



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:34 PM GMT

PDB ID : 1DFA
Title : CRYSTAL STRUCTURE OF PI-SCEI IN C2 SPACE GROUP
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Deposited on : 1999-11-18
Resolution : 2.00 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>

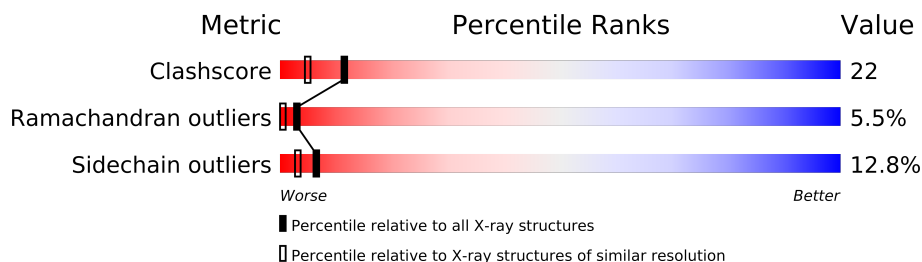
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 2.00 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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	454	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4482 atoms, of which 1113 are hydrogens 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 PI-SCEI ENDONUCLEASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	C	H	N	O	S	728	0	0
			3906	2011	729	547	605	14			

- Molecule 2 is water.

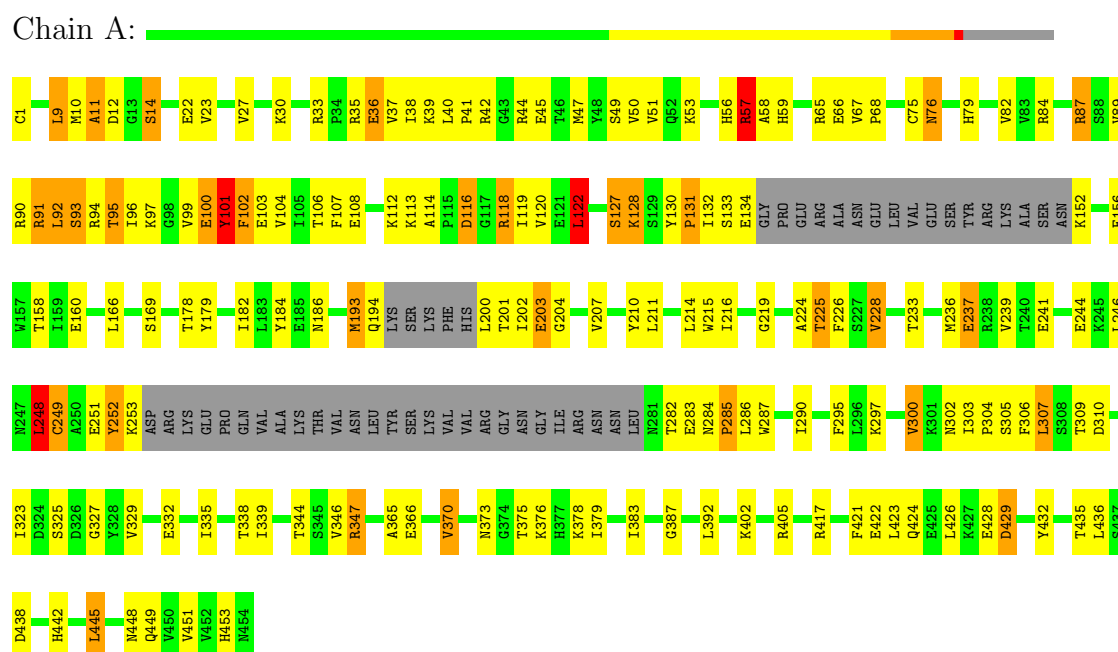
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	192	Total	H	O	384	0
			576	384	192		

3 Residue-property plots

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.

Note EDS was not executed.

• Molecule 1: PI-SCEI ENDONUCLEASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.60Å 76.00Å 71.40Å 90.00° 111.30° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.210 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4482	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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	0.65	0/3235	0.90	8/4364 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	TYR	N-CA-C	6.63	128.89	111.00
1	A	122	LEU	CA-CB-CG	5.99	129.07	115.30
1	A	91	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	445	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	57	ARG	N-CA-C	5.39	125.56	111.00
1	A	65	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	347	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	103	GLU	N-CA-C	5.08	124.72	111.00

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	3177	729	2431	124	0
2	A	192	384	0	7	0
All	All	3369	1113	2431	124	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 22.

All (124) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:370:VAL:HG13	1:A:373:ASN:HA	1.41	0.98
1:A:84:ARG:NH1	1:A:178:THR:HG21	1.93	0.84
1:A:92:LEU:HD23	1:A:95:THR:HA	1.59	0.84
1:A:91:ARG:NH2	1:A:102:PHE:HB2	1.91	0.84
1:A:297:LYS:HB2	1:A:302:ASN:HB2	1.62	0.81
1:A:92:LEU:HD22	1:A:104:VAL:HG21	1.64	0.80
1:A:202:ILE:HG22	1:A:203:GLU:HG3	1.67	0.77
1:A:1:CYS:HA	1:A:76:ASN:ND2	1.99	0.76
1:A:116:ASP:HB2	1:A:118:ARG:NH1	2.00	0.76
1:A:44:ARG:HA	1:A:429:ASP:O	1.86	0.75
1:A:252:TYR:O	1:A:253:LYS:HG3	1.87	0.75
1:A:41:PRO:O	1:A:42:ARG:HD3	1.87	0.74
1:A:130:TYR:CD2	1:A:131:PRO:HD2	2.23	0.73
1:A:39:LYS:HB3	1:A:435:THR:HB	1.74	0.70
1:A:49:SER:HB3	1:A:424:GLN:HB2	1.71	0.70
1:A:297:LYS:HB2	1:A:302:ASN:CB	2.22	0.69
1:A:344:THR:HG23	1:A:347:ARG:NH1	2.09	0.67
1:A:92:LEU:HB2	1:A:104:VAL:HG22	1.76	0.67
1:A:228:VAL:HB	1:A:236:MET:SD	2.35	0.67
1:A:248:LEU:O	1:A:249:CYS:HB2	1.94	0.67
1:A:215:TRP:CD1	1:A:219:GLY:HA3	2.30	0.67
1:A:215:TRP:HB2	1:A:226:PHE:HE2	1.60	0.66
1:A:45:GLU:O	1:A:428:GLU:HA	1.96	0.66
1:A:282:THR:OG1	1:A:284:ASN:HB2	1.96	0.65
1:A:92:LEU:HD22	1:A:104:VAL:CG2	2.27	0.64
1:A:101:TYR:HD2	1:A:128:LYS:HE2	1.61	0.64
1:A:251:GLU:HG3	1:A:252:TYR:CD2	2.33	0.64
1:A:112:LYS:HB2	1:A:122:LEU:HD21	1.80	0.64
1:A:1:CYS:O	1:A:75:CYS:HA	1.97	0.63
1:A:370:VAL:HG13	1:A:373:ASN:CA	2.22	0.63
1:A:57:ARG:NH1	1:A:66:GLU:HA	2.12	0.63
1:A:50:VAL:HG22	1:A:423:LEU:HD11	1.82	0.62
1:A:370:VAL:CG1	1:A:373:ASN:HA	2.23	0.62
1:A:225:THR:HA	1:A:252:TYR:HB3	1.81	0.62
1:A:50:VAL:HG22	1:A:423:LEU:CD1	2.30	0.61
1:A:120:VAL:HG21	1:A:166:LEU:HD12	1.83	0.60
1:A:216:ILE:HD11	1:A:295:PHE:HD2	1.66	0.60
1:A:248:LEU:HD12	1:A:252:TYR:OH	2.00	0.60
1:A:92:LEU:HD21	1:A:96:ILE:O	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:35:ARG:HG3	1:A:436:LEU:HD21	1.84	0.60
1:A:207:VAL:O	1:A:211:LEU:HG	2.03	0.59
1:A:224:ALA:O	1:A:252:TYR:HB3	2.03	0.58
1:A:99:VAL:HG12	1:A:100:GLU:HG2	1.86	0.58
1:A:79:HIS:O	1:A:160:GLU:HA	2.03	0.58
1:A:442:HIS:HD2	2:A:502:HOH:O	1.87	0.57
1:A:297:LYS:HB2	1:A:302:ASN:CG	2.24	0.57
1:A:27:VAL:HG23	1:A:35:ARG:HB2	1.86	0.56
1:A:87:ARG:NH2	1:A:107:PHE:O	2.39	0.56
1:A:182:ILE:HG21	1:A:309:THR:HG22	1.87	0.56
1:A:11:ALA:HB2	1:A:27:VAL:O	2.06	0.55
1:A:297:LYS:CB	1:A:302:ASN:HB2	2.35	0.55
1:A:365:ALA:HB1	1:A:379:ILE:HD11	1.87	0.55
1:A:438:ASP:O	1:A:442:HIS:HE1	1.91	0.54
1:A:287:TRP:CE3	1:A:290:ILE:HD12	2.42	0.54
1:A:237:GLU:O	1:A:241:GLU:HB2	2.08	0.54
1:A:53:LYS:HE3	1:A:421:PHE:O	2.09	0.53
1:A:207:VAL:HG23	1:A:246:LEU:HD13	1.91	0.52
1:A:204:GLY:O	1:A:207:VAL:HG22	2.09	0.52
1:A:228:VAL:HG21	1:A:239:VAL:HG21	1.91	0.52
1:A:23:VAL:HG13	1:A:37:VAL:O	2.10	0.52
1:A:304:PRO:HB2	1:A:306:PHE:CE2	2.45	0.51
1:A:210:TYR:CE2	1:A:214:LEU:HD22	2.45	0.51
1:A:286:LEU:O	1:A:290:ILE:HG13	2.10	0.51
1:A:442:HIS:CD2	2:A:502:HOH:O	2.63	0.50
1:A:96:ILE:HG22	1:A:97:LYS:N	2.26	0.49
1:A:448:ASN:O	1:A:449:GLN:HB2	2.12	0.49
1:A:51:VAL:HG13	1:A:422:GLU:HG3	1.93	0.49
1:A:91:ARG:NH2	1:A:102:PHE:CB	2.67	0.49
1:A:297:LYS:N	1:A:300:VAL:O	2.44	0.49
1:A:120:VAL:HG21	1:A:166:LEU:CD1	2.43	0.49
1:A:225:THR:HA	1:A:252:TYR:CB	2.43	0.49
1:A:179:TYR:CE2	1:A:417:ARG:HB2	2.49	0.48
1:A:193:MET:HG2	1:A:194:GLN:N	2.30	0.47
1:A:303:ILE:HD11	1:A:346:VAL:HG13	1.96	0.47
1:A:36:GLU:CD	1:A:36:GLU:N	2.68	0.46
1:A:1:CYS:HB3	1:A:79:HIS:CD2	2.49	0.46
1:A:297:LYS:HB3	1:A:300:VAL:HG12	1.97	0.46
1:A:35:ARG:HB3	1:A:436:LEU:HG	1.98	0.46
1:A:49:SER:O	1:A:423:LEU:HA	2.16	0.46
1:A:87:ARG:NH1	2:A:560:HOH:O	2.49	0.46
1:A:252:TYR:C	1:A:253:LYS:HG3	2.35	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:335:ILE:HG22	2:A:615:HOH:O	2.16	0.45
1:A:184:TYR:OH	1:A:186:ASN:ND2	2.48	0.45
1:A:10:MET:N	1:A:14:SER:O	2.50	0.45
1:A:82:VAL:HG23	2:A:521:HOH:O	2.15	0.45
1:A:57:ARG:HD2	1:A:67:VAL:HG22	1.99	0.45
1:A:344:THR:HG23	1:A:347:ARG:CZ	2.46	0.45
1:A:236:MET:HB3	2:A:611:HOH:O	2.15	0.45
1:A:366:GLU:O	1:A:379:ILE:HG13	2.17	0.45
1:A:112:LYS:HB2	1:A:122:LEU:CD2	2.46	0.44
1:A:233:THR:HG21	2:A:642:HOH:O	2.16	0.44
1:A:99:VAL:HG12	1:A:100:GLU:N	2.32	0.44
1:A:108:GLU:HB2	1:A:134:GLU:HA	2.00	0.44
1:A:96:ILE:O	1:A:97:LYS:HG3	2.17	0.44
1:A:202:ILE:O	1:A:203:GLU:HB2	2.18	0.44
1:A:23:VAL:HG13	1:A:38:ILE:HA	1.98	0.44
1:A:82:VAL:HG13	1:A:453:HIS:HB2	2.00	0.44
1:A:92:LEU:HG	1:A:96:ILE:HB	2.00	0.44
1:A:49:SER:HB2	1:A:426:LEU:HD11	1.99	0.44
1:A:114:ALA:HB1	1:A:116:ASP:OD2	2.18	0.43
1:A:108:GLU:HB2	1:A:134:GLU:CA	2.49	0.43
1:A:246:LEU:O	1:A:248:LEU:HD23	2.18	0.43
1:A:102:PHE:N	1:A:102:PHE:CD1	2.84	0.43
1:A:90:ARG:O	1:A:91:ARG:HB2	2.19	0.42
1:A:47:MET:O	1:A:426:LEU:HB2	2.19	0.42
1:A:127:SER:OG	1:A:128:LYS:N	2.47	0.42
1:A:89:VAL:HG22	1:A:90:ARG:N	2.35	0.42
1:A:402:LYS:O	1:A:402:LYS:HG2	2.20	0.42
1:A:130:TYR:HD2	1:A:131:PRO:HD2	1.78	0.42
1:A:370:VAL:O	1:A:370:VAL:HG12	2.20	0.42
1:A:30:LYS:NZ	1:A:451:VAL:HG11	2.35	0.42
1:A:56:HIS:N	1:A:56:HIS:ND1	2.68	0.42
1:A:9:LEU:HA	1:A:9:LEU:HD23	1.93	0.42
1:A:284:ASN:HA	1:A:285:PRO:HD2	1.88	0.41
1:A:327:GLY:HA2	1:A:338:THR:O	2.19	0.41
1:A:104:VAL:O	1:A:127:SER:O	2.39	0.41
1:A:307:LEU:HA	1:A:307:LEU:HD12	1.70	0.41
1:A:89:VAL:HG23	1:A:106:THR:HG22	2.02	0.41
1:A:202:ILE:HA	1:A:202:ILE:HD13	1.90	0.41
1:A:432:TYR:N	1:A:432:TYR:CD1	2.89	0.41
1:A:41:PRO:C	1:A:42:ARG:HD3	2.41	0.40
1:A:99:VAL:N	1:A:102:PHE:CZ	2.89	0.40
1:A:323:ILE:HG13	1:A:339:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:SER:OG	1:A:96:ILE:HD11	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	397/454 (87%)	337 (85%)	38 (10%)	22 (6%)	3 0

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	100	GLU
1	A	127	SER
1	A	128	LYS
1	A	131	PRO
1	A	133	SER
1	A	375	THR
1	A	93	SER
1	A	132	ILE
1	A	248	LEU
1	A	370	VAL
1	A	376	LYS
1	A	378	LYS
1	A	101	TYR
1	A	249	CYS
1	A	332	GLU
1	A	58	ALA
1	A	201	THR
1	A	11	ALA
1	A	203	GLU
1	A	285	PRO
1	A	387	GLY

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	344/392 (88%)	300 (87%)	44 (13%)	6 3

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	12	ASP
1	A	14	SER
1	A	22	GLU
1	A	33	ARG
1	A	36	GLU
1	A	40	LEU
1	A	59	HIS
1	A	68	PRO
1	A	76	ASN
1	A	87	ARG
1	A	92	LEU
1	A	94	ARG
1	A	95	THR
1	A	102	PHE
1	A	113	LYS
1	A	116	ASP
1	A	118	ARG
1	A	119	ILE
1	A	122	LEU
1	A	152	LYS
1	A	156	GLU
1	A	158	THR
1	A	169	SER
1	A	193	MET
1	A	200	LEU
1	A	225	THR
1	A	228	VAL
1	A	237	GLU
1	A	244	GLU
1	A	248	LEU

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Mol	Chain	Res	Type
1	A	252	TYR
1	A	283	GLU
1	A	300	VAL
1	A	305	SER
1	A	307	LEU
1	A	310	ASP
1	A	325	SER
1	A	329	VAL
1	A	383	ILE
1	A	392	LEU
1	A	405	ARG
1	A	429	ASP
1	A	445	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	79	HIS
1	A	186	ASN
1	A	188	HIS
1	A	333	HIS
1	A	393	ASN
1	A	442	HIS

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.