



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:13 PM GMT

PDB ID : 2CDR
Title : Crystal structures of caspase-3 in complex with aza-peptide epoxide inhibitors.
Authors : Ganesan, R.; Jelakovic, S.; Campbell, A.J.; Li, Z.Z.; Asgian, J.L.; Powers, J.C.; Gruetter, M.G.
Deposited on : 2006-01-27
Resolution : 1.70 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>

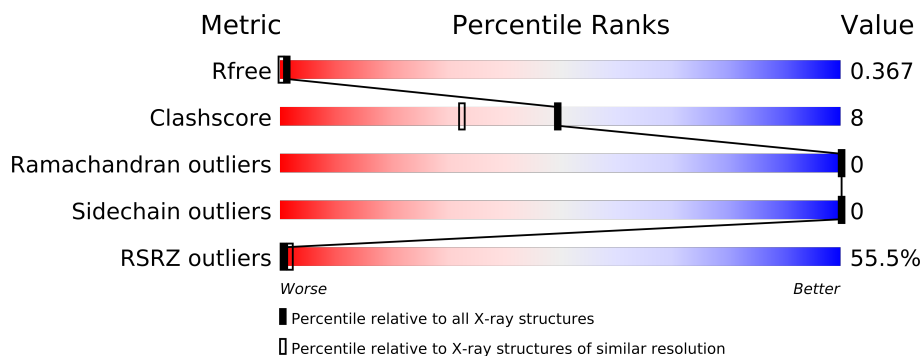
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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}	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (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. 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	147	
2	B	103	
3	I	5	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2429 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 CASPASE-3 SUBUNIT P17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1161	716	208	228	9			

- Molecule 2 is a protein called CASPASE-3 SUBUNIT P12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	103	Total	C	N	O	S	0	0	0
			843	547	135	154	7			

- Molecule 3 is a protein called AZA-PEPTIDE EXPOXIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	5	Total	C	N	O	0	0	0
			62	42	6	14			

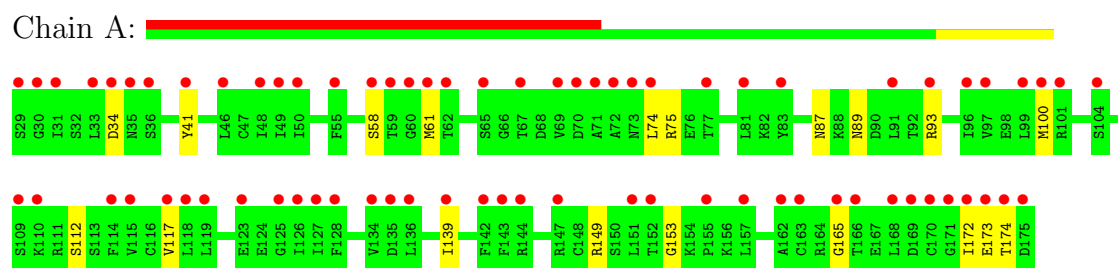
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	126	Total	O	0	0
			126	126		
4	A	231	Total	O	0	0
			231	231		
4	I	6	Total	O	0	0
			6	6		

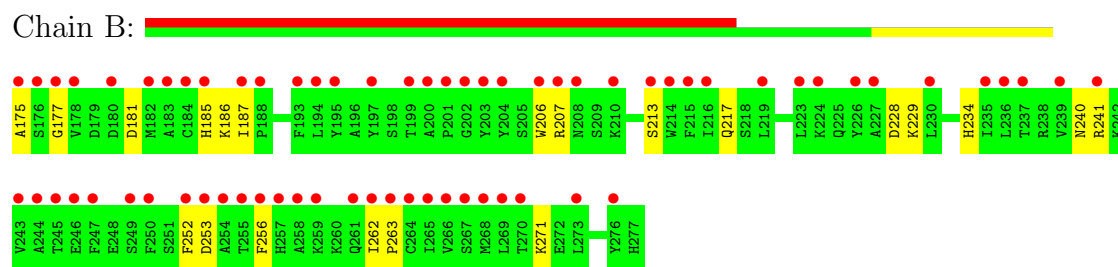
3 Residue-property plots

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.

• Molecule 1: CASPASE-3 SUBUNIT P17



• Molecule 2: CASPASE-3 SUBUNIT P12



• Molecule 3: AZA-PEPTIDE EXPOXIDE



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	67.47Å 83.78Å 96.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.49 – 1.70 19.80 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.49-1.70) 95.6 (19.80-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.177 , 0.204 0.368 , 0.367	Depositor DCC
R_{free} test set	2876 reflections (9.97%)	DCC
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 28859 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	2429	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MY1, PHQ

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	0.29	0/1176	0.58	0/1574
2	B	0.34	0/868	0.63	0/1171
3	I	0.25	0/23	0.62	0/30
All	All	0.31	0/2067	0.60	0/2775

There are no bond length outliers.

There are no bond angle outliers.

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	1161	0	1152	19	12
2	B	843	0	807	13	15
3	I	62	0	44	3	0
4	A	231	0	0	8	6
4	B	126	0	0	6	4
4	I	6	0	0	0	0
All	All	2429	0	2003	31	21

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 8.

All (31) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:185:HIS:O	4:B:2044:HOH:O	1.77	1.01
1:A:61:MET:HG2	3:I:905:MY1:H20	1.48	0.92
1:A:174:THR:OG1	4:A:2221:HOH:O	1.60	0.74
2:B:185:HIS:HB2	4:B:2044:HOH:O	1.88	0.74
1:A:87:ASN:HB2	4:A:2121:HOH:O	1.89	0.71
2:B:241:ARG:NH1	4:B:2096:HOH:O	2.19	0.70
2:B:252:PHE:HB2	4:B:2110:HOH:O	1.90	0.70
2:B:175:ALA:N	4:B:2028:HOH:O	2.27	0.67
2:B:228:ASP:OD1	2:B:229:LYS:HG3	1.97	0.64
1:A:100:MET:HG3	1:A:139:ILE:HG23	1.84	0.59
2:B:177:GLY:HA3	4:B:2035:HOH:O	2.04	0.58
1:A:74:LEU:HD13	1:A:117:VAL:HG11	1.87	0.57
1:A:153:GLY:HA3	4:A:2196:HOH:O	2.07	0.54
1:A:149:ARG:HH11	1:A:149:ARG:HA	1.74	0.53
1:A:165:GLY:HA2	3:I:905:MY1:H27	1.94	0.50
2:B:240:ASN:OD1	2:B:263:PRO:HB2	2.12	0.50
1:A:93:ARG:NH1	4:A:2131:HOH:O	2.45	0.50
2:B:206:TRP:HH2	2:B:256:PHE:HB3	1.76	0.50
2:B:213:SER:O	2:B:217:GLN:HG3	2.12	0.49
2:B:207:ARG:HA	2:B:213:SER:HA	1.96	0.47
1:A:34:ASP:OD1	2:B:271:LYS:HE2	2.15	0.46
2:B:262:ILE:O	2:B:262:ILE:HG23	2.15	0.46
1:A:89:ASN:O	4:A:2124:HOH:O	2.20	0.46
1:A:75:ARG:HD2	4:A:2121:HOH:O	2.16	0.45
1:A:149:ARG:NH1	1:A:149:ARG:HB3	2.32	0.45
1:A:149:ARG:HH11	1:A:149:ARG:CA	2.31	0.43
1:A:89:ASN:HB3	4:A:2038:HOH:O	2.18	0.43
1:A:153:GLY:CA	4:A:2196:HOH:O	2.65	0.43
1:A:74:LEU:CD1	1:A:117:VAL:HG11	2.48	0.42
1:A:41:TYR:HB2	1:A:112:SER:OG	2.21	0.41
1:A:61:MET:SD	3:I:905:MY1:H19	2.60	0.41

All (21) 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	Distance(Å)	Clash(Å)
1:A:58:SER:OG	2:B:253:ASP:OD2[2_665]	1.16	1.04
1:A:173:GLU:OE2	2:B:186:LYS:CG[3_656]	1.49	0.71
1:A:173:GLU:OE2	2:B:186:LYS:CD[3_656]	1.53	0.67
1:A:172:ILE:N	2:B:187:ILE:O[3_656]	1.59	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:234:HIS:CE1	2:B:234:HIS:CE1[3.656]	1.74	0.46
1:A:172:ILE:O	2:B:187:ILE:N[3.656]	1.75	0.45
1:A:173:GLU:CD	2:B:186:LYS:CG[3.656]	1.76	0.44
2:B:234:HIS:NE2	2:B:234:HIS:NE2[3.656]	1.78	0.42
4:A:2126:HOH:O	4:B:2043:HOH:O[6.554]	1.79	0.41
4:A:2063:HOH:O	4:B:2060:HOH:O[2.665]	1.85	0.35
1:A:58:SER:OG	2:B:253:ASP:CG[2.665]	1.86	0.34
1:A:174:THR:CG2	2:B:187:ILE:CG2[3.656]	1.87	0.33
1:A:89:ASN:N	2:B:181:ASP:OD2[6.554]	1.90	0.30
4:A:2085:HOH:O	4:A:2085:HOH:O[3.656]	1.91	0.29
1:A:173:GLU:OE1	2:B:185:HIS:O[3.656]	2.00	0.20
4:A:2156:HOH:O	4:A:2156:HOH:O[3.656]	2.06	0.14
1:A:87:ASN:ND2	2:B:181:ASP:O[6.554]	2.09	0.11
4:A:2079:HOH:O	4:B:2045:HOH:O[6.554]	2.09	0.11
2:B:234:HIS:CE1	2:B:234:HIS:NE2[3.656]	2.13	0.07
1:A:173:GLU:OE1	2:B:186:LYS:CG[3.656]	2.14	0.06
4:A:2059:HOH:O	4:B:2107:HOH:O[2.665]	2.17	0.03

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	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
2	B	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
3	I	1/5 (20%)	1 (100%)	0	0	100	100
All	All	247/255 (97%)	241 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	132/132 (100%)	132 (100%)	0	100	100
2	B	90/90 (100%)	90 (100%)	0	100	100
3	I	3/3 (100%)	3 (100%)	0	100	100
All	All	225/225 (100%)	225 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN

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	147/147 (100%)	2.16	73 (49%) ⓘ ⓘ	12, 18, 29, 56	0
2	B	103/103 (100%)	2.57	67 (65%) ⓘ ⓘ	11, 15, 28, 34	0
3	I	4/5 (80%)	2.33	1 (25%) ⓘ ⓘ	23, 26, 31, 31	0
All	All	254/255 (99%)	2.33	141 (55%) ⓘ ⓘ	11, 17, 29, 56	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	LEU	7.0
2	B	204	TYR	6.5
2	B	256	PHE	6.3
1	A	172	ILE	6.0
1	A	61	MET	5.3
2	B	183	ALA	5.3
2	B	180	ASP	5.1
2	B	252	PHE	4.9
2	B	210	LYS	4.8
1	A	173	GLU	4.8
2	B	206	TRP	4.6
1	A	128	PHE	4.5
1	A	170	CYS	4.5
2	B	262	ILE	4.5
1	A	175	ASP	4.4
2	B	200	ALA	4.4
2	B	250	PHE	4.3
2	B	255	THR	4.2
2	B	246	GLU	4.2
2	B	247	PHE	4.2
1	A	174	THR	4.1
2	B	215	PHE	4.1
2	B	203	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
3	I	904	VAL	3.9
2	B	235	ILE	3.9
2	B	184	CYS	3.8
1	A	30	GLY	3.7
2	B	266	VAL	3.6
1	A	60	GLY	3.6
2	B	253	ASP	3.5
1	A	33	LEU	3.5
1	A	62	THR	3.5
2	B	264	CYS	3.4
2	B	199	THR	3.4
1	A	151	LEU	3.4
1	A	96	ILE	3.4
1	A	136	LEU	3.4
2	B	185	HIS	3.4
1	A	169	ASP	3.4
1	A	152	THR	3.4
2	B	261	GLN	3.3
1	A	46	LEU	3.3
1	A	171	GLY	3.3
2	B	201	PRO	3.3
1	A	162	ALA	3.3
1	A	34	ASP	3.3
2	B	214	TRP	3.3
2	B	270	THR	3.2
1	A	119	LEU	3.2
2	B	176	SER	3.2
1	A	36	SER	3.2
2	B	265	ILE	3.2
2	B	243	VAL	3.1
2	B	208	ASN	3.1
1	A	29	SER	3.1
1	A	59	THR	3.1
2	B	216	ILE	3.1
1	A	155	PRO	3.0
1	A	127	ILE	3.0
2	B	177	GLY	3.0
1	A	123	GLU	3.0
1	A	110	LYS	3.0
1	A	91	LEU	2.9
1	A	100	MET	2.9
2	B	227	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	147	ARG	2.9
2	B	219	LEU	2.9
1	A	139	ILE	2.9
1	A	31	ILE	2.8
1	A	163	CYS	2.8
1	A	143	PHE	2.8
2	B	245	THR	2.8
2	B	223	LEU	2.8
2	B	187	ILE	2.8
2	B	276	TYR	2.8
1	A	118	LEU	2.8
1	A	55	PHE	2.8
2	B	175	ALA	2.7
2	B	230	LEU	2.7
2	B	202	GLY	2.7
2	B	239	VAL	2.7
2	B	178	VAL	2.7
1	A	58	SER	2.7
2	B	273	LEU	2.6
2	B	193	PHE	2.6
2	B	263	PRO	2.6
1	A	72	ALA	2.6
1	A	115	VAL	2.6
1	A	114	PHE	2.6
2	B	195	TYR	2.5
2	B	241	ARG	2.5
2	B	249	SER	2.5
2	B	257	HIS	2.5
2	B	254	ALA	2.5
1	A	165	GLY	2.5
1	A	97	VAL	2.5
2	B	258	ALA	2.5
1	A	142	PHE	2.5
2	B	213	SER	2.5
1	A	35	ASN	2.5
1	A	50	ILE	2.5
1	A	83	TYR	2.5
2	B	244	ALA	2.5
1	A	69	VAL	2.4
1	A	134	VAL	2.4
2	B	182	MET	2.4
1	A	93	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	135	ASP	2.3
1	A	73	ASN	2.3
2	B	197	TYR	2.3
2	B	188	PRO	2.3
1	A	49	ILE	2.2
1	A	125	GLY	2.2
2	B	224	LYS	2.2
2	B	259	LYS	2.2
1	A	104	SER	2.2
1	A	67	THR	2.2
1	A	166	THR	2.2
2	B	267	SER	2.2
1	A	99	LEU	2.2
2	B	269	LEU	2.2
1	A	77	THR	2.2
2	B	236	LEU	2.1
2	B	226	TYR	2.1
1	A	71	ALA	2.1
2	B	268	MET	2.1
1	A	157	LEU	2.1
2	B	207	ARG	2.1
1	A	48	ILE	2.1
1	A	109	SER	2.1
2	B	194	LEU	2.1
2	B	237	THR	2.1
1	A	117	VAL	2.1
1	A	70	ASP	2.0
1	A	65	SER	2.0
1	A	41	TYR	2.0
1	A	74	LEU	2.0
1	A	101	ARG	2.0
1	A	144	ARG	2.0
1	A	126	ILE	2.0
1	A	81	LEU	2.0

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.