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wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 10:04 AM EDT

PDB ID	:	6I04
Title	:	Crystal structure of Sema domain of the Met receptor in complex with FAB
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	:	2018-10-25
Resolution	:	3.10 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 (i)) were used in the production of this report:

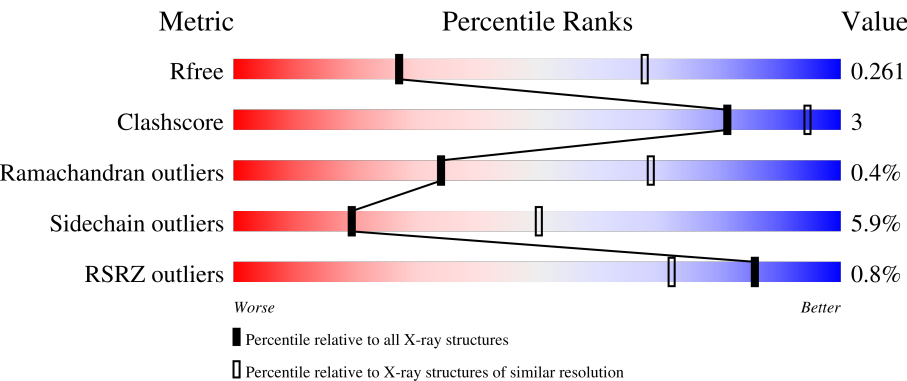|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.10 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	Percentile Ranks	Value
Rfree		0.261
Clashscore		3
Ramachandran outliers		0.4%
Sidechain outliers		5.9%
RSRZ outliers		0.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	552	69% 10% • 20%
1	B	552	70% 8% • 22%
2	C	230	83% 9% 7%
2	H	230	83% 8% 8%
3	D	214	90% 9% •

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Mol	Chain	Length	Quality of chain
3	L	214	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 13366 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 Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3512	2241	588	662	21			
1	B	432	Total	C	N	O	S	0	0	0
			3439	2194	576	648	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	565	GLY	-	expression tag	UNP P08581
A	566	GLY	-	expression tag	UNP P08581
A	567	GLY	-	expression tag	UNP P08581
A	568	GLY	-	expression tag	UNP P08581
A	569	GLY	-	expression tag	UNP P08581
A	570	SER	-	expression tag	UNP P08581
A	571	HIS	-	expression tag	UNP P08581
A	572	HIS	-	expression tag	UNP P08581
A	573	HIS	-	expression tag	UNP P08581
A	574	HIS	-	expression tag	UNP P08581
A	575	HIS	-	expression tag	UNP P08581
A	576	HIS	-	expression tag	UNP P08581
B	565	GLY	-	expression tag	UNP P08581
B	566	GLY	-	expression tag	UNP P08581
B	567	GLY	-	expression tag	UNP P08581
B	568	GLY	-	expression tag	UNP P08581
B	569	GLY	-	expression tag	UNP P08581
B	570	SER	-	expression tag	UNP P08581
B	571	HIS	-	expression tag	UNP P08581
B	572	HIS	-	expression tag	UNP P08581
B	573	HIS	-	expression tag	UNP P08581
B	574	HIS	-	expression tag	UNP P08581
B	575	HIS	-	expression tag	UNP P08581
B	576	HIS	-	expression tag	UNP P08581

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	211	Total	C	N	O	S	0	0	0
			1588	1016	255	312	5			
2	C	214	Total	C	N	O	S	0	0	0
			1609	1028	259	317	5			

- Molecule 3 is a protein called Fab light chain.

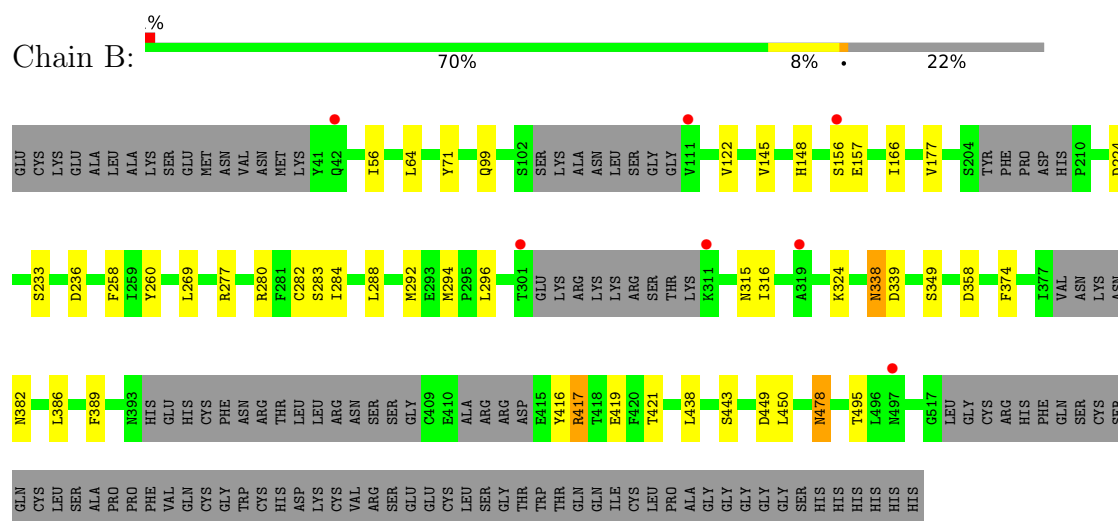| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1609	1009	270	325	5			
3	D	212	Total	C	N	O	S	0	0	0
			1609	1009	270	325	5			

3 Residue-property plots ⓘ

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.
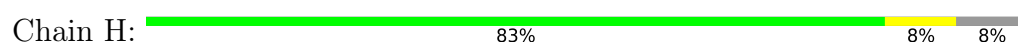
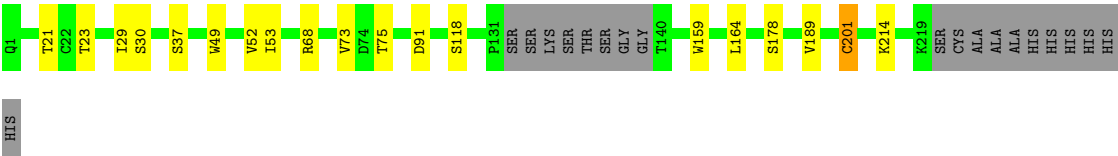• Molecule 1: Hepatocyte growth factor receptor

Chain A:

• Molecule 1: Hepatocyte growth factor receptor

Chain B:

• Molecule 2: Fab heavy chain

Chain H:

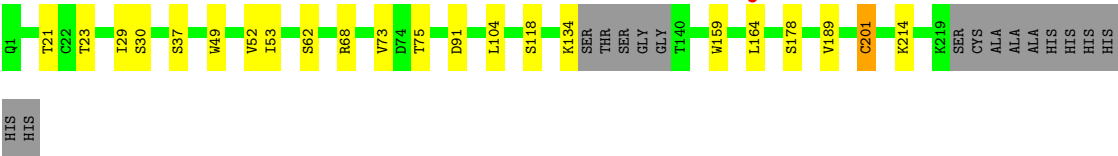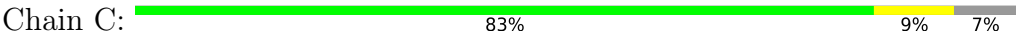Q1 T21 C22 T23 I29 S30 S37 W49 V52 I53 R68 V73 D74 T75 D91 S118 P131 SER SER LYS SER THR SER GLY GLY T140 W159 L164 S178 V189 C201 K214 K219 SER CYS ALA ALA HIS HIS HIS HIS

HIS

• Molecule 2: Fab heavy chain

Chain C:

83%9%7%

Q1 T21 C22 T23 I29 S30 S37 W49 V52 I53 S62 R68 V73 D74 T75 D91 L104 S118 K134 SER THR SER GLY GLY T140 W159 L164 S178 V189 C201 K214 K219 SER CYS ALA ALA ALA HIS HIS HIS

HIS HIS

• Molecule 3: Fab light chain

Chain L:

91%8%

D1 S30 S31 W32 L33 L47 V58 D70 F71 T72 L136 Y140 P141 N158 T172 S176 L179 E187 K190 S202 G212 GLU CYS

• Molecule 3: Fab light chain

Chain D:

90%9%

D1 S30 S31 W32 L33 L47 V58 D70 F71 T72 L136 Y140 P141 R142 E143 N158 T172 S176 L179 K190 S202 S208 G212 GLU CYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.93Å 85.50Å 101.30Å 77.49° 88.58° 68.76°	Depositor
Resolution (Å)	29.56 – 3.10 29.56 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.56-3.10) 97.1 (29.56-3.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.202 , 0.261 0.206 , 0.261	Depositor DCC
R_{free} test set	1983 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	83.1	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13366	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

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	0.65	0/3594	0.74	0/4875
1	B	0.64	0/3518	0.74	0/4772
2	C	0.65	0/1650	0.78	0/2256
2	H	0.64	0/1629	0.77	0/2229
3	D	0.66	0/1645	0.75	0/2235
3	L	0.65	0/1645	0.76	0/2235
All	All	0.65	0/13681	0.75	0/18602

There are no bond length outliers.

There are no bond angle outliers.

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	3512	0	3406	21	0
1	B	3439	0	3336	22	0
2	C	1609	0	1603	11	0
2	H	1588	0	1580	9	0
3	D	1609	0	1570	4	0
3	L	1609	0	1570	4	0
All	All	13366	0	13065	69	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 3.

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The worst 5 of 69 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:B:338:ASN:C	1:B:338:ASN:HD22	1.81	0.84
1:A:338:ASN:HD22	1:A:338:ASN:C	1.83	0.82
1:A:338:ASN:HD22	1:A:339:ASP:N	1.84	0.75
1:B:338:ASN:HD22	1:B:339:ASP:N	1.90	0.68
2:H:29:ILE:HD11	2:H:75:THR:HA	1.79	0.65

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	430/552 (78%)	406 (94%)	21 (5%)	3 (1%)	22	57
1	B	418/552 (76%)	399 (96%)	18 (4%)	1 (0%)	47	79
2	C	210/230 (91%)	201 (96%)	9 (4%)	0	100	100
2	H	207/230 (90%)	198 (96%)	9 (4%)	0	100	100
3	D	210/214 (98%)	198 (94%)	11 (5%)	1 (0%)	29	64
3	L	210/214 (98%)	195 (93%)	14 (7%)	1 (0%)	29	64
All	All	1685/1992 (85%)	1597 (95%)	82 (5%)	6 (0%)	34	69

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	104	LYS
1	A	478	ASN
1	B	478	ASN
3	L	30	SER

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	399/495 (81%)	367 (92%)	32 (8%)	12	40
1	B	392/495 (79%)	373 (95%)	19 (5%)	25	58
2	C	188/199 (94%)	179 (95%)	9 (5%)	25	58
2	H	185/199 (93%)	177 (96%)	8 (4%)	29	62
3	D	183/185 (99%)	172 (94%)	11 (6%)	19	49
3	L	183/185 (99%)	172 (94%)	11 (6%)	19	49
All	All	1530/1758 (87%)	1440 (94%)	90 (6%)	19	50

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	236	ASP
2	C	23	THR
1	B	283	SER
1	B	417	ARG
2	C	178	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
1	B	338	ASN

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.

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5.5 Carbohydrates ⓘ

There are no monosaccharides 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, 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(Å²)	Q<0.9
1	A	442/552 (80%)	-0.13	4 (0%)	84	69	60, 94, 131, 163	0
1	B	432/552 (78%)	-0.08	7 (1%)	72	51	68, 97, 131, 160	0
2	C	214/230 (93%)	-0.36	1 (0%)	91	81	52, 77, 116, 137	0
2	H	211/230 (91%)	-0.47	0	100	100	53, 76, 104, 134	0
3	D	212/214 (99%)	-0.34	1 (0%)	91	81	62, 85, 108, 120	0
3	L	212/214 (99%)	-0.46	1 (0%)	91	81	55, 82, 105, 116	0
All	All	1723/1992 (86%)	-0.25	14 (0%)	86	72	52, 88, 123, 163	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	ASP	3.6
1	A	393	ASN	3.0
1	B	319	ALA	2.9
1	B	111	VAL	2.9
1	A	41	TYR	2.6

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.