Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 02:20 PM EDT

PDB ID	:	3Q9U
Title	:	In silico and in vitro co-evolution of a high affinity complementary protein-protein interface
Authors	:	Karanicolas, J.; Corn, J.E.; Chen, I.; Joachimiak, L.A.; Dym, O.; Chung, S.; Albeck, S.; Unger, T.; Hu, W.; Liu, G.; Delbecq, S.; Montelione, G.T.; Spiegel, C.; Liu, D.; Baker, D.; Israel Structural Proteomics Center (ISPC)
Deposited on	:	2011-01-10
Resolution	:	2.30 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 (i) 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 (1)) were used in the production of this report:

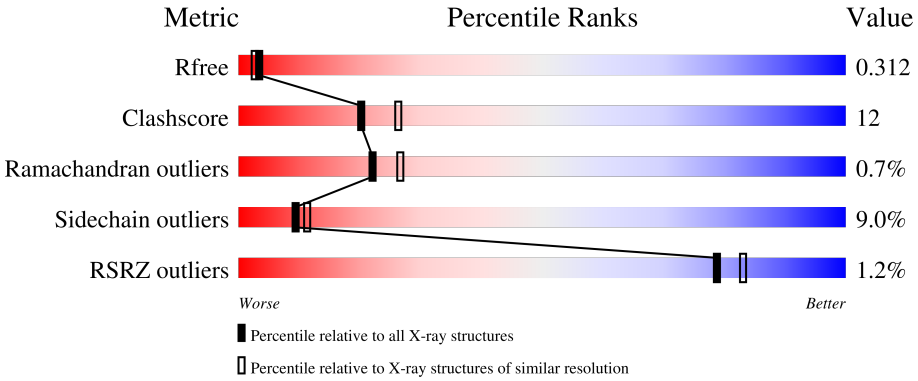
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.90Å 57.62Å 58.23Å 89.96° 90.14° 113.44°	Depositor
Resolution (Å)	37.74 – 2.30 37.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	86.2 (37.74-2.30) 86.2 (37.74-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.240 , 0.318 0.235 , 0.312	Depositor DCC
R_{free} test set	1263 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 40.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4617	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.57% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

3 Model quality

3.1 Standard geometry

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

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	0.51	0/1141	0.67	0/1546
1	B	0.48	0/1116	0.64	1/1513 (0.1%)
2	C	0.45	0/1170	0.63	0/1592
2	D	0.43	0/1174	0.60	0/1599
All	All	0.47	0/4601	0.64	1/6250 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	69	LEU	CA-CB-CG	6.44	130.11	115.30

There are no chirality outliers.

There are no planarity outliers.

3.2 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	1115	0	1141	31	0
1	B	1090	0	1117	32	0
2	C	1156	0	1136	18	0
2	D	1160	0	1141	34	0
3	A	48	0	28	0	0
3	B	48	0	28	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4617	0	4591	114	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 (114) 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:D:-3:ALA:HA	2:D:-2:PHE:HB2	1.08	1.04
2:D:-3:ALA:HA	2:D:-2:PHE:CB	1.93	0.98
2:D:-3:ALA:CA	2:D:-2:PHE:HB2	1.96	0.95
2:D:113:GLN:HG2	2:D:116:ILE:HD12	1.63	0.81
1:B:57:GLU:O	1:B:63:LYS:HA	1.82	0.80
1:A:13:ARG:O	1:A:17:THR:HB	1.88	0.74
2:D:49:GLU:O	2:D:53:VAL:HG13	1.89	0.73
1:A:23:ALA:HB2	1:A:75:ILE:HD12	1.72	0.71
2:D:136:THR:HG23	2:D:139:ASP:H	1.56	0.71
2:D:113:GLN:O	2:D:117:VAL:HG23	1.91	0.69
2:C:148:ASP:O	2:C:152:ILE:HG23	1.94	0.68
2:D:135:LEU:HD22	2:D:139:ASP:HB3	1.76	0.67
1:B:137:LEU:O	1:B:138:LEU:HD23	1.96	0.66
2:D:5:LYS:HB3	2:D:21:LEU:HD11	1.78	0.66
1:B:122:LEU:HD22	1:B:122:LEU:H	1.62	0.63
2:C:29:ASN:HD21	2:C:60:ASP:H	1.47	0.63
2:D:55:LEU:C	2:D:57:ASN:H	2.03	0.62
2:C:138:PHE:HE1	2:C:154:GLN:HG3	1.66	0.59
2:C:113:GLN:HG2	2:C:116:ILE:HD12	1.85	0.59
1:B:62:ARG:HH11	1:B:62:ARG:HB3	1.68	0.58
1:B:67:SER:OG	1:B:69:LEU:HD12	2.03	0.58
1:A:19:TYR:O	1:A:20:LYS:HE2	2.03	0.58
2:D:22:MET:CE	2:D:57:ASN:HD22	2.16	0.58
2:D:29:ASN:HD21	2:D:60:ASP:H	1.50	0.58
2:C:117:VAL:HG12	2:C:152:ILE:HD11	1.85	0.58
1:B:105:GLN:HB3	3:B:1070:COA:O5P	2.04	0.57
1:B:101:VAL:HG13	1:B:123:ILE:O	2.05	0.56
1:B:74:LYS:HG2	1:B:75:ILE:N	2.20	0.56
1:A:67:SER:O	1:A:70:ASP:HB2	2.06	0.55
1:B:133:GLU:HA	1:B:133:GLU:OE2	2.06	0.55
1:B:51:PRO:HB2	1:B:64:CYS:SG	2.46	0.55
1:B:122:LEU:H	1:B:122:LEU:CD2	2.19	0.55
1:B:8:THR:O	1:B:12:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ILE:C	1:B:97:LYS:H	2.10	0.54
2:D:55:LEU:C	2:D:57:ASN:N	2.61	0.54
1:B:105:GLN:HE22	1:B:130:MET:H	1.55	0.54
1:A:2:ARG:HB3	1:A:2:ARG:CZ	2.37	0.54
2:C:138:PHE:C	2:C:138:PHE:CD2	2.81	0.54
2:C:147:GLU:H	2:C:147:GLU:CD	2.10	0.54
1:B:73:ASP:OD1	1:B:74:LYS:N	2.41	0.53
2:D:22:MET:HE1	2:D:57:ASN:HD22	1.73	0.53
1:A:2:ARG:HB2	1:A:2:ARG:NH1	2.24	0.52
1:B:134:HIS:CD2	1:B:138:LEU:HD12	2.45	0.52
2:D:61:VAL:HG22	2:D:92:ALA:HB2	1.92	0.52
1:B:131:MET:HG2	1:B:135:LYS:HD2	1.90	0.52
1:A:84:PRO:HG3	1:A:107:ASN:O	2.10	0.50
1:B:123:ILE:HD12	1:B:123:ILE:N	2.26	0.50
2:D:29:ASN:HD21	2:D:60:ASP:N	2.09	0.50
2:D:140:ILE:O	2:D:144:GLN:HG3	2.11	0.50
1:A:2:ARG:CZ	1:A:2:ARG:CB	2.89	0.50
1:B:129:CYS:HG	3:B:1070:COA:HS1	1.60	0.50
2:D:148:ASP:HA	2:D:151:GLU:OE2	2.12	0.49
1:B:91:VAL:O	1:B:95:ILE:HD12	2.13	0.49
1:B:101:VAL:HG12	1:B:102:VAL:N	2.28	0.49
1:A:21:LYS:HG2	1:A:76:GLU:OE1	2.13	0.49
1:B:58:GLU:HA	1:B:62:ARG:O	2.13	0.49
1:B:92:ALA:O	1:B:96:LYS:HG3	2.13	0.48
2:C:117:VAL:CG1	2:C:152:ILE:HD11	2.42	0.48
1:B:111:PRO:C	1:B:113:ALA:N	2.66	0.48
1:A:111:PRO:C	1:A:113:ALA:N	2.64	0.48
2:D:136:THR:CG2	2:D:139:ASP:H	2.24	0.48
1:A:44:GLU:O	1:A:44:GLU:HG3	2.14	0.48
2:D:79:GLY:HA3	2:D:113:GLN:NE2	2.29	0.48
1:A:23:ALA:CB	1:A:75:ILE:HD12	2.43	0.47
1:B:100:LYS:N	1:B:100:LYS:HD3	2.29	0.47
2:C:31:THR:HA	2:C:36:LEU:O	2.14	0.47
1:A:105:GLN:HE22	1:A:130:MET:H	1.63	0.46
1:A:111:PRO:C	1:A:113:ALA:H	2.17	0.46
2:D:135:LEU:HD22	2:D:139:ASP:CB	2.44	0.46
1:A:102:VAL:HG23	1:A:122:LEU:HD13	1.97	0.46
2:D:39:LEU:HD23	2:D:71:PRO:HG2	1.98	0.45
2:D:127:VAL:CG2	2:D:153:LEU:O	2.65	0.45
1:A:29:PRO:HD3	1:A:56:TYR:CE1	2.52	0.45
1:A:83:ASN:OD1	1:A:85:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:138:PHE:CE1	2:C:154:GLN:HG3	2.50	0.45
1:A:109:TYR:CE2	1:A:113:ALA:HB3	2.52	0.44
2:C:-2:PHE:CE1	2:C:0:GLN:HB2	2.53	0.44
2:D:110:LEU:HG	2:D:140:ILE:HG21	1.99	0.44
1:B:111:PRO:C	1:B:113:ALA:H	2.20	0.44
2:C:113:GLN:O	2:C:117:VAL:HG23	2.17	0.44
2:D:136:THR:O	2:D:140:ILE:HG13	2.18	0.44
2:D:148:ASP:O	2:D:151:GLU:HB2	2.18	0.44
1:A:139:GLY:O	1:A:140:GLU:C	2.56	0.44
2:D:110:LEU:HA	2:D:144:GLN:HE22	1.83	0.44
1:B:112:LEU:HD23	2:D:102:TRP:CZ3	2.54	0.43
1:B:34:ASP:N	1:B:34:ASP:OD1	2.51	0.43
2:C:133:LEU:O	2:C:135:LEU:HD12	2.18	0.43
2:D:127:VAL:HG21	2:D:153:LEU:O	2.18	0.43
1:A:71:ILE:HA	1:A:72:PRO:HD3	1.88	0.43
2:C:20:ILE:O	2:C:24:ASN:HB2	2.19	0.43
2:C:64:SER:HA	2:C:69:ILE:O	2.19	0.42
2:D:16:ASP:O	2:D:20:ILE:HD12	2.19	0.42
2:D:115:GLU:O	2:D:119:VAL:HG23	2.19	0.42
2:C:148:ASP:O	2:C:151:GLU:HB3	2.20	0.42
1:A:18:ARG:HD2	1:A:19:TYR:CE1	2.54	0.42
1:A:31:PRO:HD2	1:A:32:GLU:OE1	2.19	0.42
1:A:121:GLY:HA3	1:A:122:LEU:HA	1.88	0.42
1:A:59:VAL:HG23	1:A:64:CYS:HB2	2.02	0.41
1:A:19:TYR:C	1:A:20:LYS:HE2	2.39	0.41
1:B:42:LEU:HD23	1:B:42:LEU:HA	1.86	0.41
2:D:100:ALA:HB3	2:D:102:TRP:CE3	2.55	0.41
1:A:30:LYS:HA	1:A:31:PRO:HD3	1.89	0.41
2:D:127:VAL:HG22	2:D:127:VAL:O	2.20	0.41
1:A:65:TYR:HA	1:A:66:PRO:HD3	1.88	0.41
1:B:39:MET:HG2	1:B:60:LEU:HD12	2.02	0.41
1:A:2:ARG:NH1	1:A:2:ARG:CB	2.84	0.41
1:A:83:ASN:OD1	1:A:85:ALA:HB3	2.20	0.41
2:D:72:LEU:HD11	2:D:84:VAL:HG13	2.02	0.41
2:C:115:GLU:O	2:C:119:VAL:HG23	2.20	0.41
1:A:22:ILE:HD11	1:A:47:TYR:CD2	2.55	0.41
1:B:81:PHE:CZ	1:B:105:GLN:HG3	2.56	0.40
1:A:2:ARG:HB2	1:A:2:ARG:HH11	1.86	0.40
1:B:136:ARG:HG2	1:B:136:ARG:O	2.21	0.40
2:C:142:ILE:HG22	2:C:143:ASN:N	2.35	0.40

There are no symmetry-related clashes.

3.3 Torsion angles (i)

3.3.1 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	134/141 (95%)	126 (94%)	8 (6%)	0	100 100
1	B	132/141 (94%)	120 (91%)	10 (8%)	2 (2%)	10 10
2	C	155/158 (98%)	150 (97%)	5 (3%)	0	100 100
2	D	156/158 (99%)	146 (94%)	8 (5%)	2 (1%)	12 12
All	All	577/598 (96%)	542 (94%)	31 (5%)	4 (1%)	22 26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	-2	PHE
1	B	120	ALA
1	B	96	LYS
2	D	56	LYS

3.3.2 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	117/118 (99%)	106 (91%)	11 (9%)	8 10
1	B	114/118 (97%)	102 (90%)	12 (10%)	7 8
2	C	117/117 (100%)	108 (92%)	9 (8%)	13 16
2	D	117/117 (100%)	107 (92%)	10 (8%)	10 13
All	All	465/470 (99%)	423 (91%)	42 (9%)	9 11

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	15	THR
1	A	17	THR
1	A	28	SER
1	A	32	GLU
1	A	37	ILE
1	A	67	SER
1	A	75	ILE
1	A	111	PRO
1	A	112	LEU
1	A	116	GLN
1	B	10	GLU
1	B	14	GLU
1	B	15	THR
1	B	18	ARG
1	B	37	ILE
1	B	62	ARG
1	B	64	CYS
1	B	69	LEU
1	B	74	LYS
1	B	75	ILE
1	B	100	LYS
1	B	122	LEU
2	C	2	LEU
2	C	16	ASP
2	C	47	GLN
2	C	115	GLU
2	C	138	PHE
2	C	142	ILE
2	C	147	GLU
2	C	151	GLU
2	C	152	ILE
2	D	4	LYS
2	D	8	GLU
2	D	21	LEU
2	D	33	ASP
2	D	47	GLN
2	D	53	VAL
2	D	56	LYS
2	D	110	LEU
2	D	113	GLN
2	D	151	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	B	105	GLN
2	C	29	ASN
2	C	47	GLN
2	C	80	HIS
2	C	123	HIS
2	D	29	ASN
2	D	47	GLN
2	D	57	ASN
2	D	123	HIS
2	D	144	GLN

3.3.3 RNA

There are no RNA molecules in this entry.

3.4 Non-standard residues in protein, DNA, RNA chains

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

3.5 Carbohydrates

There are no monosaccharides in this entry.

3.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - 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.

3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 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	138/141 (97%)	-0.15	0	100	100	17, 31, 58, 89	0
1	B	136/141 (96%)	-0.27	1 (0%)	87	91	19, 38, 75, 87	0
2	C	157/158 (99%)	-0.15	3 (1%)	66	73	20, 37, 68, 106	4 (2%)
2	D	158/158 (100%)	-0.17	3 (1%)	66	73	22, 39, 62, 84	3 (1%)
All	All	589/598 (98%)	-0.18	7 (1%)	79	83	17, 37, 67, 106	7 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	0	GLN	3.8
2	C	138	PHE	2.8
1	B	61	GLY	2.2
2	D	25	GLY	2.2
2	C	142	ILE	2.1
2	D	20	ILE	2.1
2	C	2	LEU	2.0

4.2 Non-standard residues in protein, DNA, RNA chains

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

4.3 Carbohydrates

There are no monosaccharides in this entry.

4.4 Ligands

LIGAND-RSR INFOmissingINFO

4.5 Other polymers (i)

There are no such residues in this entry.