wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:23 PM GMT

PDB ID	:	1FCC
Title	:	CRYSTAL STRUCTURE OF THE C2 FRAGMENT OF STREPTOCOCCAL PROTEIN G IN COMPLEX WITH THE FC DOMAIN OF HUMAN IGG
Authors	:	Sauer-Eriksson, A.E.; Kleywegt, G.J.; Uhlen, M.; Jones, T.A.
Deposited on	:	1995-01-17
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

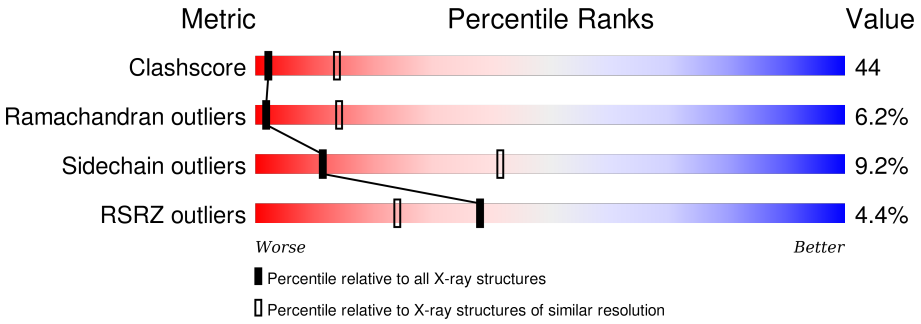
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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 <=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	206	36% 53% 10%
1	B	206	10% 38% 52% 9%
2	C	56	2% 34% 59% 7%
2	D	56	36% 57% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4180 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 MO61 FC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1656	1054	281	314	7			
1	B	206	Total	C	N	O	S	0	0	0
			1656	1054	281	314	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	GLN	GLU	CONFLICT	UNP P01857
A	283	GLN	GLU	CONFLICT	UNP P01857
A	294	GLN	GLU	CONFLICT	UNP P01857
A	312	ASN	ASP	CONFLICT	UNP P01857
A	315	ASP	ASN	CONFLICT	UNP P01857
A	356	GLU	ASP	CONFLICT	UNP P01857
A	358	MET	LEU	CONFLICT	UNP P01857
B	272	GLN	GLU	CONFLICT	UNP P01857
B	283	GLN	GLU	CONFLICT	UNP P01857
B	294	GLN	GLU	CONFLICT	UNP P01857
B	312	ASN	ASP	CONFLICT	UNP P01857
B	315	ASP	ASN	CONFLICT	UNP P01857
B	356	GLU	ASP	CONFLICT	UNP P01857
B	358	MET	LEU	CONFLICT	UNP P01857

- Molecule 2 is a protein called STREPTOCOCCAL PROTEIN G (C2 FRAGMENT).

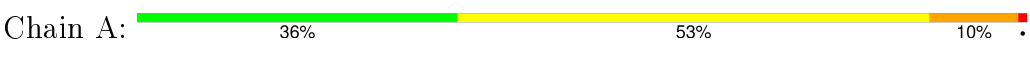
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	56	Total	C	N	O	0	0	0
			434	271	67	96			
2	D	56	Total	C	N	O	0	0	0
			434	271	67	96			

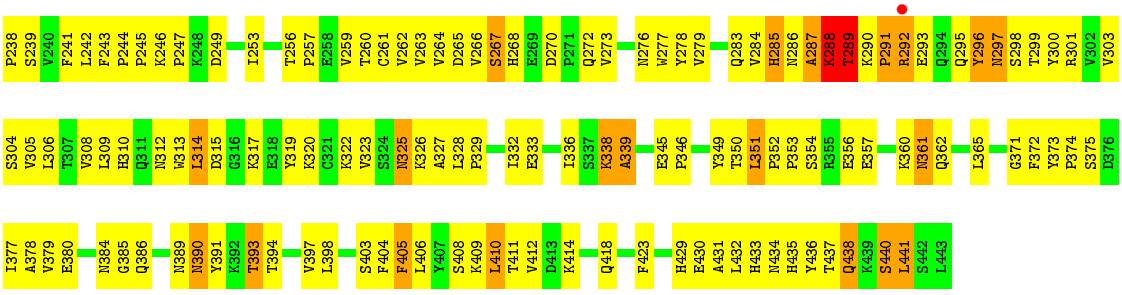
3 Residue-property plots (i)

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.

- Molecule 1: IGG1 MO61 FC

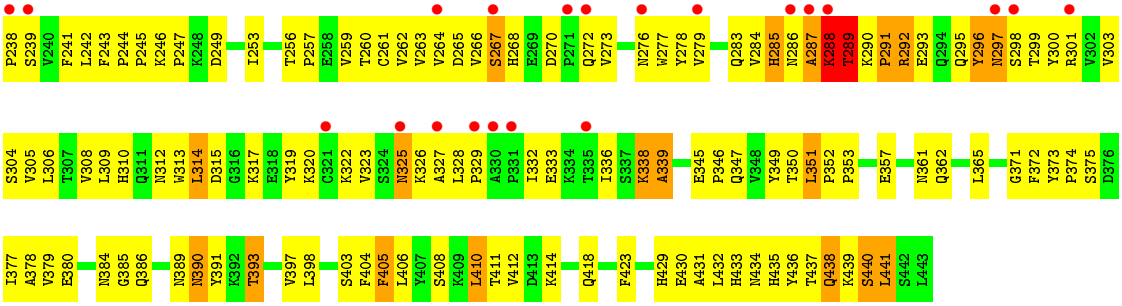
Chain A:





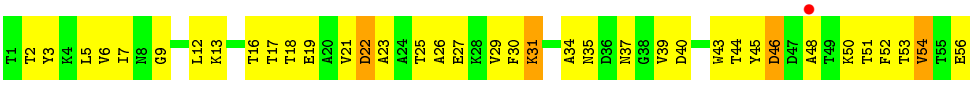
- Molecule 1: IGG1 MO61 FC

Chain B:



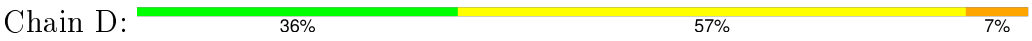
- Molecule 2: STREPTOCOCCAL PROTEIN G (C2 FRAGMENT)

Chain C:



- Molecule 2: STREPTOCOCCAL PROTEIN G (C2 FRAGMENT)

Chain D:




T1
T2
Y3
K4
L5
V6
I7
N8
G9
L12
K13
T16
T17
T18
E19
A20
V21
D22
A23
A24
T25
A26
E27
K28
V29
F30
K31
A34
N35
V39
D40
W43
T44
Y45
D46
D47
A48
T49
K50
T51
F52
T53
V54
T55
E56

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	110.60Å 110.60Å 160.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 18.35 – 3.20	Depositor EDS
% Data completeness (in resolution range)	72.0 (8.00-3.20) 72.7 (18.35-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.289 , 0.357 0.294 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	87.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 58.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 12297 reflections	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	4180	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.80	1/1702 (0.1%)	0.94	1/2316 (0.0%)
1	B	0.81	1/1702 (0.1%)	0.94	1/2316 (0.0%)
2	C	0.73	0/440	0.92	0/597
2	D	0.73	0/440	0.92	0/597
All	All	0.79	2/4284 (0.0%)	0.94	2/5826 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	GLU	CG-CD	5.22	1.59	1.51
1	A	293	GLU	CG-CD	5.20	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	288	LYS	N-CA-C	-8.45	88.18	111.00
1	A	288	LYS	N-CA-C	-8.44	88.20	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1656	0	1630	161	1
1	B	1656	0	1630	159	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	434	0	415	39	1
2	D	434	0	415	40	0
All	All	4180	0	4090	368	2

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 44.

The worst 5 of 368 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:357:GLU:HG3	1:B:349:TYR:CZ	1.85	1.10
1:A:371:GLY:HA2	1:A:403:SER:OG	1.73	0.89
1:A:357:GLU:HG3	1:B:349:TYR:OH	1.72	0.89
1:B:371:GLY:HA2	1:B:403:SER:OG	1.73	0.87
1:B:375:SER:HB3	1:B:404:PHE:CZ	2.10	0.86

All (2) 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)
1:A:286:ASN:OD1	1:A:361:ASN:ND2[5_544]	1.95	0.25
2:C:37:ASN:ND2	2:C:37:ASN:ND2[7_555]	2.18	0.02

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	204/206 (99%)	171 (84%)	19 (9%)	14 (7%)	1 10
1	B	204/206 (99%)	171 (84%)	19 (9%)	14 (7%)	1 10
2	C	54/56 (96%)	45 (83%)	7 (13%)	2 (4%)	4 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	54/56 (96%)	45 (83%)	7 (13%)	2 (4%)	4 29
All	All	516/524 (98%)	432 (84%)	52 (10%)	32 (6%)	2 14

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	LYS
1	A	291	PRO
1	A	292	ARG
1	A	298	SER
2	C	46	ASP

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	193/193 (100%)	175 (91%)	18 (9%)	11 41
1	B	193/193 (100%)	175 (91%)	18 (9%)	11 41
2	C	46/46 (100%)	42 (91%)	4 (9%)	13 45
2	D	46/46 (100%)	42 (91%)	4 (9%)	13 45
All	All	478/478 (100%)	434 (91%)	44 (9%)	11 41

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	22	ASP
1	B	288	LYS
2	D	19	GLU
2	C	31	LYS
1	B	256	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	32	GLN
1	B	276	ASN
1	B	311	GLN
1	A	390	ASN
1	A	418	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 carbohydrates in this entry.

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

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, 95^{th} 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	206/206 (100%)	-0.18	1 (0%) 91 87	2, 37, 83, 125	0
1	B	206/206 (100%)	0.33	21 (10%) 9 5	2, 37, 83, 125	0
2	C	56/56 (100%)	0.01	1 (1%) 71 58	2, 39, 73, 86	0
2	D	56/56 (100%)	0.00	0 100 100	2, 39, 73, 86	0
All	All	524/524 (100%)	0.06	23 (4%) 38 24	2, 38, 83, 125	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	SER	7.0
1	B	239	SER	6.1
1	B	238	PRO	5.0
1	B	330	ALA	4.0
1	B	331	PRO	3.7

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.