



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:05 PM UTC

PDB ID : 5HCG / pdb_00005hcg
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

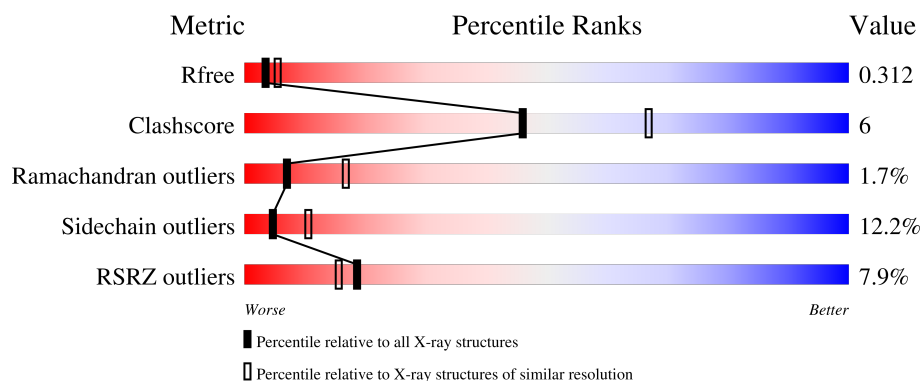
1 Overall quality at a glance

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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (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 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 $\leq 5\%$. 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	6% 69% 24% • •
2	L	334	9% 74% 22% • •

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			

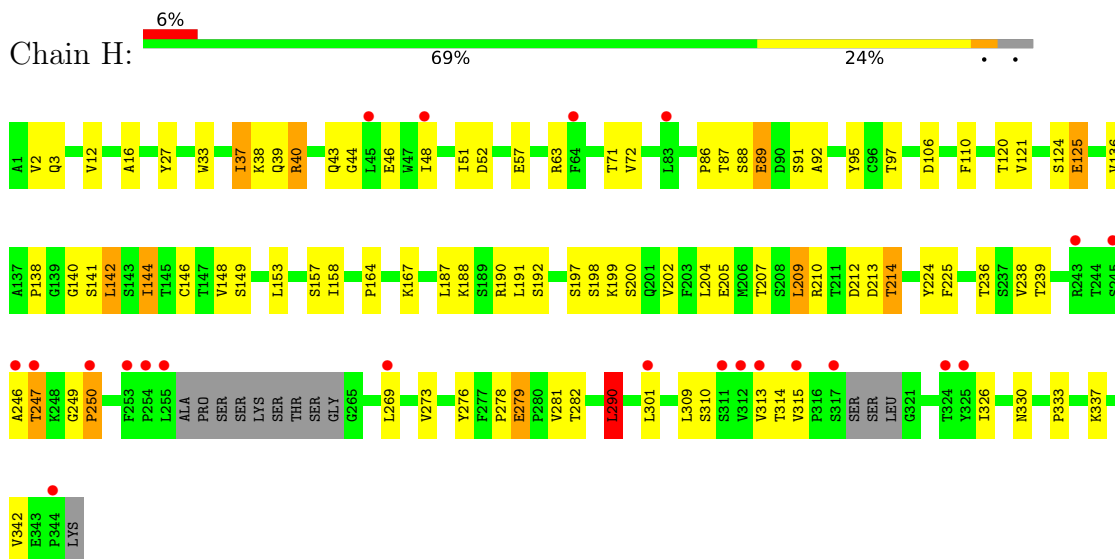
- Molecule 3 is water.

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

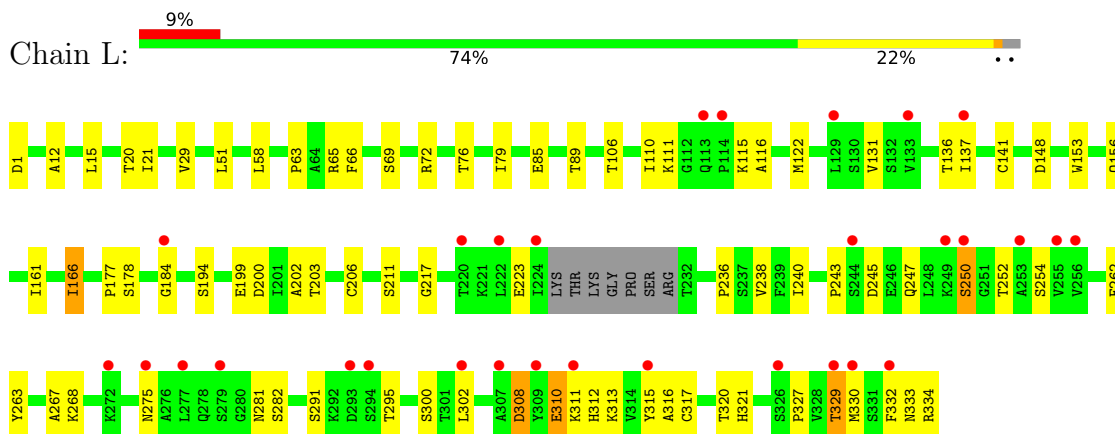
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: 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 49.16 – 2.68	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.16-2.68) 99.9 (49.16-2.68)	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 (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.5	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

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	H	0.90	1/2592 (0.0%)	1.31	17/3528 (0.5%)
2	L	0.89	1/2541 (0.0%)	1.28	8/3456 (0.2%)
All	All	0.89	2/5133 (0.0%)	1.30	25/6984 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	43	GLN	CA-C	5.81	1.56	1.52
2	L	51	LEU	CA-C	-5.73	1.48	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	249	GLY	CA-C-N	9.17	131.30	119.84
1	H	249	GLY	C-N-CA	9.17	131.30	119.84
1	H	246	ALA	CA-C-N	6.75	133.86	121.70
1	H	246	ALA	C-N-CA	6.75	133.86	121.70
1	H	250	PRO	N-CA-CB	6.69	110.28	103.25
2	L	245	ASP	CA-C-N	6.32	128.66	120.44
2	L	245	ASP	C-N-CA	6.32	128.66	120.44
1	H	106	ASP	N-CA-C	-6.17	104.46	112.23
1	H	89	GLU	N-CA-C	-6.12	106.36	113.88
2	L	177	PRO	CA-C-N	6.07	130.41	120.63
2	L	177	PRO	C-N-CA	6.07	130.41	120.63
1	H	125	GLU	CB-CG-CD	6.02	122.83	112.60
1	H	188	LYS	CA-C-N	5.88	128.43	120.38
1	H	188	LYS	C-N-CA	5.88	128.43	120.38
1	H	330	ASN	CA-CB-CG	5.76	118.36	112.60
1	H	37	ILE	CA-C-N	5.62	130.41	122.09
1	H	37	ILE	C-N-CA	5.62	130.41	122.09
1	H	214	THR	N-CA-C	-5.62	100.65	109.25
2	L	89	THR	CB-CA-C	5.59	118.87	109.48
1	H	213	ASP	N-CA-C	-5.46	105.84	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	197	SER	CA-C-N	5.37	127.42	120.44
1	H	197	SER	C-N-CA	5.37	127.42	120.44
2	L	327	PRO	CA-C-N	5.28	129.59	122.93
2	L	327	PRO	C-N-CA	5.28	129.59	122.93
2	L	184	GLY	N-CA-C	5.21	117.36	112.04

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	30	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	56	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 6.

All (56) 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	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:39:GLN:O	1:H:40:ARG:HB2	2.17	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
1:H:164:PRO:HB2	1:H:167:LYS:HD2	2.02	0.42
1:H:224:TYR:O	1:H:225:PHE:C	2.63	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:138:PRO:C	1:H:140:GLY:H	2.28	0.41
1:H:214:THR:HG23	1:H:239:THR:HA	2.02	0.41
1:H:87:THR:C	1:H:89:GLU:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	6	15
2	L	323/334 (97%)	295 (91%)	23 (7%)	5 (2%)	8	19
All	All	649/679 (96%)	590 (91%)	48 (7%)	11 (2%)	7	17

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
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%)	240 (86%)	40 (14%)	3	7
2	L	277/285 (97%)	249 (90%)	28 (10%)	7	16
All	All	557/579 (96%)	489 (88%)	68 (12%)	5	10

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	37	ILE
1	H	46	GLU
1	H	51	ILE
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	136	VAL
1	H	141	SER
1	H	142	LEU
1	H	144	ILE
1	H	148	VAL
1	H	149	SER
1	H	153	LEU
1	H	157	SER
1	H	187	LEU
1	H	198	SER
1	H	199	LYS
1	H	200	SER
1	H	209	LEU
1	H	210	ARG
1	H	212	ASP
1	H	236	THR

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Mol	Chain	Res	Type
1	H	247	THR
1	H	269	LEU
1	H	279	GLU
1	H	282	THR
1	H	290	LEU
1	H	301	LEU
1	H	309	LEU
1	H	310	SER
1	H	314	THR
1	H	315	VAL
1	H	326	ILE
1	H	337	LYS
1	H	342	VAL
2	L	1	ASP
2	L	15	LEU
2	L	20	THR
2	L	29	VAL
2	L	69	SER
2	L	76	THR
2	L	85	GLU
2	L	110	ILE
2	L	131	VAL
2	L	137	ILE
2	L	166	ILE
2	L	178	SER
2	L	199	GLU
2	L	200	ASP
2	L	203	THR
2	L	211	SER
2	L	223	GLU
2	L	238	VAL
2	L	250	SER
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	329	THR
2	L	330	MET
2	L	333	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
1	H	65	GLN
1	H	104	ASN
1	H	163	GLN
1	H	295	HIS
1	H	330	ASN
2	L	42	GLN
2	L	113	GLN
2	L	121	GLN
2	L	155	GLN
2	L	156	GLN
2	L	171	ASN
2	L	260	ASN
2	L	261	ASN
2	L	283	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 oligosaccharides 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 ⓘ

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%)	0.62	22 (6%)	24 21	29, 66, 113, 129	0
2	L	327/334 (97%)	0.62	30 (9%)	14 12	31, 71, 116, 134	0
All	All	659/679 (97%)	0.62	52 (7%)	18 15	29, 69, 114, 134	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	269	LEU	5.8
1	H	324	THR	4.1
2	L	224	ILE	4.0
2	L	113	GLN	3.9
1	H	315	VAL	3.6
2	L	277	LEU	3.3
2	L	309	TYR	3.2
1	H	255	LEU	3.1
1	H	48	ILE	3.1
2	L	315	TYR	3.1
2	L	114	PRO	2.8
1	H	246	ALA	2.6
1	H	313	VAL	2.6
1	H	250	PRO	2.6
2	L	220	THR	2.5
2	L	332	PHE	2.5
2	L	279	SER	2.4
1	H	83	LEU	2.3
2	L	137	ILE	2.3
2	L	255	VAL	2.3
1	H	301	LEU	2.3
1	H	247	THR	2.3
1	H	344	PRO	2.3
1	H	253	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	307	ALA	2.3
1	H	45	LEU	2.3
1	H	64	PHE	2.3
1	H	325	TYR	2.3
2	L	293	ASP	2.3
1	H	312	VAL	2.3
2	L	133	VAL	2.3
2	L	275	ASN	2.2
2	L	329	THR	2.2
2	L	184	GLY	2.2
2	L	250	SER	2.2
1	H	245	SER	2.2
1	H	311	SER	2.2
2	L	244	SER	2.2
1	H	254	PRO	2.1
2	L	311	LYS	2.1
2	L	330	MET	2.1
2	L	326	SER	2.1
2	L	129	LEU	2.1
2	L	222	LEU	2.1
2	L	302	LEU	2.1
1	H	243	ARG	2.0
1	H	317	SER	2.0
2	L	249	LYS	2.0
2	L	253	ALA	2.0
2	L	272	LYS	2.0
2	L	294	SER	2.0
2	L	256	VAL	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 oligosaccharides 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.