



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 09:51 PM GMT

PDB ID : 1E4K
Title : CRYSTAL STRUCTURE OF SOLUBLE HUMAN IGG1 FC FRAGMENT-FC-GAMMA RECEPTOR III COMPLEX
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Deposited on : 2000-07-07
Resolution : 3.20 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

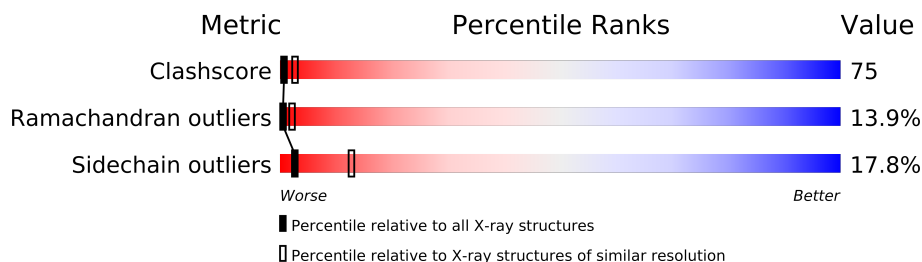
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	225	
1	B	225	
2	C	176	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5042 atoms, of which 0 are hydrogen and 0 are deuterium.

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 FC FRAGMENT OF HUMAN IGG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1719	1094	291	326	8			
1	B	216	Total	C	N	O	S	0	0	0
			1719	1094	291	326	8			

- Molecule 2 is a protein called LOW AFFINITY IMMUNOGLOBULIN GAMMA FC RECEPTOR III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	172	Total	C	N	O	S	0	0	0
			1384	877	237	266	4			

- Molecule 3 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	9	Total	C	N	O	0	0
			110	62	4	44		

- Molecule 4 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	9	Total	C	N	O	0	0
			110	62	4	44		

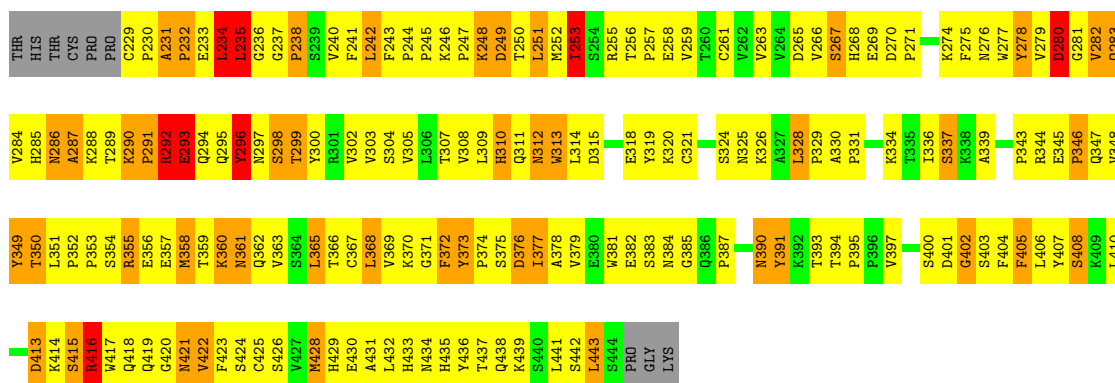
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

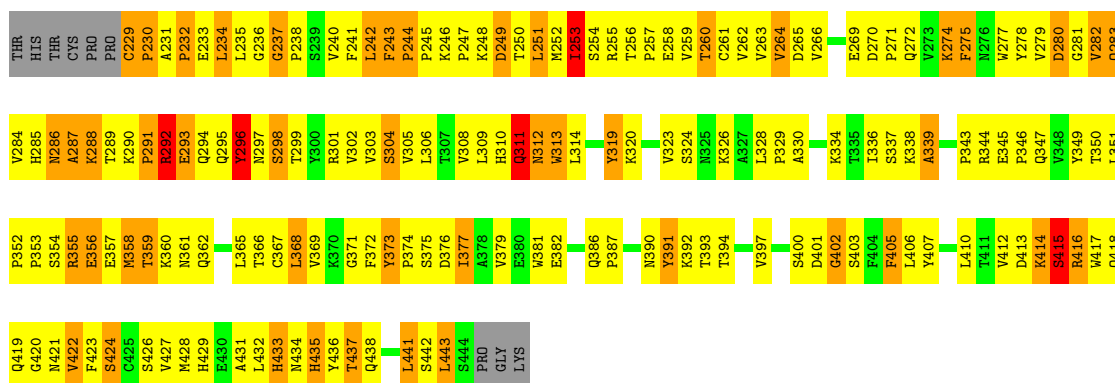
• Molecule 1: FC FRAGMENT OF HUMAN IGG1

Chain A:



• Molecule 1: FC FRAGMENT OF HUMAN IGG1

Chain B:



• Molecule 2: LOW AFFINITY IMMUNOGLOBULIN GAMMA FC RECEPTOR III

Chain C:



L121	Q122	N123	G124	K125	D126	R127	K128	Y129	F130	H131	H132	N133	S134	D135	F136	H137	I138	P139	K140	A141	T142	L143	K144	D145	S146	G147	S148	Y149	F150	C151	R152	G153	L154	V155	K158	N159	V160	S161	S162	V165	W166	I167	T168	I169	T170	Q171	G172											
M60	N61	D62	E65	Y66	R67	C68	Q69	T70	N71	L72	S73	T74	L75	S76	D77	P78	Y79	Q80	L81	E82	Y83	H84	T85	G86	W87	L88	L89	L90	Q91	R92	P93	R94	W95	Y96	F97	K98	E99	E100	D101	P102	I103	H104	L105	R106	C107	H108	S109	W110	K111	N112	T113	A114	L115	H116	K117	V118	T119	Y120

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	115.32Å 115.32Å 299.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 3.20	Depositor
% Data completeness (in resolution range)	94.9 (100.00-3.20)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.271 , 0.357	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5042	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, GLA, GAL, FUC, FUL, MAN

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	0.66	0/1767	0.99	7/2408 (0.3%)
1	B	0.88	3/1767 (0.2%)	1.00	1/2408 (0.0%)
2	C	0.77	0/1422	1.03	4/1933 (0.2%)
All	All	0.77	3/4956 (0.1%)	1.00	12/6749 (0.2%)

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	B	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	GLU	CG-CD	7.51	1.63	1.51
1	B	292	ARG	N-CA	6.11	1.58	1.46
1	B	293	GLU	CB-CG	5.44	1.62	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	CYS	CA-CB-SG	7.16	126.89	114.00
1	A	234	LEU	C-N-CA	6.88	138.91	121.70
2	C	42	ASN	N-CA-C	-6.46	93.56	111.00
2	C	88	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	328	LEU	CA-CB-CG	5.83	128.72	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	296	TYR	Sidechain
1	B	319	TYR	Sidechain
1	B	373	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1719	0	1689	297	0
1	B	1719	0	1690	256	0
2	C	1384	0	1324	208	0
3	A	110	0	94	9	0
4	B	110	0	94	19	0
All	All	5042	0	4891	748	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 75.

The worst 5 of 748 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:805:MAN:O3	3:A:806:NAG:H2	1.34	1.25
1:A:232:PRO:O	1:A:233:GLU:HG2	1.43	1.17
1:B:245:PRO:HA	4:B:807:GAL:H61	1.18	1.13
1:B:258:GLU:O	4:B:807:GAL:H62	1.47	1.13
2:C:116:HIS:HB2	2:C:154:LEU:HB2	1.30	1.11

There are no symmetry-related clashes.

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	214/225 (95%)	147 (69%)	35 (16%)	32 (15%)	0	1
1	B	214/225 (95%)	154 (72%)	30 (14%)	30 (14%)	0	2
2	C	170/176 (97%)	131 (77%)	18 (11%)	21 (12%)	1	3
All	All	598/626 (96%)	432 (72%)	83 (14%)	83 (14%)	0	2

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ALA
1	A	232	PRO
1	A	235	LEU
1	A	283	GLN
1	A	291	PRO

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	200/208 (96%)	163 (82%)	37 (18%)	2	11
1	B	200/208 (96%)	165 (82%)	35 (18%)	3	13
2	C	156/160 (98%)	129 (83%)	27 (17%)	3	13
All	All	556/576 (96%)	457 (82%)	99 (18%)	2	13

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	259	VAL
1	B	301	ARG
2	C	112	ASN
1	B	264	VAL
1	B	282	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	421	ASN
1	A	438	GLN
1	B	438	GLN
1	A	418	GLN
2	C	108	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

18 carbohydrates are 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	NAG	A	801	1,3	12,14,15	0.80	0	15,19,21	0.89	0
3	FUC	A	802	3	9,10,11	0.62	0	10,14,16	0.93	0
3	NAG	A	803	3	12,14,15	0.67	0	15,19,21	0.76	0
3	BMA	A	804	3	10,11,12	0.81	0	11,15,17	1.07	1 (9%)
3	MAN	A	805	3	10,11,12	0.58	0	11,15,17	1.04	2 (18%)
3	NAG	A	806	3	12,14,15	0.75	0	15,19,21	0.84	0
3	GLA	A	807	3	10,11,12	0.35	0	11,15,17	1.01	1 (9%)
3	MAN	A	808	3	10,11,12	0.53	0	11,15,17	0.78	0
3	NAG	A	809	3	12,14,15	0.68	0	15,19,21	0.93	1 (6%)
4	NAG	B	801	1,4	12,14,15	0.73	0	15,19,21	1.28	3 (20%)
4	FUL	B	802	4	9,10,11	0.80	0	10,14,16	1.00	1 (10%)
4	NAG	B	803	4	12,14,15	0.64	0	15,19,21	0.96	2 (13%)
4	BMA	B	804	4	10,11,12	0.59	0	11,15,17	1.47	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	B	805	4	10,11,12	0.50	0	11,15,17	0.72	0
4	NAG	B	806	4	12,14,15	0.78	0	15,19,21	1.18	2 (13%)
4	GAL	B	807	4	10,11,12	0.41	0	11,15,17	1.03	1 (9%)
4	MAN	B	808	4	10,11,12	0.58	0	11,15,17	1.01	1 (9%)
4	NAG	B	809	4	12,14,15	0.72	0	15,19,21	1.06	1 (6%)

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	NAG	A	801	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	802	3	-	0/0/17/20	1/1/1/1
3	NAG	A	803	3	-	0/6/23/26	0/1/1/1
3	BMA	A	804	3	-	0/2/19/22	0/1/1/1
3	MAN	A	805	3	-	0/2/19/22	0/1/1/1
3	NAG	A	806	3	-	0/6/23/26	0/1/1/1
3	GLA	A	807	3	-	0/2/19/22	0/1/1/1
3	MAN	A	808	3	-	0/2/19/22	0/1/1/1
3	NAG	A	809	3	-	0/6/23/26	0/1/1/1
4	NAG	B	801	1,4	-	0/6/23/26	0/1/1/1
4	FUL	B	802	4	-	0/0/17/20	0/1/1/1
4	NAG	B	803	4	-	0/6/23/26	0/1/1/1
4	BMA	B	804	4	-	0/2/19/22	0/1/1/1
4	MAN	B	805	4	-	0/2/19/22	0/1/1/1
4	NAG	B	806	4	-	0/6/23/26	0/1/1/1
4	GAL	B	807	4	-	0/2/19/22	0/1/1/1
4	MAN	B	808	4	-	0/2/19/22	0/1/1/1
4	NAG	B	809	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	804	BMA	C4-C3-C2	-3.21	106.20	110.50
4	B	801	NAG	C3-C4-C5	-2.94	104.95	110.20
3	A	809	NAG	C2-N2-C7	-2.84	118.31	123.09
4	B	806	NAG	C3-C2-N2	-2.79	107.52	111.76
4	B	801	NAG	C2-N2-C7	-2.49	118.91	123.09

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	FUC	C1-C2-C3-C4-C5-O5

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.