



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:18 AM UTC

PDB ID : 6FAB / pdb_00006fab
Title : THREE-DIMENSIONAL STRUCTURE OF MURINE ANTI-P-AZOPHENYLARSONATE FAB 36-71. 1. X-RAY CRYSTALLOGRAPHY, SITE-DIRECTED MUTAGENESIS, AND MODELING OF THE COMPLEX WITH HAPTEN
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Deposited on : 1991-01-17
Resolution : 1.90 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

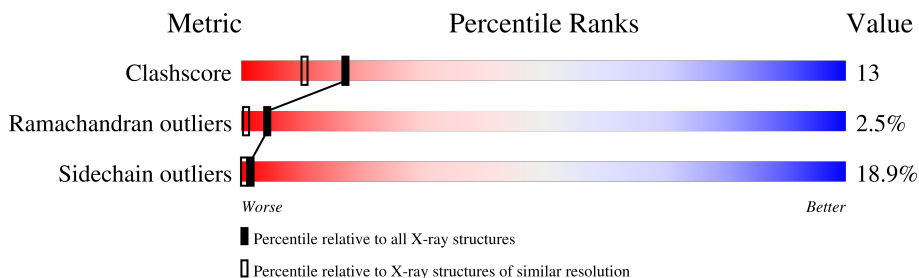
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	L	214	
2	H	222	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3409 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 IGG1-KAPPA 36-71 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1660	1026	284	343	7			

- Molecule 2 is a protein called IGG1-KAPPA 36-71 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1679	1057	279	336	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	32	Total	O	0	0
			32	32		
3	H	38	Total	O	0	0
			38	38		

3 Residue-property plots

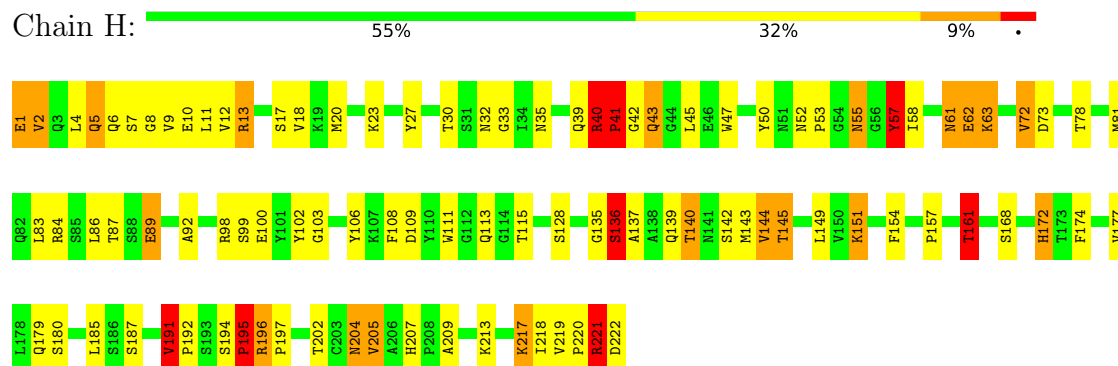
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: IGG1-KAPPA 36-71 FAB (LIGHT CHAIN)



• Molecule 2: IGG1-KAPPA 36-71 FAB (HEAVY CHAIN)



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	67.13Å 73.05Å 46.78Å 90.00° 104.48° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.209 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3409	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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	6/1693 (0.4%)	2.29	98/2293 (4.3%)
2	H	1.17	2/1721 (0.1%)	2.15	60/2345 (2.6%)
All	All	1.23	8/3414 (0.2%)	2.22	158/4638 (3.4%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	44	ILE	CA-CB	7.69	1.65	1.54
1	L	198	HIS	CD2-NE2	-6.86	1.30	1.37
1	L	205	ILE	CA-CB	6.58	1.61	1.54
2	H	205	VAL	CA-CB	6.42	1.63	1.54
1	L	83	ILE	CA-CB	6.37	1.61	1.54
1	L	51	THR	CA-C	-5.95	1.45	1.53
2	H	207	HIS	CD2-NE2	-5.87	1.31	1.37
1	L	189	HIS	CD2-NE2	-5.37	1.31	1.37

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	154	GLU	N-CA-C	14.58	131.83	110.10
1	L	156	GLN	N-CA-C	12.68	124.84	111.14
1	L	138	ASN	OD1-CG-ND2	-12.19	110.41	122.60
2	H	57	TYR	N-CA-C	12.11	136.59	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	170	ASP	CA-CB-CG	11.46	124.06	112.60
1	L	161	ASN	OD1-CG-ND2	-10.81	111.79	122.60
2	H	222	ASP	CA-CB-CG	10.77	123.37	112.60
1	L	170	ASP	O-C-N	-10.48	109.20	122.20
2	H	58	ILE	N-CA-C	10.46	124.05	108.46
1	L	154	GLU	CA-C-O	10.39	132.76	120.92
1	L	213	GLU	N-CA-C	-9.84	95.14	109.11
2	H	40	ARG	N-CA-C	-9.47	97.71	109.65
1	L	51	THR	CA-CB-OG1	-9.05	96.02	109.60
1	L	90	GLN	OE1-CD-NE2	-9.02	113.58	122.60
2	H	135	GLY	O-C-N	9.00	132.36	122.82
1	L	42	GLY	N-CA-C	8.92	127.15	115.47
1	L	17	ASP	CA-CB-CG	8.88	121.48	112.60
2	H	151	LYS	CA-C-O	-8.64	111.21	120.71
2	H	43	GLN	N-CA-C	8.38	128.64	110.80
1	L	29	ILE	N-CA-CB	-8.33	101.52	112.26
2	H	109	ASP	CA-CB-CG	8.24	120.84	112.60
2	H	151	LYS	O-C-N	-8.23	113.49	122.38
2	H	151	LYS	N-CA-C	8.17	126.41	110.56
1	L	52	SER	CA-CB-OG	8.00	127.11	111.10
2	H	32	ASN	OD1-CG-ND2	-7.92	114.68	122.60
1	L	117	ILE	CB-CA-C	-7.83	98.17	110.69
1	L	34	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	L	198	HIS	CB-CG-CD2	-7.62	121.29	131.20
2	H	61	ASN	OD1-CG-ND2	-7.50	115.10	122.60
1	L	3	GLN	OE1-CD-NE2	-7.48	115.12	122.60
2	H	55	ASN	CA-CB-CG	7.41	120.01	112.60
1	L	175	MET	CG-SD-CE	-7.41	84.59	100.90
1	L	212	ASN	OD1-CG-ND2	-7.24	115.36	122.60
1	L	210	ASN	CA-CB-CG	7.24	119.83	112.60
1	L	211	ARG	N-CA-C	7.19	119.12	111.28
1	L	51	THR	CA-CB-CG2	6.99	122.39	110.50
1	L	51	THR	O-C-N	6.98	131.68	122.47
1	L	117	ILE	N-CA-C	-6.86	97.67	108.86
2	H	143	MET	N-CA-C	-6.84	99.82	110.42
1	L	205	ILE	CB-CA-C	6.83	120.33	110.98
1	L	119	PRO	CA-C-N	6.80	126.84	119.90
1	L	119	PRO	C-N-CA	6.80	126.84	119.90
1	L	138	ASN	CB-CG-ND2	6.77	126.55	116.40
2	H	217	LYS	CA-CB-CG	-6.76	100.58	114.10
1	L	212	ASN	CA-CB-CG	-6.74	105.86	112.60
1	L	103	LYS	CG-CD-CE	6.71	126.74	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	39	GLN	OE1-CD-NE2	-6.70	115.90	122.60
2	H	89	GLU	CA-CB-CG	6.67	127.45	114.10
1	L	154	GLU	CB-CA-C	-6.64	99.54	109.90
1	L	170	ASP	N-CA-C	-6.62	100.10	110.36
2	H	39	GLN	CG-CD-NE2	6.56	126.24	116.40
1	L	167	ASP	CA-CB-CG	-6.54	106.06	112.60
1	L	29	ILE	CB-CA-C	6.54	119.31	111.20
1	L	31	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	L	37	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	L	117	ILE	CA-CB-CG2	6.50	121.54	110.50
1	L	114	THR	N-CA-C	-6.49	98.14	108.73
2	H	73	ASP	N-CA-C	-6.48	96.60	107.80
2	H	61	ASN	CB-CG-ND2	6.42	126.03	116.40
2	H	174	PHE	CA-CB-CG	-6.41	107.39	113.80
2	H	207	HIS	CB-CG-CD2	-6.32	122.98	131.20
2	H	161	THR	N-CA-CB	-6.31	100.57	111.55
1	L	28	ASP	CA-CB-CG	6.30	118.90	112.60
1	L	94	LEU	CA-C-O	-6.25	114.20	120.64
1	L	112	ALA	N-CA-CB	6.19	121.39	110.37
2	H	174	PHE	CA-C-N	6.18	126.20	119.90
2	H	174	PHE	C-N-CA	6.18	126.20	119.90
1	L	208	SER	CA-C-O	-6.16	114.67	121.33
1	L	27	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	L	206	VAL	N-CA-CB	-6.12	99.89	111.21
2	H	72	VAL	N-CA-CB	-6.10	103.97	112.52
2	H	180	SER	CA-C-O	6.07	129.35	122.37
1	L	117	ILE	CA-CB-CG1	-6.07	100.09	110.40
2	H	204	ASN	OD1-CG-ND2	-6.06	116.54	122.60
1	L	198	HIS	CB-CG-ND1	6.05	131.77	122.70
1	L	57	GLY	CA-C-O	6.04	131.09	120.57
1	L	51	THR	CB-CA-C	-5.99	103.49	111.63
1	L	153	SER	CA-C-O	-5.97	111.97	120.51
1	L	92	ASN	O-C-N	-5.96	114.50	122.49
2	H	209	ALA	N-CA-C	5.96	119.82	112.54
2	H	109	ASP	N-CA-C	5.96	120.62	113.23
1	L	29	ILE	CA-CB-CG2	5.93	120.57	110.50
2	H	43	GLN	CA-C-O	-5.91	112.05	120.51
1	L	21	ILE	O-C-N	-5.88	116.83	123.18
1	L	111	ALA	N-CA-C	5.87	120.23	112.72
2	H	1	GLU	N-CA-C	-5.84	94.64	111.00
1	L	206	VAL	CB-CA-C	5.83	119.67	110.81
2	H	154	PHE	O-C-N	-5.81	117.31	121.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	58	VAL	N-CA-CB	-5.77	103.14	111.21
1	L	107	LYS	CG-CD-CE	5.76	124.55	111.30
2	H	172	HIS	CB-CG-CD2	-5.76	123.72	131.20
2	H	219	VAL	O-C-N	-5.75	116.63	121.40
1	L	154	GLU	CA-CB-CG	5.74	125.58	114.10
1	L	155	ARG	CA-CB-CG	5.73	125.55	114.10
1	L	1	ASP	CA-CB-CG	5.72	118.32	112.60
1	L	38	GLN	CA-CB-CG	-5.71	102.67	114.10
1	L	103	LYS	CA-CB-CG	5.71	125.51	114.10
1	L	137	ASN	N-CA-C	5.66	118.62	109.40
2	H	5	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	L	137	ASN	OD1-CG-ND2	-5.61	116.99	122.60
2	H	136	SER	N-CA-CB	-5.61	101.01	110.49
2	H	219	VAL	N-CA-CB	-5.60	107.97	111.83
1	L	153	SER	CA-C-N	5.59	128.71	120.82
1	L	153	SER	C-N-CA	5.59	128.71	120.82
1	L	189	HIS	CB-CG-CD2	-5.58	123.94	131.20
1	L	203	SER	N-CA-C	-5.58	102.74	109.72
1	L	147	LYS	CA-CB-CG	5.53	125.16	114.10
1	L	163	TRP	CD1-CG-CD2	5.51	115.12	106.30
1	L	187	GLU	N-CA-C	5.49	119.69	113.15
2	H	221	ARG	CA-CB-CG	5.49	125.08	114.10
1	L	117	ILE	N-CA-CB	5.48	122.07	111.93
1	L	163	TRP	CE2-CD2-CG	-5.47	100.64	107.20
1	L	98	PHE	CA-CB-CG	5.46	119.26	113.80
2	H	113	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	L	35	TRP	CG-CD1-NE1	-5.43	103.15	110.20
2	H	195	PRO	CA-N-CD	-5.42	104.41	112.00
1	L	209	PHE	N-CA-C	-5.41	100.49	108.99
1	L	148	TRP	CE2-CD2-CG	-5.41	100.71	107.20
1	L	75	ILE	N-CA-C	-5.37	100.02	107.80
1	L	43	THR	CA-C-N	-5.33	115.53	122.94
1	L	43	THR	C-N-CA	-5.33	115.53	122.94
1	L	112	ALA	CB-CA-C	-5.33	99.67	110.17
1	L	52	SER	N-CA-C	-5.33	100.07	109.02
1	L	73	LEU	CA-C-O	-5.32	115.07	120.71
1	L	159	VAL	N-CA-CB	-5.32	104.99	111.21
1	L	83	ILE	N-CA-C	-5.28	100.15	108.23
1	L	163	TRP	CG-CD1-NE1	-5.24	103.39	110.20
1	L	161	ASN	CB-CG-ND2	5.22	124.24	116.40
1	L	22	SER	CA-CB-OG	5.22	121.55	111.10
1	L	19	VAL	O-C-N	-5.21	117.56	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	202	THR	CA-CB-OG1	-5.21	101.78	109.60
2	H	42	GLY	CA-C-N	5.20	131.48	121.54
2	H	42	GLY	C-N-CA	5.20	131.48	121.54
1	L	155	ARG	CB-CG-CD	5.20	123.25	111.30
1	L	58	VAL	N-CA-C	-5.18	97.68	108.88
2	H	111	TRP	CE2-CD2-CG	-5.18	100.98	107.20
2	H	185	LEU	CA-CB-CG	5.14	134.31	116.30
2	H	220	PRO	CA-C-N	5.14	131.36	121.54
2	H	220	PRO	C-N-CA	5.14	131.36	121.54
1	L	116	SER	O-C-N	-5.14	117.31	123.27
2	H	135	GLY	CA-C-N	5.12	131.31	121.54
2	H	135	GLY	C-N-CA	5.12	131.31	121.54
2	H	128	SER	N-CA-C	-5.11	101.38	109.76
2	H	6	GLN	N-CA-C	5.09	118.36	110.17
2	H	137	ALA	N-CA-C	-5.09	102.38	109.96
2	H	191	VAL	O-C-N	-5.08	117.05	121.57
1	L	50	PHE	CA-CB-CG	5.08	118.88	113.80
1	L	96	ARG	N-CA-C	-5.06	102.37	109.96
1	L	139	PHE	CA-CB-CG	5.05	118.86	113.80
2	H	81	MET	CG-SD-CE	-5.04	89.81	100.90
2	H	145	THR	N-CA-C	-5.04	101.48	109.59
2	H	195	PRO	N-CA-C	5.04	122.85	112.47
1	L	54	SER	CA-C-O	5.04	125.92	120.43
2	H	207	HIS	CA-C-N	5.03	124.63	119.05
2	H	207	HIS	C-N-CA	5.03	124.63	119.05
1	L	211	ARG	CA-C-N	-5.01	115.70	123.17
1	L	211	ARG	C-N-CA	-5.01	115.70	123.17
2	H	87	THR	CA-CB-OG1	-5.01	102.09	109.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	106	TYR	Sidechain
1	L	155	ARG	Peptide
1	L	192	TYR	Sidechain

5.2 Too-close contacts

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	1660	0	1590	52	0
2	H	1679	0	1636	37	0
3	H	38	0	0	2	0
3	L	32	0	0	1	0
All	All	3409	0	3226	83	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 13.

All (83) 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:192:PRO:HB2	2:H:195:PRO:HD2	1.54	0.88
1:L:213:GLU:HG3	2:H:136:SER:HB3	1.63	0.80
1:L:52:SER:HB3	1:L:64:GLY:HA3	1.64	0.78
1:L:48:ILE:HG21	1:L:52:SER:HA	1.66	0.78
2:H:161:THR:HG22	2:H:204:ASN:HB2	1.64	0.77
1:L:47:LEU:HA	1:L:58:VAL:HG11	1.65	0.77
1:L:31:ASN:HB3	1:L:51:THR:HB	1.67	0.77
2:H:196:ARG:HG2	2:H:197:PRO:HA	1.66	0.75
2:H:140:THR:HB	2:H:144:VAL:HA	1.74	0.70
2:H:144:VAL:HG23	2:H:191:VAL:HG23	1.75	0.69
1:L:160:LEU:HD13	2:H:177:VAL:CG2	2.24	0.68
1:L:50:PHE:HD2	2:H:102:TYR:HE2	1.45	0.64
1:L:147:LYS:HA	1:L:155:ARG:HG2	1.80	0.64
2:H:2:VAL:HB	2:H:27:TYR:HD2	1.62	0.63
2:H:35:ASN:HD22	2:H:47:TRP:HE1	1.46	0.63
1:L:48:ILE:CG2	1:L:52:SER:HA	2.27	0.62
1:L:155:ARG:HB3	1:L:156:GLN:HG2	1.82	0.62
1:L:52:SER:HB3	1:L:64:GLY:CA	2.29	0.62
1:L:145:ASN:OD1	1:L:147:LYS:HE2	2.01	0.60
1:L:24:ARG:HB3	1:L:24:ARG:NH1	2.18	0.59
1:L:160:LEU:HD13	2:H:177:VAL:HG23	1.85	0.58
1:L:2:ILE:HG21	1:L:29:ILE:HD11	1.86	0.57
1:L:154:GLU:HA	3:L:637:HOH:O	2.05	0.57
1:L:149:LYS:HA	1:L:153:SER:O	2.05	0.56
2:H:53:PRO:HB3	2:H:72:VAL:HG21	1.87	0.56
2:H:35:ASN:ND2	2:H:47:TRP:HE1	2.05	0.55
2:H:13:ARG:HD2	3:H:629:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2:ILE:HD13	1:L:29:ILE:HD11	1.88	0.55
1:L:52:SER:HB3	1:L:64:GLY:C	2.31	0.55
1:L:90:GLN:HE22	1:L:93:ALA:H	1.53	0.54
2:H:8:GLY:HA3	2:H:20:MET:HA	1.90	0.53
1:L:112:ALA:HA	1:L:200:THR:HG21	1.91	0.53
1:L:189:HIS:O	1:L:211:ARG:HD3	2.09	0.53
2:H:172:HIS:O	2:H:187:SER:HA	2.11	0.51
1:L:160:LEU:HD13	2:H:177:VAL:HG21	1.92	0.51
1:L:4:MET:HE3	1:L:23:CYS:SG	2.51	0.51
1:L:148:TRP:H	1:L:155:ARG:HG2	1.76	0.50
2:H:40:ARG:NH2	2:H:89:GLU:HA	2.26	0.50
2:H:62:GLU:O	2:H:63:LYS:HB2	2.11	0.49
1:L:145:ASN:HB3	1:L:197:THR:HB	1.94	0.49
1:L:31:ASN:O	1:L:51:THR:HB	2.13	0.49
1:L:90:GLN:NE2	1:L:92:ASN:H	2.11	0.48
2:H:41:PRO:HD3	2:H:92:ALA:HA	1.96	0.48
1:L:50:PHE:O	1:L:51:THR:HG22	2.13	0.48
1:L:2:ILE:HG21	1:L:29:ILE:CD1	2.44	0.48
2:H:83:LEU:HB3	2:H:86:LEU:HD21	1.97	0.47
2:H:9:VAL:HG12	2:H:12:VAL:HG13	1.95	0.47
2:H:12:VAL:HG11	2:H:18:VAL:CG1	2.44	0.47
2:H:139:GLN:HG2	2:H:140:THR:N	2.28	0.47
1:L:34:ASN:HD22	1:L:49:TYR:HA	1.81	0.46
2:H:62:GLU:HA	2:H:62:GLU:OE1	2.16	0.46
1:L:39:LYS:HG3	1:L:40:PRO:HD2	1.98	0.46
1:L:24:ARG:HA	1:L:69:THR:O	2.15	0.45
2:H:98:ARG:O	2:H:108:PHE:HA	2.16	0.45
1:L:107:LYS:HD2	1:L:140:TYR:OH	2.16	0.45
2:H:33:GLY:HA3	2:H:50:TYR:CE1	2.51	0.45
1:L:52:SER:O	1:L:53:ARG:HB3	2.16	0.45
2:H:140:THR:HG21	2:H:145:THR:OG1	2.17	0.45
1:L:8:PRO:HG3	1:L:11:LEU:HD23	1.99	0.44
1:L:51:THR:O	1:L:52:SER:HB2	2.18	0.44
1:L:212:ASN:HD22	1:L:212:ASN:HA	1.70	0.44
2:H:23:LYS:HG2	2:H:78:THR:HG23	1.99	0.44
1:L:66:GLY:HA3	1:L:71:TYR:HA	2.00	0.43
1:L:117:ILE:CG1	1:L:207:LYS:HB3	2.48	0.43
2:H:179:GLN:HG3	3:H:657:HOH:O	2.16	0.43
1:L:55:GLN:NE2	1:L:59:PRO:O	2.51	0.43
1:L:183:LYS:NZ	1:L:187:GLU:OE1	2.52	0.43
2:H:17:SER:OG	2:H:84:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:50:PHE:CD2	2:H:102:TYR:HE2	2.31	0.43
1:L:207:LYS:HD3	1:L:207:LYS:HA	1.83	0.43
2:H:2:VAL:HB	2:H:27:TYR:CD2	2.48	0.43
1:L:115:VAL:HG12	1:L:207:LYS:HG3	2.00	0.42
1:L:117:ILE:HD12	1:L:117:ILE:O	2.19	0.42
1:L:31:ASN:HB3	1:L:51:THR:CB	2.44	0.42
1:L:10:SER:OG	1:L:103:LYS:HE3	2.20	0.42
1:L:150:ILE:HD11	1:L:179:LEU:HD11	2.02	0.42
2:H:52:ASN:ND2	2:H:55:ASN:HB2	2.35	0.41
1:L:90:GLN:HE21	1:L:92:ASN:H	1.67	0.41
2:H:196:ARG:HE	2:H:196:ARG:HB3	1.54	0.41
2:H:40:ARG:HH11	2:H:40:ARG:HD3	1.75	0.41
2:H:217:LYS:HG2	2:H:218:ILE:N	2.35	0.41
1:L:161:ASN:ND2	1:L:177:SER:OG	2.55	0.40
1:L:167:ASP:CG	1:L:169:LYS:HZ2	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	212/214 (99%)	198 (93%)	11 (5%)	3 (1%)	9	3
2	H	220/222 (99%)	199 (90%)	13 (6%)	8 (4%)	2	0
All	All	432/436 (99%)	397 (92%)	24 (6%)	11 (2%)	4	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	43	GLN
2	H	136	SER
2	H	142	SER

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Mol	Chain	Res	Type
2	H	221	ARG
1	L	200	THR
2	H	63	LYS
2	H	103	GLY
1	L	112	ALA
2	H	57	TYR
1	L	50	PHE
2	H	41	PRO

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	191/191 (100%)	151 (79%)	40 (21%)	1	0
2	H	190/190 (100%)	158 (83%)	32 (17%)	2	0
All	All	381/381 (100%)	309 (81%)	72 (19%)	1	0

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	7	ILE
1	L	9	SER
1	L	10	SER
1	L	11	LEU
1	L	20	SER
1	L	27	GLN
1	L	29	ILE
1	L	30	ASN
1	L	43	THR
1	L	44	ILE
1	L	46	LEU
1	L	47	LEU
1	L	53	ARG
1	L	58	VAL

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Mol	Chain	Res	Type
1	L	74	THR
1	L	81	GLU
1	L	83	ILE
1	L	90	GLN
1	L	97	THR
1	L	103	LYS
1	L	105	GLU
1	L	117	ILE
1	L	143	ASP
1	L	147	LYS
1	L	154	GLU
1	L	155	ARG
1	L	165	ASP
1	L	169	LYS
1	L	179	LEU
1	L	184	ASP
1	L	191	SER
1	L	199	LYS
1	L	200	THR
1	L	203	SER
1	L	205	ILE
1	L	208	SER
1	L	210	ASN
1	L	212	ASN
1	L	214	CYS
2	H	1	GLU
2	H	2	VAL
2	H	4	LEU
2	H	5	GLN
2	H	7	SER
2	H	10	GLU
2	H	11	LEU
2	H	13	ARG
2	H	30	THR
2	H	40	ARG
2	H	41	PRO
2	H	45	LEU
2	H	57	TYR
2	H	61	ASN
2	H	62	GLU
2	H	99	SER
2	H	100	GLU

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Mol	Chain	Res	Type
2	H	115	THR
2	H	140	THR
2	H	144	VAL
2	H	149	LEU
2	H	151	LYS
2	H	157	PRO
2	H	161	THR
2	H	168	SER
2	H	191	VAL
2	H	194	SER
2	H	195	PRO
2	H	196	ARG
2	H	205	VAL
2	H	213	LYS
2	H	221	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	31	ASN
1	L	34	ASN
1	L	90	GLN
1	L	161	ASN
1	L	212	ASN
2	H	43	GLN
2	H	61	ASN

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

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.