



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:49 AM UTC

PDB ID : 1HIN / pdb_00001hin
Title : STRUCTURAL EVIDENCE FOR INDUCED FIT AS A MECHANISM FOR
ANTIBODY-ANTIGEN RECOGNITION
Authors : Rini, J.M.; Wilson, I.A.
Deposited on : 1992-07-08
Resolution : 3.10 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

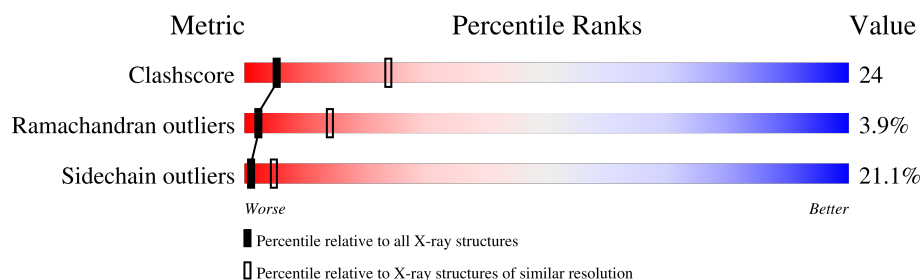
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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	L	217	
2	H	220	
3	P	8	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3432 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	L	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	H	220	Total	C	N	O	S	0	0	0
			1664	1047	276	333	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	227	PRO	-	insertion	GB 533229

- Molecule 3 is a protein called INFLUENZA HEMAGGLUTININ HA1 (STRAIN X47) (RESIDUES 100-107).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	8	Total	C	N	O	0	0	0
			66	42	8	16			

- Molecule 4 is water.

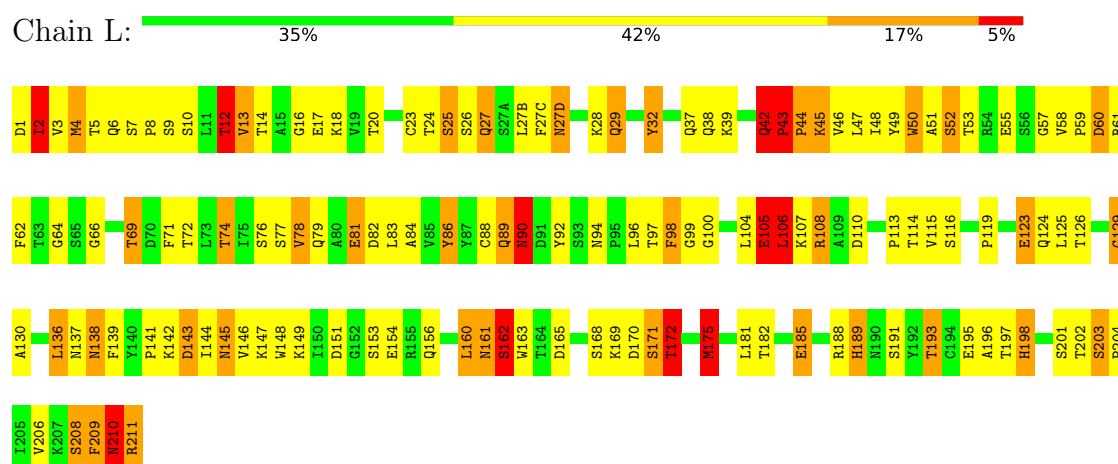
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	11	Total	O	0	0
			11	11		
4	H	11	Total	O	0	0
			11	11		

3 Residue-property plots

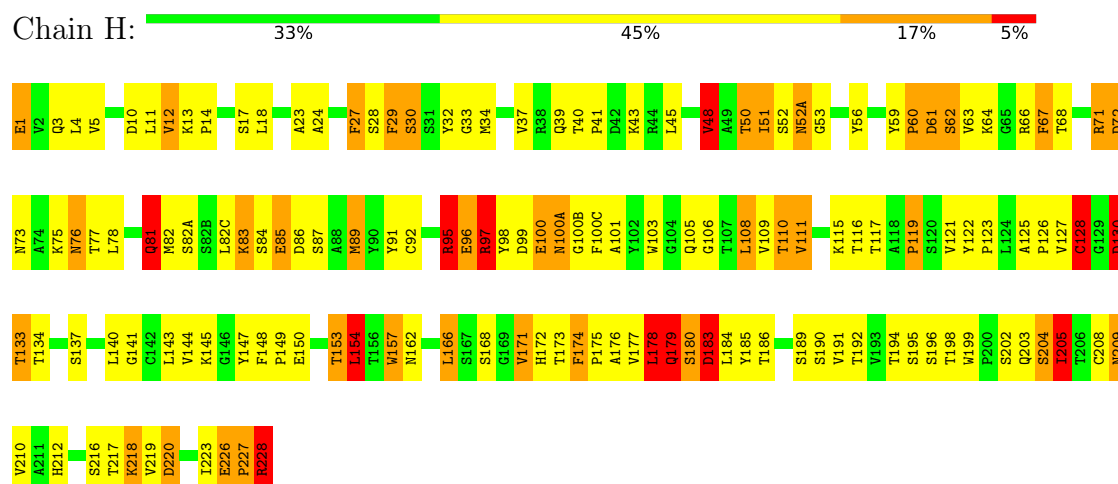
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

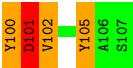


• Molecule 2: IGG2A-KAPPA 17/9 FAB (HEAVY CHAIN)



• Molecule 3: INFLUENZA HEMAGGLUTININ HA1 (STRAIN X47) (RESIDUES 100-107)





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	63.50Å 73.40Å 62.70Å 90.00° 117.10° 90.00°	Depositor
Resolution (Å)	8.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3432	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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	L	1.28	9/1718 (0.5%)	2.31	92/2334 (3.9%)
2	H	1.31	7/1705 (0.4%)	2.25	79/2322 (3.4%)
3	P	1.54	2/68 (2.9%)	2.63	4/92 (4.3%)
All	All	1.30	18/3491 (0.5%)	2.29	175/4748 (3.7%)

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	L	0	2
2	H	0	1
All	All	0	3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	217	THR	CA-CB	8.82	1.65	1.53
2	H	212	HIS	CD2-NE2	-7.04	1.30	1.37
1	L	27	GLN	CA-CB	-7.03	1.42	1.53
2	H	121	VAL	CA-CB	6.98	1.62	1.53
1	L	143	ASP	CA-CB	6.91	1.61	1.52
1	L	189	HIS	CD2-NE2	-6.83	1.30	1.37
2	H	12	VAL	CA-CB	6.69	1.64	1.54
2	H	171	VAL	CA-CB	6.31	1.62	1.54
1	L	2	ILE	CA-CB	6.28	1.61	1.54
1	L	182	THR	CA-CB	6.01	1.63	1.53
3	P	101	ASP	CG-OD2	-5.87	1.14	1.25
1	L	198	HIS	CD2-NE2	-5.76	1.31	1.37
1	L	198	HIS	CG-ND1	-5.56	1.32	1.38
3	P	102	VAL	CA-CB	5.19	1.60	1.54
1	L	13	VAL	CA-CB	5.11	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	27(C)	PHE	N-CA	-5.11	1.39	1.46
2	H	212	HIS	CG-ND1	-5.06	1.32	1.38
2	H	172	HIS	CD2-NE2	-5.05	1.32	1.37

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	101	ASP	CA-CB-CG	-15.16	97.44	112.60
1	L	145	ASN	OD1-CG-ND2	-14.56	108.03	122.60
1	L	143	ASP	CA-CB-CG	12.86	125.45	112.60
2	H	183	ASP	CA-CB-CG	12.18	124.78	112.60
1	L	145	ASN	CA-CB-CG	11.32	123.92	112.60
1	L	209	PHE	CA-CB-CG	11.16	124.96	113.80
1	L	145	ASN	CB-CG-ND2	10.93	132.80	116.40
2	H	220	ASP	CA-CB-CG	10.43	123.03	112.60
2	H	130	ASP	CA-CB-CG	10.12	122.72	112.60
1	L	81	GLU	CB-CG-CD	9.63	128.97	112.60
1	L	60	ASP	CA-CB-CG	9.54	122.14	112.60
1	L	138	ASN	OD1-CG-ND2	-9.51	113.09	122.60
2	H	95	ARG	CD-NE-CZ	-9.33	111.34	124.40
2	H	10	ASP	CA-CB-CG	9.31	121.91	112.60
2	H	171	VAL	N-CA-C	9.08	120.88	108.89
2	H	73	ASN	OD1-CG-ND2	-8.98	113.62	122.60
2	H	27	PHE	CA-CB-CG	8.78	122.58	113.80
1	L	208	SER	CA-CB-OG	8.54	128.17	111.10
1	L	45	LYS	CA-CB-CG	8.47	131.05	114.10
1	L	42	GLN	CA-C-N	8.24	128.86	120.38
1	L	42	GLN	C-N-CA	8.24	128.86	120.38
1	L	151	ASP	CA-CB-CG	8.10	120.69	112.60
1	L	188	ARG	N-CA-C	-7.99	104.50	112.97
1	L	139	PHE	CA-CB-CG	7.97	121.77	113.80
2	H	111	VAL	N-CA-CB	-7.97	101.28	111.64
2	H	174	PHE	CA-CB-CG	-7.96	105.84	113.80
2	H	127	VAL	CA-C-N	7.84	136.51	121.54
2	H	127	VAL	C-N-CA	7.84	136.51	121.54
2	H	228	ARG	CA-CB-CG	7.77	129.65	114.10
1	L	204	PRO	N-CA-C	7.74	123.49	110.95
2	H	67	PHE	CA-CB-CG	7.51	121.31	113.80
1	L	198	HIS	ND1-CG-CD2	7.49	113.59	106.10
2	H	212	HIS	ND1-CG-CD2	7.38	113.48	106.10
2	H	52(A)	ASN	N-CA-C	7.38	121.97	113.19
2	H	179	GLN	CA-CB-CG	7.33	128.76	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	98	PHE	CA-CB-CG	7.28	121.08	113.80
3	P	101	ASP	CA-C-N	-7.26	116.36	123.04
3	P	101	ASP	C-N-CA	-7.26	116.36	123.04
2	H	52(A)	ASN	CA-CB-CG	7.24	119.84	112.60
2	H	61	ASP	CA-CB-CG	-7.21	105.39	112.60
1	L	156	GLN	CB-CG-CD	7.19	124.82	112.60
2	H	192	THR	CA-CB-OG1	-7.18	98.83	109.60
1	L	161	ASN	CA-CB-CG	7.11	119.71	112.60
1	L	171	SER	CA-C-O	7.05	129.56	120.81
1	L	210	ASN	CA-CB-CG	7.04	119.64	112.60
1	L	42	GLN	OE1-CD-NE2	-7.01	115.59	122.60
2	H	162	ASN	CA-CB-CG	7.00	119.60	112.60
1	L	69	THR	CB-CA-C	6.98	122.51	110.23
1	L	27	GLN	CG-CD-NE2	-6.90	106.05	116.40
1	L	14	THR	O-C-N	-6.84	113.49	122.59
1	L	78	VAL	N-CA-C	6.79	119.42	109.63
1	L	172	THR	N-CA-CB	-6.78	100.41	110.85
1	L	26	SER	CA-C-O	6.75	127.86	120.90
1	L	175	MET	CG-SD-CE	-6.74	86.08	100.90
2	H	100	GLU	CA-CB-CG	-6.74	100.62	114.10
2	H	127	VAL	CA-C-O	6.70	129.16	120.78
1	L	146	VAL	N-CA-C	-6.69	99.51	108.35
1	L	129	GLY	CA-C-O	-6.66	114.90	121.76
1	L	172	THR	OG1-CB-CG2	6.64	122.59	109.30
1	L	27	GLN	OE1-CD-NE2	6.61	129.21	122.60
1	L	119	PRO	CA-C-N	6.61	126.56	119.76
1	L	119	PRO	C-N-CA	6.61	126.56	119.76
2	H	40	THR	CA-C-N	6.59	126.84	119.32
2	H	40	THR	C-N-CA	6.59	126.84	119.32
2	H	111	VAL	CB-CA-C	6.58	120.12	110.77
1	L	42	GLN	N-CA-C	6.57	117.94	109.72
2	H	43	LYS	N-CA-C	6.57	120.60	112.58
1	L	105	GLU	CB-CG-CD	6.56	123.76	112.60
2	H	29	PHE	CA-CB-CG	6.56	120.36	113.80
1	L	137	ASN	N-CA-C	6.55	120.20	109.72
1	L	113	PRO	N-CA-C	6.55	121.79	111.38
1	L	89	GLN	OE1-CD-NE2	-6.53	116.07	122.60
1	L	3	VAL	O-C-N	6.49	130.70	123.10
1	L	43	PRO	N-CA-C	-6.49	102.78	110.70
2	H	76	ASN	CA-CB-CG	-6.49	106.11	112.60
1	L	147	LYS	CB-CG-CD	-6.47	96.42	111.30
1	L	138	ASN	CB-CG-ND2	6.40	126.01	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	203	SER	CA-C-N	6.40	127.40	119.98
1	L	203	SER	C-N-CA	6.40	127.40	119.98
1	L	39	LYS	CA-C-N	6.35	126.38	119.90
1	L	39	LYS	C-N-CA	6.35	126.38	119.90
1	L	43	PRO	CA-N-CD	-6.35	103.11	112.00
2	H	128	CYS	N-CA-C	6.30	124.23	110.80
2	H	154	LEU	CD1-CG-CD2	-6.27	97.00	110.80
2	H	173	THR	CA-C-O	6.24	126.85	120.24
1	L	2	ILE	N-CA-C	-6.23	99.45	108.36
2	H	111	VAL	CA-C-O	6.21	126.85	120.39
1	L	27	GLN	CB-CG-CD	-6.17	102.11	112.60
1	L	79	GLN	OE1-CD-NE2	-6.13	116.47	122.60
1	L	25	SER	N-CA-CB	-6.09	100.67	111.08
2	H	52(A)	ASN	OD1-CG-ND2	-6.08	116.52	122.60
2	H	179	GLN	OE1-CD-NE2	-6.08	116.52	122.60
2	H	226	GLU	CA-C-O	-6.07	113.06	119.13
2	H	128	CYS	N-CA-CB	-6.05	100.26	110.49
1	L	153	SER	CA-CB-OG	-6.04	99.02	111.10
2	H	205	ILE	N-CA-C	-6.04	99.42	108.12
2	H	110	THR	CA-CB-OG1	-6.00	100.60	109.60
2	H	203	GLN	CA-CB-CG	5.92	125.93	114.10
1	L	69	THR	N-CA-CB	-5.91	96.89	110.83
2	H	128	CYS	CA-C-O	5.90	128.95	120.51
1	L	198	HIS	CG-CD2-NE2	-5.90	101.30	107.20
2	H	172	HIS	ND1-CG-CD2	5.89	111.99	106.10
2	H	218	LYS	N-CA-C	-5.87	100.71	110.17
2	H	154	LEU	N-CA-C	5.86	119.47	107.69
2	H	50	THR	CA-CB-CG2	5.86	120.45	110.50
2	H	226	GLU	CA-CB-CG	5.85	125.81	114.10
1	L	52	SER	N-CA-CB	-5.84	100.62	110.49
2	H	204	SER	CA-CB-OG	5.81	122.73	111.10
2	H	212	HIS	CB-CG-CD2	-5.80	123.66	131.20
2	H	96	GLU	O-C-N	5.80	129.97	122.43
1	L	172	THR	CA-CB-OG1	-5.71	101.03	109.60
1	L	53	THR	CA-C-N	5.69	128.79	120.71
1	L	53	THR	C-N-CA	5.69	128.79	120.71
1	L	189	HIS	CA-CB-CG	-5.68	108.12	113.80
1	L	79	GLN	CG-CD-NE2	5.66	124.89	116.40
2	H	100(C)	PHE	CA-CB-CG	5.64	119.44	113.80
1	L	48	ILE	O-C-N	-5.62	116.97	122.93
2	H	212	HIS	CG-CD2-NE2	-5.61	101.59	107.20
2	H	228	ARG	CG-CD-NE	5.61	124.34	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	81	GLU	CA-CB-CG	5.61	125.31	114.10
2	H	95	ARG	NH1-CZ-NH2	-5.60	112.02	119.30
1	L	162	SER	CA-CB-OG	5.59	122.28	111.10
2	H	72	ASP	CA-CB-CG	-5.59	107.01	112.60
2	H	39	GLN	CG-CD-NE2	5.58	124.76	116.40
1	L	196	ALA	CA-C-N	-5.57	114.59	122.94
1	L	196	ALA	C-N-CA	-5.57	114.59	122.94
2	H	81	GLN	CB-CG-CD	5.56	122.06	112.60
1	L	50	TRP	CG-CD1-NE1	-5.51	103.03	110.20
2	H	153	THR	CB-CA-C	5.51	119.30	109.65
1	L	27(D)	ASN	CA-CB-CG	5.51	118.11	112.60
1	L	171	SER	N-CA-C	5.40	119.15	112.24
2	H	178	LEU	N-CA-CB	-5.38	102.66	110.84
2	H	216	SER	CA-C-N	-5.37	115.48	123.11
2	H	216	SER	C-N-CA	-5.37	115.48	123.11
2	H	180	SER	CA-CB-OG	5.35	121.80	111.10
1	L	52	SER	CA-CB-OG	5.32	121.73	111.10
2	H	43	LYS	CA-CB-CG	-5.31	103.48	114.10
1	L	44	PRO	CB-CA-C	5.30	118.02	111.23
1	L	106	LEU	N-CA-C	5.29	118.84	109.96
1	L	202	THR	O-C-N	5.29	127.73	122.12
1	L	12	THR	CA-CB-OG1	-5.28	101.68	109.60
1	L	210	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	L	108	ARG	CB-CG-CD	-5.25	99.22	111.30
2	H	82(C)	LEU	CA-C-O	5.25	126.31	120.43
2	H	202	SER	CA-C-N	5.24	129.58	122.19
2	H	202	SER	C-N-CA	5.24	129.58	122.19
2	H	39	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	L	211	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	L	148	TRP	CE2-CD2-CG	-5.20	100.95	107.20
2	H	100(A)	ASN	OD1-CG-ND2	-5.20	117.40	122.60
2	H	96	GLU	CA-C-N	5.20	131.47	121.54
2	H	96	GLU	C-N-CA	5.20	131.47	121.54
2	H	60	PRO	CA-N-CD	-5.19	104.73	112.00
1	L	203	SER	O-C-N	-5.19	118.39	121.71
2	H	48	VAL	N-CA-C	5.18	116.64	111.00
2	H	227	PRO	N-CA-C	-5.18	101.81	112.47
1	L	50	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	L	210	ASN	N-CA-C	-5.17	99.79	110.80
1	L	188	ARG	CA-CB-CG	5.13	124.37	114.10
1	L	123	GLU	CB-CG-CD	5.12	121.31	112.60
1	L	149	LYS	CB-CG-CD	-5.11	99.54	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	179	GLN	CB-CG-CD	5.10	121.27	112.60
1	L	90	ASN	CA-CB-CG	5.09	117.69	112.60
1	L	48	ILE	N-CA-CB	-5.09	102.72	110.86
2	H	37	VAL	O-C-N	-5.09	117.58	123.07
1	L	57	GLY	N-CA-C	-5.08	107.65	114.25
1	L	123	GLU	CA-CB-CG	5.07	124.24	114.10
1	L	94	ASN	CA-CB-CG	5.07	117.67	112.60
2	H	43	LYS	N-CA-CB	-5.05	104.79	112.47
2	H	97	ARG	NE-CZ-NH1	5.04	126.54	121.50
2	H	157	TRP	CE2-CD2-CG	-5.04	101.16	107.20
1	L	42	GLN	CG-CD-NE2	5.02	123.93	116.40
3	P	105	TYR	CA-CB-CG	5.02	122.94	113.90
2	H	100(B)	GLY	CA-C-N	-5.02	106.17	117.20
2	H	83	LYS	CA-C-O	-5.00	115.81	121.72

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	95	ARG	Sidechain
1	L	32	TYR	Sidechain
1	L	86	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	L	1680	0	1612	70	0
2	H	1664	0	1616	100	0
3	P	66	0	51	4	0
4	H	11	0	0	0	0
4	L	11	0	0	0	0
All	All	3432	0	3279	162	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 24.

All (162) 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)
2:H:11:LEU:HD13	2:H:110:THR:HG22	1.56	0.87
1:L:181:LEU:HD22	1:L:185:GLU:HG2	1.56	0.86
2:H:126:PRO:HG2	2:H:128:CYS:HA	1.60	0.84
2:H:166:LEU:HD13	2:H:191:VAL:HG21	1.61	0.83
1:L:83:LEU:HD11	1:L:106:LEU:HB3	1.58	0.83
1:L:66:GLY:HA3	1:L:71:PHE:HA	1.61	0.81
2:H:137:SER:HA	2:H:194:THR:HA	1.63	0.80
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.66	0.78
2:H:4:LEU:HA	2:H:23:ALA:O	1.87	0.74
1:L:47:LEU:HA	1:L:58:VAL:HG21	1.69	0.74
1:L:38:GLN:O	1:L:84:ALA:HB1	1.89	0.73
1:L:20:THR:HG23	1:L:72:THR:HG23	1.75	0.69
2:H:154:LEU:HD12	2:H:210:VAL:HG22	1.75	0.68
2:H:130:ASP:HA	2:H:137:SER:O	1.94	0.68
2:H:84:SER:HA	2:H:111:VAL:HG13	1.75	0.67
1:L:49:TYR:CD2	2:H:100(A):ASN:HB2	2.29	0.67
1:L:160:LEU:HD11	2:H:177:VAL:HG11	1.77	0.66
2:H:140:LEU:HD22	2:H:223:ILE:HG21	1.77	0.66
2:H:228:ARG:HH11	2:H:228:ARG:HB2	1.59	0.66
2:H:34:MET:HB2	2:H:78:LEU:HD13	1.77	0.65
1:L:162:SER:HB2	2:H:174:PHE:HB3	1.77	0.65
2:H:63:VAL:HG13	2:H:67:PHE:CD2	2.31	0.65
1:L:138:ASN:HA	1:L:172:THR:HG23	1.80	0.64
1:L:20:THR:OG1	1:L:74:THR:HG23	1.97	0.64
1:L:25:SER:OG	1:L:69:THR:HA	1.97	0.64
2:H:119:PRO:HB2	2:H:144:VAL:HG13	1.78	0.64
1:L:12:THR:HG23	1:L:107:LYS:HG2	1.79	0.64
1:L:28:LYS:O	1:L:29:GLN:HB2	1.98	0.64
1:L:193:THR:HG23	1:L:206:VAL:HG13	1.81	0.63
2:H:100(A):ASN:N	2:H:100(A):ASN:HD22	1.97	0.61
2:H:100:GLU:HG2	3:P:105:TYR:CD2	2.36	0.61
2:H:11:LEU:HA	2:H:110:THR:O	2.01	0.60
1:L:17:GLU:O	1:L:78:VAL:HG12	2.02	0.60
1:L:108:ARG:HG3	1:L:171:SER:HB2	1.83	0.59
1:L:38:GLN:NE2	1:L:44:PRO:HD3	2.18	0.59
2:H:60:PRO:O	2:H:64:LYS:HG3	2.02	0.59
2:H:1:GLU:OE1	2:H:3:GLN:HB2	2.03	0.59
2:H:4:LEU:HB3	2:H:92:CYS:SG	2.42	0.58
1:L:38:GLN:HA	1:L:42:GLN:OE1	2.04	0.58
1:L:13:VAL:CG2	1:L:78:VAL:HG11	2.33	0.58
2:H:51:ILE:HG12	2:H:52:SER:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82:MET:HE1	2:H:109:VAL:HG21	1.86	0.58
2:H:134:THR:N	2:H:137:SER:HG	2.01	0.58
2:H:171:VAL:HA	2:H:190:SER:O	2.03	0.58
2:H:27:PHE:HE2	2:H:32:TYR:HB2	1.69	0.57
2:H:24:ALA:HB1	2:H:27:PHE:HE1	1.69	0.57
2:H:52(A):ASN:HD21	3:P:102:VAL:HG22	1.68	0.57
1:L:47:LEU:O	1:L:55:GLU:HB2	2.05	0.56
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.40	0.56
2:H:85:GLU:H	2:H:85:GLU:CD	2.13	0.56
2:H:66:ARG:HB3	2:H:82(A):SER:O	2.06	0.55
1:L:89:GLN:HE21	1:L:96:LEU:HB3	1.71	0.55
2:H:14:PRO:HG3	2:H:111:VAL:HG22	1.88	0.55
2:H:33:GLY:HA2	2:H:71:ARG:HH12	1.70	0.55
1:L:18:LYS:HG2	1:L:76:SER:HA	1.88	0.55
1:L:43:PRO:HD2	2:H:105:GLN:HE21	1.72	0.54
1:L:25:SER:HB2	1:L:27:GLN:O	2.07	0.54
2:H:144:VAL:O	2:H:186:THR:HA	2.07	0.54
2:H:134:THR:N	2:H:137:SER:OG	2.41	0.54
2:H:140:LEU:HD22	2:H:223:ILE:CG2	2.37	0.53
1:L:193:THR:CG2	1:L:206:VAL:HG13	2.38	0.53
1:L:12:THR:HA	1:L:105:GLU:O	2.08	0.53
2:H:52(A):ASN:HA	2:H:71:ARG:NH1	2.23	0.53
2:H:83:LYS:HE2	2:H:86:ASP:OD1	2.09	0.52
1:L:2:ILE:HD13	1:L:90:ASN:ND2	2.24	0.52
2:H:29:PHE:HB2	2:H:76:ASN:HD21	1.74	0.52
2:H:179:GLN:O	2:H:183:ASP:N	2.43	0.52
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.93	0.51
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.92	0.51
1:L:2:ILE:HG23	1:L:27:GLN:HB2	1.92	0.51
2:H:199:TRP:HB2	2:H:205:ILE:HD13	1.92	0.51
2:H:178:LEU:HD13	2:H:185:TYR:CZ	2.46	0.51
1:L:46:VAL:HG23	2:H:101:ALA:HA	1.93	0.50
2:H:33:GLY:O	2:H:95:ARG:HB2	2.12	0.50
2:H:116:THR:HA	2:H:148:PHE:O	2.12	0.50
1:L:82:ASP:O	1:L:104:LEU:HD12	2.12	0.50
1:L:115:VAL:HG22	1:L:136:LEU:HG	1.94	0.49
1:L:185:GLU:O	1:L:189:HIS:HD2	1.95	0.49
1:L:124:GLN:HG2	1:L:129:GLY:O	2.11	0.49
1:L:27(D):ASN:HB3	1:L:92:TYR:HE1	1.77	0.49
2:H:52(A):ASN:ND2	2:H:97:ARG:HH21	2.11	0.49
1:L:8:PRO:HB2	1:L:10:SER:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:209:ASN:HA	2:H:220:ASP:HA	1.93	0.49
1:L:5:THR:O	1:L:23:CYS:HA	2.12	0.49
1:L:51:ALA:HB2	1:L:71:PHE:HE2	1.78	0.48
2:H:97:ARG:HD2	2:H:98:TYR:CE1	2.47	0.48
2:H:12:VAL:O	2:H:111:VAL:HA	2.13	0.48
3:P:100:TYR:CD1	3:P:100:TYR:O	2.67	0.48
2:H:48:VAL:O	2:H:63:VAL:HG11	2.14	0.48
2:H:83:LYS:HG2	2:H:86:ASP:OD2	2.13	0.47
1:L:32:TYR:HE2	2:H:100:GLU:HB3	1.79	0.47
1:L:4:MET:HB3	1:L:99:GLY:HA2	1.96	0.47
2:H:27:PHE:CE2	2:H:29:PHE:HA	2.50	0.47
1:L:16:GLY:HA2	1:L:77:SER:OG	2.15	0.47
1:L:61:ARG:HA	1:L:76:SER:OG	2.13	0.47
2:H:140:LEU:HB3	2:H:223:ILE:HD13	1.96	0.47
1:L:142:LYS:HG2	1:L:163:TRP:CZ2	2.50	0.47
2:H:3:GLN:O	2:H:24:ALA:HA	2.15	0.47
2:H:92:CYS:SG	2:H:92:CYS:O	2.73	0.46
2:H:157:TRP:CZ3	2:H:208:CYS:HB2	2.50	0.46
2:H:96:GLU:HG3	2:H:100(A):ASN:HD21	1.80	0.46
2:H:143:LEU:HG	2:H:145:LYS:HG2	1.96	0.46
1:L:160:LEU:HD12	1:L:161:ASN:H	1.81	0.46
2:H:179:GLN:OE1	2:H:184:LEU:HB2	2.16	0.46
2:H:176:ALA:HA	2:H:186:THR:O	2.16	0.46
2:H:27:PHE:CE2	2:H:32:TYR:HB2	2.50	0.46
1:L:2:ILE:O	1:L:97:THR:HG21	2.17	0.45
2:H:145:LYS:NZ	2:H:179:GLN:HE21	2.13	0.45
1:L:59:PRO:HD2	1:L:62:PHE:HE2	1.81	0.45
1:L:37:GLN:HG2	1:L:38:GLN:N	2.30	0.45
1:L:110:ASP:OD1	1:L:141:PRO:HD3	2.17	0.45
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.98	0.45
1:L:52:SER:HA	1:L:64:GLY:HA3	1.97	0.45
2:H:18:LEU:HD23	2:H:109:VAL:HG13	1.98	0.45
2:H:89:MET:HA	2:H:108:LEU:HA	1.98	0.45
2:H:89:MET:HE3	2:H:108:LEU:HB2	1.98	0.45
1:L:144:ILE:HD12	1:L:198:HIS:HD2	1.82	0.45
1:L:13:VAL:HG22	1:L:78:VAL:HG11	1.98	0.45
1:L:160:LEU:HD11	2:H:177:VAL:CG1	2.46	0.44
2:H:72:ASP:CG	2:H:75:LYS:HB2	2.42	0.44
2:H:148:PHE:HB2	2:H:184:LEU:CD2	2.48	0.44
1:L:27(B):LEU:HD22	1:L:92:TYR:HB3	1.98	0.44
1:L:161:ASN:HB3	1:L:175:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:126:PRO:C	2:H:128:CYS:H	2.25	0.44
1:L:50:TRP:NE1	2:H:100:GLU:O	2.50	0.44
1:L:66:GLY:CA	1:L:71:PHE:HA	2.38	0.44
1:L:59:PRO:HD2	1:L:62:PHE:CE2	2.53	0.43
2:H:18:LEU:CD2	2:H:109:VAL:HG13	2.48	0.43
2:H:148:PHE:HB2	2:H:184:LEU:HD22	2.01	0.43
1:L:88:CYS:SG	1:L:99:GLY:HA3	2.58	0.43
2:H:134:THR:O	2:H:137:SER:N	2.52	0.43
1:L:114:THR:HG22	2:H:133:THR:HG22	2.01	0.43
2:H:81:GLN:HE22	2:H:82(A):SER:HB2	1.83	0.43
2:H:87:SER:HA	2:H:109:VAL:O	2.19	0.43
2:H:18:LEU:HB3	2:H:82:MET:HE3	2.00	0.43
1:L:170:ASP:OD1	1:L:172:THR:HB	2.19	0.42
2:H:83:LYS:HG2	2:H:86:ASP:CG	2.44	0.42
2:H:154:LEU:CD1	2:H:210:VAL:HG22	2.47	0.42
2:H:126:PRO:C	2:H:128:CYS:N	2.77	0.42
2:H:145:LYS:HZ1	2:H:179:GLN:HE21	1.66	0.42
2:H:30:SER:O	2:H:52(A):ASN:HB2	2.20	0.42
1:L:185:GLU:O	1:L:185:GLU:HG3	2.15	0.42
2:H:59:TYR:OH	2:H:68:THR:HA	2.20	0.42
2:H:174:PHE:HA	2:H:175:PRO:HD2	1.84	0.42
1:L:125:LEU:HD21	1:L:130:ALA:HB2	2.02	0.41
1:L:2:ILE:HD12	1:L:2:ILE:N	2.35	0.41
2:H:34:MET:CB	2:H:78:LEU:HD13	2.45	0.41
1:L:42:GLN:HA	1:L:43:PRO:HD2	1.97	0.41
1:L:18:LYS:NZ	1:L:20:THR:OG1	2.52	0.41
2:H:62:SER:O	2:H:66:ARG:NH2	2.47	0.41
2:H:96:GLU:CB	2:H:100(A):ASN:ND2	2.83	0.41
1:L:37:GLN:HG3	1:L:86:TYR:CE2	2.55	0.41
2:H:52:SER:HB2	3:P:101:ASP:OD1	2.21	0.41
2:H:125:ALA:HB2	2:H:223:ILE:HG23	2.03	0.41
2:H:141:GLY:HA2	2:H:189:SER:O	2.21	0.41
2:H:178:LEU:HA	2:H:185:TYR:HA	2.03	0.41
2:H:89:MET:HG2	2:H:91:TYR:CE2	2.56	0.40
2:H:122:TYR:HA	2:H:123:PRO:HD2	1.97	0.40
1:L:209:PHE:O	1:L:210:ASN:HB2	2.21	0.40
1:L:90:ASN:HB3	1:L:97:THR:OG1	2.22	0.40
2:H:95:ARG:HD3	2:H:95:ARG:HA	1.70	0.40
1:L:4:MET:HE1	1:L:25:SER:HB3	2.03	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	L	215/217 (99%)	188 (87%)	22 (10%)	5 (2%)	5	23
2	H	218/220 (99%)	187 (86%)	19 (9%)	12 (6%)	1	9
3	P	6/8 (75%)	6 (100%)	0	0	100	100
All	All	439/445 (99%)	381 (87%)	41 (9%)	17 (4%)	2	14

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	29	GLN
2	H	149	PRO
2	H	180	SER
2	H	183	ASP
2	H	195	SER
2	H	196	SER
2	H	227	PRO
1	L	201	SER
2	H	106	GLY
2	H	128	CYS
2	H	179	GLN
1	L	60	ASP
1	L	210	ASN
2	H	30	SER
2	H	56	TYR
1	L	100	GLY
2	H	53	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	194/194 (100%)	155 (80%)	39 (20%)	1	5
2	H	187/187 (100%)	146 (78%)	41 (22%)	1	4
3	P	7/7 (100%)	5 (71%)	2 (29%)	0	1
All	All	388/388 (100%)	306 (79%)	82 (21%)	1	5

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	2	ILE
1	L	4	MET
1	L	6	GLN
1	L	7	SER
1	L	9	SER
1	L	12	THR
1	L	24	THR
1	L	42	GLN
1	L	43	PRO
1	L	45	LYS
1	L	74	THR
1	L	81	GLU
1	L	90	ASN
1	L	98	PHE
1	L	105	GLU
1	L	106	LEU
1	L	116	SER
1	L	123	GLU
1	L	126	THR
1	L	136	LEU
1	L	143	ASP
1	L	145	ASN
1	L	154	GLU
1	L	160	LEU
1	L	162	SER
1	L	165	ASP
1	L	168	SER
1	L	169	LYS
1	L	172	THR
1	L	175	MET

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Mol	Chain	Res	Type
1	L	185	GLU
1	L	191	SER
1	L	193	THR
1	L	195	GLU
1	L	197	THR
1	L	203	SER
1	L	208	SER
1	L	211	ARG
2	H	1	GLU
2	H	5	VAL
2	H	13	LYS
2	H	17	SER
2	H	28	SER
2	H	41	PRO
2	H	45	LEU
2	H	48	VAL
2	H	50	THR
2	H	51	ILE
2	H	61	ASP
2	H	62	SER
2	H	71	ARG
2	H	77	THR
2	H	81	GLN
2	H	85	GLU
2	H	89	MET
2	H	97	ARG
2	H	99	ASP
2	H	103	TRP
2	H	108	LEU
2	H	115	LYS
2	H	117	THR
2	H	119	PRO
2	H	130	ASP
2	H	133	THR
2	H	150	GLU
2	H	153	THR
2	H	154	LEU
2	H	166	LEU
2	H	168	SER
2	H	178	LEU
2	H	179	GLN
2	H	198	THR

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Mol	Chain	Res	Type
2	H	204	SER
2	H	205	ILE
2	H	209	ASN
2	H	218	LYS
2	H	219	VAL
2	H	226	GLU
2	H	228	ARG
3	P	100	TYR
3	P	101	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	38	GLN
1	L	89	GLN
1	L	145	ASN
1	L	210	ASN
2	H	39	GLN
2	H	81	GLN
2	H	100(A)	ASN
2	H	105	GLN
2	H	172	HIS
2	H	179	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 oligosaccharides 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 [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.