



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:19 PM GMT

PDB ID : 4K0C
Title : Crystal Structure of the computationally designed serine hydrolase. Northeast Structural Genomics Consortium (NESG) Target OR317
Authors : Kuzin, A.; Lew, S.; Rajagopalan, S.; Seetharaman, J.; Maglaqui, M.; Xiao, R.; Lee, D.; Everett, J.K.; Acton, T.B.; Baker, D.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2013-04-03
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

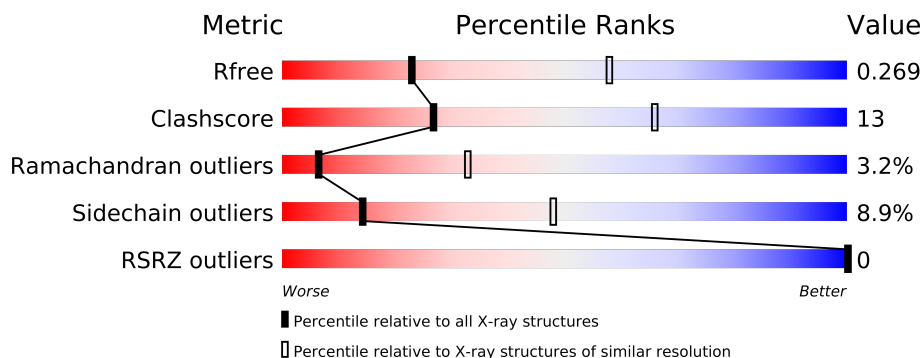
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	167	
1	B	167	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2368 atoms, of which 0 are hydrogen and 0 are deuterium.

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 designed serine hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	Se	0	0	0
			1179	734	218	224	2	1			
1	B	161	Total	C	N	O	S	Se	0	0	0
			1189	740	221	225	2	1			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	30.03Å 76.03Å 128.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.29 – 3.00 37.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.9 (37.29-3.00) 89.5 (37.29-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1269)	Depositor
R, R_{free}	0.181 , 0.257 0.192 , 0.269	Depositor DCC
R_{free} test set	286 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 26.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 5695 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2368	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.44	0/1191	0.61	0/1608
1	B	0.47	0/1202	0.67	1/1623 (0.1%)
All	All	0.46	0/2393	0.64	1/3231 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	VAL	C-N-CD	-6.51	106.27	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1179	0	1218	30	0
1	B	1189	0	1225	34	0
All	All	2368	0	2443	63	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (63) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:161:GLU:H	1:B:162:HIS:HA	1.48	0.79
1:B:13:GLU:OE2	1:B:40:LYS:NZ	2.20	0.74
1:A:65:ALA:HB1	1:A:68:LEU:HB2	1.71	0.71
1:B:113:PRO:HB3	1:B:114:GLY:HA3	1.73	0.70
1:A:14:PHE:O	1:A:69:PRO:HG2	1.97	0.65
1:A:112:VAL:HG21	1:A:146:HIS:CE1	2.32	0.64
1:A:28:LYS:HA	1:A:46:GLN:HE22	1.64	0.62
1:B:161:GLU:N	1:B:162:HIS:HA	2.15	0.61
1:B:65:ALA:HB1	1:B:68:LEU:HB2	1.84	0.60
1:B:117:VAL:HG23	1:B:118:GLY:H	1.68	0.58
1:A:112:VAL:HG22	1:A:113:PRO:HD2	1.85	0.58
1:A:79:LEU:HD23	1:A:84:ALA:HB2	1.88	0.55
1:B:134:LYS:HE2	1:B:162:HIS:HD2	1.71	0.55
1:B:113:PRO:CB	1:B:114:GLY:HA3	2.37	0.55
1:B:115:ALA:HA	1:B:116:TRP:C	2.27	0.55
1:B:6:ASP:OD2	1:B:159:ARG:NH2	2.39	0.54
1:B:126:ARG:HA	1:B:129:MSE:HB2	1.90	0.53
1:B:149:GLU:O	1:B:153:GLU:HG2	2.08	0.53
1:A:133:ILE:HG23	1:A:142:VAL:HG21	1.89	0.53
1:B:113:PRO:HD2	1:B:146:HIS:HA	1.91	0.53
1:B:156:ARG:O	1:B:160:LEU:HD13	2.10	0.52
1:B:106:LYS:HZ2	1:B:139:THR:HB	1.75	0.52
1:A:112:VAL:HG11	1:A:146:HIS:ND1	2.25	0.51
1:A:17:ASP:HB2	1:A:107:THR:O	2.10	0.51
1:B:112:VAL:HG11	1:B:129:MSE:HE1	1.92	0.51
1:B:133:ILE:HD13	1:B:142:VAL:HG11	1.92	0.51
1:A:124:ALA:O	1:A:128:VAL:HG13	2.12	0.50
1:A:130:VAL:HA	1:A:133:ILE:HD12	1.93	0.50
1:B:48:GLU:O	1:B:52:ILE:HG13	2.11	0.50
1:A:91:LYS:NZ	1:A:94:LYS:HD3	2.27	0.50
1:A:121:PRO:HB3	1:B:66:GLY:HA2	1.93	0.49
1:A:97:LEU:HD11	1:A:133:ILE:HA	1.94	0.48
1:A:146:HIS:CE1	1:A:155:CYS:HB2	2.48	0.48
1:B:106:LYS:NZ	1:B:139:THR:HB	2.28	0.48
1:A:84:ALA:HA	1:A:88:THR:HG21	1.95	0.48
1:B:16:GLY:O	1:B:70:VAL:HG12	2.15	0.47
1:A:52:ILE:HD13	1:A:61:ALA:HB1	1.96	0.47
1:B:112:VAL:HA	1:B:113:PRO:O	2.14	0.47
1:A:78:VAL:HG23	1:A:79:LEU:HG	1.96	0.47
1:A:25:ASN:HB2	1:A:55:ILE:O	2.14	0.47
1:B:116:TRP:O	1:B:118:GLY:N	2.48	0.46
1:A:22:ALA:HB2	1:A:116:TRP:CE2	2.50	0.46
1:B:126:ARG:NE	1:B:155:CYS:SG	2.89	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:57:VAL:HG21	1:A:82:GLU:HG2	1.96	0.45
1:B:14:PHE:CE2	1:B:16:GLY:HA3	2.51	0.45
1:B:117:VAL:O	1:B:120:LEU:HB2	2.17	0.45
1:A:2:ALA:HB1	1:A:140:LEU:O	2.17	0.45
1:A:140:LEU:HD12	1:A:140:LEU:HA	1.68	0.44
1:B:115:ALA:HA	1:B:117:VAL:HG22	2.01	0.42
1:A:97:LEU:HD13	1:A:136:ALA:HB2	2.01	0.42
1:B:115:ALA:CA	1:B:117:VAL:HG22	2.50	0.42
1:B:106:LYS:HG2	1:B:139:THR:O	2.20	0.42
1:A:82:GLU:HB2	1:A:83:PRO:HD2	2.00	0.42
1:A:156:ARG:O	1:A:160:LEU:HB2	2.19	0.42
1:A:121:PRO:HB2	1:A:124:ALA:HB3	2.00	0.42
1:B:138:ASP:C	1:B:140:LEU:H	2.23	0.42
1:B:78:VAL:O	1:B:88:THR:HG21	2.20	0.41
1:B:140:LEU:HA	1:B:140:LEU:HD12	1.74	0.41
1:A:89:VAL:HG11	1:A:125:VAL:HG13	2.03	0.40
1:A:144:GLY:O	1:A:146:HIS:HD2	2.04	0.40
1:B:153:GLU:O	1:B:157:ARG:HG3	2.21	0.40
1:B:17:ASP:N	1:B:107:THR:OG1	2.53	0.40
1:A:112:VAL:HG13	1:A:113:PRO:HD2	2.03	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	158/167 (95%)	144 (91%)	10 (6%)	4 (2%)	9	40
1	B	159/167 (95%)	141 (89%)	12 (8%)	6 (4%)	5	27
All	All	317/334 (95%)	285 (90%)	22 (7%)	10 (3%)	6	33

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	PRO
1	B	113	PRO
1	B	117	VAL
1	A	16	GLY
1	B	83	PRO
1	B	116	TRP
1	B	114	GLY
1	A	31	ALA
1	B	115	ALA
1	A	117	VAL

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	118/123 (96%)	108 (92%)	10 (8%)	15	51
1	B	119/123 (97%)	108 (91%)	11 (9%)	13	46
All	All	237/246 (96%)	216 (91%)	21 (9%)	14	48

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	12	THR
1	A	13	GLU
1	A	29	LEU
1	A	88	THR
1	A	91	LYS
1	A	111	THR
1	A	112	VAL
1	A	129	MSE
1	A	155	CYS
1	B	29	LEU
1	B	33	VAL
1	B	85	SER
1	B	88	THR
1	B	90	ARG
1	B	111	THR

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Mol	Chain	Res	Type
1	B	116	TRP
1	B	126	ARG
1	B	128	VAL
1	B	139	THR
1	B	162	HIS

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 chains 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, 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	160/167 (95%)	-0.22	0 100 100	12, 26, 67, 90	0
1	B	161/167 (96%)	-0.18	0 100 100	17, 33, 61, 83	0
All	All	321/334 (96%)	-0.20	0 100 100	12, 29, 64, 90	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.