wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 05:00 PM EDT

PDB ID	:	5O1R
Title	:	human Fab 5H2 bound to NHBA-C3 from Neisseria meningitidis serogroup B
Authors	:	Malito, E.; Maritan, M.
Deposited on	:	2017-05-19
Resolution	:	2.86 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

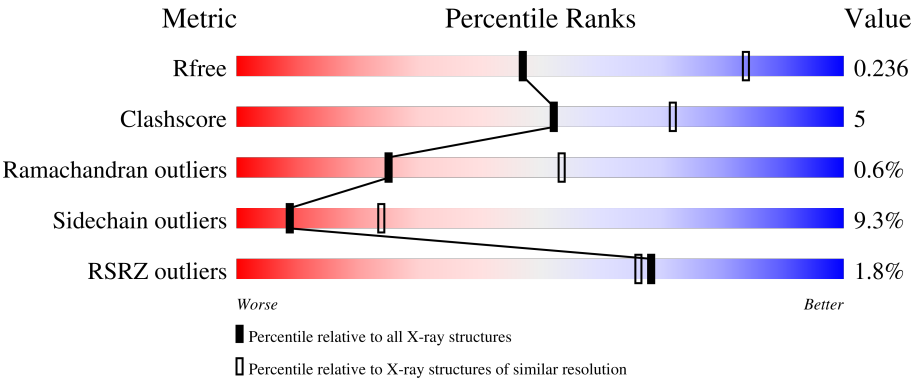
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.86 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	A	127	80% 9% • 9%
1	B	127	75% 14% • 9%
2	H	265	67% 15% • 15%
2	I	265	3% 68% 13% • 17%
3	L	213	79% 19% ••

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Mol	Chain	Length	Quality of chain
3	M	213	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8356 atoms, of which 30 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 GNA2132.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	0	0
			862	540	152	168	2			
1	B	115	Total	C	N	O	S	0	1	0
			869	544	153	170	2			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	MET	-	initiating methionine	UNP Q9JPP1
A	310	ALA	-	expression tag	UNP Q9JPP1
A	311	SER	-	expression tag	UNP Q9JPP1
A	428	LEU	-	expression tag	UNP Q9JPP1
A	429	GLU	-	expression tag	UNP Q9JPP1
A	430	HIS	-	expression tag	UNP Q9JPP1
A	431	HIS	-	expression tag	UNP Q9JPP1
A	432	HIS	-	expression tag	UNP Q9JPP1
A	433	HIS	-	expression tag	UNP Q9JPP1
A	434	HIS	-	expression tag	UNP Q9JPP1
A	435	HIS	-	expression tag	UNP Q9JPP1
B	309	MET	-	initiating methionine	UNP Q9JPP1
B	310	ALA	-	expression tag	UNP Q9JPP1
B	311	SER	-	expression tag	UNP Q9JPP1
B	428	LEU	-	expression tag	UNP Q9JPP1
B	429	GLU	-	expression tag	UNP Q9JPP1
B	430	HIS	-	expression tag	UNP Q9JPP1
B	431	HIS	-	expression tag	UNP Q9JPP1
B	432	HIS	-	expression tag	UNP Q9JPP1
B	433	HIS	-	expression tag	UNP Q9JPP1
B	434	HIS	-	expression tag	UNP Q9JPP1
B	435	HIS	-	expression tag	UNP Q9JPP1

- Molecule 2 is a protein called IGH@ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	0	0
			1675	1055	278	336	6			
2	I	221	Total	C	N	O	S	0	0	0
			1641	1036	272	328	5			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	29	VAL	ILE	conflict	UNP Q6GMX6
H	31	SER	-	insertion	UNP Q6GMX6
H	32	GLY	-	insertion	UNP Q6GMX6
H	33	SER	GLY	conflict	UNP Q6GMX6
H	34	SER	TYR	conflict	UNP Q6GMX6
H	37	THR	SER	conflict	UNP Q6GMX6
H	42	THR	PRO	conflict	UNP Q6GMX6
H	43	PRO	ALA	conflict	UNP Q6GMX6
H	52	TYR	ARG	conflict	UNP Q6GMX6
H	53	THR	ILE	conflict	UNP Q6GMX6
H	54	SER	TYR	conflict	UNP Q6GMX6
H	55	TYR	THR	conflict	UNP Q6GMX6
H	60	LYS	ASN	conflict	UNP Q6GMX6
H	71	LEU	MET	conflict	UNP Q6GMX6
H	75	MET	THR	conflict	UNP Q6GMX6
H	85	LYS	SER	conflict	UNP Q6GMX6
H	96	PHE	TYR	conflict	UNP Q6GMX6
H	100	ASP	GLY	conflict	UNP Q6GMX6
H	103	ASP	-	insertion	UNP Q6GMX6
H	104	VAL	-	insertion	UNP Q6GMX6
H	105	ALA	-	insertion	UNP Q6GMX6
H	106	SER	-	insertion	UNP Q6GMX6
H	107	GLY	-	insertion	UNP Q6GMX6
H	108	SER	THR	conflict	UNP Q6GMX6
H	109	SER	TYR	conflict	UNP Q6GMX6
H	112	PHE	TYR	conflict	UNP Q6GMX6
H	220	ARG	LYS	conflict	UNP Q6GMX6
H	229	GLY	-	expression tag	UNP Q6GMX6
H	230	SER	-	expression tag	UNP Q6GMX6
H	231	GLU	-	expression tag	UNP Q6GMX6
H	232	ASN	-	expression tag	UNP Q6GMX6
H	233	LEU	-	expression tag	UNP Q6GMX6
H	234	TYR	-	expression tag	UNP Q6GMX6
H	235	PHE	-	expression tag	UNP Q6GMX6
H	236	GLN	-	expression tag	UNP Q6GMX6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	237	GLY	-	expression tag	UNP Q6GMX6
H	238	SER	-	expression tag	UNP Q6GMX6
H	239	TRP	-	expression tag	UNP Q6GMX6
H	240	SER	-	expression tag	UNP Q6GMX6
H	241	HIS	-	expression tag	UNP Q6GMX6
H	242	PRO	-	expression tag	UNP Q6GMX6
H	243	GLN	-	expression tag	UNP Q6GMX6
H	244	PHE	-	expression tag	UNP Q6GMX6
H	245	GLU	-	expression tag	UNP Q6GMX6
H	246	LYS	-	expression tag	UNP Q6GMX6
H	247	GLY	-	expression tag	UNP Q6GMX6
H	248	GLY	-	expression tag	UNP Q6GMX6
H	249	SER	-	expression tag	UNP Q6GMX6
H	250	GLY	-	expression tag	UNP Q6GMX6
H	251	GLY	-	expression tag	UNP Q6GMX6
H	252	GLY	-	expression tag	UNP Q6GMX6
H	253	SER	-	expression tag	UNP Q6GMX6
H	254	GLY	-	expression tag	UNP Q6GMX6
H	255	GLY	-	expression tag	UNP Q6GMX6
H	256	GLY	-	expression tag	UNP Q6GMX6
H	257	SER	-	expression tag	UNP Q6GMX6
H	258	TRP	-	expression tag	UNP Q6GMX6
H	259	SER	-	expression tag	UNP Q6GMX6
H	260	HIS	-	expression tag	UNP Q6GMX6
H	261	PRO	-	expression tag	UNP Q6GMX6
H	262	GLN	-	expression tag	UNP Q6GMX6
H	263	PHE	-	expression tag	UNP Q6GMX6
H	264	GLU	-	expression tag	UNP Q6GMX6
H	265	LYS	-	expression tag	UNP Q6GMX6
I	29	VAL	ILE	conflict	UNP Q6GMX6
I	31	SER	-	insertion	UNP Q6GMX6
I	32	GLY	-	insertion	UNP Q6GMX6
I	33	SER	GLY	conflict	UNP Q6GMX6
I	34	SER	TYR	conflict	UNP Q6GMX6
I	37	THR	SER	conflict	UNP Q6GMX6
I	42	THR	PRO	conflict	UNP Q6GMX6
I	43	PRO	ALA	conflict	UNP Q6GMX6
I	52	TYR	ARG	conflict	UNP Q6GMX6
I	53	THR	ILE	conflict	UNP Q6GMX6
I	54	SER	TYR	conflict	UNP Q6GMX6
I	55	TYR	THR	conflict	UNP Q6GMX6
I	60	LYS	ASN	conflict	UNP Q6GMX6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	71	LEU	MET	conflict	UNP Q6GMX6
I	75	MET	THR	conflict	UNP Q6GMX6
I	85	LYS	SER	conflict	UNP Q6GMX6
I	96	PHE	TYR	conflict	UNP Q6GMX6
I	100	ASP	GLY	conflict	UNP Q6GMX6
I	103	ASP	-	insertion	UNP Q6GMX6
I	104	VAL	-	insertion	UNP Q6GMX6
I	105	ALA	-	insertion	UNP Q6GMX6
I	106	SER	-	insertion	UNP Q6GMX6
I	107	GLY	-	insertion	UNP Q6GMX6
I	108	SER	THR	conflict	UNP Q6GMX6
I	109	SER	TYR	conflict	UNP Q6GMX6
I	112	PHE	TYR	conflict	UNP Q6GMX6
I	220	ARG	LYS	conflict	UNP Q6GMX6
I	229	GLY	-	expression tag	UNP Q6GMX6
I	230	SER	-	expression tag	UNP Q6GMX6
I	231	GLU	-	expression tag	UNP Q6GMX6
I	232	ASN	-	expression tag	UNP Q6GMX6
I	233	LEU	-	expression tag	UNP Q6GMX6
I	234	TYR	-	expression tag	UNP Q6GMX6
I	235	PHE	-	expression tag	UNP Q6GMX6
I	236	GLN	-	expression tag	UNP Q6GMX6
I	237	GLY	-	expression tag	UNP Q6GMX6
I	238	SER	-	expression tag	UNP Q6GMX6
I	239	TRP	-	expression tag	UNP Q6GMX6
I	240	SER	-	expression tag	UNP Q6GMX6
I	241	HIS	-	expression tag	UNP Q6GMX6
I	242	PRO	-	expression tag	UNP Q6GMX6
I	243	GLN	-	expression tag	UNP Q6GMX6
I	244	PHE	-	expression tag	UNP Q6GMX6
I	245	GLU	-	expression tag	UNP Q6GMX6
I	246	LYS	-	expression tag	UNP Q6GMX6
I	247	GLY	-	expression tag	UNP Q6GMX6
I	248	GLY	-	expression tag	UNP Q6GMX6
I	249	SER	-	expression tag	UNP Q6GMX6
I	250	GLY	-	expression tag	UNP Q6GMX6
I	251	GLY	-	expression tag	UNP Q6GMX6
I	252	GLY	-	expression tag	UNP Q6GMX6
I	253	SER	-	expression tag	UNP Q6GMX6
I	254	GLY	-	expression tag	UNP Q6GMX6
I	255	GLY	-	expression tag	UNP Q6GMX6
I	256	GLY	-	expression tag	UNP Q6GMX6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	257	SER	-	expression tag	UNP Q6GMX6
I	258	TRP	-	expression tag	UNP Q6GMX6
I	259	SER	-	expression tag	UNP Q6GMX6
I	260	HIS	-	expression tag	UNP Q6GMX6
I	261	PRO	-	expression tag	UNP Q6GMX6
I	262	GLN	-	expression tag	UNP Q6GMX6
I	263	PHE	-	expression tag	UNP Q6GMX6
I	264	GLU	-	expression tag	UNP Q6GMX6
I	265	LYS	-	expression tag	UNP Q6GMX6

- Molecule 3 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1602	998	272	327	5			
3	M	212	Total	C	N	O	S	0	0	0
			1611	1003	273	330	5			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	GLU	ASP	conflict	UNP Q6GMX0
L	3	VAL	GLN	conflict	UNP Q6GMX0
L	7	THR	SER	conflict	UNP Q6GMX0
L	28	SER	ASN	conflict	UNP Q6GMX0
L	30	SER	ASN	conflict	UNP Q6GMX0
L	38	GLN	LEU	conflict	UNP Q6GMX0
L	42	THR	LYS	conflict	UNP Q6GMX0
L	45	LYS	ASN	conflict	UNP Q6GMX0
L	48	THR	ILE	conflict	UNP Q6GMX0
L	55	GLY	GLN	conflict	UNP Q6GMX0
L	71	LEU	PHE	conflict	UNP Q6GMX0
L	81	GLU	ASP	conflict	UNP Q6GMX0
L	93	GLY	ASN	conflict	UNP Q6GMX0
L	94	SER	ILE	conflict	UNP Q6GMX0
L	?	-	LEU	deletion	UNP Q6GMX0
L	99	GLN	GLY	conflict	UNP Q6GMX0
L	102	LYS	ASN	conflict	UNP Q6GMX0
L	103	LEU	VAL	conflict	UNP Q6GMX0
L	106	ARG	LYS	conflict	UNP Q6GMX0
M	1	GLU	ASP	conflict	UNP Q6GMX0
M	3	VAL	GLN	conflict	UNP Q6GMX0

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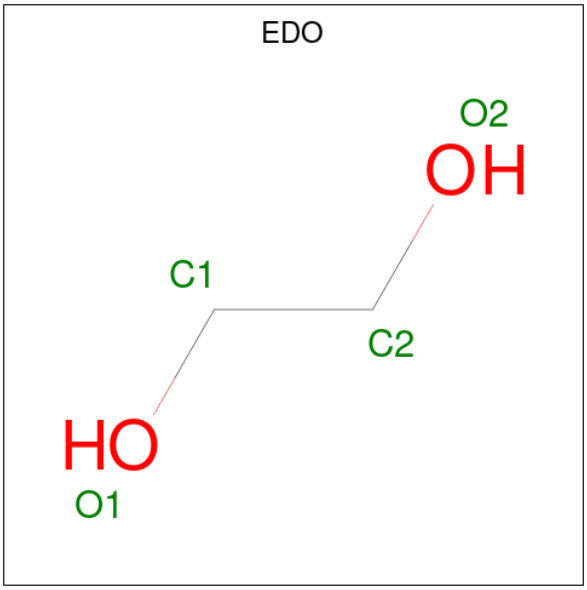
Chain	Residue	Modelled	Actual	Comment	Reference
M	7	THR	SER	conflict	UNP Q6GMX0
M	28	SER	ASN	conflict	UNP Q6GMX0
M	30	SER	ASN	conflict	UNP Q6GMX0
M	38	GLN	LEU	conflict	UNP Q6GMX0
M	42	THR	LYS	conflict	UNP Q6GMX0
M	45	LYS	ASN	conflict	UNP Q6GMX0
M	48	THR	ILE	conflict	UNP Q6GMX0
M	55	GLY	GLN	conflict	UNP Q6GMX0
M	71	LEU	PHE	conflict	UNP Q6GMX0
M	81	GLU	ASP	conflict	UNP Q6GMX0
M	93	GLY	ASN	conflict	UNP Q6GMX0
M	94	SER	ILE	conflict	UNP Q6GMX0
M	?	-	LEU	deletion	UNP Q6GMX0
M	99	GLN	GLY	conflict	UNP Q6GMX0
M	102	LYS	ASN	conflict	UNP Q6GMX0
M	103	LEU	VAL	conflict	UNP Q6GMX0
M	106	ARG	LYS	conflict	UNP Q6GMX0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	H	1	Total	C	H	O	0	0
			10	2	6	2		
4	I	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	M	1	Total	C	H	O	0	0
			10	2	6	2		
4	M	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is water.

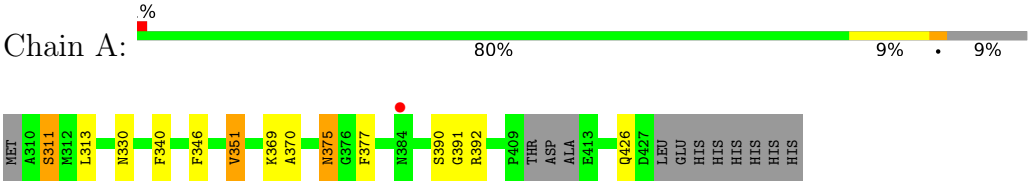
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	B	5	Total	O	0	0
			5	5		
5	H	11	Total	O	0	0
			11	11		
5	I	8	Total	O	0	0
			8	8		
5	L	10	Total	O	0	0
			10	10		
5	M	10	Total	O	0	0
			10	10		

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.

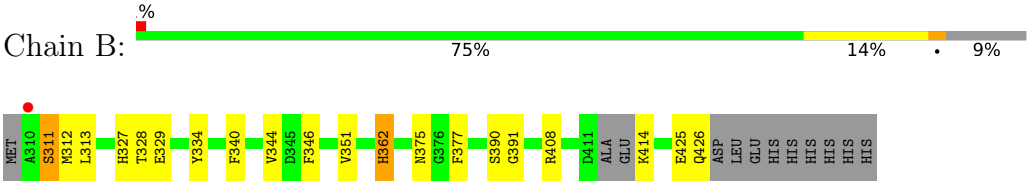
• Molecule 1: GNA2132

Chain A:



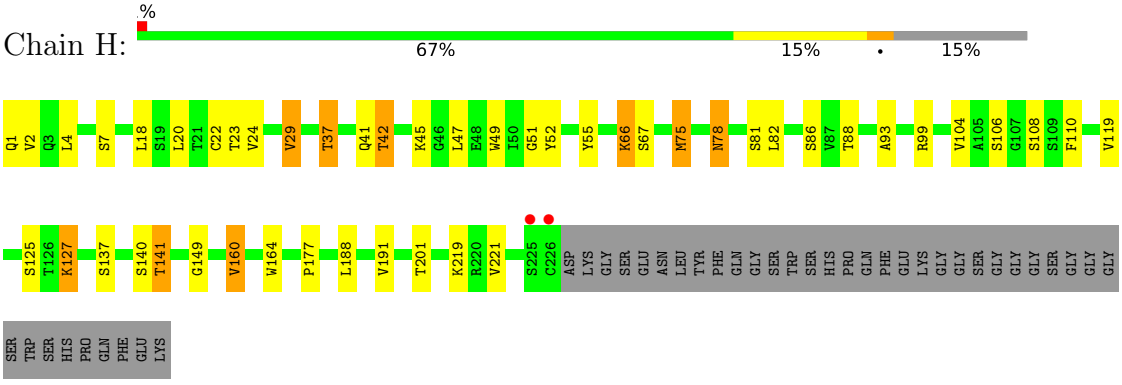
• Molecule 1: GNA2132

Chain B:



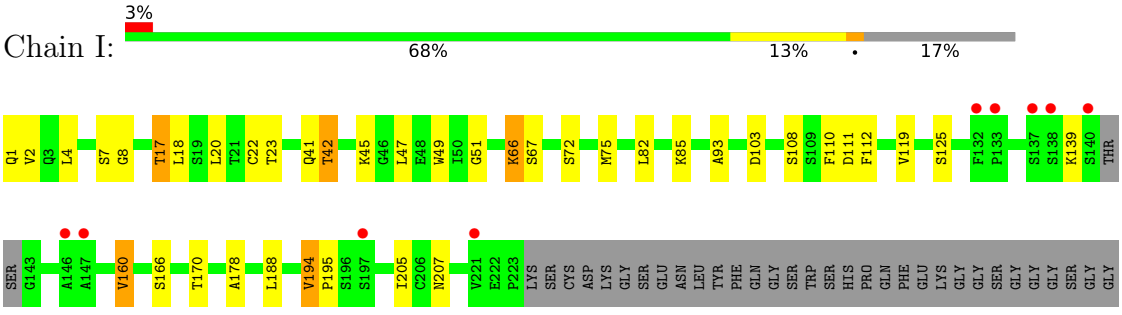
• Molecule 2: IGH@ protein

Chain H:



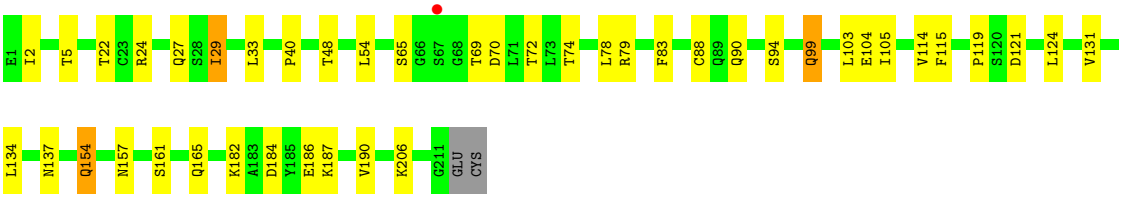
• Molecule 2: IGH@ protein

Chain I:



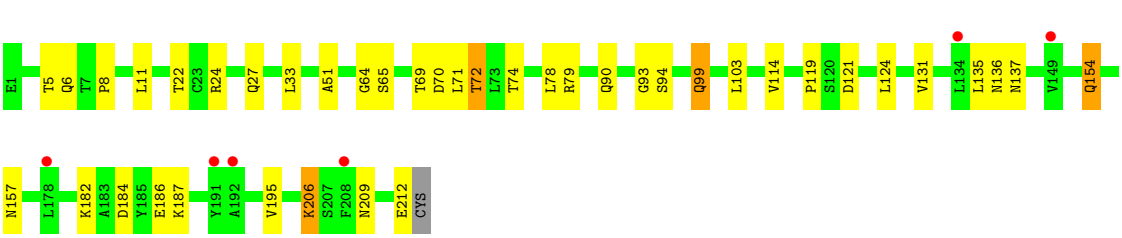
• Molecule 3: Uncharacterized protein

Chain L:



• Molecule 3: Uncharacterized protein

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.45Å 119.45Å 364.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	78.74 – 2.86 78.74 – 2.86	Depositor EDS
% Data completeness (in resolution range)	100.0 (78.74-2.86) 100.0 (78.74-2.86)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.178 , 0.222 0.190 , 0.236	Depositor DCC
R_{free} test set	1775 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	77.1	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 61.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8356	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: EDO

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	0.51	0/882	0.73	0/1181
1	B	0.53	0/889	0.76	0/1191
2	H	0.54	0/1715	0.81	1/2337 (0.0%)
2	I	0.53	0/1680	0.82	2/2289 (0.1%)
3	L	0.48	0/1635	0.78	0/2222
3	M	0.49	0/1644	0.74	0/2234
All	All	0.51	0/8445	0.78	3/11454 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	110	PHE	C-N-CA	6.05	136.83	121.70
2	I	110	PHE	C-N-CA	5.79	136.18	121.70
2	I	111	ASP	N-CA-CB	-5.16	101.32	110.60

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	862	0	805	4	0
1	B	869	0	811	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1675	0	1653	19	0
2	I	1641	0	1617	14	0
3	L	1602	0	1562	23	0
3	M	1611	0	1568	23	0
4	A	4	6	6	0	0
4	H	4	6	6	1	0
4	I	4	6	6	0	0
4	M	8	12	12	0	0
5	A	2	0	0	0	0
5	B	5	0	0	0	0
5	H	11	0	0	0	0
5	I	8	0	0	0	0
5	L	10	0	0	0	0
5	M	10	0	0	0	0
All	All	8326	30	8046	89	0

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 5.

The worst 5 of 89 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:L:105:ILE:H	3:L:165:GLN:HE22	1.19	0.89
3:M:99:GLN:HE21	3:M:99:GLN:H	1.22	0.84
1:B:311:SER:HB2	1:B:375:ASN:HD21	1.41	0.84
3:L:99:GLN:HE21	3:L:99:GLN:H	1.23	0.84
3:M:90:GLN:NE2	3:M:93:GLY:H	1.75	0.83

There are no symmetry-related clashes.

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	111/127 (87%)	105 (95%)	6 (5%)	0	100	100
1	B	112/127 (88%)	108 (96%)	4 (4%)	0	100	100
2	H	224/265 (84%)	216 (96%)	6 (3%)	2 (1%)	17	43
2	I	217/265 (82%)	208 (96%)	7 (3%)	2 (1%)	17	43
3	L	209/213 (98%)	202 (97%)	6 (3%)	1 (0%)	29	57
3	M	210/213 (99%)	203 (97%)	6 (3%)	1 (0%)	29	57
All	All	1083/1210 (90%)	1042 (96%)	35 (3%)	6 (1%)	25	53

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	66	LYS
2	I	66	LYS
2	I	139	LYS
3	L	137	ASN
3	M	137	ASN

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	83/94 (88%)	74 (89%)	9 (11%)	6	17
1	B	84/94 (89%)	74 (88%)	10 (12%)	5	13
2	H	195/224 (87%)	173 (89%)	22 (11%)	6	16
2	I	190/224 (85%)	173 (91%)	17 (9%)	9	26
3	L	183/186 (98%)	168 (92%)	15 (8%)	11	29
3	M	184/186 (99%)	171 (93%)	13 (7%)	14	36
All	All	919/1008 (91%)	833 (91%)	86 (9%)	9	23

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	205	ILE

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Mol	Chain	Res	Type
3	L	154	GLN
3	L	24	ARG
3	L	72	THR
3	M	27	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	136	ASN
3	M	157	ASN
3	M	209	ASN
3	M	159	GLN
3	L	37	GLN

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)

5 ligands 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	$\#\|Z\|>2$
4	EDO	A	501	-	3,3,3	1.10	0	2,2,2	0.13	0
4	EDO	H	301	-	3,3,3	0.86	0	2,2,2	0.10	0
4	EDO	M	302	-	3,3,3	0.67	0	2,2,2	0.16	0
4	EDO	M	301	-	3,3,3	0.45	0	2,2,2	0.42	0
4	EDO	I	301	-	3,3,3	0.96	0	2,2,2	0.04	0

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
4	EDO	A	501	-	-	0/1/1/1	-
4	EDO	H	301	-	-	0/1/1/1	-
4	EDO	M	302	-	-	1/1/1/1	-
4	EDO	M	301	-	-	0/1/1/1	-
4	EDO	I	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	301	EDO	O1-C1-C2-O2
4	M	302	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	301	EDO	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	A	115/127 (90%)	0.23	1 (0%)	84	84	62, 83, 127, 155	0
1	B	115/127 (90%)	0.20	1 (0%)	84	84	58, 77, 127, 147	0
2	H	226/265 (85%)	0.04	2 (0%)	84	84	58, 77, 115, 158	0
2	I	221/265 (83%)	0.29	9 (4%)	37	31	47, 78, 129, 161	0
3	L	211/213 (99%)	0.20	1 (0%)	91	90	62, 85, 116, 137	0
3	M	212/213 (99%)	0.29	6 (2%)	53	48	55, 78, 134, 150	0
All	All	1100/1210 (90%)	0.21	20 (1%)	68	66	47, 80, 127, 161	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	140	SER	5.9
1	B	310	ALA	4.4
3	M	191	TYR	4.3
2	H	226	CYS	4.0
1	A	384	ASN	3.4

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 (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, 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
4	EDO	I	301	4/4	0.46	0.23	101,104,104,104	0
4	EDO	H	301	4/4	0.80	0.16	103,104,104,104	0
4	EDO	A	501	4/4	0.81	0.36	68,74,75,75	0
4	EDO	M	302	4/4	0.87	0.16	99,102,106,106	0
4	EDO	M	301	4/4	0.89	0.15	71,71,77,77	0

6.5 Other polymers (i)

There are no such residues in this entry.