



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:05 AM UTC

PDB ID : 8FAB / pdb_00008fab
Title : CRYSTAL STRUCTURE OF THE FAB FRAGMENT FROM THE HUMAN MYELOMA IMMUNOGLOBULIN IGG HIL AT 1.8 ANGSTROMS RESOLUTION
Authors : Saul, F.A.; Poljak, R.J.
Deposited on : 1992-03-23
Resolution : 1.80 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

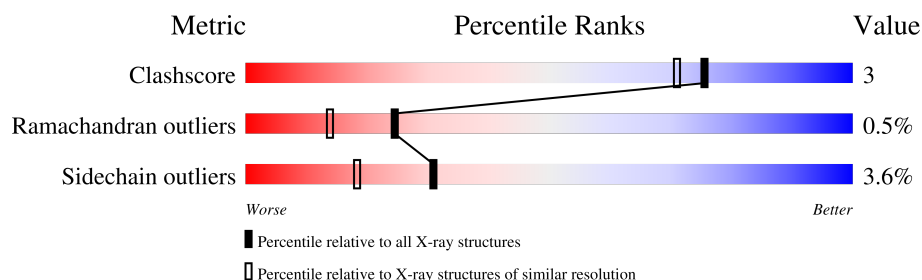
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	212	 83% 13% . .
1	C	212	 83% 12% . .
2	B	224	 77% 17% . .
2	D	224	 81% 16% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7073 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-LAMBDA HIL FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1544	966	259	314	5			
1	C	206	Total	C	N	O	S	0	0	0
			1544	966	259	314	5			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ARG	SER	conflict	PIR S25738
A	24	ALA	GLY	conflict	PIR S25738
A	25	ASN	ASP	conflict	PIR S25738
A	26	ALA	THR	conflict	PIR S25738
A	28	PRO	GLY	conflict	PIR S25738
A	29	ASN	ASP	conflict	PIR S25738
A	30	GLN	LYS	conflict	PIR S25738
A	33	TYR	CYS	conflict	PIR S25738
A	41	ARG	HIS	conflict	PIR S25738
A	42	ALA	SER	conflict	PIR S25738
A	45	MET	LEU	conflict	PIR S25738
A	48	TYR	PHE	conflict	PIR S25738
A	49	LYS	GLN	conflict	PIR S25738
A	51	THR	SER	conflict	PIR S25738
A	52	GLN	LYS	conflict	PIR S25738
A	59	GLN	GLU	conflict	PIR S25738
A	63	SER	GLY	conflict	PIR S25738
A	65	THR	ASN	conflict	PIR S25738
A	68	THR	ASN	conflict	PIR S25738
A	70	VAL	ALA	conflict	PIR S25738
A	77	VAL	THR	conflict	PIR S25738
A	80	GLU	MET	conflict	PIR S25738
A	92	ASN	SER	conflict	PIR S25738
A	94	ALA	THR	conflict	PIR S25738
A	95	SER	ALA	conflict	PIR S25738

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Chain	Residue	Modelled	Actual	Comment	Reference
A	96	ILE	VAL	conflict	PIR S25738
A	155	ILE	VAL	conflict	PIR S25738
C	19	ARG	SER	conflict	PIR S25738
C	24	ALA	GLY	conflict	PIR S25738
C	25	ASN	ASP	conflict	PIR S25738
C	26	ALA	THR	conflict	PIR S25738
C	28	PRO	GLY	conflict	PIR S25738
C	29	ASN	ASP	conflict	PIR S25738
C	30	GLN	LYS	conflict	PIR S25738
C	33	TYR	CYS	conflict	PIR S25738
C	41	ARG	HIS	conflict	PIR S25738
C	42	ALA	SER	conflict	PIR S25738
C	45	MET	LEU	conflict	PIR S25738
C	48	TYR	PHE	conflict	PIR S25738
C	49	LYS	GLN	conflict	PIR S25738
C	51	THR	SER	conflict	PIR S25738
C	52	GLN	LYS	conflict	PIR S25738
C	59	GLN	GLU	conflict	PIR S25738
C	63	SER	GLY	conflict	PIR S25738
C	65	THR	ASN	conflict	PIR S25738
C	68	THR	ASN	conflict	PIR S25738
C	70	VAL	ALA	conflict	PIR S25738
C	77	VAL	THR	conflict	PIR S25738
C	80	GLU	MET	conflict	PIR S25738
C	92	ASN	SER	conflict	PIR S25738
C	94	ALA	THR	conflict	PIR S25738
C	95	SER	ALA	conflict	PIR S25738
C	96	ILE	VAL	conflict	PIR S25738
C	155	ILE	VAL	conflict	PIR S25738

- Molecule 2 is a protein called IGG1-LAMBDA HIL FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	1
			1635	1042	279	307	7			
2	D	222	Total	C	N	O	S	0	0	0
			1682	1068	287	320	7			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	LYS	GLN	conflict	EMBL Y14737

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	GLN	GLU	conflict	EMBL Y14737
B	7	ALA	SER	conflict	EMBL Y14737
B	23	ILE	ALA	conflict	EMBL Y14737
B	50	VAL	ALA	conflict	EMBL Y14737
B	54	ASN	ASP	conflict	EMBL Y14737
B	57	ARG	ASN	conflict	EMBL Y14737
B	58	THR	LYS	conflict	EMBL Y14737
B	61	GLY	ALA	conflict	EMBL Y14737
B	77	ARG	ASN	conflict	EMBL Y14737
B	88	THR	ALA	conflict	EMBL Y14737
B	?	-	ARG	deletion	EMBL Y14737
B	?	-	GLU	deletion	EMBL Y14737
B	?	-	GLY	deletion	EMBL Y14737
B	?	-	ARG	deletion	EMBL Y14737
B	?	-	TRP	deletion	EMBL Y14737
B	?	-	VAL	deletion	EMBL Y14737
B	99	ASP	TYR	conflict	EMBL Y14737
B	100	PRO	THR	conflict	EMBL Y14737
B	101	ASP	THR	conflict	EMBL Y14737
B	102	ILE	VAL	conflict	EMBL Y14737
B	103	LEU	THR	conflict	EMBL Y14737
B	?	-	ILE	deletion	EMBL Y14737
B	105	ALA	GLY	conflict	EMBL Y14737
B	106	PHE	TYR	conflict	EMBL Y14737
B	107	SER	TYR	conflict	EMBL Y14737
B	115	VAL	THR	conflict	EMBL Y14737
B	218	LYS	ARG	conflict	EMBL Y14737
D	3	LYS	GLN	conflict	EMBL Y14737
D	6	GLN	GLU	conflict	EMBL Y14737
D	7	ALA	SER	conflict	EMBL Y14737
D	23	ILE	ALA	conflict	EMBL Y14737
D	50	VAL	ALA	conflict	EMBL Y14737
D	54	ASN	ASP	conflict	EMBL Y14737
D	57	ARG	ASN	conflict	EMBL Y14737
D	58	THR	LYS	conflict	EMBL Y14737
D	61	GLY	ALA	conflict	EMBL Y14737
D	77	ARG	ASN	conflict	EMBL Y14737
D	88	THR	ALA	conflict	EMBL Y14737
D	?	-	ARG	deletion	EMBL Y14737
D	?	-	GLU	deletion	EMBL Y14737
D	?	-	GLY	deletion	EMBL Y14737
D	?	-	ARG	deletion	EMBL Y14737

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	TRP	deletion	EMBL Y14737
D	?	-	VAL	deletion	EMBL Y14737
D	99	ASP	TYR	conflict	EMBL Y14737
D	100	PRO	THR	conflict	EMBL Y14737
D	101	ASP	THR	conflict	EMBL Y14737
D	102	ILE	VAL	conflict	EMBL Y14737
D	103	LEU	THR	conflict	EMBL Y14737
D	?	-	ILE	deletion	EMBL Y14737
D	105	ALA	GLY	conflict	EMBL Y14737
D	106	PHE	TYR	conflict	EMBL Y14737
D	107	SER	TYR	conflict	EMBL Y14737
D	115	VAL	THR	conflict	EMBL Y14737
D	218	LYS	ARG	conflict	EMBL Y14737

- Molecule 3 is water.

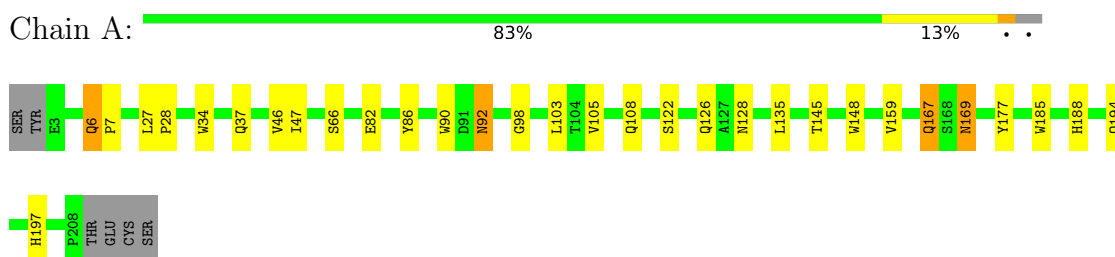
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	177	Total O 177 177	0	0
3	B	155	Total O 155 155	0	0
3	C	187	Total O 187 187	0	0
3	D	149	Total O 149 149	0	0

3 Residue-property plots [i](#)

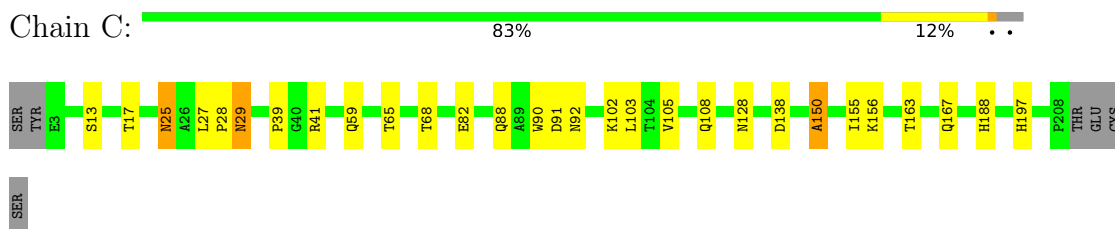
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

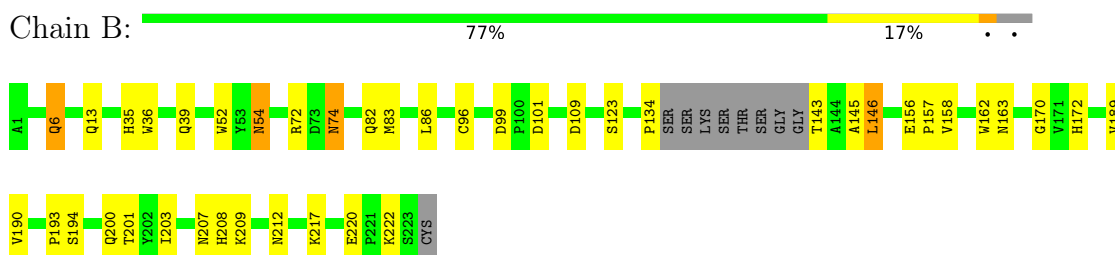
- Molecule 1: IGG1-LAMBDA HIL FAB (LIGHT CHAIN)



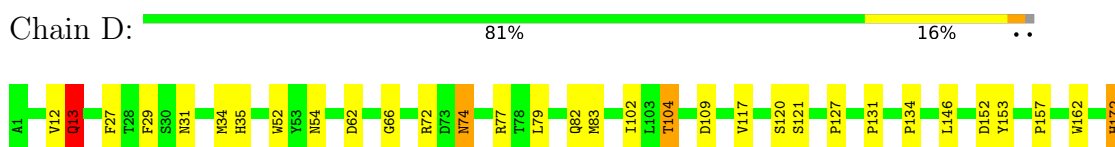
- Molecule 1: IGG1-LAMBDA HIL FAB (LIGHT CHAIN)



- Molecule 2: IGG1-LAMBDA HIL FAB (HEAVY CHAIN)



- Molecule 2: IGG1-LAMBDA HIL 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.60Å 127.42Å 66.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7073	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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	0.87	3/1582 (0.2%)	1.66	23/2164 (1.1%)
1	C	0.85	2/1582 (0.1%)	1.63	16/2164 (0.7%)
2	B	0.93	4/1677 (0.2%)	1.64	26/2285 (1.1%)
2	D	0.92	3/1725 (0.2%)	1.65	21/2349 (0.9%)
All	All	0.89	12/6566 (0.2%)	1.64	86/8962 (1.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	35	HIS	CD2-NE2	-7.10	1.30	1.37
1	A	197	HIS	CD2-NE2	-6.52	1.30	1.37
2	B	222	LYS	C-N	-6.49	1.24	1.33
2	B	35	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	188	HIS	CD2-NE2	-6.11	1.31	1.37
1	C	188	HIS	CD2-NE2	-5.97	1.31	1.37
2	B	172	HIS	CD2-NE2	-5.88	1.31	1.37
1	C	197	HIS	CD2-NE2	-5.71	1.31	1.37
2	B	208	HIS	CD2-NE2	-5.70	1.31	1.37
2	D	172	HIS	CD2-NE2	-5.70	1.31	1.37
2	D	208	HIS	CD2-NE2	-5.24	1.32	1.37
1	A	46	VAL	CA-CB	5.11	1.60	1.54

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	29	ASN	CA-CB-CG	9.07	121.67	112.60
1	A	6	GLN	OE1-CD-NE2	-8.78	113.82	122.60
1	A	167	GLN	OE1-CD-NE2	-8.62	113.98	122.60
2	D	172	HIS	CB-CG-CD2	-7.96	120.85	131.20
2	D	74	ASN	OD1-CG-ND2	-7.53	115.07	122.60
2	D	212	ASN	CA-CB-CG	7.41	120.00	112.60
2	B	54	ASN	OD1-CG-ND2	-7.25	115.36	122.60
1	C	167	GLN	OE1-CD-NE2	-7.21	115.39	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	172	HIS	CB-CG-ND1	7.01	133.22	122.70
1	A	197	HIS	CB-CG-CD2	-6.93	122.19	131.20
2	B	200	GLN	N-CA-C	6.92	120.25	109.52
1	A	7	PRO	O-C-N	-6.91	117.90	121.15
2	B	109	ASP	CA-CB-CG	6.90	119.50	112.60
2	D	82	GLN	OE1-CD-NE2	-6.76	115.84	122.60
1	C	25	ASN	CA-CB-CG	-6.74	105.86	112.60
2	B	74	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	A	92	ASN	CA-CB-CG	6.67	119.27	112.60
2	B	101	ASP	CA-CB-CG	6.49	119.09	112.60
2	B	36	TRP	CG-CD2-CE3	6.21	140.11	133.90
2	D	197	LEU	N-CA-C	6.17	119.65	111.75
1	A	108	GLN	OE1-CD-NE2	-6.16	116.44	122.60
2	D	31	ASN	OD1-CG-ND2	-6.16	116.44	122.60
2	D	54	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	C	91	ASP	CA-CB-CG	5.97	118.57	112.60
2	B	220	GLU	CA-C-N	5.97	125.99	119.90
2	B	220	GLU	C-N-CA	5.97	125.99	119.90
1	C	41	ARG	N-CA-C	5.95	119.64	110.42
2	D	35	HIS	CB-CG-CD2	-5.95	123.47	131.20
1	C	17	THR	CA-CB-OG1	-5.93	100.71	109.60
1	C	92	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	188	HIS	CB-CG-CD2	-5.92	123.50	131.20
1	A	167	GLN	N-CA-C	-5.88	101.28	110.17
2	D	35	HIS	CA-CB-CG	5.84	119.64	113.80
1	A	105	VAL	N-CA-C	-5.83	98.82	107.51
2	B	13	GLN	CA-C-N	5.79	125.80	119.89
2	B	13	GLN	C-N-CA	5.79	125.80	119.89
2	D	109	ASP	CA-CB-CG	5.78	118.38	112.60
2	B	54	ASN	CB-CG-ND2	5.77	125.05	116.40
2	B	52	TRP	CG-CD2-CE3	5.76	139.66	133.90
1	A	197	HIS	CB-CG-ND1	5.73	131.30	122.70
1	C	128	ASN	CA-CB-CG	-5.73	106.87	112.60
2	B	207	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	C	197	HIS	CB-CG-CD2	-5.67	123.83	131.20
2	D	13	GLN	OE1-CD-NE2	-5.67	116.94	122.60
1	A	92	ASN	N-CA-C	5.64	122.81	110.80
1	A	128	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	C	188	HIS	CB-CG-CD2	-5.63	123.88	131.20
2	B	52	TRP	CB-CG-CD1	-5.63	118.45	126.90
1	A	126	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	C	150	ALA	N-CA-C	-5.56	98.29	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	99	ASP	CA-C-N	5.56	124.91	118.85
2	B	99	ASP	C-N-CA	5.56	124.91	118.85
1	C	108	GLN	N-CA-C	-5.55	103.13	108.07
2	D	174	PHE	CA-C-N	5.52	125.53	119.90
2	D	174	PHE	C-N-CA	5.52	125.53	119.90
1	A	185	TRP	CG-CD2-CE3	5.51	139.41	133.90
1	A	6	GLN	CA-C-N	5.51	123.62	119.66
1	A	6	GLN	C-N-CA	5.51	123.62	119.66
2	B	6	GLN	OE1-CD-NE2	-5.47	117.13	122.60
2	D	66	GLY	N-CA-C	-5.43	108.61	115.08
2	D	152	ASP	N-CA-C	5.43	118.61	111.28
1	C	105	VAL	N-CA-C	-5.32	99.58	107.51
2	B	156	GLU	CB-CG-CD	5.32	121.64	112.60
1	C	88	GLN	OE1-CD-NE2	-5.32	117.28	122.60
2	D	62	ASP	N-CA-C	5.28	117.78	111.71
2	D	27	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	148	TRP	CE2-CD2-CG	-5.24	100.91	107.20
1	A	194	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	A	27	LEU	CA-C-N	5.22	125.53	119.47
1	A	27	LEU	C-N-CA	5.22	125.53	119.47
2	B	162	TRP	CG-CD2-CE3	5.21	139.12	133.90
2	B	123	SER	N-CA-C	-5.21	102.75	110.46
1	A	185	TRP	CB-CG-CD1	-5.17	119.15	126.90
1	C	163	THR	CA-CB-OG1	-5.16	101.86	109.60
1	C	138	ASP	N-CA-C	5.15	118.69	111.74
2	B	35	HIS	CB-CG-CD2	-5.13	124.53	131.20
2	B	145	ALA	N-CA-C	-5.11	101.07	109.40
2	D	162	TRP	CE2-CD2-CG	-5.11	101.07	107.20
2	B	172	HIS	CB-CG-CD2	-5.10	124.57	131.20
2	D	52	TRP	CE2-CD2-CG	-5.09	101.09	107.20
2	B	36	TRP	CE2-CD2-CG	-5.08	101.10	107.20
2	B	212	ASN	OD1-CG-ND2	-5.08	117.52	122.60
2	D	102	ILE	CA-CB-CG2	-5.06	101.90	110.50
2	B	52	TRP	CG-CD1-NE1	-5.06	103.63	110.20
1	A	145	THR	N-CA-C	-5.03	100.70	108.90
1	A	169	ASN	OD1-CG-ND2	-5.03	117.57	122.60

There are no chirality outliers.

There are no planarity outliers.

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	A	1544	0	1499	8	0
1	C	1544	0	1499	5	0
2	B	1635	0	1613	14	0
2	D	1682	0	1660	13	0
3	A	177	0	0	0	0
3	B	155	0	0	1	0
3	C	187	0	0	3	0
3	D	149	0	0	2	0
All	All	7073	0	6271	38	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 3.

All (38) 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:B:6:GLN:HE21	2:B:96:CYS:H	1.31	0.79
1:A:135:LEU:HD13	2:B:189:VAL:HG21	1.69	0.74
1:C:150:ALA:HB2	1:C:155:ILE:HD11	1.74	0.70
2:B:72:ARG:HE	2:B:74:ASN:HD21	1.40	0.68
1:C:59:GLN:HG2	3:C:216:HOH:O	1.94	0.65
1:A:37:GLN:HE22	2:B:39:GLN:HE22	1.45	0.64
2:B:170:GLY:O	2:B:190:VAL:HA	2.02	0.59
2:D:72:ARG:HE	2:D:74:ASN:HD21	1.53	0.57
2:B:6:GLN:HE21	2:B:96:CYS:N	2.01	0.56
2:B:72:ARG:HE	2:B:74:ASN:ND2	2.03	0.55
1:A:167:GLN:HB2	1:A:169:ASN:OD1	2.07	0.54
1:A:82:GLU:HG3	1:A:103:LEU:O	2.08	0.53
2:B:6:GLN:NE2	2:B:96:CYS:H	2.03	0.53
2:D:131:PRO:HD3	2:D:217:LYS:HD2	1.90	0.53
2:D:191:THR:HG21	3:D:258:HOH:O	2.10	0.51
1:C:82:GLU:HG3	1:C:103:LEU:O	2.10	0.50
2:D:83:MET:HE1	2:D:117:VAL:HG21	1.95	0.48
3:C:377:HOH:O	2:D:172:HIS:HE1	1.96	0.47
2:D:72:ARG:HE	2:D:74:ASN:ND2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:ILE:HA	2:B:217:LYS:O	2.15	0.46
1:C:39:PRO:HD3	3:C:304:HOH:O	2.16	0.46
2:D:34:MET:HB3	2:D:79:LEU:HD22	1.99	0.45
2:B:72:ARG:NE	2:B:74:ASN:HD21	2.11	0.45
2:D:127:PRO:HB3	2:D:153:TYR:HB3	1.99	0.45
2:D:13:GLN:HA	2:D:120:SER:O	2.17	0.44
2:D:134:PRO:HD3	2:D:146:LEU:HD23	1.99	0.44
1:A:6:GLN:HE22	1:A:86:TYR:HA	1.83	0.44
2:B:143:THR:N	3:B:302:HOH:O	2.51	0.43
1:A:34:TRP:HB2	1:A:47:ILE:HB	2.00	0.43
2:B:163:ASN:HA	2:B:203:ILE:HG13	1.99	0.43
2:B:83:MET:HE2	2:B:86:LEU:HD21	2.01	0.42
1:A:6:GLN:HE21	1:A:98:GLY:HA3	1.84	0.42
2:B:134:PRO:HD3	2:B:146:LEU:HB3	2.00	0.42
2:D:72:ARG:NE	2:D:74:ASN:HD21	2.18	0.41
1:C:27:LEU:N	1:C:28:PRO:HD2	2.36	0.41
2:D:209:LYS:HB2	3:D:299:HOH:O	2.21	0.41
2:D:29:PHE:CD2	2:D:77:ARG:HA	2.56	0.41
1:A:159:VAL:HA	1:A:177:TYR:O	2.21	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	A	204/212 (96%)	194 (95%)	8 (4%)	2 (1%)	12	4
1	C	204/212 (96%)	195 (96%)	8 (4%)	1 (0%)	24	14
2	B	211/224 (94%)	207 (98%)	4 (2%)	0	100	100
2	D	220/224 (98%)	212 (96%)	7 (3%)	1 (0%)	24	14
All	All	839/872 (96%)	808 (96%)	27 (3%)	4 (0%)	24	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	TRP
1	C	90	TRP
1	A	92	ASN
2	D	104	THR

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	173/180 (96%)	170 (98%)	3 (2%)	53	45
1	C	173/180 (96%)	166 (96%)	7 (4%)	28	15
2	B	181/189 (96%)	172 (95%)	9 (5%)	22	10
2	D	187/189 (99%)	180 (96%)	7 (4%)	30	18
All	All	714/738 (97%)	688 (96%)	26 (4%)	31	18

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PRO
1	A	66	SER
1	A	122	SER
2	B	54	ASN
2	B	82	GLN
2	B	146	LEU
2	B	157	PRO
2	B	158	VAL
2	B	193	PRO
2	B	194	SER
2	B	201	THR
2	B	209	LYS
1	C	13	SER
1	C	25	ASN
1	C	29	ASN
1	C	65	THR

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Mol	Chain	Res	Type
1	C	68	THR
1	C	102	LYS
1	C	156	LYS
2	D	12	VAL
2	D	13	GLN
2	D	104	THR
2	D	121	SER
2	D	157	PRO
2	D	197	LEU
2	D	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	30	GLN
1	A	52	GLN
1	A	78	GLN
1	A	126	GLN
2	B	39	GLN
2	B	54	ASN
2	B	74	ASN
2	B	179	GLN
1	C	29	ASN
1	C	37	GLN
1	C	78	GLN
1	C	88	GLN
1	C	126	GLN
1	C	194	GLN
2	D	31	ASN
2	D	39	GLN
2	D	74	ASN
2	D	207	ASN

5.3.3 RNA ⓘ

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.