



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:08 pm GMT

PDB ID : 5HCG
Title : CRYSTAL STRUCTURE OF FREE-CODV.
Authors : Vallee, F.; Dupuy, A.; Rak, A.
Deposited on : 2016-01-04
Resolution : 2.68 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

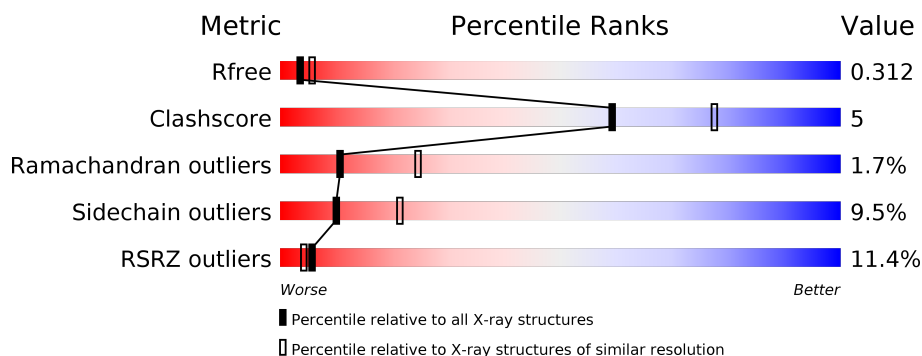
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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}	100719	3050 (2.70-2.66)
Clashscore	112137	3418 (2.70-2.66)
Ramachandran outliers	110173	3367 (2.70-2.66)
Sidechain outliers	110143	3367 (2.70-2.66)
RSRZ outliers	101464	3069 (2.70-2.66)

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 $\leq 5\%$. 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	H	345	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>..</div> </div> </div>
2	L	334	<div> <div>12%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5102 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 CODV heavy-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	332	Total	C	N	O	S	0	0	0
			2530	1600	419	500	11			

- Molecule 2 is a protein called CODV light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	327	Total	C	N	O	S	0	0	0
			2485	1558	417	501	9			

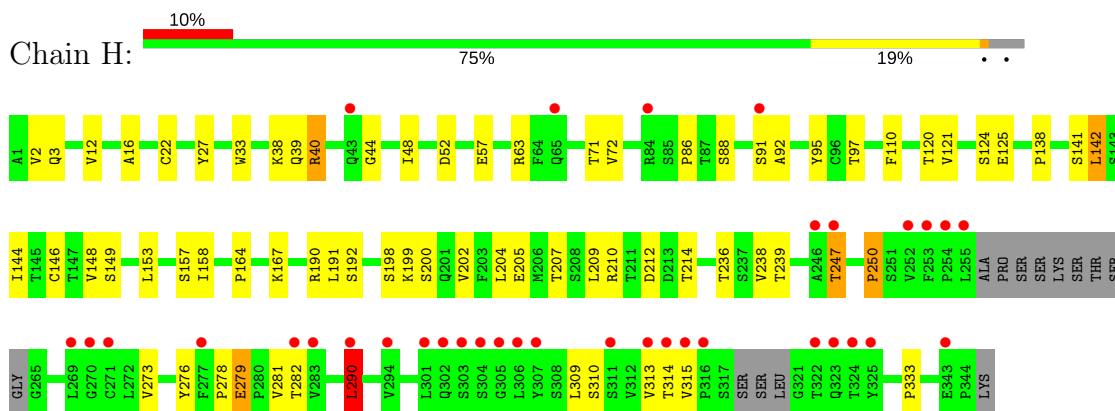
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	42	Total	O	0	0
			42	42		
3	L	45	Total	O	0	0
			45	45		

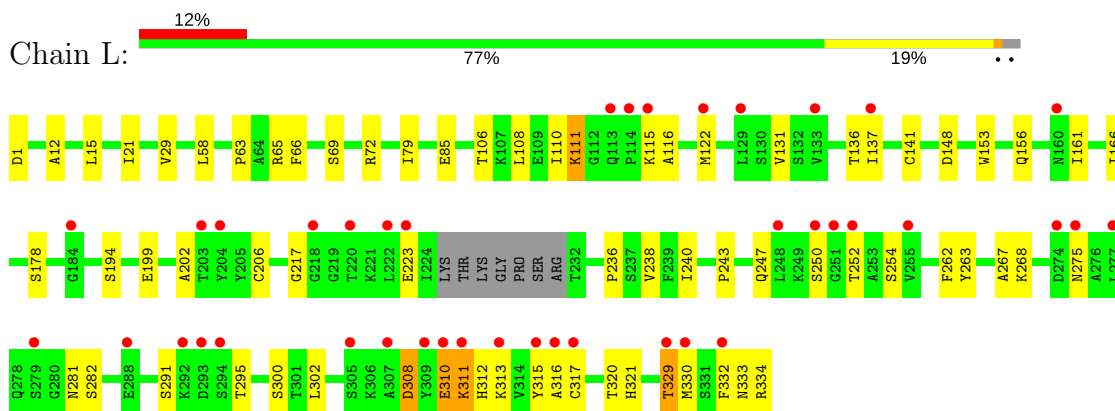
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: CODV heavy-chain



• Molecule 2: CODV light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	70.92Å 70.92Å 272.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.16 – 2.68 47.07 – 2.68	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.16-2.68) 100.0 (47.07-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.229 , 0.296 0.238 , 0.312	Depositor DCC
R_{free} test set	1006 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5102	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	H	0.52	0/2592	0.78	1/3528 (0.0%)
2	L	0.52	0/2541	0.74	0/3456
All	All	0.52	0/5133	0.76	1/6984 (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	250	PRO	N-CA-CB	5.81	110.28	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	H	2530	0	2439	27	0
2	L	2485	0	2398	27	0
3	H	42	0	0	0	0
3	L	45	0	0	0	0
All	All	5102	0	4837	53	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.

All (53) 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)
2:L:141:CYS:HG	2:L:206:CYS:HG	1.27	0.80
2:L:315:TYR:HB2	2:L:332:PHE:CE2	2.31	0.65
1:H:142:LEU:HD12	1:H:238:VAL:HG11	1.82	0.62
2:L:12:ALA:HB1	2:L:111:LYS:HB3	1.82	0.61
2:L:267:ALA:HB2	2:L:321:HIS:HD2	1.67	0.60
1:H:144:ILE:HD12	1:H:204:LEU:HD23	1.86	0.58
1:H:39:GLN:HG3	1:H:44:GLY:O	2.04	0.57
1:H:190:ARG:HD2	1:H:207:THR:O	2.05	0.57
1:H:164:PRO:HB2	1:H:167:LYS:HB2	1.87	0.57
1:H:273:VAL:HG11	1:H:281:VAL:HG11	1.89	0.55
1:H:16:ALA:O	1:H:86:PRO:HD3	2.07	0.54
2:L:268:LYS:HB3	2:L:320:THR:HB	1.90	0.53
2:L:240:ILE:HD12	2:L:317:CYS:HB2	1.89	0.53
1:H:95:TYR:HE1	2:L:161:ILE:HG22	1.74	0.52
2:L:63:PRO:HB2	2:L:65:ARG:HG2	1.92	0.52
1:H:12:VAL:HG13	1:H:16:ALA:HB3	1.92	0.51
2:L:250:SER:HB2	2:L:252:THR:HG22	1.93	0.50
2:L:316:ALA:HB1	2:L:329:THR:HG22	1.93	0.49
1:H:138:PRO:HA	1:H:209:LEU:O	2.13	0.49
1:H:191:LEU:HD22	1:H:204:LEU:HD11	1.94	0.49
2:L:21:ILE:HG12	2:L:106:THR:HG21	1.95	0.48
2:L:282:SER:HB3	2:L:302:LEU:HD12	1.96	0.48
2:L:136:THR:HA	2:L:194:SER:HA	1.95	0.48
2:L:153:TRP:HB2	2:L:166:ILE:HB	1.96	0.47
1:H:2:VAL:HG22	1:H:27:TYR:HB3	1.96	0.47
2:L:308:ASP:HA	2:L:311:LYS:HE3	1.97	0.47
2:L:263:TYR:HB2	2:L:295:THR:HG22	1.98	0.46
1:H:97:THR:OG1	1:H:110:PHE:HB3	2.16	0.46
2:L:58:LEU:HD11	2:L:66:PHE:O	2.16	0.46
1:H:278:PRO:HD2	1:H:333:PRO:HB2	1.99	0.45
2:L:247:GLN:HG2	2:L:252:THR:HG23	1.98	0.45
1:H:39:GLN:O	1:H:40:ARG:HB2	2.17	0.44
1:H:276:TYR:HE2	1:H:279:GLU:HA	1.82	0.44
2:L:122:MET:HB2	2:L:217:GLY:HA2	1.99	0.44
2:L:243:PRO:HB3	2:L:254:SER:H	1.82	0.44
1:H:86:PRO:HB2	1:H:121:VAL:HG21	1.99	0.44
1:H:146:CYS:HB3	1:H:202:VAL:HB	2.00	0.44
2:L:312:HIS:HB2	2:L:315:TYR:CE1	2.54	0.43
2:L:313:LYS:HG3	2:L:334:ARG:HE	1.83	0.43
1:H:290:LEU:HD23	1:H:313:VAL:HG21	2.00	0.43
2:L:236:PRO:HB3	2:L:262:PHE:CD2	2.54	0.42
1:H:38:LYS:HB2	1:H:48:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164:PRO:HB2	1:H:167:LYS:HD2	2.02	0.42
1:H:158:ILE:HG13	1:H:202:VAL:HG21	2.01	0.42
1:H:214:THR:HG23	1:H:239:THR:HG22	2.02	0.41
1:H:214:THR:HG23	1:H:239:THR:HA	2.02	0.41
1:H:192:SER:HB3	1:H:205:GLU:HB2	2.02	0.41
1:H:33:TRP:CH2	1:H:52:ASP:HB2	2.56	0.41
2:L:156:GLN:O	2:L:202:ALA:HB1	2.21	0.41
2:L:311:LYS:HD2	2:L:312:HIS:CE1	2.56	0.40
2:L:317:CYS:O	2:L:329:THR:HA	2.21	0.40
1:H:40:ARG:HG3	1:H:92:ALA:HB2	2.03	0.40
2:L:66:PHE:CD1	2:L:79:ILE:HG12	2.56	0.40

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	H	326/345 (94%)	295 (90%)	25 (8%)	6 (2%)	10	23
2	L	323/334 (97%)	295 (91%)	23 (7%)	5 (2%)	12	28
All	All	649/679 (96%)	590 (91%)	48 (7%)	11 (2%)	11	24

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	250	PRO
2	L	115	LYS
2	L	116	ALA
2	L	72	ARG
2	L	148	ASP
1	H	40	ARG
1	H	124	SER

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Mol	Chain	Res	Type
1	H	125	GLU
1	H	247	THR
2	L	310	GLU
1	H	290	LEU

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	H	280/294 (95%)	251 (90%)	29 (10%)	8	17
2	L	277/285 (97%)	253 (91%)	24 (9%)	12	25
All	All	557/579 (96%)	504 (90%)	53 (10%)	10	21

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	22	CYS
1	H	57	GLU
1	H	63	ARG
1	H	71	THR
1	H	72	VAL
1	H	88	SER
1	H	91	SER
1	H	120	THR
1	H	141	SER
1	H	142	LEU
1	H	148	VAL
1	H	149	SER
1	H	153	LEU
1	H	157	SER
1	H	198	SER
1	H	199	LYS
1	H	200	SER
1	H	210	ARG

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Mol	Chain	Res	Type
1	H	212	ASP
1	H	236	THR
1	H	247	THR
1	H	279	GLU
1	H	282	THR
1	H	290	LEU
1	H	309	LEU
1	H	310	SER
1	H	314	THR
1	H	315	VAL
2	L	1	ASP
2	L	15	LEU
2	L	29	VAL
2	L	69	SER
2	L	85	GLU
2	L	108	LEU
2	L	110	ILE
2	L	111	LYS
2	L	131	VAL
2	L	137	ILE
2	L	178	SER
2	L	199	GLU
2	L	223	GLU
2	L	238	VAL
2	L	275	ASN
2	L	281	ASN
2	L	291	SER
2	L	300	SER
2	L	308	ASP
2	L	310	GLU
2	L	311	LYS
2	L	329	THR
2	L	330	MET
2	L	333	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	104	ASN
2	L	113	GLN
2	L	121	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	H	332/345 (96%)	0.55	35 (10%) 7 5	29, 66, 113, 129	0
2	L	327/334 (97%)	0.61	40 (12%) 5 3	31, 71, 116, 134	0
All	All	659/679 (97%)	0.58	75 (11%) 6 4	29, 69, 114, 134	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	269	LEU	8.5
2	L	293	ASP	7.4
1	H	315	VAL	6.0
1	H	306	LEU	5.9
2	L	310	GLU	5.7
2	L	251	GLY	5.7
2	L	311	LYS	5.6
2	L	252	THR	5.4
1	H	253	PHE	5.4
1	H	324	THR	5.2
2	L	113	GLN	5.1
2	L	114	PRO	5.1
2	L	292	LYS	4.9
1	H	294	VAL	4.8
2	L	218	GLY	4.5
1	H	247	THR	4.4
1	H	313	VAL	4.1
2	L	309	TYR	4.1
2	L	129	LEU	4.0
2	L	294	SER	4.0
2	L	315	TYR	3.9
2	L	277	LEU	3.7
2	L	220	THR	3.7
2	L	275	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
2	L	330	MET	3.6
1	H	270	GLY	3.5
1	H	255	LEU	3.4
1	H	322	THR	3.2
1	H	314	THR	3.2
1	H	323	GLN	3.2
2	L	250	SER	3.1
1	H	343	GLU	3.1
1	H	325	TYR	3.1
2	L	307	ALA	3.0
2	L	160	ASN	3.0
1	H	246	ALA	3.0
2	L	313	LYS	2.9
1	H	303	SER	2.9
1	H	305	GLY	2.9
1	H	301	LEU	2.9
2	L	222	LEU	2.9
1	H	277	PHE	2.8
2	L	184	GLY	2.8
2	L	332	PHE	2.8
1	H	43	GLN	2.7
1	H	316	PRO	2.7
1	H	290	LEU	2.7
1	H	65	GLN	2.6
1	H	282	THR	2.6
1	H	84	ARG	2.6
2	L	248	LEU	2.5
1	H	311	SER	2.4
1	H	304	SER	2.4
2	L	133	VAL	2.3
2	L	204	TYR	2.3
1	H	254	PRO	2.3
2	L	305	SER	2.3
2	L	329	THR	2.3
2	L	203	THR	2.2
2	L	274	ASP	2.2
1	H	283	VAL	2.2
2	L	279	SER	2.2
1	H	307	TYR	2.2
2	L	115	LYS	2.1
2	L	223	GLU	2.1
1	H	91	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	252	VAL	2.1
2	L	317	CYS	2.1
2	L	255	VAL	2.1
2	L	122	MET	2.1
2	L	288	GLU	2.1
2	L	137	ILE	2.1
1	H	302	GLN	2.1
2	L	316	ALA	2.1
1	H	271	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.