Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:29 AM GMT

PDB ID	:	2HEO
Title	:	General Structure-Based Approach to the Design of Protein Ligands: Application to the Design of Kv1.2 Potassium Channel Blockers.
Authors	:	Magis, C.; Gasparini, S.; Charbonnier, J.B.; Stura, E.; Le Du, M.H.; Menez, A.; Cuniasse, P.
Deposited on	:	2006-06-21
Resolution	:	1.70 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:

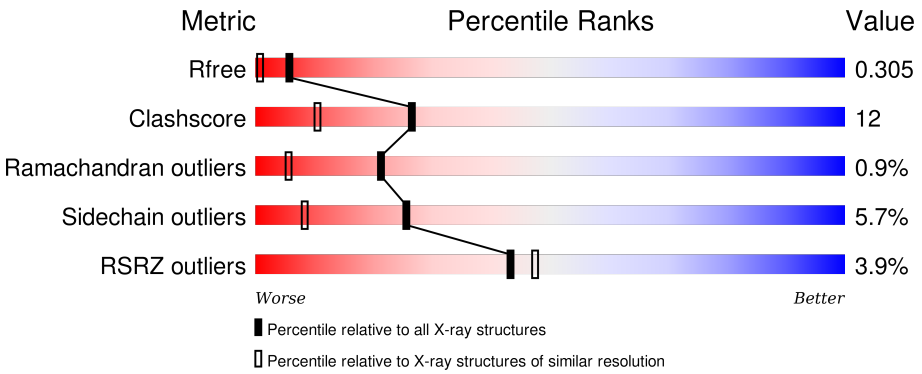
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	B	7	57% 29% 14%
1	E	7	71% 14% 14%
2	A	67	4% 66% 19% • 12%
2	D	67	3% 67% 16% • 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1409 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 DNA chain called 5'-D(*TP*CP*GP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	6	123	57	24	36	6	0	0	0
1	E	6	123	57	24	36	6	0	0	0

- Molecule 2 is a protein called Z-DNA binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	59	477	305	85	86	1	0	3	0
2	D	58	458	294	78	85	1	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	GLY	-	CLONING ARTIFACT	UNP Q9QY24
A	105	SER	-	CLONING ARTIFACT	UNP Q9QY24
A	106	HIS	-	CLONING ARTIFACT	UNP Q9QY24
A	107	MET	-	CLONING ARTIFACT	UNP Q9QY24
A	130	ALA	LYS	ENGINEERED	UNP Q9QY24
A	132	PHE	GLY	ENGINEERED	UNP Q9QY24
A	162	SER	GLU	ENGINEERED	UNP Q9QY24
A	164	LYS	ALA	ENGINEERED	UNP Q9QY24
A	165	TYR	THR	ENGINEERED	UNP Q9QY24
D	104	GLY	-	CLONING ARTIFACT	UNP Q9QY24
D	105	SER	-	CLONING ARTIFACT	UNP Q9QY24
D	106	HIS	-	CLONING ARTIFACT	UNP Q9QY24
D	107	MET	-	CLONING ARTIFACT	UNP Q9QY24
D	130	ALA	LYS	ENGINEERED	UNP Q9QY24
D	132	PHE	GLY	ENGINEERED	UNP Q9QY24
D	162	SER	GLU	ENGINEERED	UNP Q9QY24

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Chain	Residue	Modelled	Actual	Comment	Reference
D	164	LYS	ALA	ENGINEERED	UNP Q9QY24
D	165	TYR	THR	ENGINEERED	UNP Q9QY24

- Molecule 3 is water.

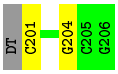
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	83	Total O 83 83	0	0
3	B	32	Total O 32 32	0	0
3	D	84	Total O 84 84	0	0
3	E	29	Total O 29 29	0	0

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: 5'-D(*TP*CP*GP*CP*GP*CP*G)-3'

Chain B:

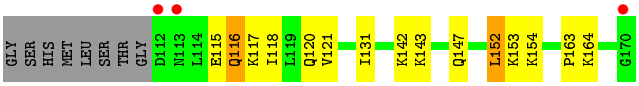


- Molecule 1: 5'-D(*TP*CP*GP*CP*GP*CP*G)-3'

Chain E:

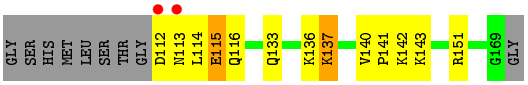
- Molecule 2: Z-DNA binding protein 1

Chain A:



- Molecule 2: Z-DNA binding protein 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	79.91Å 79.91Å 55.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.70 43.22 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.70) 99.8 (43.22-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.241 , 0.305 0.243 , 0.305	Depositor DCC
R_{free} test set	1129 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 37.7	EDS
Estimated twinning fraction	0.439 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 22200 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	1409	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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 (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	B	1.16	0/137	2.03	3/209 (1.4%)
1	E	1.32	2/137 (1.5%)	2.18	5/209 (2.4%)
2	A	0.76	1/500 (0.2%)	0.94	2/670 (0.3%)
2	D	0.65	0/466	0.74	0/630
All	All	0.86	3/1240 (0.2%)	1.27	10/1718 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	152	LEU	C-N	8.07	1.52	1.34
1	E	204	DG	C2-N3	5.65	1.37	1.32
1	E	205	DC	N1-C6	5.07	1.40	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	152	LEU	O-C-N	-11.17	104.83	122.70
1	E	204	DG	O4'-C1'-N9	-9.70	101.21	108.00
1	B	204	DG	O4'-C1'-N9	-9.26	101.52	108.00
1	E	201	DC	OP1-P-OP2	8.94	133.00	119.60
2	A	152	LEU	CA-C-N	7.48	133.65	117.20
1	B	204	DG	N3-C2-N2	-6.50	115.35	119.90
1	B	204	DG	N9-C4-C5	6.34	107.93	105.40
1	E	205	DC	C6-N1-C2	5.34	122.44	120.30
1	E	202	DG	O4'-C1'-N9	-5.32	104.27	108.00
1	E	203	DC	P-O3'-C3'	5.17	125.91	119.70

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	B	123	0	67	1	0
1	E	123	0	67	2	0
2	A	477	0	509	12	0
2	D	458	0	471	13	0
3	A	83	0	0	2	0
3	B	32	0	0	2	1
3	D	84	0	0	2	1
3	E	29	0	0	3	0
All	All	1409	0	1114	28	1

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 (28) 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:140:VAL:HG12	2:D:141:PRO:HD2	1.55	0.87
1:E:206:DG:N7	3:E:210:HOH:O	2.16	0.77
2:D:140:VAL:CG1	2:D:141:PRO:HD2	2.14	0.77
2:A:117:LYS:NZ	3:A:215:HOH:O	2.26	0.67
2:D:140:VAL:HG12	2:D:141:PRO:CD	2.27	0.65
2:D:133:GLN:O	2:D:137:LYS:HD3	1.96	0.65
3:E:46:HOH:O	2:D:142:LYS:HE3	1.97	0.63
2:D:115:GLU:HG3	2:D:151:ARG:NH1	2.14	0.62
2:A:153:LYS:HE3	3:A:235:HOH:O	1.98	0.62
2:D:140:VAL:CG1	2:D:141:PRO:CD	2.78	0.61
2:A:118:ILE:O	2:A:121:VAL:HG22	2.02	0.59
2:A:131:ILE:HG12	2:A:142:LYS:HG3	1.83	0.59
1:B:201:DC:H5"	3:B:26:HOH:O	2.02	0.58
2:A:118:ILE:O	2:A:121:VAL:CG2	2.53	0.56
2:D:136:LYS:NZ	3:D:216:HOH:O	2.40	0.54
2:D:143:LYS:NZ	3:D:191:HOH:O	2.40	0.52
2:A:116:GLN:HE21	2:A:116:GLN:HA	1.75	0.51
1:E:201:DC:H5"	3:E:211:HOH:O	2.10	0.51
2:A:116:GLN:HE21	2:A:116:GLN:CA	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:117:LYS:O	2:A:121:VAL:HG22	2.12	0.50
2:A:143:LYS:O	2:A:147:GLN:HG3	2.11	0.50
2:A:115:GLU:HG3	2:A:152:LEU:HD21	1.94	0.49
2:D:115:GLU:HG3	2:D:151:ARG:HH11	1.78	0.47
2:D:133:GLN:HE22	2:D:136:LYS:NZ	2.12	0.46
2:A:163:PRO:O	2:A:164:LYS:HB2	2.18	0.44
3:B:15:HOH:O	2:A:142:LYS:HE2	2.18	0.44
2:D:112:ASP:OD2	2:D:116:GLN:HB2	2.18	0.43
2:D:140:VAL:HG13	2:D:141:PRO:HD2	2.01	0.40

All (1) 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:B:175:HOH:O	3:D:219:HOH:O[6_665]	2.15	0.05

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
2	A	60/67 (90%)	59 (98%)	1 (2%)	0	100 100
2	D	56/67 (84%)	55 (98%)	0	1 (2%)	11 1
All	All	116/134 (87%)	114 (98%)	1 (1%)	1 (1%)	21 5

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	114	LEU

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	
2	A	56/60 (93%)	52 (93%)	4 (7%)	18	4
2	D	52/60 (87%)	49 (94%)	3 (6%)	25	8
All	All	108/120 (90%)	101 (94%)	7 (6%)	25	6

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	116	GLN
2	A	120	GLN
2	A	154[A]	LYS
2	A	154[B]	LYS
2	D	113	ASN
2	D	115	GLU
2	D	137	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	116	GLN
2	A	120	GLN
2	A	133	GLN
2	D	133	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 (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	B	6/7 (85%)	-0.16	0	100	100	28, 29, 32, 32	0
1	E	6/7 (85%)	-0.31	0	100	100	28, 30, 32, 35	0
2	A	59/67 (88%)	0.53	3 (5%)	32	34	26, 31, 41, 45	0
2	D	58/67 (86%)	0.45	2 (3%)	49	53	26, 32, 41, 45	0
All	All	129/148 (87%)	0.42	5 (3%)	43	47	26, 32, 41, 45	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	113	ASN	6.2
2	A	170	GLY	4.8
2	A	112	ASP	4.3
2	D	112	ASP	2.6
2	A	113	ASN	2.2

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.