



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:22 PM UTC

PDB ID : 1HIL / pdb_00001hil
Title : STRUCTURAL EVIDENCE FOR INDUCED FIT AS A MECHANISM FOR
ANTIGEN-ANTIBODY RECOGNITION
Authors : Rini, J.M.; Wilson, I.A.
Deposited on : 1992-07-08
Resolution : 2.00 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

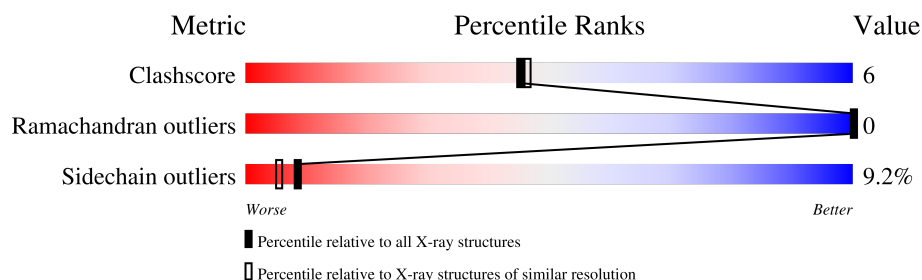
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	217	77% 16% 6%
1	C	217	71% 24% 5%
2	B	220	79% 18% .
2	D	220	75% 18% . . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6765 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	A	217	Total	C	N	O	S	0	0	0
			1680	1047	279	347	7			
1	C	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	B	214	Total	C	N	O	S	0	0	0
			1628	1028	270	323	7			
2	D	214	Total	C	N	O	S	0	0	1
			1617	1022	267	321	7			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is water.

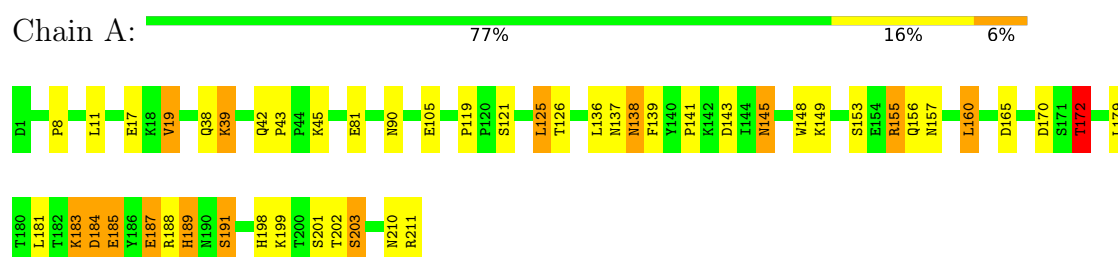
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	42	Total	O	0	0
			42	42		
3	C	39	Total	O	0	0
			39	39		
3	D	41	Total	O	0	0
			41	41		

3 Residue-property plots [i](#)

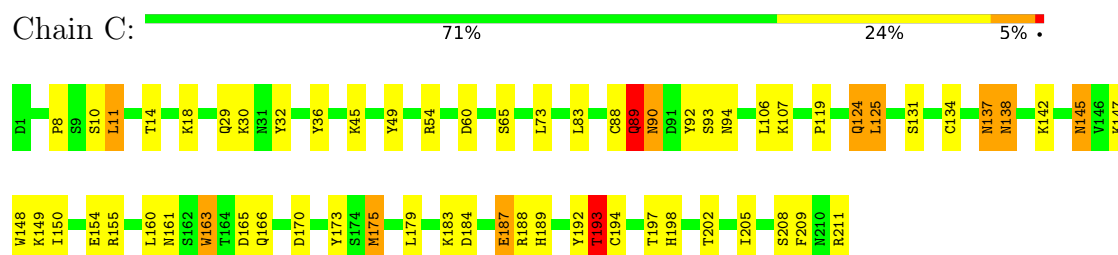
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

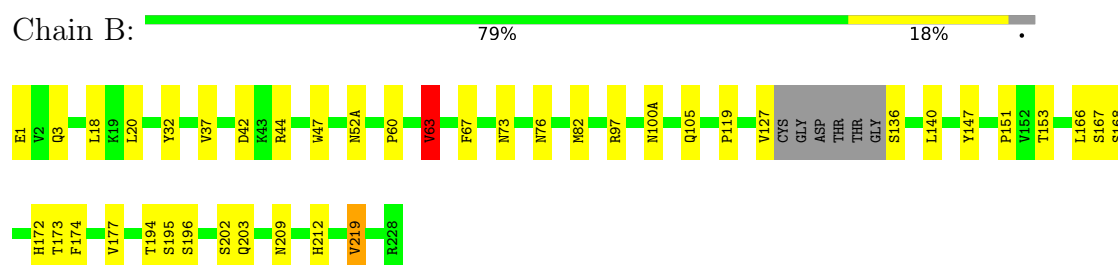
• Molecule 1: IGG2A-KAPPA 17/9 FAB (LIGHT CHAIN)



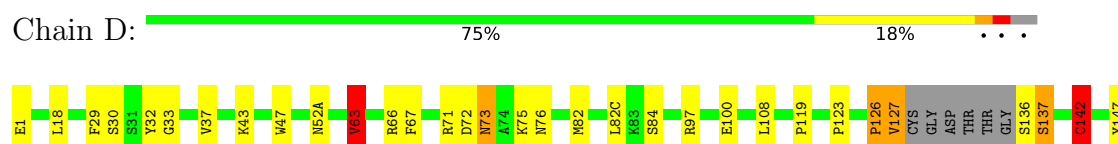
• Molecule 1: IGG2A-KAPPA 17/9 FAB (LIGHT CHAIN)



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



• Molecule 2: IGG2A-KAPPA 17/9 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	90.04Å 82.80Å 73.40Å 90.00° 122.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6765	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.00	4/1718 (0.2%)	1.65	26/2334 (1.1%)
1	C	0.99	5/1718 (0.3%)	1.70	30/2334 (1.3%)
2	B	0.99	1/1668 (0.1%)	1.68	25/2270 (1.1%)
2	D	1.03	7/1657 (0.4%)	1.65	23/2258 (1.0%)
All	All	1.01	17/6761 (0.3%)	1.67	104/9196 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	VAL	CA-CB	7.75	1.65	1.54
2	D	126	PRO	C-N	-6.60	1.24	1.33
2	B	172	HIS	CD2-NE2	-6.31	1.30	1.37
2	D	212	HIS	CG-ND1	-6.29	1.31	1.38
2	D	227	PRO	C-N	-6.25	1.24	1.33
1	C	198	HIS	CD2-NE2	-6.21	1.31	1.37
2	D	172	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	198	HIS	CD2-NE2	-5.96	1.31	1.37
2	D	212	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	189	HIS	CD2-NE2	-5.87	1.31	1.37
1	C	189	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	198	HIS	CG-ND1	-5.48	1.32	1.38
2	D	123	PRO	CA-CB	-5.27	1.47	1.53
1	C	88	CYS	CA-CB	-5.24	1.45	1.53
1	C	189	HIS	CG-ND1	-5.24	1.32	1.38
1	C	193	THR	CA-CB	5.09	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	172	HIS	CG-ND1	-5.05	1.32	1.38

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	29	GLN	OE1-CD-NE2	-11.41	111.19	122.60
1	C	165	ASP	CA-CB-CG	10.46	123.06	112.60
2	B	63	VAL	N-CA-CB	-10.28	98.17	112.35
1	C	145	ASN	CA-CB-CG	10.27	122.87	112.60
1	A	145	ASN	CA-CB-CG	9.49	122.09	112.60
1	A	184	ASP	CA-CB-CG	9.38	121.97	112.60
2	B	105	GLN	OE1-CD-NE2	-9.18	113.42	122.60
2	D	156	THR	N-CA-CB	-9.10	95.86	111.69
1	A	198	HIS	ND1-CG-CD2	8.38	114.48	106.10
1	C	124	GLN	OE1-CD-NE2	-8.27	114.33	122.60
2	B	172	HIS	ND1-CG-CD2	8.20	114.30	106.10
1	C	30	LYS	CB-CG-CD	-8.06	92.77	111.30
2	B	105	GLN	CG-CD-NE2	7.82	128.14	116.40
1	C	29	GLN	CG-CD-NE2	7.75	128.03	116.40
1	A	145	ASN	OD1-CG-ND2	-7.70	114.90	122.60
2	B	1	GLU	CB-CG-CD	7.63	125.56	112.60
2	D	73	ASN	OD1-CG-ND2	-7.59	115.01	122.60
1	C	60	ASP	CA-CB-CG	7.47	120.07	112.60
2	D	137	SER	N-CA-C	7.43	120.03	108.96
2	D	63	VAL	N-CA-CB	-7.36	99.08	111.23
1	C	138	ASN	OD1-CG-ND2	-7.29	115.31	122.60
2	D	72	ASP	CA-CB-CG	7.28	119.88	112.60
1	C	189	HIS	ND1-CG-CD2	7.22	113.32	106.10
1	C	198	HIS	ND1-CG-CD2	7.08	113.19	106.10
2	B	203	GLN	OE1-CD-NE2	-7.08	115.52	122.60
1	A	187	GLU	CA-CB-CG	-6.94	100.22	114.10
1	C	187	GLU	CA-CB-CG	-6.87	100.36	114.10
2	D	33	GLY	N-CA-C	-6.82	103.41	112.82
2	B	63	VAL	CB-CA-C	6.78	118.27	110.88
1	A	185	GLU	CB-CG-CD	6.67	123.94	112.60
2	D	212	HIS	ND1-CG-CD2	6.62	112.72	106.10
1	A	153	SER	CA-CB-OG	6.61	124.33	111.10
1	A	172	THR	N-CA-CB	-6.61	100.22	110.46
1	C	90	ASN	OD1-CG-ND2	-6.60	116.00	122.60
2	D	226	GLU	CB-CG-CD	6.60	123.82	112.60
1	A	198	HIS	CG-CD2-NE2	-6.55	100.65	107.20
1	C	89	GLN	OE1-CD-NE2	-6.51	116.08	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	173	THR	CA-CB-OG1	-6.49	99.86	109.60
2	D	162	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	165	ASP	CA-CB-CG	6.30	118.90	112.60
1	C	137	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	C	145	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	C	170	ASP	CA-CB-CG	6.18	118.78	112.60
1	C	163	TRP	CG-CD2-CE3	6.09	139.99	133.90
2	D	73	ASN	CB-CG-ND2	6.09	125.54	116.40
2	B	42	ASP	CA-CB-CG	6.09	118.69	112.60
2	D	142	CYS	CA-CB-SG	-6.07	100.44	114.40
1	C	198	HIS	CG-CD2-NE2	-5.92	101.28	107.20
2	D	75	LYS	CA-CB-CG	-5.90	102.29	114.10
2	D	198	THR	CA-CB-OG1	-5.89	100.76	109.60
1	A	17	GLU	CA-CB-CG	5.87	125.84	114.10
1	C	94	ASN	OD1-CG-ND2	-5.82	116.78	122.60
2	D	198	THR	N-CA-C	5.82	117.42	111.14
2	B	76	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	A	183	LYS	CA-C-N	5.79	128.84	120.79
1	A	183	LYS	C-N-CA	5.79	128.84	120.79
1	C	163	TRP	CB-CG-CD1	-5.77	118.25	126.90
2	B	203	GLN	CA-CB-CG	5.75	125.61	114.10
2	D	127	VAL	N-CA-C	-5.75	94.89	111.00
2	D	162	ASN	CB-CG-ND2	5.74	125.01	116.40
1	A	170	ASP	CA-CB-CG	5.72	118.32	112.60
2	B	172	HIS	CG-CD2-NE2	-5.67	101.53	107.20
2	D	126	PRO	O-C-N	-5.66	115.00	122.64
2	B	212	HIS	ND1-CG-CD2	5.64	111.74	106.10
2	B	52(A)	ASN	CA-CB-CG	5.57	118.17	112.60
2	D	212	HIS	CA-C-N	5.46	124.92	119.24
2	D	212	HIS	C-N-CA	5.46	124.92	119.24
2	B	100(A)	ASN	CB-CA-C	-5.43	110.33	116.63
1	C	163	TRP	CE2-CD2-CG	-5.40	100.72	107.20
2	B	209	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	C	189	HIS	CG-CD2-NE2	-5.38	101.82	107.20
1	A	139	PHE	CA-CB-CG	5.38	119.17	113.80
1	C	148	TRP	CG-CD1-NE1	-5.38	103.21	110.20
2	B	37	VAL	O-C-N	-5.36	117.36	123.10
1	C	161	ASN	OD1-CG-ND2	-5.34	117.26	122.60
2	B	47	TRP	CG-CD1-NE1	-5.33	103.27	110.20
1	C	198	HIS	CB-CG-CD2	-5.26	124.37	131.20
1	A	148	TRP	CG-CD1-NE1	-5.25	103.38	110.20
1	A	38	GLN	CG-CD-NE2	5.23	124.25	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	148	TRP	CE2-CD2-CG	-5.20	100.96	107.20
2	B	73	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	C	124	GLN	CG-CD-NE2	5.14	124.11	116.40
2	B	174	PHE	CA-CB-CG	-5.13	108.67	113.80
2	D	37	VAL	O-C-N	-5.12	117.62	123.10
1	A	203	SER	CA-C-N	5.11	125.11	119.90
1	A	203	SER	C-N-CA	5.11	125.11	119.90
2	D	47	TRP	CG-CD1-NE1	-5.11	103.56	110.20
2	B	140	LEU	CD1-CG-CD2	-5.10	99.58	110.80
1	A	119	PRO	CA-C-N	5.10	125.10	119.90
1	A	119	PRO	C-N-CA	5.10	125.10	119.90
2	B	219	VAL	CB-CA-C	-5.10	102.89	110.33
1	C	54	ARG	CB-CG-CD	-5.08	99.62	111.30
1	C	10	SER	CA-C-O	-5.08	115.17	121.06
1	A	126	THR	N-CA-CB	-5.07	102.41	110.22
2	B	60	PRO	N-CA-C	-5.07	103.86	111.57
1	A	153	SER	N-CA-CB	-5.06	102.17	110.52
1	A	138	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	39	LYS	N-CA-CB	-5.03	103.91	109.74
2	B	44	ARG	CB-CG-CD	-5.02	99.75	111.30
2	D	174	PHE	CA-C-N	5.02	125.02	119.90
2	D	174	PHE	C-N-CA	5.02	125.02	119.90
1	C	30	LYS	CA-CB-CG	5.01	124.12	114.10
1	A	198	HIS	CB-CG-CD2	-5.01	124.69	131.20
2	B	3	GLN	OE1-CD-NE2	-5.00	117.60	122.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	126	PRO	Peptide,Mainchain

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	1680	0	1614	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1680	0	1616	25	0
2	B	1628	0	1590	7	0
2	D	1617	0	1577	25	0
3	A	38	0	0	1	0
3	B	42	0	0	0	0
3	C	39	0	0	2	0
3	D	41	0	0	0	0
All	All	6765	0	6397	70	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 6.

All (70) 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:D:142:CYS:HG	2:D:208:CYS:HG	0.89	0.84
2:D:163:SER:H	2:D:209:ASN:HD21	1.33	0.77
2:D:142:CYS:HG	2:D:208:CYS:CB	1.99	0.75
2:D:142:CYS:SG	2:D:208:CYS:CB	2.79	0.70
1:C:106:LEU:H	1:C:166:GLN:HE22	1.40	0.69
2:D:163:SER:H	2:D:209:ASN:ND2	1.91	0.68
1:C:8:PRO:HG3	1:C:11:LEU:HG	1.76	0.68
1:A:138:ASN:HA	1:A:172:THR:HG23	1.77	0.66
1:C:125:LEU:HD12	1:C:183:LYS:HG3	1.78	0.65
2:D:32:TYR:CE2	2:D:97:ARG:HG3	2.32	0.64
2:D:30:SER:O	2:D:52(A):ASN:HB2	1.99	0.62
2:D:119:PRO:HB3	2:D:147:TYR:HB3	1.82	0.62
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.81	0.62
1:A:43:PRO:HD2	1:A:45:LYS:NZ	2.15	0.61
1:A:42:GLN:HG3	3:A:216:HOH:O	2.02	0.60
2:D:82:MET:HE2	2:D:82(C):LEU:HD21	1.85	0.59
1:A:125:LEU:HD12	1:A:183:LYS:HG3	1.86	0.58
2:D:142:CYS:CB	2:D:208:CYS:HG	2.16	0.56
1:A:138:ASN:HA	1:A:172:THR:CG2	2.33	0.56
1:A:43:PRO:HD2	1:A:45:LYS:HZ1	1.70	0.56
1:C:150:ILE:HD11	1:C:179:LEU:HD21	1.86	0.56
1:C:187:GLU:HA	1:C:211:ARG:NH2	2.21	0.55
1:C:184:ASP:HB3	1:C:188:ARG:NH2	2.22	0.55
3:C:237:HOH:O	2:D:43:LYS:HD2	2.06	0.54
1:C:32:TYR:HB2	1:C:92:TYR:HB2	1.90	0.54
2:D:156:THR:HG22	2:D:209:ASN:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:TRP:CD1	1:C:175:MET:HG3	2.42	0.53
2:B:20:LEU:HG	2:B:82:MET:HE2	1.91	0.53
2:D:71:ARG:HE	2:D:73:ASN:HD21	1.55	0.53
1:C:8:PRO:CG	1:C:11:LEU:HG	2.39	0.53
1:C:184:ASP:HB3	1:C:188:ARG:HH22	1.73	0.52
2:B:18:LEU:HB3	2:B:82:MET:HE3	1.93	0.51
1:A:137:ASN:HB3	1:A:138:ASN:HD22	1.76	0.51
1:C:124:GLN:NE2	3:C:219:HOH:O	2.41	0.51
2:D:63:VAL:HG13	2:D:67:PHE:HB2	1.93	0.51
1:C:149:LYS:HB2	1:C:193:THR:HG23	1.93	0.49
2:D:71:ARG:NE	2:D:73:ASN:HD21	2.12	0.48
2:D:156:THR:HG22	2:D:209:ASN:HD22	1.77	0.48
1:A:141:PRO:HG2	1:A:199:LYS:HD3	1.95	0.48
1:C:137:ASN:HB3	1:C:138:ASN:HD22	1.79	0.48
2:B:63:VAL:HG13	2:B:67:PHE:HB2	1.96	0.47
2:D:71:ARG:HE	2:D:73:ASN:ND2	2.12	0.47
2:D:142:CYS:CB	2:D:208:CYS:SG	3.02	0.47
2:B:194:THR:HG22	2:B:196:SER:H	1.80	0.46
1:A:8:PRO:HG3	1:A:11:LEU:HD13	1.97	0.46
1:A:191:SER:OG	1:A:210:ASN:ND2	2.49	0.46
1:C:124:GLN:NE2	1:C:131:SER:H	2.15	0.45
1:C:49:TYR:CD2	2:D:100:GLU:HG3	2.52	0.45
1:C:149:LYS:HA	1:C:154:GLU:HA	1.98	0.45
1:C:150:ILE:HD12	1:C:155:ARG:HD2	1.98	0.45
1:C:142:LYS:HD3	1:C:173:TYR:CE2	2.51	0.45
2:D:66:ARG:HH11	2:D:66:ARG:HD2	1.66	0.44
1:A:155:ARG:HH11	1:A:155:ARG:HB2	1.82	0.44
1:C:138:ASN:HD21	2:D:172:HIS:HE1	1.67	0.43
1:A:39:LYS:HE2	1:A:81:GLU:O	2.18	0.43
1:A:155:ARG:HB2	1:A:155:ARG:NH1	2.34	0.42
1:A:185:GLU:O	1:A:189:HIS:HD2	2.03	0.42
2:D:226:GLU:H	2:D:226:GLU:CD	2.27	0.42
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.84	0.42
1:A:160:LEU:HD11	2:B:177:VAL:HG23	2.01	0.42
2:D:29:PHE:CD2	2:D:76:ASN:HA	2.55	0.42
1:C:124:GLN:HE22	1:C:131:SER:H	1.69	0.41
1:C:134:CYS:SG	1:C:194:CYS:CB	3.09	0.41
2:B:32:TYR:CE2	2:B:97:ARG:HG3	2.56	0.41
1:C:160:LEU:HD22	2:D:177:VAL:HG23	2.03	0.41
1:C:192:TYR:HB2	1:C:209:PHE:CE1	2.56	0.41
2:D:142:CYS:SG	2:D:208:CYS:HB2	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:TYR:OH	1:C:89:GLN:NE2	2.54	0.40
1:C:119:PRO:HB3	1:C:209:PHE:CE2	2.57	0.40
1:A:188:ARG:HE	1:A:188:ARG:HB3	1.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/217 (99%)	211 (98%)	4 (2%)	0	100	100
1	C	215/217 (99%)	212 (99%)	3 (1%)	0	100	100
2	B	210/220 (96%)	204 (97%)	6 (3%)	0	100	100
2	D	210/220 (96%)	204 (97%)	6 (3%)	0	100	100
All	All	850/874 (97%)	831 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	194/194 (100%)	172 (89%)	22 (11%)	5	3
1	C	194/194 (100%)	174 (90%)	20 (10%)	7	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	183/187 (98%)	172 (94%)	11 (6%)	17	14
2	D	182/187 (97%)	166 (91%)	16 (9%)	9	6
All	All	753/762 (99%)	684 (91%)	69 (9%)	8	5

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	90	ASN
1	A	105	GLU
1	A	121	SER
1	A	125	LEU
1	A	136	LEU
1	A	143	ASP
1	A	145	ASN
1	A	149	LYS
1	A	155	ARG
1	A	156	GLN
1	A	157	ASN
1	A	160	LEU
1	A	172	THR
1	A	179	LEU
1	A	181	LEU
1	A	184	ASP
1	A	187	GLU
1	A	191	SER
1	A	201	SER
1	A	202	THR
1	A	203	SER
2	B	63	VAL
2	B	127	VAL
2	B	136	SER
2	B	151	PRO
2	B	153	THR
2	B	166	LEU
2	B	167	SER
2	B	168	SER
2	B	195	SER
2	B	202	SER
2	B	219	VAL
1	C	11	LEU

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Mol	Chain	Res	Type
1	C	14	THR
1	C	18	LYS
1	C	45	LYS
1	C	65	SER
1	C	73	LEU
1	C	83	LEU
1	C	89	GLN
1	C	90	ASN
1	C	93	SER
1	C	107	LYS
1	C	125	LEU
1	C	145	ASN
1	C	147	LYS
1	C	175	MET
1	C	193	THR
1	C	197	THR
1	C	202	THR
1	C	205	ILE
1	C	208	SER
2	D	1	GLU
2	D	18	LEU
2	D	63	VAL
2	D	84	SER
2	D	108	LEU
2	D	127	VAL
2	D	136	SER
2	D	137	SER
2	D	142	CYS
2	D	151	PRO
2	D	154	LEU
2	D	156	THR
2	D	179	GLN
2	D	202	SER
2	D	219	VAL
2	D	226	GLU

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

Mol	Chain	Res	Type
1	A	38	GLN
1	A	138	ASN
1	A	189	HIS

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Mol	Chain	Res	Type
1	A	210	ASN
2	B	39	GLN
2	B	76	ASN
1	C	89	GLN
1	C	124	GLN
1	C	138	ASN
1	C	166	GLN
2	D	73	ASN
2	D	76	ASN
2	D	209	ASN

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.