45
1:H:169:LYS:O	1:H:170:ASP:HB3	2.15	0.45
1:H:18:LYS:HB3	1:H:18:LYS:HE2	1.77	0.45
1:H:48:ILE:HD12	1:H:64:GLY:N	2.31	0.45
2:L:29:PHE:HB2	2:L:76:ASN:ND2	2.31	0.45
1:H:8:PRO:O	1:H:102:THR:HG23	2.17	0.44
2:L:89:MET:CE	2:L:108:LEU:HB2	2.47	0.44
2:L:179:GLN:O	2:L:183:ASP:N	2.50	0.44
1:J:8:PRO:O	1:J:102:THR:HG23	2.17	0.44
1:H:161:ASN:HD22	1:H:177:SER:HA	1.83	0.44
2:L:12:VAL:O	2:L:111:VAL:HA	2.18	0.44
2:M:166:LEU:HD11	2:M:205:ILE:HD12	1.99	0.44
2:M:69:ILE:HD13	2:M:69:ILE:HG21	1.62	0.44
2:M:75:LYS:O	2:M:77:THR:HG23	2.18	0.44
2:L:100:GLU:HG2	3:P:105:TYR:CD1	2.53	0.44
2:L:60:PRO:O	2:L:62:SER:N	2.51	0.44
1:J:14:THR:O	1:J:17:GLU:HG2	2.18	0.44
2:L:27:PHE:HD2	2:L:32:TYR:CD1	2.37	0.43
2:L:33:GLY:HA2	2:L:71:ARG:HH12	1.83	0.43
2:L:211:ALA:HB2	2:L:218:LYS:HG2	2.00	0.43
2:M:179:GLN:HG3	2:M:180:SER:N	2.32	0.43
2:L:63:VAL:HG13	2:L:67:PHE:CD2	2.53	0.43
2:M:4:LEU:HB3	2:M:92:CYS:SG	2.59	0.43
1:J:125:LEU:HD22	1:J:183:LYS:HG3	2.01	0.43
1:H:146:VAL:HG12	1:H:175:MET:HE1	2.00	0.42
1:J:145:ASN:HB2	1:J:197:THR:HB	2.01	0.42
2:M:4:LEU:HD22	2:M:34:MET:HE1	2.00	0.42
2:M:149:PRO:HD2	2:M:214:ALA:HB1	2.00	0.42
2:L:141:GLY:HA2	2:L:189:SER:O	2.18	0.42
2:L:51:ILE:HG23	2:L:71:ARG:HH11	1.84	0.42
1:J:95:PRO:HA	2:M:47:TRP:CZ3	2.54	0.42
1:H:86:TYR:O	1:H:101:GLY:HA2	2.19	0.42
1:H:30:LYS:HD2	1:H:50:TRP:HB3	2.00	0.42
1:J:33:LEU:HD22	1:J:71:PHE:CG	2.54	0.42
1:J:125:LEU:HD21	1:J:130:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:195:GLU:HG3	1:J:204:PRO:HB2	2.02	0.42
2:M:38:ARG:HD3	2:M:90:TYR:CE2	2.54	0.42
2:M:95:ARG:HD2	2:M:95:ARG:HA	1.86	0.42
2:M:148:PHE:CE2	2:M:149:PRO:HB3	2.55	0.42
1:H:28:LYS:HG3	1:H:32:TYR:OH	2.20	0.41
1:J:125:LEU:HD23	1:J:125:LEU:HA	1.88	0.41
2:M:17:SER:OG	2:M:82(A):SER:HA	2.19	0.41
2:M:27:PHE:HD2	2:M:32:TYR:HD2	1.66	0.41
2:M:82(C):LEU:HD23	2:M:82(C):LEU:HA	1.83	0.41
1:H:120:PRO:HD3	1:H:132:VAL:HG22	2.02	0.41
1:J:28:LYS:HB2	1:J:32:TYR:OH	2.20	0.41
1:J:13:VAL:HG12	1:J:19:VAL:HG11	2.02	0.41
1:J:147:LYS:HE3	1:J:147:LYS:HB2	1.64	0.41
2:M:56:TYR:CE2	4:R:103:PRO:HB3	2.55	0.41
2:M:66:ARG:HG2	2:M:82(B):SER:HB2	2.03	0.41
1:J:185:GLU:O	1:J:189:HIS:HD2	2.04	0.41
1:H:115:VAL:HG12	1:H:207:LYS:HG2	2.02	0.41
1:J:110:ASP:HB3	1:J:200:THR:CG2	2.50	0.41
2:L:38:ARG:NH1	2:L:46:GLU:OE1	2.54	0.41
2:L:93:ALA:HA	2:L:102:TYR:O	2.21	0.41
1:J:66:GLY:HA3	1:J:70:ASP:O	2.21	0.41
2:L:3:GLN:O	2:L:24:ALA:HA	2.19	0.41
2:M:169:GLY:O	2:M:191:VAL:HA	2.20	0.40
2:M:29:PHE:CD2	2:M:76:ASN:HA	2.56	0.40
2:M:38:ARG:HD3	2:M:90:TYR:CZ	2.57	0.40
2:L:60:PRO:C	2:L:62:SER:H	2.29	0.40
1:J:161:ASN:HB3	1:J:175:MET:HE3	2.04	0.40
2:L:15:GLY:N	2:L:82(C):LEU:O	2.54	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	H	215/217 (99%)	203 (94%)	10 (5%)	2 (1%)	14	41
1	J	215/217 (99%)	201 (94%)	13 (6%)	1 (0%)	24	54
2	L	211/220 (96%)	191 (90%)	19 (9%)	1 (0%)	24	54
2	M	211/220 (96%)	189 (90%)	16 (8%)	6 (3%)	4	15
3	P	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	R	8/10 (80%)	8 (100%)	0	0	100	100
All	All	867/893 (97%)	798 (92%)	59 (7%)	10 (1%)	10	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	214	ALA
2	L	16	GLY
2	M	163	SER
1	H	170	ASP
1	J	51	ALA
2	M	28	SER
2	M	73	ASN
2	M	175	PRO
1	H	59	PRO
2	M	9	GLY

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	H	194/194 (100%)	159 (82%)	35 (18%)	2	6
1	J	194/194 (100%)	168 (87%)	26 (13%)	4	12
2	L	182/187 (97%)	161 (88%)	21 (12%)	5	18
2	M	182/187 (97%)	156 (86%)	26 (14%)	3	11
3	P	7/7 (100%)	7 (100%)	0	100	100
4	R	8/8 (100%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	767/777 (99%)	659 (86%)	108 (14%)	3 11

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	2	ILE
1	H	4	MET
1	H	5	THR
1	H	11	LEU
1	H	12	THR
1	H	19	VAL
1	H	21	MET
1	H	24	THR
1	H	45	LYS
1	H	47	LEU
1	H	48	ILE
1	H	59	PRO
1	H	61	ARG
1	H	65	SER
1	H	70	ASP
1	H	76	SER
1	H	78	VAL
1	H	90	ASN
1	H	107	LYS
1	H	108	ARG
1	H	146	VAL
1	H	150	ILE
1	H	153	SER
1	H	154	GLU
1	H	156	GLN
1	H	162	SER
1	H	164	THR
1	H	168	SER
1	H	172	THR
1	H	183	LYS
1	H	185	GLU
1	H	201	SER
1	H	202	THR
1	H	207	LYS
1	H	211	ARG
2	L	13	LYS
2	L	21	SER

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Mol	Chain	Res	Type
2	L	30	SER
2	L	57	THR
2	L	62	SER
2	L	64	LYS
2	L	77	THR
2	L	78	LEU
2	L	107	THR
2	L	115	LYS
2	L	138	VAL
2	L	151	PRO
2	L	153	THR
2	L	166	LEU
2	L	183	ASP
2	L	186	THR
2	L	187	LEU
2	L	193	VAL
2	L	196	SER
2	L	218	LYS
2	L	223	ILE
1	J	2	ILE
1	J	12	THR
1	J	19	VAL
1	J	21	MET
1	J	24	THR
1	J	28	LYS
1	J	37	GLN
1	J	43	PRO
1	J	47	LEU
1	J	55	GLU
1	J	56	SER
1	J	63	THR
1	J	65	SER
1	J	78	VAL
1	J	83	LEU
1	J	93	SER
1	J	108	ARG
1	J	116	SER
1	J	134	CYS
1	J	172	THR
1	J	181	LEU
1	J	191	SER
1	J	194	CYS

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Mol	Chain	Res	Type
1	J	197	THR
1	J	208	SER
1	J	211	ARG
2	M	21	SER
2	M	28	SER
2	M	30	SER
2	M	40	THR
2	M	52	SER
2	M	52(A)	ASN
2	M	63	VAL
2	M	69	ILE
2	M	70	SER
2	M	84	SER
2	M	92	CYS
2	M	105	GLN
2	M	127	VAL
2	M	140	LEU
2	M	142	CYS
2	M	152	VAL
2	M	153	THR
2	M	171	VAL
2	M	173	THR
2	M	175	PRO
2	M	177	VAL
2	M	187	LEU
2	M	202	SER
2	M	217	THR
2	M	219	VAL
2	M	222	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	161	ASN
1	H	189	HIS
1	H	190	ASN
1	H	198	HIS
2	L	39	GLN
2	L	76	ASN
2	L	81	GLN
2	L	162	ASN
2	L	179	GLN

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Mol	Chain	Res	Type
1	J	31	ASN
1	J	37	GLN
1	J	79	GLN
1	J	138	ASN
1	J	161	ASN
1	J	189	HIS
2	M	76	ASN
2	M	100(A)	ASN
2	M	179	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.