



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 02:54 AM BST

PDB ID : 6SS5
Title : Structure of the arginase-2-inhibitory human antigen-binding fragment Fab C0020187
Authors : Burschowsky, D.; Addyman, A.; Fiedler, S.; Groves, M.; Haynes, S.; See-wooruthun, C.; Carr, M.
Deposited on : 2019-09-06
Resolution : 1.78 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

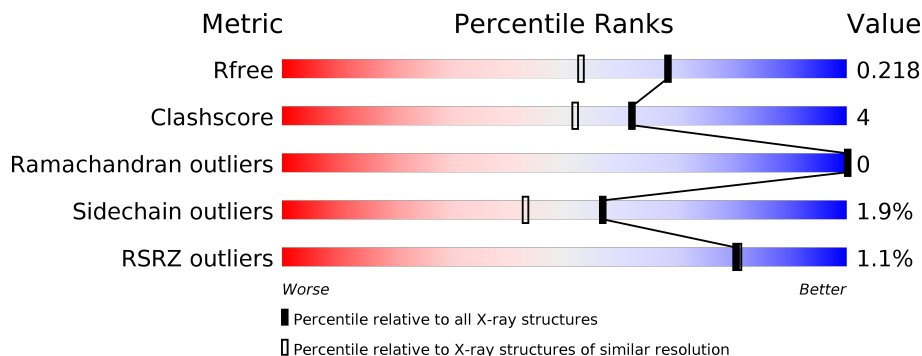
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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))
R_{free}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	HHH	233	
2	LLL	220	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7106 atoms, of which 3359 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 Fab C0020187 heavy chain (IgG1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	HHH	227	3398	1070	1685	293	338	12	99	5	0

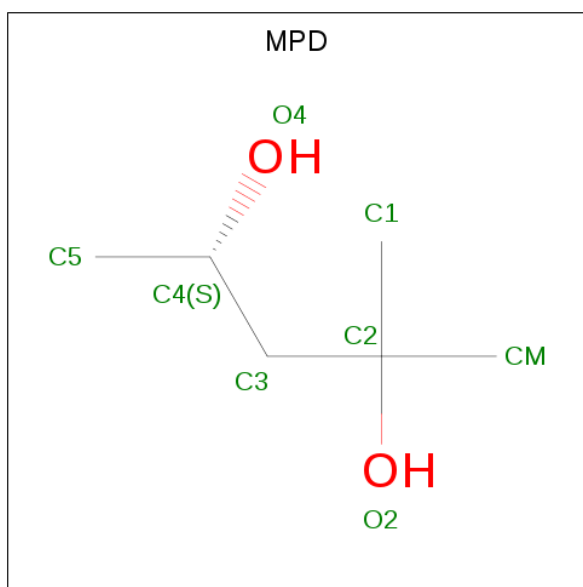
- Molecule 2 is a protein called Fab C0020187 light chain (IgG1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	LLL	216	3250	1028	1598	275	342	7	110	7	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

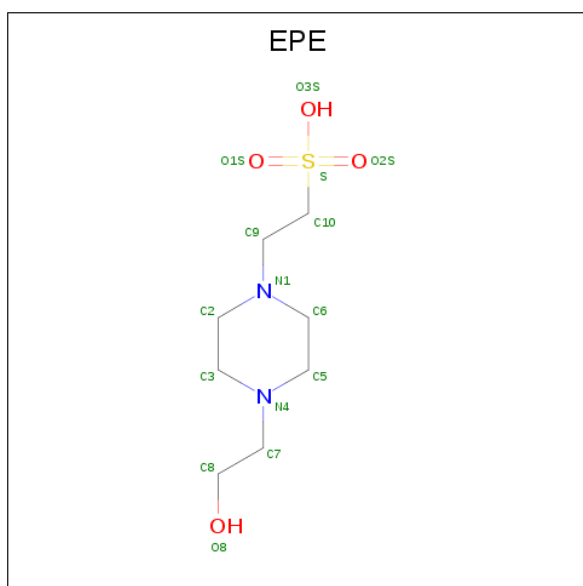
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	HHH	3	Total	Cl	0	0
			3	3		
3	LLL	2	Total	Cl	0	0
			2	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



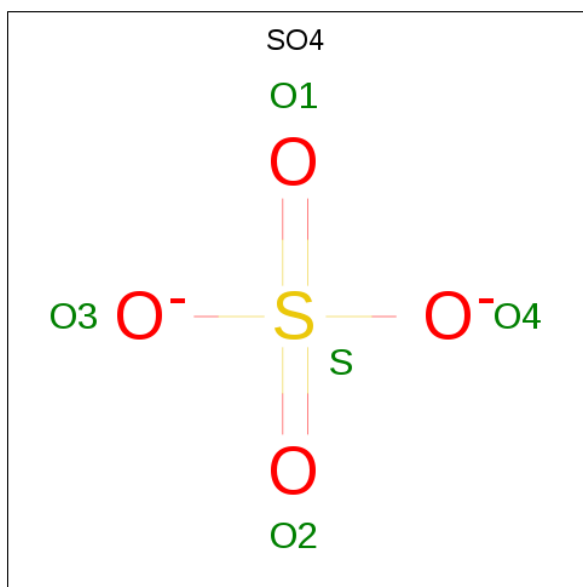
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	HHH	1	Total	C	H	O	1	0
			22	6	14	2		
4	LLL	1	Total	C	H	O	1	0
			22	6	14	2		
4	LLL	1	Total	C	H	O	1	0
			22	6	14	2		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	LLL	1	Total	C	H	N	O	S	1	0
			32	8	17	2	4	1		
5	LLL	1	Total	C	H	N	O	S	1	0
			32	8	17	2	4	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	LLL	1	Total	O S	0	0
			5	4 1		

- Molecule 7 is water.

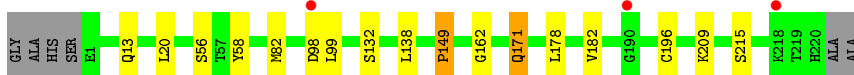
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	HHH	138	Total	O	0	0
			138	138		
7	LLL	180	Total	O	0	1
			180	180		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: Fab C0020187 heavy chain (IgG1)

Chain HHH:  90% 6% ..



- Molecule 2: Fab C0020187 light chain (IgG1)

Chain LLL:  87% 10% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.32Å 103.37Å 164.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.35 – 1.78 49.31 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.35-1.78) 99.4 (49.31-1.69)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.178 , 0.216 0.187 , 0.218	Depositor DCC
R_{free} test set	3004 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtrriage
Anisotropy	0.642	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7106	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: MPD, EPE, SO4, CL

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	HHH	0.76	0/1750	0.92	1/2378 (0.0%)
2	LLL	0.81	0/1691	0.90	1/2307 (0.0%)
All	All	0.79	0/3441	0.91	2/4685 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	HHH	149	PRO	N-CA-CB	-6.55	95.39	102.60
2	LLL	61	ARG	CB-CA-C	-6.26	97.87	110.40

There are no chirality outliers.

There are no planarity outliers.

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	HHH	1713	1685	1676	10	0
2	LLL	1652	1598	1587	19	0
3	HHH	3	0	0	0	0
3	LLL	2	0	0	0	0
4	HHH	8	14	14	0	0
4	LLL	16	28	28	1	0
5	LLL	30	34	36	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	LLL	5	0	0	0	0
7	HHH	138	0	0	3	1
7	LLL	180	0	0	8	3
All	All	3747	3359	3341	30	3

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 4.

The worst 5 of 30 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:LLL:195[A]:GLN:NE2	7:LLL:403:HOH:O	1.82	1.12
2:LLL:17[B]:GLN:OE1	7:LLL:401:HOH:O	1.77	1.02
2:LLL:10:SER:OG	7:LLL:402:HOH:O	1.80	0.98
2:LLL:199:GLU:OE1	7:LLL:404:HOH:O	2.08	0.72
2:LLL:17[A]:GLN:NE2	7:LLL:408:HOH:O	2.25	0.70

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LLL:559:HOH:O	7:LLL:568:HOH:O[4_555]	1.74	0.46
7:LLL:575:HOH:O	7:LLL:580:HOH:O[8_455]	2.00	0.20
7:HHH:532:HOH:O	7:LLL:452:HOH:O[8_555]	2.07	0.13

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	HHH	230/233 (99%)	225 (98%)	5 (2%)	0	100 100
2	LLL	221/220 (100%)	214 (97%)	7 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	451/453 (100%)	439 (97%)	12 (3%)	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	HHH	193/190 (102%)	188 (97%)	5 (3%)	46	29
2	LLL	188/184 (102%)	186 (99%)	2 (1%)	73	65
All	All	381/374 (102%)	374 (98%)	7 (2%)	57	45

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HHH	171	GLN
2	LLL	66	LYS
1	HHH	215	SER
1	HHH	99	LEU
2	LLL	47	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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
4	MPD	LLL	306	-	7,7,7	0.29	0	9,10,10	0.67	0
5	EPE	LLL	301	-	15,15,15	1.92	2 (13%)	18,20,20	2.13	5 (27%)
4	MPD	LLL	305	-	7,7,7	0.62	0	9,10,10	0.82	0
4	MPD	HHH	304	-	7,7,7	0.27	0	9,10,10	0.86	0
6	SO4	LLL	307	-	4,4,4	1.08	1 (25%)	6,6,6	0.44	0
5	EPE	LLL	302	-	15,15,15	1.91	1 (6%)	18,20,20	1.50	2 (11%)

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
4	MPD	LLL	306	-	-	1/5/5/5	-
4	MPD	LLL	305	-	-	0/5/5/5	-
4	MPD	HHH	304	-	-	0/5/5/5	-
5	EPE	LLL	301	-	-	6/9/19/19	0/1/1/1
5	EPE	LLL	302	-	-	3/9/19/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	LLL	302	EPE	C10-S	-6.94	1.67	1.77
5	LLL	301	EPE	C10-S	-6.11	1.68	1.77
5	LLL	301	EPE	C5-N4	2.63	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	LLL	307	SO4	O2-S	2.12	1.57	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	LLL	301	EPE	O2S-S-C10	5.76	113.84	106.92
5	LLL	302	EPE	O2S-S-C10	3.76	111.44	106.92
5	LLL	301	EPE	C7-N4-C5	3.44	120.03	111.23
5	LLL	302	EPE	O3S-S-C10	3.23	110.99	105.77
5	LLL	301	EPE	O1S-S-C10	3.13	110.69	106.92

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	LLL	306	MPD	CM-C2-C3-C4
5	LLL	301	EPE	C10-C9-N1-C6
5	LLL	301	EPE	C9-C10-S-O2S
5	LLL	301	EPE	C9-C10-S-O3S
5	LLL	302	EPE	C9-C10-S-O1S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	LLL	305	MPD	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	HHH	227/233 (97%)	-0.15	3 (1%) 77 77	25, 35, 54, 89	0
2	LLL	216/220 (98%)	-0.04	2 (0%) 84 84	23, 31, 50, 94	0
All	All	443/453 (97%)	-0.09	5 (1%) 80 81	23, 33, 51, 94	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	LLL	2	GLN	3.9
1	HHH	218	LYS	3.1
1	HHH	98	ASP	2.6
1	HHH	190	GLY	2.3
2	LLL	190	ARG	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EPE	LLL	302	15/15	0.83	0.20	68,95,107,110	1
4	MPD	LLL	306	8/8	0.86	0.17	57,69,73,73	1
4	MPD	HHH	304	8/8	0.90	0.12	65,69,77,86	1
5	EPE	LLL	301	15/15	0.94	0.12	40,55,65,68	1
4	MPD	LLL	305	8/8	0.95	0.12	41,45,50,51	1
3	CL	HHH	302	1/1	0.97	0.04	62,62,62,62	0
6	SO4	LLL	307	5/5	0.97	0.10	38,39,51,52	0
3	CL	LLL	304	1/1	0.97	0.04	45,45,45,45	0
3	CL	HHH	303	1/1	0.98	0.05	53,53,53,53	0
3	CL	LLL	303	1/1	0.99	0.07	37,37,37,37	0
3	CL	HHH	301	1/1	0.99	0.04	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.