wwPDB X-ray Structure Validation Summary Report (i)

Jun 1, 2021 – 12:11 PM EDT

PDB ID	:	7KE1
Title	:	Factor H enhancing human antibody fragment (Fab) to meningococcal Factor H binding protein
Authors	:	Beernink, P.T.; Sands, N.
Deposited on	:	2020-10-09
Resolution	:	1.50 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 (i) symbol.

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

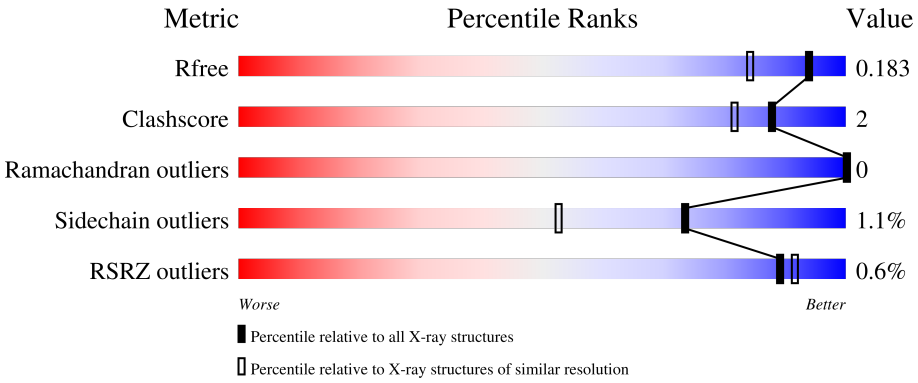
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.19
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.19

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 <=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	B	217	% 92% 7% ·
1	D	217	92% 7% ·
2	A	235	89% · 8%
2	C	235	89% · 8%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14285 atoms, of which 6659 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.

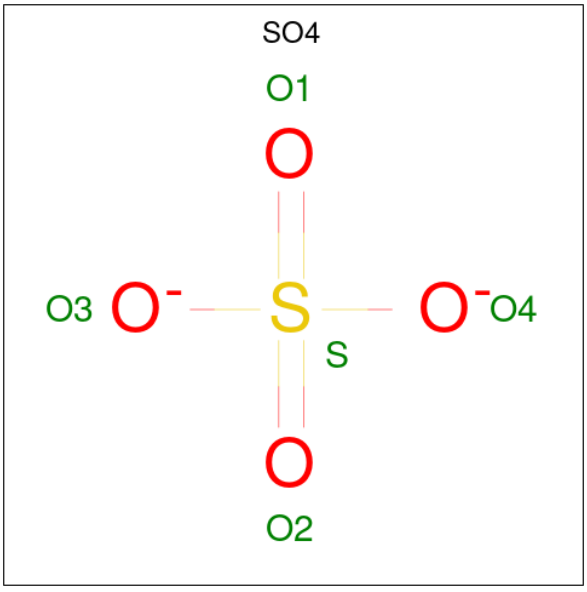
- Molecule 1 is a protein called Immunoglobulin gamma, kappa light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	214	Total	C	H	N	O	S	0	13	0
			3375	1068	1680	280	342	5			
1	D	214	Total	C	H	N	O	S	0	12	0
			3376	1067	1682	283	339	5			

- Molecule 2 is a protein called Immunoglobulin gamma, heavy chain Fd fragment.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	217	Total	C	H	N	O	S	0	10	0
			3303	1044	1651	272	325	11			
2	C	216	Total	C	H	N	O	S	0	9	0
			3294	1042	1646	274	322	10			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0

- Molecule 5 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Li 1 1	0	0
5	C	1	Total Li 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	220	Total O 220 220	0	0
7	A	238	Total O 238 238	0	0

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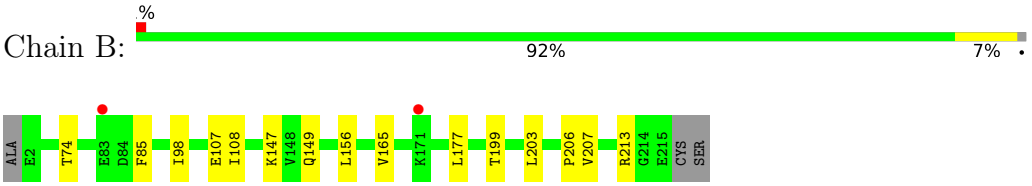
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	214	Total O 214 214	0	0
7	C	226	Total O 226 226	0	0

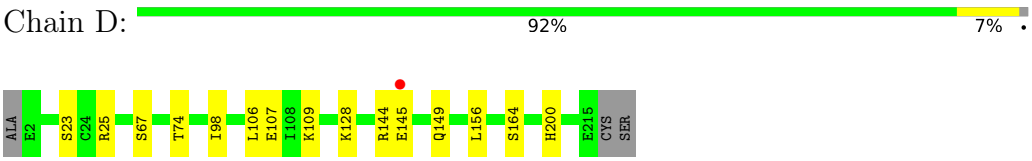
3 Residue-property plots (i)

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.

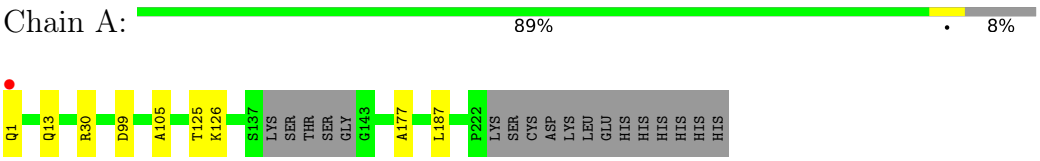
• Molecule 1: Immunoglobulin gamma, kappa light chain



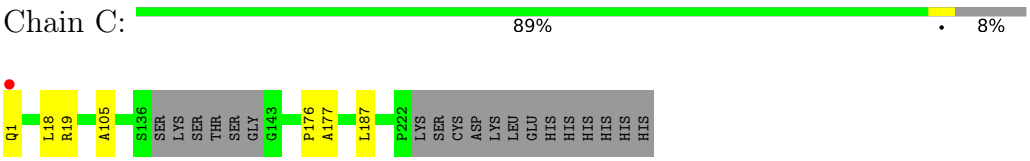
• Molecule 1: Immunoglobulin gamma, kappa light chain



• Molecule 2: Immunoglobulin gamma, heavy chain Fd fragment



• Molecule 2: Immunoglobulin gamma, heavy chain Fd fragment



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.77Å 97.26Å 70.47Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	70.47 – 1.50 70.47 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (70.47-1.50) 98.0 (70.47-1.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.162 , 0.183 0.162 , 0.183	Depositor DCC
R_{free} test set	1441 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 30.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.006 for l,k,-h 0.159 for h,-k,-l 0.021 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14285	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, NA, LI, 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	B	0.61	1/1770 (0.1%)	0.75	0/2404
1	D	0.57	0/1766	0.74	2/2396 (0.1%)
2	A	0.56	0/1719	0.72	0/2342
2	C	0.60	3/1712 (0.2%)	0.74	1/2333 (0.0%)
All	All	0.59	4/6967 (0.1%)	0.74	3/9475 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	213	ARG	C-O	-6.14	1.11	1.23
2	C	19[A]	ARG	C-O	5.75	1.34	1.23
2	C	19[B]	ARG	C-O	5.75	1.34	1.23
2	C	18	LEU	C-O	-5.28	1.13	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	144	ARG	C-N-CA	-6.02	106.65	121.70
1	D	25	ARG	NE-CZ-NH1	-5.57	117.52	120.30
2	C	1	GLN	CB-CA-C	5.34	121.09	110.40

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	B	1695	1680	1680	10	0
1	D	1694	1682	1682	8	0
2	A	1652	1651	1651	6	0
2	C	1648	1646	1646	5	0
3	A	10	0	0	0	0
3	B	15	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
7	A	238	0	0	4	0
7	B	220	0	0	2	1
7	C	226	0	0	2	1
7	D	214	0	0	2	0
All	All	7626	6659	6659	27	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 2.

The worst 5 of 27 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)
3:C:301:SO4:O2	7:C:401:HOH:O	2.08	0.72
1:B:199[A]:THR:HG21	7:B:536:HOH:O	1.90	0.71
1:B:199[A]:THR:HG22	1:B:206:PRO:HG3	1.72	0.69
2:A:126:LYS:HE2	7:A:420:HOH:O	1.94	0.65
1:D:74[B]:THR:HG23	7:D:496:HOH:O	2.02	0.59

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)
7:B:420:HOH:O	7:C:441:HOH:O[1_656]	1.86	0.34

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	B	225/217 (104%)	220 (98%)	5 (2%)	0	100	100
1	D	224/217 (103%)	220 (98%)	4 (2%)	0	100	100
2	A	223/235 (95%)	219 (98%)	4 (2%)	0	100	100
2	C	221/235 (94%)	218 (99%)	3 (1%)	0	100	100
All	All	893/904 (99%)	877 (98%)	16 (2%)	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	B	198/187 (106%)	197 (100%)	1 (0%)	88	78
1	D	197/187 (105%)	193 (98%)	4 (2%)	55	25
2	A	193/200 (96%)	189 (98%)	4 (2%)	53	23
2	C	191/200 (96%)	191 (100%)	0	100	100
All	All	779/774 (101%)	770 (99%)	9 (1%)	73	48

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	109	LYS
1	D	128	LYS
2	A	13[B]	GLN

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Mol	Chain	Res	Type
2	A	99	ASP
1	D	106	LEU

Sometimes 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, 4 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
3	SO4	A	302	-	4,4,4	0.16	0	6,6,6	0.11	0
3	SO4	A	301	-	4,4,4	0.24	0	6,6,6	0.26	0
3	SO4	B	303	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	D	301	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	B	301	-	4,4,4	0.31	0	6,6,6	0.20	0
3	SO4	C	301	-	4,4,4	0.52	0	6,6,6	0.12	0
3	SO4	B	302	-	4,4,4	0.16	0	6,6,6	0.11	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	SO4	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

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	B	214/217 (98%)	-0.38	2 (0%)	84	87	13, 20, 33, 52	0
1	D	214/217 (98%)	-0.41	1 (0%)	91	93	14, 21, 35, 50	0
2	A	217/235 (92%)	-0.51	1 (0%)	91	93	12, 19, 32, 55	0
2	C	216/235 (91%)	-0.46	1 (0%)	91	93	14, 21, 34, 46	0
All	All	861/904 (95%)	-0.44	5 (0%)	89	91	12, 20, 34, 55	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1	GLN	3.7
2	A	1	GLN	2.9
1	D	145	GLU	2.8
1	B	83	GLU	2.5
1	B	171	LYS	2.1

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 monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
3	SO4	C	301	5/5	0.81	0.15	50,61,64,93	0
5	LI	A	303	1/1	0.86	0.66	21,21,21,21	0
3	SO4	A	302	5/5	0.93	0.13	57,63,70,78	0
4	NA	B	304	1/1	0.94	0.09	31,31,31,31	0
3	SO4	B	303	5/5	0.94	0.07	53,57,64,67	0
5	LI	C	302	1/1	0.94	0.68	16,16,16,16	0
6	CL	A	304	1/1	0.94	0.05	50,50,50,50	0
3	SO4	B	302	5/5	0.96	0.10	50,65,66,66	0
3	SO4	D	301	5/5	0.97	0.13	43,49,54,56	0
3	SO4	A	301	5/5	0.97	0.07	39,40,41,47	0
3	SO4	B	301	5/5	0.99	0.11	33,37,40,42	0

6.5 Other polymers (i)

There are no such residues in this entry.