



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:59 PM GMT

PDB ID : 4IML
Title : CrossFab binding to human Angiopoietin 2
Authors : Fenn, S.; Schiller, C.; Griesse, J.; Hopfner, K.-P.; Kettenberger, H.
Deposited on : 2013-01-03
Resolution : 2.93 Å(reported)

This is a full wwPDB validation 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>

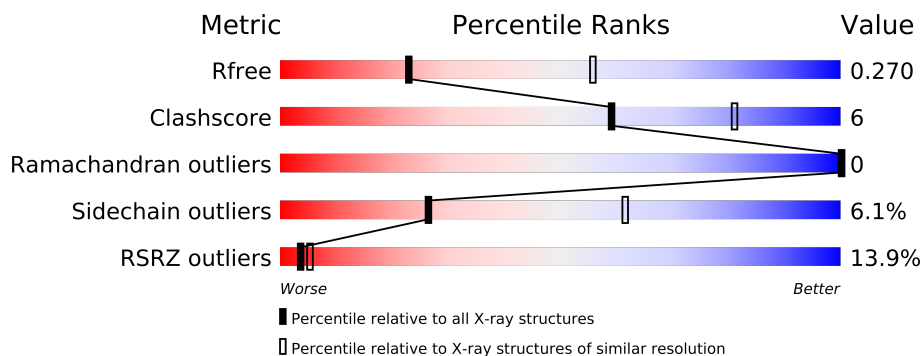
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 2.93 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}	66092	1424 (2.98-2.90)
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RSRZ outliers	66119	1425 (2.98-2.90)

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.

Mol	Chain	Length	Quality of chain
1	A	245	
1	H	245	
2	B	213	
2	L	213	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	B	301	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6743 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 Crossed heavy chain (VH-Ckappa).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	234	Total	C	N	O	S	81	0	0
			1816	1142	305	360	9			
1	A	234	Total	C	N	O	S	95	0	0
			1816	1142	305	360	9			

- Molecule 2 is a protein called Crossed light chain (VL-CH1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	18	0	0
			1540	961	260	315	4			
2	B	212	Total	C	N	O	S	16	0	0
			1552	968	262	317	5			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	2	Total	O	0	0
			2	2		
4	L	2	Total	O	0	0
			2	2		
4	A	2	Total	O	0	0
			2	2		
4	B	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.75Å 80.55Å 158.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.13 – 2.93 44.13 – 2.93	Depositor EDS
% Data completeness (in resolution range)	98.6 (44.13-2.93) 98.7 (44.13-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.237 , 0.269 0.239 , 0.270	Depositor DCC
R_{free} test set	1060 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 21186 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6743	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.94 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.2315e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.24	0/1863	0.47	0/2532
1	H	0.23	0/1863	0.46	1/2532 (0.0%)
2	B	0.23	0/1591	0.46	0/2176
2	L	0.23	0/1579	0.45	0/2162
All	All	0.23	0/6896	0.46	1/9402 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	223	LEU	CA-CB-CG	5.80	128.63	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1816	0	0	15	0
1	H	1816	0	0	14	0
2	B	1552	0	0	5	0
2	L	1540	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	0	0	0
3	H	6	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	H	2	0	0	0	0
4	L	2	0	0	0	0
All	All	6743	0	0	40	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 6.

All (40) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:173:ASP:N	1:A:213:VAL:CG2	2.21	1.04
1:A:213:VAL:O	1:A:214:TYR:CG	2.36	0.79
1:A:213:VAL:O	1:A:214:TYR:CD1	2.38	0.77
1:A:173:ASP:CA	1:A:213:VAL:CG2	2.68	0.72
1:H:212:LYS:O	1:H:232:ASN:ND2	2.26	0.69
2:L:30:LYS:NZ	2:L:90:TRP:O	2.29	0.65
1:H:12:LYS:NZ	1:H:17:SER:O	2.31	0.63
1:H:32:TYR:OH	1:H:106:ASP:OD2	2.20	0.60
1:A:67:ARG:NH1	1:A:90:ASP:OD2	2.35	0.60
1:H:159:ASN:OD1	1:H:160:ASN:ND2	2.35	0.59
2:B:38:LYS:NZ	2:B:80:GLY:O	2.36	0.58
2:L:124:SER:OG	2:L:125:SER:N	2.38	0.56
1:A:172:VAL:O	1:A:175:ALA:N	2.39	0.55
1:H:146:GLN:O	1:H:149:SER:OG	2.24	0.54
1:A:180:ASN:ND2	1:A:202:THR:O	2.42	0.53
2:B:194:ASN:ND2	2:B:205:ASP:OD1	2.43	0.52
1:A:213:VAL:C	1:A:214:TYR:CG	2.81	0.49
1:A:146:GLN:O	1:A:149:SER:OG	2.30	0.49
2:B:141:ASP:OD1	2:B:168:GLN:NE2	2.46	0.49
2:L:197:HIS:ND1	2:L:200:SER:OG	2.47	0.48
1:H:67:ARG:NH1	1:H:90:ASP:OD2	2.47	0.48
1:H:207:ASP:O	1:H:211:HIS:ND1	2.46	0.48
1:H:106:ASP:OD1	1:H:107:SER:N	2.47	0.48
2:B:126:LYS:O	2:B:130:GLY:N	2.47	0.47
1:H:143:SER:OG	2:L:120:PRO:O	2.33	0.46
1:A:77:SER:O	1:A:77:SER:OG	2.32	0.46
1:A:60:TYR:OH	1:A:70:MET:N	2.50	0.45
1:A:208:TYR:O	1:A:214:TYR:OH	2.35	0.44
1:H:165:GLU:OE1	1:H:165:GLU:N	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:52:ASN:O	1:A:56:GLY:N	2.52	0.43
1:H:50:TRP:NE1	2:L:95:ASP:OD2	2.52	0.42
1:H:52:ASN:O	1:H:56:GLY:N	2.52	0.42
1:H:173:ASP:OD2	1:H:173:ASP:N	2.53	0.42
2:B:130:GLY:C	2:B:132:THR:N	2.73	0.41
1:A:133:ALA:N	1:A:162:TYR:O	2.54	0.41
2:L:125:SER:O	2:L:128:THR:OG1	2.39	0.41
1:A:170:TRP:NE1	1:A:199:SER:OG	2.54	0.41
2:L:28:GLY:N	2:L:67:GLY:O	2.54	0.40
2:L:124:SER:O	2:L:127:SER:OG	2.39	0.40
1:H:73:ASP:OD1	1:H:75:SER:OG	2.40	0.40

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	232/245 (95%)	223 (96%)	9 (4%)	0	100	100
1	H	232/245 (95%)	225 (97%)	7 (3%)	0	100	100
2	B	210/213 (99%)	203 (97%)	7 (3%)	0	100	100
2	L	208/213 (98%)	198 (95%)	10 (5%)	0	100	100
All	All	882/916 (96%)	849 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	199/208 (96%)	188 (94%)	11 (6%)	30	67
1	H	199/208 (96%)	185 (93%)	14 (7%)	21	53
2	B	180/181 (99%)	170 (94%)	10 (6%)	30	66
2	L	178/181 (98%)	167 (94%)	11 (6%)	26	61
All	All	756/778 (97%)	710 (94%)	46 (6%)	26	61

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LYS
1	H	43	GLN
1	H	72	ARG
1	H	87	ARG
1	H	88	SER
1	H	172	VAL
1	H	173	ASP
1	H	189	ASP
1	H	203	LEU
1	H	209	GLU
1	H	213	VAL
1	H	218	VAL
1	H	219	THR
1	H	223	LEU
2	L	12	VAL
2	L	69	THR
2	L	89	VAL
2	L	105	VAL
2	L	106	THR
2	L	126	LYS
2	L	156	LEU
2	L	157	THR
2	L	175	LEU
2	L	201	ASN
2	L	209	GLU
1	A	1	GLN
1	A	72	ARG
1	A	89	ASP
1	A	125	VAL
1	A	148	LYS
1	A	173	ASP
1	A	186	THR
1	A	190	SER

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Mol	Chain	Res	Type
1	A	192	ASP
1	A	201	LEU
1	A	223	LEU
2	B	27	ILE
2	B	44	VAL
2	B	47	VAL
2	B	110	SER
2	B	158	SER
2	B	172	LEU
2	B	176	SER
2	B	190	THR
2	B	192	ILE
2	B	201	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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
3	GOL	B	301	-	5,5,5	0.34	0	5,5,5	0.29	0
3	GOL	H	301	-	5,5,5	0.35	0	5,5,5	0.27	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
3	GOL	B	301	-	-	0/4/4/4	0/0/0/0
3	GOL	H	301	-	-	0/4/4/4	0/0/0/0

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.

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(Å ²)	Q<0.9
1	A	234/245 (95%)	0.91	41 (17%) 2 3	32, 70, 134, 161	24 (10%)
1	H	234/245 (95%)	0.71	28 (11%) 5 7	31, 74, 111, 127	21 (8%)
2	B	212/213 (99%)	0.88	30 (14%) 3 5	24, 57, 147, 253	4 (1%)
2	L	210/213 (98%)	0.63	25 (11%) 5 7	27, 56, 136, 180	5 (2%)
All	All	890/916 (97%)	0.78	124 (13%) 4 5	24, 64, 131, 253	54 (6%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	127	SER	9.0
2	B	128	THR	7.8
2	B	188	THR	7.3
2	B	189	GLN	7.2
2	B	212	SER	6.5
2	B	185	SER	6.3
1	A	222	GLY	6.0
2	B	129	SER	6.0
2	B	130	GLY	5.8
2	B	125	SER	5.7
2	B	3	GLY	5.5
2	B	156	LEU	5.3
1	H	128	SER	5.3
1	A	230	SER	5.1
2	L	128	THR	4.8
1	A	228	THR	4.6
1	H	190	SER	4.6
2	B	135	LEU	4.4
2	B	190	THR	4.4
2	B	213	CYS	4.3
1	A	140	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	158	LEU	4.3
1	A	208	TYR	4.2
1	A	190	SER	4.2
2	B	131	GLY	4.1
2	B	210	PRO	4.1
2	L	185	SER	4.0
1	A	219	THR	4.0
1	A	163	PRO	4.0
1	A	214	TYR	3.9
2	L	180	THR	3.9
2	L	127	SER	3.9
2	L	1	GLN	3.8
2	B	155	ALA	3.8
1	A	174	ASN	3.8
1	A	200	THR	3.8
2	B	182	PRO	3.7
2	L	157	THR	3.6
1	A	154	VAL	3.6
1	H	86	LEU	3.6
2	L	125	SER	3.6
2	B	211	LYS	3.6
1	A	196	SER	3.6
2	B	181	VAL	3.6
2	L	208	VAL	3.5
1	A	157	LEU	3.5
2	L	112	SER	3.5
1	A	176	LEU	3.5
2	B	126	LYS	3.5
2	B	2	PRO	3.4
1	A	224	SER	3.3
2	L	186	LEU	3.3
1	A	129	SER	3.3
1	A	227	VAL	3.2
2	L	181	VAL	3.2
2	L	129	SER	3.1
1	H	14	PRO	3.1
2	B	134	ALA	3.1
1	A	211	HIS	3.0
1	H	178	SER	3.0
2	L	130	GLY	3.0
2	L	133	ALA	2.9
1	A	151	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	170	TRP	2.8
1	H	144	ASP	2.7
1	A	128	SER	2.7
2	L	182	PRO	2.7
1	A	232	ASN	2.7
1	H	192	ASP	2.7
2	B	208	VAL	2.7
1	H	212	LYS	2.6
2	L	191	TYR	2.6
1	H	158	LEU	2.6
1	H	163	PRO	2.6
1	A	195	TYR	2.6
1	A	160	ASN	2.5
1	A	192	ASP	2.5
1	A	223	LEU	2.5
1	H	189	ASP	2.5
1	H	149	SER	2.5
2	L	156	LEU	2.5
1	H	130	ALA	2.5
1	A	138	PHE	2.5
2	L	210	PRO	2.4
1	A	162	TYR	2.4
1	H	57	GLY	2.4
1	A	134	ALA	2.4
1	A	171	LYS	2.4
1	A	152	ALA	2.4
1	H	177	GLN	2.4
1	A	218	VAL	2.4
2	L	152	ASN	2.4
1	A	194	THR	2.4
1	A	220	HIS	2.3
1	A	197	LEU	2.3
2	L	134	ALA	2.3
1	H	165	GLU	2.3
1	H	222	GLY	2.3
1	H	126	THR	2.3
2	L	132	THR	2.3
1	H	127	VAL	2.3
2	L	3	GLY	2.2
2	B	187	GLY	2.2
1	H	129	SER	2.2
1	H	191	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	187	GLY	2.2
1	H	185	VAL	2.2
1	H	223	LEU	2.2
1	A	213	VAL	2.1
1	A	186	THR	2.1
1	H	234	GLY	2.1
2	B	123	PRO	2.1
1	H	228	THR	2.1
2	L	155	ALA	2.1
1	H	154	VAL	2.1
1	A	135	PRO	2.1
1	H	174	ASN	2.1
2	B	159	GLY	2.1
1	H	166	ALA	2.0
2	L	131	GLY	2.0
2	B	132	THR	2.0
2	B	136	GLY	2.0
2	B	158	SER	2.0
1	A	173	ASP	2.0

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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	B	301	6/6	0.24	2.95	47,49,51,54	0
3	GOL	H	301	6/6	0.16	-0.36	43,44,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.