



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:38 pm BST

PDB ID : 8FAB
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

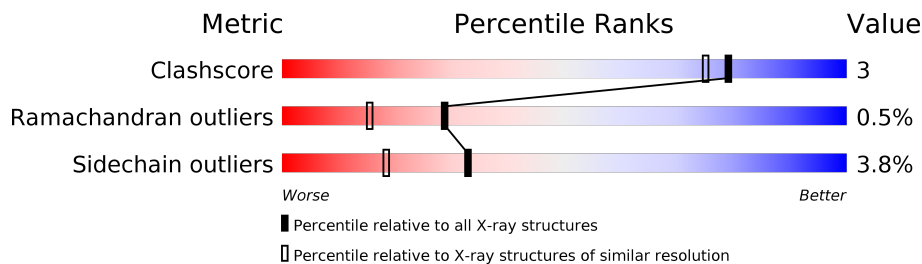
1 Overall quality at a glance

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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (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 on 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	
1	C	212	
2	B	224	
2	D	224	

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
			Total	C	N	O	S			
1	A	206	1544	966	259	314	5	0	0	0
1	C	206	1544	966	259	314	5	0	0	0

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
			Total	C	N	O	S			
2	B	215	1635	1042	279	307	7	0	0	1
2	D	222	1682	1068	287	320	7	0	0	0

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

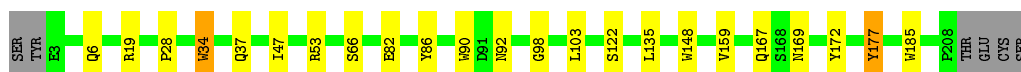
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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)

Chain A: 




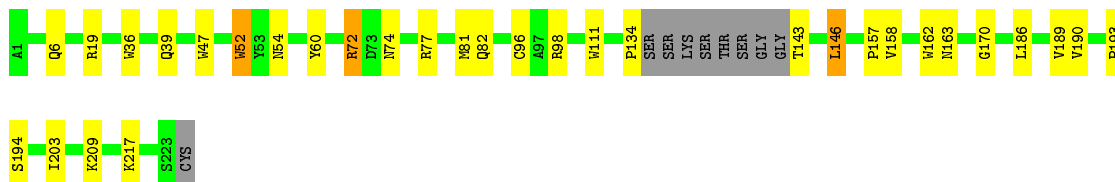
- Molecule 1: IGG1-LAMBDA HIL FAB (LIGHT CHAIN)

Chain C: 




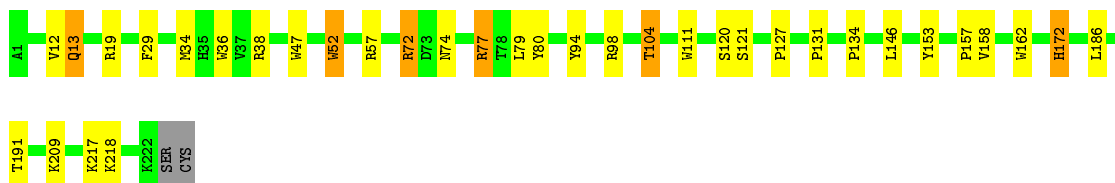
- Molecule 2: IGG1-LAMBDA HIL FAB (HEAVY CHAIN)

Chain B: 



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

Chain D: 



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	7073	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.71	0/1582	1.37	15/2164 (0.7%)
1	C	0.70	0/1582	1.39	16/2164 (0.7%)
2	B	0.78	0/1677	1.53	30/2285 (1.3%)
2	D	0.78	0/1725	1.48	26/2349 (1.1%)
All	All	0.74	0/6566	1.44	87/8962 (1.0%)

There are no bond length outliers.

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	60	TYR	CB-CG-CD2	-12.65	113.41	121.00
1	A	148	TRP	CD1-CG-CD2	9.95	114.26	106.30
2	B	98	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	A	53	ARG	NE-CZ-NH2	-9.39	115.61	120.30
2	B	52	TRP	CD1-CG-CD2	8.75	113.30	106.30
2	D	77	ARG	NE-CZ-NH2	-8.70	115.95	120.30
2	D	36	TRP	CD1-CG-CD2	8.47	113.07	106.30
2	D	162	TRP	CD1-CG-CD2	8.42	113.04	106.30
2	B	77	ARG	NE-CZ-NH2	-8.16	116.22	120.30
2	B	162	TRP	CD1-CG-CD2	8.09	112.78	106.30
1	A	148	TRP	CE2-CD2-CG	-7.99	100.91	107.30
2	D	47	TRP	CD1-CG-CD2	7.85	112.58	106.30
2	D	52	TRP	CD1-CG-CD2	7.85	112.58	106.30
2	D	162	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	C	148	TRP	CD1-CG-CD2	7.78	112.53	106.30
2	B	98	ARG	NE-CZ-NH2	-7.78	116.41	120.30
2	D	52	TRP	CE2-CD2-CG	-7.77	101.09	107.30
2	B	36	TRP	CE2-CD2-CG	-7.75	101.10	107.30
2	D	111	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	C	34	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	C	185	TRP	CD1-CG-CD2	7.68	112.44	106.30
2	B	162	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	A	185	TRP	CE2-CD2-CG	-7.50	101.30	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	A	19	ARG	NE-CZ-NH2	-7.42	116.59	120.30
2	B	47	TRP	CD1-CG-CD2	7.10	111.98	106.30
2	D	72	ARG	NE-CZ-NH1	7.08	123.84	120.30
2	D	57	ARG	NE-CZ-NH2	-7.06	116.77	120.30
2	D	36	TRP	CE2-CD2-CG	-7.06	101.65	107.30
2	B	52	TRP	CE2-CD2-CG	-7.03	101.67	107.30
1	C	148	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	A	34	TRP	CD1-CG-CD2	6.95	111.86	106.30
2	B	36	TRP	CG-CD2-CE3	6.91	140.11	133.90
2	B	111	TRP	CD1-CG-CD2	6.75	111.70	106.30
2	B	36	TRP	CD1-CG-CD2	6.74	111.69	106.30
1	C	19	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	185	TRP	CE2-CD2-CG	-6.64	101.99	107.30
2	B	47	TRP	CE2-CD2-CG	-6.59	102.03	107.30
2	B	52	TRP	CB-CG-CD1	-6.57	118.45	127.00
2	B	77	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	B	52	TRP	CG-CD1-NE1	-6.47	103.63	110.10
2	B	52	TRP	CG-CD2-CE3	6.40	139.66	133.90
2	D	47	TRP	CE2-CD2-CG	-6.40	102.18	107.30
2	D	111	TRP	CE2-CD2-CG	-6.34	102.23	107.30
1	A	34	TRP	CE2-CD2-CG	-6.32	102.25	107.30
2	B	111	TRP	CE2-CD2-CG	-6.30	102.26	107.30
2	B	186	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	148	TRP	CG-CD1-NE1	-6.25	103.85	110.10
1	A	172	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	C	48	TYR	CB-CG-CD1	-6.22	117.27	121.00
2	B	19	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	D	19	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	185	TRP	CG-CD2-CE3	6.12	139.41	133.90
1	C	34	TRP	CE2-CD2-CG	-6.12	102.40	107.30
2	B	60	TYR	CG-CD2-CE2	-6.07	116.44	121.30
2	B	72	ARG	NE-CZ-NH2	-6.07	117.27	120.30
2	D	38	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	185	TRP	CB-CG-CD1	-6.04	119.15	127.00
2	D	80	TYR	CB-CG-CD2	-5.99	117.41	121.00
2	B	72	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	C	77	VAL	CG1-CB-CG2	-5.99	101.32	110.90
1	C	34	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	A	53	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	B	162	TRP	CG-CD2-CE3	5.79	139.12	133.90
1	A	19	ARG	NE-CZ-NH1	5.66	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	52	TRP	CG-CD1-NE1	-5.61	104.49	110.10
2	D	36	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	C	172	TYR	CB-CG-CD2	-5.52	117.69	121.00
2	D	111	TRP	CG-CD1-NE1	-5.51	104.59	110.10
1	C	85	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	A	177	TYR	CB-CG-CD2	-5.43	117.74	121.00
2	D	94	TYR	CB-CG-CD2	-5.38	117.77	121.00
2	D	77	ARG	NE-CZ-NH1	5.37	122.98	120.30
2	D	158	VAL	CG1-CB-CG2	-5.37	102.31	110.90
1	C	189	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	D	98	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	3	GLU	CA-C-N	5.27	128.79	117.20
2	D	98	ARG	NE-CZ-NH2	-5.27	117.67	120.30
2	B	162	TRP	CG-CD1-NE1	-5.24	104.86	110.10
2	B	47	TRP	CG-CD2-CE3	5.21	138.59	133.90
2	D	47	TRP	CG-CD1-NE1	-5.20	104.90	110.10
2	D	186	LEU	CA-CB-CG	5.17	127.20	115.30
2	B	60	TYR	CB-CG-CD1	5.11	124.06	121.00
2	B	81	MET	CA-CB-CG	-5.06	104.69	113.30
1	C	148	TRP	CG-CD1-NE1	-5.06	105.04	110.10
2	B	162	TRP	CB-CG-CD1	-5.04	120.44	127.00
1	C	185	TRP	CB-CG-CD1	-5.04	120.45	127.00

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	13	0
2	D	1682	0	1660	12	0
3	A	177	0	0	0	0
3	B	155	0	0	1	0
3	C	187	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	149	0	0	2	0
All	All	7073	0	6271	36	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 (36) 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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	204/212 (96%)	194 (95%)	8 (4%)	2 (1%)	15	5
1	C	204/212 (96%)	195 (96%)	8 (4%)	1 (0%)	29	15
2	B	211/224 (94%)	207 (98%)	4 (2%)	0	100	100
2	D	220/224 (98%)	212 (96%)	7 (3%)	1 (0%)	29	15
All	All	839/872 (96%)	808 (96%)	27 (3%)	4 (0%)	29	15

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 [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	173/180 (96%)	170 (98%)	3 (2%)	60	51
1	C	173/180 (96%)	166 (96%)	7 (4%)	31	16
2	B	181/189 (96%)	172 (95%)	9 (5%)	24	10
2	D	187/189 (99%)	179 (96%)	8 (4%)	29	14
All	All	714/738 (97%)	687 (96%)	27 (4%)	33	18

All (27) 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	52	TRP
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	209	LYS
1	C	13	SER
1	C	29	ASN
1	C	65	THR
1	C	68	THR
1	C	88	GLN
1	C	102	LYS
1	C	156	LYS
2	D	12	VAL
2	D	13	GLN
2	D	52	TRP
2	D	104	THR
2	D	121	SER
2	D	157	PRO
2	D	172	HIS
2	D	218	LYS

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

Mol	Chain	Res	Type
1	A	6	GLN
1	A	37	GLN
2	B	54	ASN
2	B	74	ASN
1	C	88	GLN
2	D	31	ASN
2	D	74	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 carbohydrates 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.