



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 06:18 AM UTC

PDB ID : 1FIG / pdb_00001fig
Title : ROUTES TO CATALYSIS: STRUCTURE OF A CATALYTIC ANTIBODY
AND COMPARISON WITH ITS NATURAL COUNTERPART
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Deposited on : 1994-01-07
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

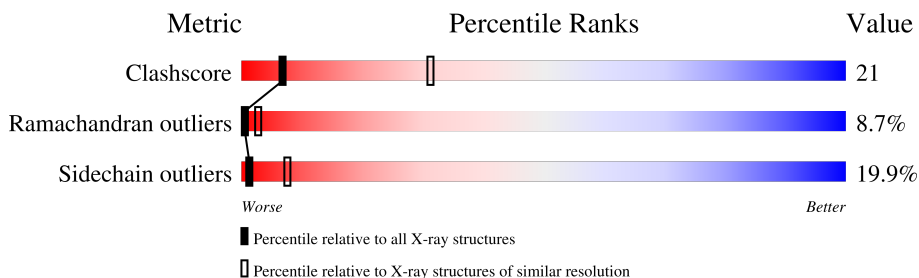
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	L	215	
2	H	216	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3284 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.

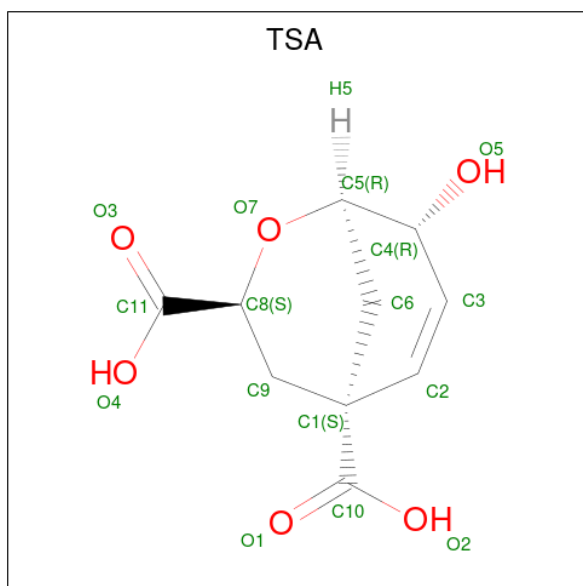
- Molecule 1 is a protein called IGG1-KAPPA 1F7 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	215	1635	1014	272	341	8	0	0	0

- Molecule 2 is a protein called IGG1-KAPPA 1F7 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	216	1632	1033	272	321	6	0	0	0

- Molecule 3 is 8-HYDROXY-2-OXA-BICYCLO[3.3.1]NON-6-ENE-3,5-DICARBOXYLIC ACID (CCD ID: TSA) (formula: C₁₀H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	H	1	16	10	6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O 1 1	0	0

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	37.10Å 63.30Å 178.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-3.00)	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	3284	wwPDB-VP
Average B, all atoms (Å ²)	3.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TSA

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	1.19	7/1671 (0.4%)	2.42	106/2269 (4.7%)
2	H	1.29	11/1676 (0.7%)	2.48	119/2289 (5.2%)
All	All	1.24	18/3347 (0.5%)	2.45	225/4558 (4.9%)

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	3
2	H	0	2
All	All	0	5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	32	HIS	CD2-NE2	-7.71	1.29	1.37
2	H	212	HIS	CD2-NE2	-7.70	1.29	1.37
2	H	204	THR	CA-CB	7.19	1.65	1.53
1	L	198	HIS	CD2-NE2	-7.04	1.30	1.37
2	H	172	HIS	CD2-NE2	-6.96	1.30	1.37

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	62	PHE	N-CA-C	13.65	128.36	110.88
2	H	135	ASN	CA-CB-CG	13.22	125.82	112.60
2	H	138	VAL	N-CA-C	13.00	126.35	109.58
1	L	138	ASN	N-CA-C	12.40	126.53	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	H	209	ASN	CA-CB-CG	11.97	124.57	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	147	TYR	Sidechain
2	H	75	SER	Peptide
1	L	119	PRO	Peptide
1	L	186	TYR	Sidechain
1	L	58	VAL	Peptide

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	1635	0	1563	78	0
2	H	1632	0	1596	66	0
3	H	16	0	10	5	0
4	H	1	0	0	0	0
All	All	3284	0	3169	138	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 21.

The worst 5 of 138 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\AA)	Clash overlap (\AA)
1:L:149:LYS:HA	1:L:153:SER:HA	1.54	0.87
1:L:150:ILE:HB	1:L:154:GLU:HB3	1.55	0.86
1:L:11:MET:SD	1:L:104:LEU:HG	2.18	0.84
1:L:19:VAL:HG12	1:L:75:ILE:HB	1.60	0.82
2:H:89:VAL:HG12	2:H:108:LEU:HG	1.64	0.80

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	213/215 (99%)	170 (80%)	30 (14%)	13 (6%)	1	7
2	H	214/216 (99%)	159 (74%)	31 (14%)	24 (11%)	0	1
All	All	427/431 (99%)	329 (77%)	61 (14%)	37 (9%)	0	3

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	29	SER
1	L	211	ARG
2	H	74	SER
2	H	76	SER
2	H	84	SER

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	186/186 (100%)	151 (81%)	35 (19%)	1	9
2	H	185/185 (100%)	146 (79%)	39 (21%)	1	6
All	All	371/371 (100%)	297 (80%)	74 (20%)	1	7

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	151	PRO

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Mol	Chain	Res	Type
2	H	213	PRO
2	H	162	ASN
2	H	191	VAL
1	L	170	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	81	HIS
2	H	209	ASN
1	L	145	ASN
1	L	198	HIS
2	H	5	GLN

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TSA	H	224	-	16,17,17	3.03	7 (43%)	16,26,26	2.38	4 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TSA	H	224	-	-	1/10/34/34	1/3/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	224	TSA	C9-C8	7.21	1.66	1.52
3	H	224	TSA	O7-C8	5.16	1.53	1.43
3	H	224	TSA	C6-C1	-4.87	1.47	1.55
3	H	224	TSA	C8-C11	3.68	1.56	1.52
3	H	224	TSA	C4-C3	-2.57	1.44	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	224	TSA	O7-C8-C11	7.11	121.15	107.72
3	H	224	TSA	O4-C11-C8	3.00	120.51	112.71
3	H	224	TSA	C5-C4-C3	2.39	114.47	108.83
3	H	224	TSA	O2-C10-O1	-2.14	117.02	123.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	224	TSA	O3-C11-C8-O7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	224	TSA	C1-C2-C3-C4-C5-C8-C9-O7

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	224	TSA	5	0

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.