



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:02 PM GMT

PDB ID : 4QQL
Title : Crystal structure of C1QL3 in P1 space group
Authors : Ressler, S.; Brunger, A.T.
Deposited on : 2014-06-27
Resolution : 2.39 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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

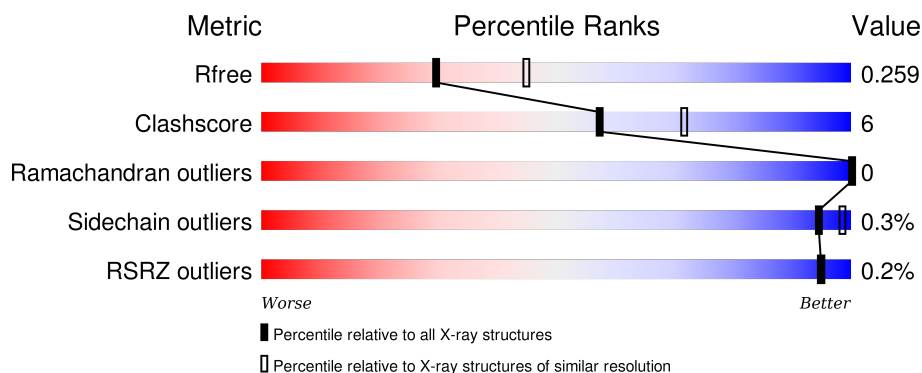
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	A	137	<div> <div>83%</div> <div>12%</div> <div>5%</div> </div>
1	B	137	<div> <div>%</div> <div>82%</div> <div>12%</div> <div>5%</div> </div>
1	C	137	<div> <div>86%</div> <div>9%</div> <div>.</div> </div>
1	D	137	<div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
1	E	137	<div> <div>82%</div> <div>12%</div> <div>5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	137	
1	G	137	
1	H	137	
1	I	137	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	D	203	-	-	-	X
2	MG	E	202	-	-	-	X
2	MG	F	201	-	-	-	X
2	MG	F	202	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 19068 atoms, of which 8847 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 Complement C1q-like protein 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	130	Total 2014	C 658	H 981	N 173	O 197	S 5	0	3	0
1	B	130	Total 2022	C 660	H 986	N 173	O 198	S 5	0	4	0
1	C	131	Total 2037	C 665	H 994	N 174	O 199	S 5	0	4	0
1	D	130	Total 2022	C 660	H 986	N 173	O 198	S 5	0	4	0
1	E	130	Total 2022	C 660	H 986	N 173	O 198	S 5	0	4	0
1	F	130	Total 2002	C 655	H 974	N 170	O 198	S 5	0	3	0
1	G	130	Total 2001	C 655	H 973	N 170	O 198	S 5	0	3	0
1	H	130	Total 2001	C 655	H 973	N 170	O 198	S 5	0	3	0
1	I	131	Total 2037	C 665	H 994	N 174	O 199	S 5	0	4	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	D	5	Total	Mg	0	0
			5	5		
2	E	4	Total	Mg	0	0
			4	4		
2	H	3	Total	Mg	0	0
			3	3		
2	B	3	Total	Mg	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	2	Total 2	Mg 2	0	0
2	C	1	Total 1	Mg 1	0	0
2	A	3	Total 3	Mg 3	0	0
2	F	2	Total 2	Mg 2	0	0


- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total 92	O 92	0	0
3	B	106	Total 106	O 106	0	0
3	C	93	Total 93	O 93	0	0
3	D	106	Total 106	O 106	0	0
3	E	100	Total 100	O 100	0	0
3	F	79	Total 79	O 79	0	0
3	G	77	Total 77	O 77	0	0
3	H	158	Total 158	O 158	0	0
3	I	75	Total 75	O 75	0	0

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 errors 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: Complement C1q-like protein 3

Chain A: 




- Molecule 1: Complement C1q-like protein 3

Chain B: 




- Molecule 1: Complement C1q-like protein 3

Chain C: 




- Molecule 1: Complement C1q-like protein 3

Chain D: 




- Molecule 1: Complement C1q-like protein 3

Chain E: 

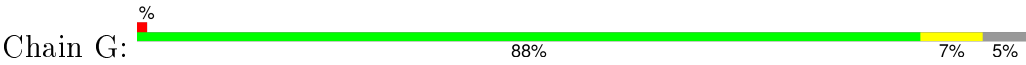


- Molecule 1: Complement C1q-like protein 3

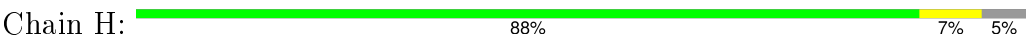
Chain F: 



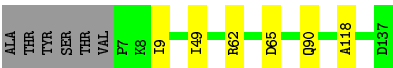
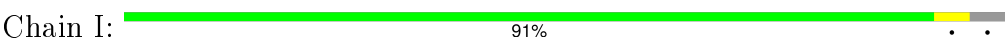
● Molecule 1: Complement C1q-like protein 3



● Molecule 1: Complement C1q-like protein 3



● Molecule 1: Complement C1q-like protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.59Å 82.60Å 86.20Å 61.44° 84.50° 74.93°	Depositor
Resolution (Å)	46.34 – 2.39 49.79 – 2.39	Depositor EDS
% Data completeness (in resolution range)	64.6 (46.34-2.39) 55.2 (49.79-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.224 , 0.259 0.237 , 0.259	Depositor DCC
R_{free} test set	1568 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.1	EDS
Estimated twinning fraction	0.000 for -h,-k,-k+l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30972 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19068	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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 78.76 % 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 6.4577e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.25	0/1068	0.44	0/1444
1	B	0.27	0/1074	0.46	0/1452
1	C	0.26	0/1082	0.47	0/1463
1	D	0.28	0/1074	0.47	0/1452
1	E	0.27	0/1074	0.47	0/1452
1	F	0.26	0/1063	0.46	0/1438
1	G	0.25	0/1063	0.45	0/1438
1	H	0.26	0/1063	0.46	0/1438
1	I	0.27	0/1082	0.50	0/1463
All	All	0.26	0/9643	0.46	0/13040

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 [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	A	1033	981	979	14	1
1	B	1036	986	984	18	0
1	C	1043	994	992	13	0
1	D	1036	986	984	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1036	986	984	16	0
1	F	1028	974	971	10	0
1	G	1028	973	971	9	0
1	H	1028	973	971	8	0
1	I	1043	994	992	4	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	5	0	0	0	0
2	E	4	0	0	0	0
2	F	2	0	0	0	0
2	G	1	0	0	0	0
2	H	3	0	0	0	0
2	I	2	0	0	0	0
3	A	92	0	0	7	0
3	B	106	0	0	18	0
3	C	93	0	0	12	0
3	D	106	0	0	19	0
3	E	100	0	0	10	1
3	F	79	0	0	7	0
3	G	77	0	0	8	0
3	H	158	0	0	6	1
3	I	75	0	0	2	1
All	All	10221	8847	8828	109	2

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.

The worst 5 of 109 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:E:26:LYS:NZ	3:E:357:HOH:O	1.91	1.04
1:B:17:ARG:NH1	3:B:385:HOH:O	1.95	0.99
1:B:15:LEU:O	3:B:376:HOH:O	1.85	0.94
1:G:98:SER:O	3:G:368:HOH:O	1.84	0.94
1:I:62[A]:ARG:NH1	1:I:118:ALA:O	2.06	0.89

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:320:HOH:O	3:I:320:HOH:O[1_655]	1.72	0.48
1:A:26:LYS:NZ	3:H:364:HOH:O[1_554]	2.13	0.07

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	131/137 (96%)	127 (97%)	4 (3%)	0	100	100
1	B	132/137 (96%)	128 (97%)	4 (3%)	0	100	100
1	C	133/137 (97%)	129 (97%)	4 (3%)	0	100	100
1	D	132/137 (96%)	128 (97%)	4 (3%)	0	100	100
1	E	132/137 (96%)	128 (97%)	4 (3%)	0	100	100
1	F	131/137 (96%)	127 (97%)	4 (3%)	0	100	100
1	G	131/137 (96%)	127 (97%)	4 (3%)	0	100	100
1	H	131/137 (96%)	127 (97%)	4 (3%)	0	100	100
1	I	133/137 (97%)	129 (97%)	4 (3%)	0	100	100
All	All	1186/1233 (96%)	1150 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	108/112 (96%)	107 (99%)	1 (1%)	84	93
1	B	109/112 (97%)	109 (100%)	0	100	100
1	C	110/112 (98%)	110 (100%)	0	100	100
1	D	109/112 (97%)	109 (100%)	0	100	100
1	E	109/112 (97%)	109 (100%)	0	100	100
1	F	108/112 (96%)	107 (99%)	1 (1%)	84	93
1	G	108/112 (96%)	107 (99%)	1 (1%)	84	93
1	H	108/112 (96%)	108 (100%)	0	100	100
1	I	110/112 (98%)	110 (100%)	0	100	100
All	All	979/1008 (97%)	976 (100%)	3 (0%)	94	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LEU
1	F	49	ILE
1	G	9	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	124	ASN
1	G	77	ASN
1	F	36	ASN
1	D	91	ASN
1	G	36	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.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	130/137 (94%)	-0.25	0 100 100	14, 19, 23, 26	0
1	B	130/137 (94%)	-0.17	1 (0%) 87 87	15, 22, 30, 34	0
1	C	131/137 (95%)	-0.32	0 100 100	14, 19, 23, 27	0
1	D	130/137 (94%)	-0.21	0 100 100	14, 19, 25, 29	0
1	E	130/137 (94%)	-0.22	0 100 100	16, 19, 24, 29	0
1	F	130/137 (94%)	-0.31	0 100 100	15, 18, 25, 29	0
1	G	130/137 (94%)	-0.06	1 (0%) 87 87	16, 24, 35, 40	0
1	H	130/137 (94%)	-0.21	0 100 100	15, 19, 24, 26	0
1	I	131/137 (95%)	-0.30	0 100 100	15, 19, 23, 29	0
All	All	1172/1233 (95%)	-0.23	2 (0%) 95 95	14, 19, 29, 40	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	49	ILE	4.2
1	B	124	ASN	2.4

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 ⓘ

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	F	202	1/1	0.99	0.15	3.32	15,15,15,15	0
2	MG	E	202	1/1	0.96	0.19	2.68	20,20,20,20	0
2	MG	F	201	1/1	0.97	0.15	2.60	19,19,19,19	0
2	MG	D	203	1/1	0.97	0.15	2.01	14,14,14,14	0
2	MG	H	203	1/1	0.95	0.17	1.81	20,20,20,20	0
2	MG	I	201	1/1	0.88	0.12	0.59	20,20,20,20	0
2	MG	B	203	1/1	0.98	0.12	0.08	13,13,13,13	0
2	MG	A	201	1/1	0.95	0.08	-0.95	19,19,19,19	0
2	MG	D	202	1/1	0.97	0.09	-1.15	15,15,15,15	0
2	MG	B	202	1/1	0.94	0.09	-1.33	16,16,16,16	0
2	MG	B	201	1/1	0.88	0.10	-1.58	17,17,17,17	0
2	MG	A	202	1/1	0.86	0.09	-1.68	18,18,18,18	0
2	MG	D	201	1/1	0.86	0.10	-1.75	18,18,18,18	0
2	MG	A	203	1/1	0.97	0.07	-2.29	16,16,16,16	0
2	MG	E	204	1/1	0.97	0.09	-2.36	23,23,23,23	0
2	MG	H	201	1/1	0.75	0.08	-2.36	20,20,20,20	0
2	MG	E	203	1/1	0.99	0.07	-2.57	21,21,21,21	0
2	MG	C	201	1/1	0.95	0.09	-2.91	22,22,22,22	0
2	MG	E	201	1/1	0.97	0.09	-2.98	17,17,17,17	0
2	MG	D	205	1/1	0.95	0.07	-3.84	20,20,20,20	0
2	MG	D	204	1/1	0.96	0.05	-5.92	17,17,17,17	0
2	MG	H	202	1/1	0.98	0.12	-	22,22,22,22	0
2	MG	I	202	1/1	0.93	0.09	-	23,23,23,23	0
2	MG	G	201	1/1	0.94	0.15	-	21,21,21,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.