



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 04:32 PM BST

PDB ID : 6HYG
Title : Heteromeric tandem IgG4/IgG1 Fc
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Deposited on : 2018-10-21
Resolution : 2.31 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
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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

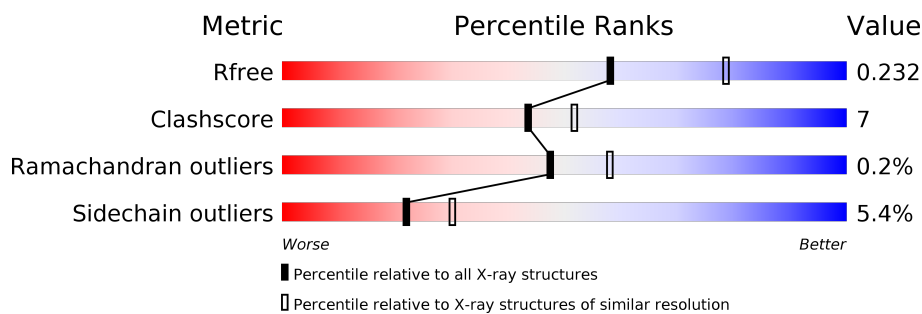
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	492	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3419 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 IgHG1 and IgHG4 hybrid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3325	2109	560	642	14			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

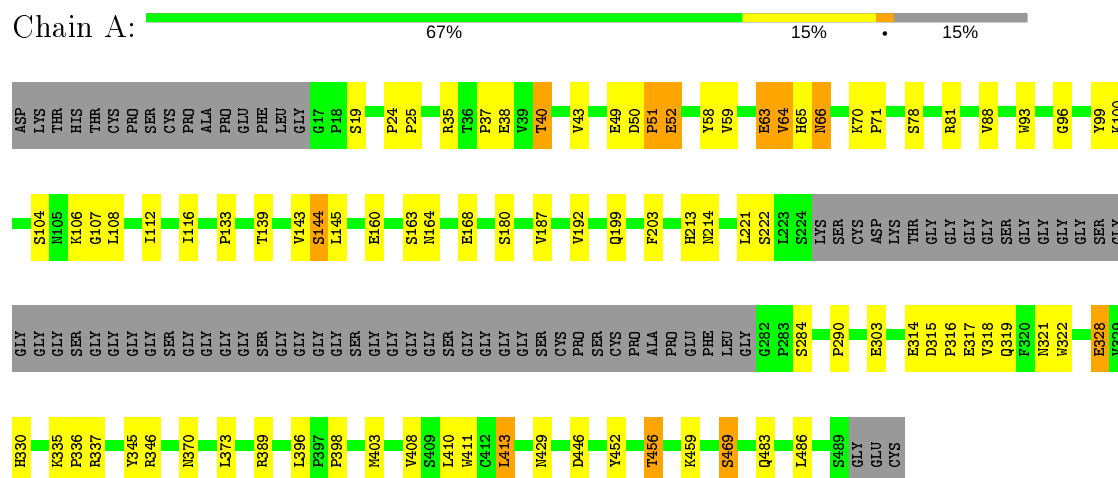
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total	O	0	0
			92	92		

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.

- Molecule 1: IgHG1 and IgHG4 hybrid



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.12Å 63.25Å 77.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.28 – 2.31 29.28 – 2.31	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.28-2.31) 99.7 (29.28-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.258 , 0.277 0.199 , 0.232	Depositor DCC
R_{free} test set	1410 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.357 for -h,-k,l	Xtriage
Reported twinning fraction	0.507 for H, K, L 0.493 for h,-k,-l	Depositor
Outliers	0 of 29204 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3419	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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

5.1 Standard geometry

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

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	1.08	13/3414 (0.4%)	1.23	4/4643 (0.1%)

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
1	A	0	4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	VAL	C-O	13.75	1.49	1.23
1	A	63	GLU	CD-OE2	10.12	1.36	1.25
1	A	328	GLU	CD-OE2	7.60	1.34	1.25
1	A	330	HIS	CB-CG	7.24	1.63	1.50
1	A	164	ASN	C-O	6.55	1.35	1.23
1	A	168	GLU	CD-OE2	6.44	1.32	1.25
1	A	65	HIS	CG-ND1	5.80	1.51	1.38
1	A	65	HIS	CD2-NE2	5.56	1.53	1.42
1	A	168	GLU	C-O	5.50	1.33	1.23
1	A	160	GLU	CD-OE2	5.48	1.31	1.25
1	A	429	ASN	C-O	5.47	1.33	1.23
1	A	163	SER	C-O	5.29	1.33	1.23
1	A	144	SER	C-O	5.26	1.33	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GLU	CB-CA-C	6.21	122.81	110.40
1	A	51	PRO	N-CA-C	-5.47	97.87	112.10
1	A	328	GLU	CB-CA-C	5.28	120.95	110.40
1	A	346	ARG	NE-CZ-NH2	-5.13	117.74	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	GLY	Peptide
1	A	315	ASP	Peptide
1	A	50	ASP	Peptide
1	A	64	VAL	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	3325	0	3244	44	0
2	A	2	0	0	0	0
3	A	92	0	0	6	1
All	All	3419	0	3244	44	1

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 7.

All (44) 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)
1:A:321:ASN:ND2	1:A:328:GLU:OE1	2.18	0.76
1:A:398:PRO:HG3	1:A:408:VAL:HG13	1.70	0.73
1:A:40:THR:CG2	3:A:612:HOH:O	2.43	0.65
1:A:456:THR:CG2	3:A:658:HOH:O	2.50	0.60
1:A:403:MET:O	1:A:459:LYS:HE3	2.02	0.59
1:A:316:PRO:HB2	1:A:317:GLU:HA	1.85	0.58
1:A:335:LYS:HB3	1:A:336:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PRO:CG	1:A:143:VAL:HG13	2.34	0.58
1:A:398:PRO:CG	1:A:408:VAL:HG13	2.34	0.58
1:A:133:PRO:HG3	1:A:143:VAL:HG13	1.87	0.57
1:A:413:LEU:HG	1:A:452:TYR:CE2	2.40	0.56
1:A:389:ARG:NH2	1:A:446:ASP:O	2.38	0.56
1:A:96:GLY:HA2	3:A:622:HOH:O	2.07	0.55
1:A:25:PRO:HA	1:A:38:GLU:O	2.06	0.55
1:A:37:PRO:HG2	1:A:88:VAL:O	2.08	0.54
1:A:58:TYR:HB2	1:A:100:LYS:HB3	1.90	0.53
1:A:213:HIS:HD2	1:A:214:ASN:ND2	2.06	0.52
1:A:318:VAL:HG22	1:A:370:ASN:HD22	1.74	0.52
1:A:40:THR:HG22	3:A:612:HOH:O	2.07	0.52
1:A:396:LEU:HB2	1:A:411:TRP:HB2	1.91	0.51
1:A:410:LEU:HB3	1:A:486:LEU:HD23	1.91	0.51
1:A:456:THR:HG23	3:A:658:HOH:O	2.12	0.50
1:A:40:THR:HG23	3:A:612:HOH:O	2.10	0.48
1:A:410:LEU:HB3	1:A:486:LEU:CD2	2.44	0.48
1:A:403:MET:O	1:A:459:LYS:NZ	2.46	0.47
1:A:403:MET:O	1:A:459:LYS:CE	2.62	0.47
1:A:24:PRO:HB3	1:A:116:ILE:HD11	1.97	0.46
1:A:469:SER:HB3	1:A:483:GLN:HG2	1.98	0.46
1:A:192:VAL:HG11	1:A:203:PHE:CE1	2.51	0.45
1:A:187:VAL:HB	1:A:452:TYR:CD1	2.52	0.45
1:A:51:PRO:HB2	1:A:52:GLU:HA	1.99	0.45
1:A:187:VAL:HG11	1:A:452:TYR:CE2	2.52	0.45
1:A:337:ARG:HD2	1:A:345:TYR:CD2	2.52	0.45
1:A:43:VAL:O	1:A:81:ARG:HA	2.17	0.44
1:A:59:VAL:HG22	1:A:99:TYR:CD2	2.52	0.44
1:A:93:TRP:CD1	1:A:93:TRP:C	2.91	0.44
1:A:70:LYS:HB3	1:A:71:PRO:HD2	2.00	0.43
1:A:322:TRP:O	1:A:328:GLU:HA	2.18	0.43
1:A:66:ASN:N	1:A:66:ASN:OD1	2.50	0.43
1:A:24:PRO:HB3	1:A:116:ILE:CD1	2.49	0.43
1:A:290:PRO:HA	1:A:303:GLU:O	2.19	0.42
1:A:108:LEU:HD21	1:A:112:ILE:HG12	2.03	0.41
1:A:145:LEU:HB3	1:A:221:LEU:HD23	2.03	0.41
1:A:318:VAL:HG22	1:A:370:ASN:ND2	2.35	0.40

All (1) 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)
3:A:680:HOH:O	3:A:680:HOH:O[2_555]	2.06	0.14

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	412/492 (84%)	400 (97%)	11 (3%)	1 (0%)	47 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU

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	389/428 (91%)	368 (95%)	21 (5%)	22 30

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	35	ARG
1	A	40	THR
1	A	49	GLU
1	A	52	GLU

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Mol	Chain	Res	Type
1	A	66	ASN
1	A	78	SER
1	A	104	SER
1	A	106	LYS
1	A	139	THR
1	A	144	SER
1	A	180	SER
1	A	199	GLN
1	A	222	SER
1	A	284	SER
1	A	314	GLU
1	A	319	GLN
1	A	373	LEU
1	A	413	LEU
1	A	456	THR
1	A	469	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	213	HIS
1	A	214	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.