Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:28 PM GMT

PDB ID	:	4LOT
Title	:	C1s CUB2-CCP1-CCP2
Authors	:	Wallis, R.; Venkatraman Girija, U.; Moody, P.C.E.; Marshall, J.E.
Deposited on	:	2013-07-13
Resolution	:	2.92 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

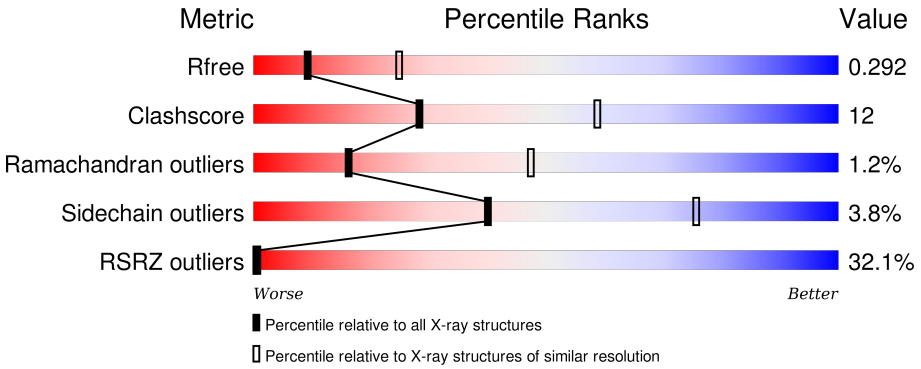
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.92 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	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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. 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	249	32% 70% 27%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1908 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 Complement C1s subcomponent heavy chain.

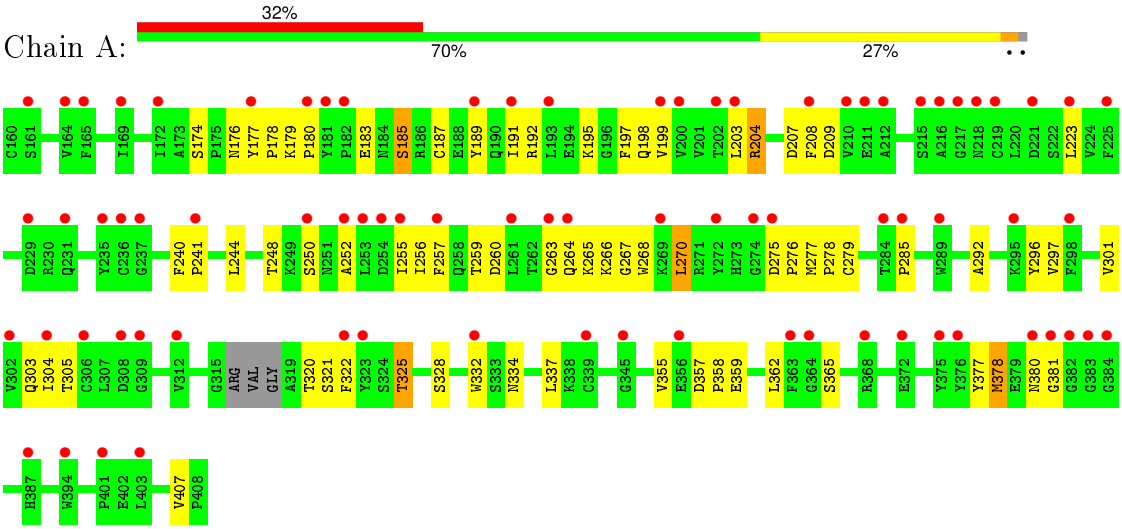
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	246	1908	1205	314	375	14	0	0	0

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 C1s subcomponent heavy chain

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.04Å 58.59Å 51.21Å 90.00° 91.12° 90.00°	Depositor
Resolution (Å)	54.22 – 2.92 54.22 – 2.85	Depositor EDS
% Data completeness (in resolution range)	92.7 (54.22-2.92) 94.0 (54.22-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.266 , 0.292 0.277 , 0.292	Depositor DCC
R_{free} test set	416 reflections (4.94%)	DCC
Wilson B-factor (Å^2)	64.5	Xtriage
Anisotropy	1.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 122.1	EDS
Estimated twinning fraction	0.050 for -h,-k,l 0.027 for -h,-k,l	Xtriage
Reported twinning fraction	0.050 for -h,-k,l	Depositor
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	3 of 9463 reflections (0.032%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	1908	wwPDB-VP
Average B, all atoms (Å^2)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.28	0/1959	0.50	0/2661

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	1908	0	1791	43	0
All	All	1908	0	1791	43	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 12.

All (43) 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:A:176:ASN:HB3	1:A:179:LYS:HD2	1.69	0.74
1:A:278:PRO:HA	1:A:297:VAL:HA	1.71	0.73
1:A:203:LEU:HD12	1:A:270:LEU:HB3	1.74	0.70
1:A:203:LEU:HD21	1:A:208:PHE:HB2	1.75	0.69
1:A:263:GLY:O	1:A:265:LYS:N	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ARG:HB3	1:A:207:ASP:HB2	1.81	0.63
1:A:189:TYR:HB2	1:A:255:ILE:HB	1.83	0.60
1:A:380:ASN:OD1	1:A:381:GLY:N	2.34	0.60
1:A:174:SER:HB3	1:A:268:TRP:H	1.69	0.58
1:A:185:SER:H	1:A:259:THR:HG1	1.53	0.55
1:A:195:LYS:HG2	1:A:328:SER:HB2	1.89	0.55
1:A:187:CYS:HB2	1:A:257:PHE:HB3	1.90	0.53
1:A:199:VAL:O	1:A:248:THR:OG1	2.21	0.53
1:A:359:GLU:OE1	1:A:359:GLU:N	2.41	0.52
1:A:362:LEU:O	1:A:365:SER:OG	2.26	0.51
1:A:378:MET:SD	1:A:380:ASN:ND2	2.84	0.51
1:A:197:PHE:HE1	1:A:276:PRO:HG3	1.76	0.51
1:A:183:GLU:HB2	1:A:260:ASP:O	2.11	0.50
1:A:301:VAL:HG22	1:A:325:THR:HG22	1.94	0.49
1:A:192:ARG:HH21	1:A:252:ALA:HB1	1.77	0.49
1:A:250:SER:OG	1:A:252:ALA:O	2.30	0.48
1:A:198:GLN:HB3	1:A:277:MET:SD	2.53	0.48
1:A:223:LEU:HB2	1:A:257:PHE:HD2	1.78	0.48
1:A:192:ARG:NH2	1:A:252:ALA:HB1	2.29	0.48
1:A:207:ASP:O	1:A:268:TRP:HA	2.15	0.46
1:A:209:ASP:HB3	1:A:267:GLY:H	1.80	0.46
1:A:279:CYS:HB3	1:A:332:TRP:CE2	2.52	0.45
1:A:303:GLN:OE1	1:A:305:THR:OG1	2.34	0.45
1:A:180:PRO:HA	1:A:265:LYS:O	2.17	0.45
1:A:275:ASP:HA	1:A:276:PRO:HD3	1.87	0.45
1:A:191:ILE:O	1:A:192:ARG:HD3	2.18	0.44
1:A:334:ASN:HB3	1:A:337:LEU:HG	2.00	0.44
1:A:223:LEU:HB2	1:A:257:PHE:CD2	2.53	0.43
1:A:177:TYR:CG	1:A:178:PRO:HA	2.53	0.43
1:A:174:SER:O	1:A:177:TYR:HB2	2.19	0.42
1:A:292:ALA:HA	1:A:296:TYR:OH	2.20	0.42
1:A:240:PHE:HA	1:A:241:PRO:HD3	1.68	0.41
1:A:266:LYS:HE2	1:A:266:LYS:HB3	1.79	0.41
1:A:357:ASP:HA	1:A:358:PRO:HD3	1.90	0.41
1:A:304:ILE:HD13	1:A:322:PHE:CE1	2.56	0.41
1:A:377:TYR:N	1:A:407:VAL:O	2.44	0.41
1:A:177:TYR:CD1	1:A:178:PRO:HA	2.56	0.40
1:A:187:CYS:O	1:A:256:ILE:HA	2.21	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	242/249 (97%)	216 (89%)	23 (10%)	3 (1%)	16 47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	A	285	PRO
1	A	378	MET

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	210/212 (99%)	202 (96%)	8 (4%)	40 76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	SER
1	A	204	ARG
1	A	244	LEU
1	A	270	LEU
1	A	320	THR
1	A	321	SER
1	A	325	THR
1	A	355	VAL

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 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

There are no carbohydrates 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, 95^{th} 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	246/249 (98%)	1.66	79 (32%) 1 0	78, 128, 193, 263	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	GLY	7.2
1	A	263	GLY	6.9
1	A	339	CYS	5.6
1	A	164	VAL	3.9
1	A	309	GLY	3.9
1	A	223	LEU	3.7
1	A	216	ALA	3.7
1	A	250	SER	3.7
1	A	189	TYR	3.7
1	A	191	ILE	3.5
1	A	382	GLY	3.4
1	A	225	PHE	3.4
1	A	363	PHE	3.3
1	A	304	ILE	3.3
1	A	323	TYR	3.3
1	A	375	TYR	3.3
1	A	302	VAL	3.2
1	A	208	PHE	3.2
1	A	295	LYS	3.2
1	A	237	GLY	3.2
1	A	376	TYR	3.1
1	A	384	GLY	3.1
1	A	312	VAL	3.0
1	A	380	ASN	3.0
1	A	364	GLY	3.0
1	A	219	CYS	3.0
1	A	372	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	368	ARG	2.9
1	A	322	PHE	2.9
1	A	394	TRP	2.8
1	A	165	PHE	2.8
1	A	387	HIS	2.8
1	A	275	ASP	2.8
1	A	345	GLY	2.8
1	A	212	ALA	2.8
1	A	257	PHE	2.7
1	A	217	GLY	2.6
1	A	306	CYS	2.6
1	A	254	ASP	2.6
1	A	332	TRP	2.6
1	A	241	PRO	2.6
1	A	169	ILE	2.6
1	A	177	TYR	2.6
1	A	289	TRP	2.6
1	A	401	PRO	2.5
1	A	215	SER	2.5
1	A	218	ASN	2.5
1	A	298	PHE	2.5
1	A	308	ASP	2.5
1	A	200	VAL	2.4
1	A	210	VAL	2.4
1	A	261	LEU	2.4
1	A	284	THR	2.4
1	A	383	GLY	2.3
1	A	211	GLU	2.3
1	A	264	GLN	2.3
1	A	356	GLU	2.3
1	A	235	TYR	2.3
1	A	202	THR	2.3
1	A	180	PRO	2.3
1	A	193	LEU	2.2
1	A	221	ASP	2.2
1	A	269	LYS	2.2
1	A	229	ASP	2.2
1	A	236	CYS	2.2
1	A	403	LEU	2.2
1	A	285	PRO	2.1
1	A	161	SER	2.1
1	A	253	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	252	ALA	2.1
1	A	272	TYR	2.1
1	A	274	GLY	2.1
1	A	231	GLN	2.1
1	A	203	LEU	2.1
1	A	181	TYR	2.1
1	A	255	ILE	2.1
1	A	199	VAL	2.0
1	A	182	PRO	2.0
1	A	172	ILE	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.