



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6HYG / pdb_00006hyg
Title : Heteromeric tandem IgG4/IgG1 Fc
Authors : Casaletto, J.B.; Geddie, M.L.; Abu-Yousif, A.O.; Masson, K.; Fulgham, A.; Boudot, A.; Maiwald, T.; Kearns, J.D.; Kohli, N.; Su, S.; Razlog, M.; Raue, A.; Kalra, A.; Hakansson, M.; Logan, D.T.; Welin, M.; Chattopadhyay, S.; Harms, B.D.; Nielsen, U.B.; Schoeberl, B.; Lugovskoy, A.A.; MacBeath, G.
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 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

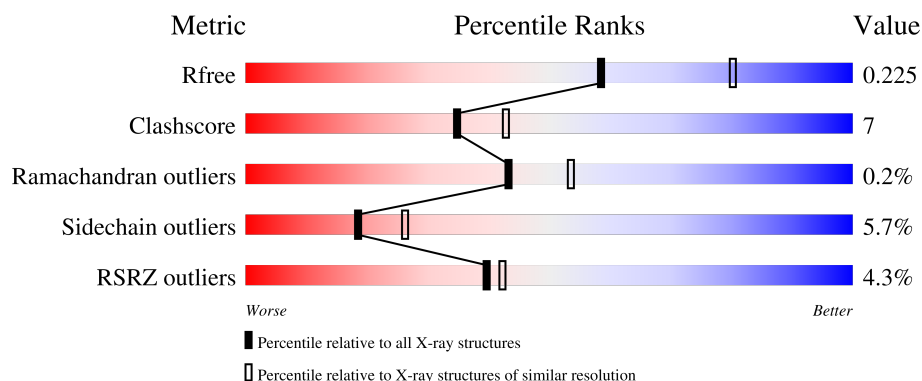
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (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 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 $\leq 5\%$. 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	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 (CCD ID: 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		

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) 99.8 (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 0.193 , 0.225	Depositor DCC
R_{free} test set	1410 reflections (4.81%)	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)	0.33 , 34.0	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	1.49	30/3414 (0.9%)	1.68	43/4643 (0.9%)

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	A	0	4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	VAL	C-O	23.04	1.49	1.23
1	A	65	HIS	CD2-NE2	14.35	1.53	1.37
1	A	65	HIS	CG-ND1	12.05	1.51	1.38
1	A	164	ASN	C-O	9.28	1.35	1.23
1	A	330	HIS	CB-CG	9.23	1.63	1.50
1	A	330	HIS	CG-ND1	8.98	1.48	1.38
1	A	163	SER	C-O	8.55	1.33	1.23
1	A	168	GLU	C-O	8.24	1.33	1.24
1	A	144	SER	C-O	7.82	1.33	1.24
1	A	64	VAL	C-N	7.32	1.43	1.33
1	A	192	VAL	C-O	7.24	1.31	1.23
1	A	451	LEU	C-O	7.01	1.32	1.23
1	A	429	ASN	C-O	6.90	1.33	1.23
1	A	433	GLU	C-O	6.82	1.32	1.24
1	A	197	TRP	C-O	6.67	1.31	1.24
1	A	383	LYS	C-O	6.58	1.31	1.23
1	A	428	SER	CA-C	-6.58	1.44	1.52
1	A	327	VAL	C-O	6.31	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	HIS	CB-CG	6.03	1.58	1.50
1	A	63	GLU	CD-OE2	6.02	1.36	1.25
1	A	467	VAL	C-O	5.91	1.30	1.24
1	A	62	VAL	C-O	5.62	1.30	1.24
1	A	409	SER	C-O	5.48	1.30	1.24
1	A	195	SER	C-O	-5.47	1.17	1.24
1	A	409	SER	CA-CB	-5.21	1.46	1.53
1	A	414	VAL	C-O	5.16	1.29	1.24
1	A	184	PHE	C-O	5.14	1.30	1.23
1	A	323	TYR	C-O	-5.04	1.18	1.24
1	A	127	GLN	C-O	5.04	1.30	1.24
1	A	459	LYS	C-O	5.00	1.30	1.24

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	PRO	CB-CA-C	7.16	123.37	111.56
1	A	429	ASN	OD1-CG-ND2	7.14	129.74	122.60
1	A	51	PRO	N-CA-C	-7.09	97.87	112.47
1	A	320	PHE	CA-C-O	-7.04	113.10	120.70
1	A	328	GLU	CB-CA-C	6.99	120.95	109.70
1	A	40	THR	CB-CA-C	6.84	122.23	109.71
1	A	63	GLU	CB-CG-CD	6.69	123.97	112.60
1	A	87	THR	CA-CB-OG1	-6.68	99.58	109.60
1	A	316	PRO	N-CA-C	-6.46	99.17	112.47
1	A	73	GLU	CB-CA-C	6.31	120.31	109.51
1	A	474	HIS	CA-C-O	-6.29	113.20	120.31
1	A	63	GLU	CB-CA-C	6.23	122.81	110.42
1	A	429	ASN	CA-CB-CG	-6.18	106.42	112.60
1	A	330	HIS	ND1-CG-CD2	-6.07	100.03	106.10
1	A	456	THR	CB-CA-C	6.06	120.00	110.19
1	A	482	THR	CA-CB-OG1	-6.01	100.59	109.60
1	A	309	VAL	CA-C-O	-5.98	113.97	120.67
1	A	63	GLU	O-C-N	5.86	130.38	122.59
1	A	65	HIS	ND1-CE1-NE2	-5.85	102.55	108.40
1	A	51	PRO	CB-CA-C	5.84	121.19	111.56
1	A	49	GLU	CB-CG-CD	5.79	122.45	112.60
1	A	395	THR	CA-CB-OG1	-5.78	100.93	109.60
1	A	143	VAL	N-CA-CB	-5.76	101.71	112.36
1	A	301	THR	CB-CA-C	5.71	121.53	111.20
1	A	154	PRO	N-CD-CG	-5.63	97.04	103.80
1	A	469	SER	CA-C-N	5.59	129.85	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	SER	C-N-CA	5.59	129.85	122.42
1	A	440	PRO	CB-CA-C	5.56	117.71	110.92
1	A	328	GLU	CB-CG-CD	5.49	121.94	112.60
1	A	460	SER	CA-C-N	5.41	127.79	120.44
1	A	460	SER	C-N-CA	5.41	127.79	120.44
1	A	414	VAL	N-CA-C	-5.34	100.42	108.12
1	A	99	TYR	CB-CA-C	5.29	118.86	110.19
1	A	24	PRO	CB-CA-C	5.26	117.34	110.92
1	A	489	SER	CA-C-O	5.23	129.69	120.80
1	A	455	LEU	CA-C-N	-5.22	115.83	122.77
1	A	455	LEU	C-N-CA	-5.22	115.83	122.77
1	A	143	VAL	CB-CA-C	5.18	119.06	110.30
1	A	125	GLU	CB-CG-CD	5.13	121.33	112.60
1	A	344	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	133	PRO	CB-CA-C	-5.10	104.30	110.98
1	A	125	GLU	O-C-N	-5.10	116.02	121.42
1	A	149	VAL	N-CA-CB	-5.07	105.05	111.64

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	49	0
2	A	2	0	0	0	0
3	A	92	0	0	6	1
All	All	3419	0	3244	49	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 (49) 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
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:93:TRP:CD1	1:A:93:TRP:C	2.91	0.48
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:51:PRO:HB2	1:A:52:GLU:HA	1.99	0.45
1:A:187:VAL:HB	1:A:452:TYR:CD1	2.52	0.45
1:A:187:VAL:HG11	1:A:452:TYR:CE2	2.52	0.45
1:A:446:ASP:C	1:A:446:ASP:OD1	2.59	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:70:LYS:HB3	1:A:71:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:TRP:O	1:A:328:GLU:HA	2.18	0.43
1:A:66:ASN:OD1	1:A:66:ASN:N	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:110:SER:C	1:A:111:SER:HG	2.28	0.41
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:397:PRO:O	1:A:398:PRO:C	2.62	0.41
1:A:451:LEU:HD12	1:A:451:LEU:C	2.46	0.41
1:A:89:LEU:O	1:A:90:HIS:C	2.64	0.40
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

5.3.1 Protein backbone

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%)	43 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU

5.3.2 Protein sidechains ⓘ

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%)	367 (94%)	22 (6%)	18	26

All (22) 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
1	A	66	ASN
1	A	139	THR
1	A	143	VAL
1	A	144	SER
1	A	180	SER
1	A	199	GLN
1	A	222	SER
1	A	284	SER
1	A	309	VAL
1	A	314	GLU
1	A	319	GLN
1	A	371	LYS
1	A	373	LEU
1	A	408	VAL
1	A	413	LEU
1	A	456	THR
1	A	469	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	213	HIS
1	A	214	ASN

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Mol	Chain	Res	Type
1	A	218	GLN
1	A	479	ASN
1	A	483	GLN

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 oligosaccharides 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	A	416/492 (84%)	0.13	18 (4%) 40 42	22, 47, 88, 126	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	PRO	4.4
1	A	316	PRO	4.3
1	A	374	PRO	4.1
1	A	109	PRO	3.3
1	A	107	GLY	3.1
1	A	65	HIS	3.0
1	A	106	LYS	2.9
1	A	371	LYS	2.8
1	A	330	HIS	2.6
1	A	314	GLU	2.5
1	A	17	GLY	2.4
1	A	224	SER	2.4
1	A	33	ILE	2.4
1	A	373	LEU	2.3
1	A	341	PHE	2.2
1	A	49	GLU	2.1
1	A	108	LEU	2.1
1	A	110	SER	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	ZN	A	501	1/1	1.00	0.01	40,40,40,40	0
2	ZN	A	502	1/1	1.00	0.01	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.