



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 07:55 AM EDT

PDB ID : 1GFW
Title : THE 2.8 ANGSTROM CRYSTAL STRUCTURE OF CASPASE-3
(APOPAIN OR CPP32)IN COMPLEX WITH AN ISATIN SULFON-
AMIDE INHIBITOR.
Authors : Concha, N.O.; Janson, C.A.
Deposited on : unknown
Resolution : 2.80 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

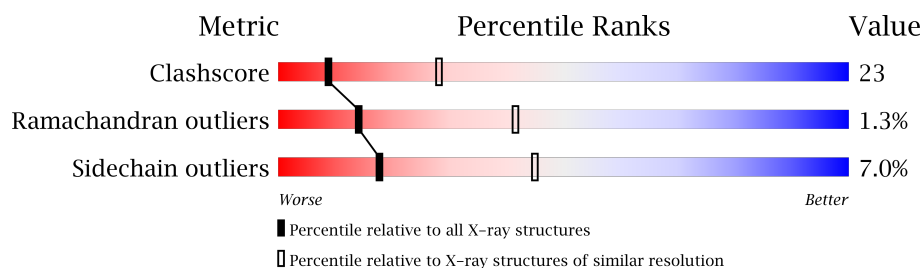
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	147	
2	B	97	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1995 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.

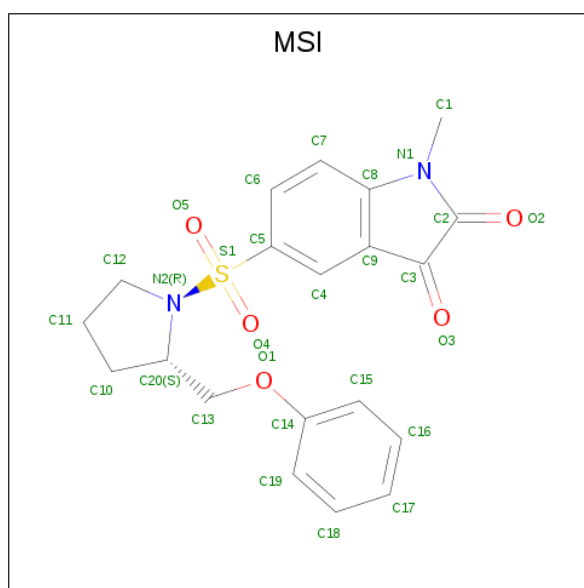
- Molecule 1 is a protein called CASPASE-3 (APOPAIN, P20).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	25	0	0
			1145	708	206	222	9			

- Molecule 2 is a protein called CASPASE-3 (APOPAIN, P10).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	93	Total	C	N	O	S	8	0	0
			777	510	125	137	5			

- Molecule 3 is 1-METHYL-5-(2-PHENOXYMETHYL-PYRROLIDINE-1-SULFONYL)-1H-INDOLE-2,3-DIONE (three-letter code: MSI) (formula: C₂₀H₂₀N₂O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	20	2	5	1		

- Molecule 4 is water.

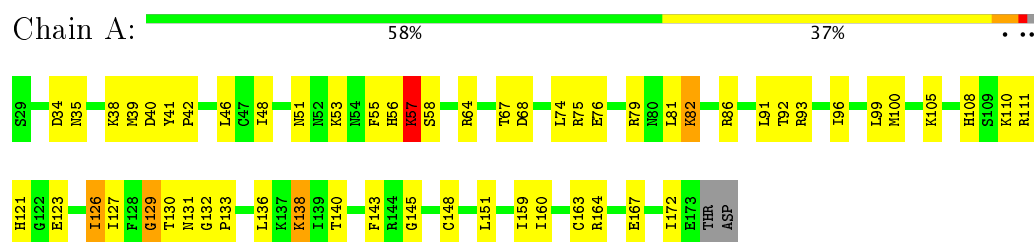
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total 28	O 28	0	0
4	B	17	Total 17	O 17	0	0

3 Residue-property plots [i](#)

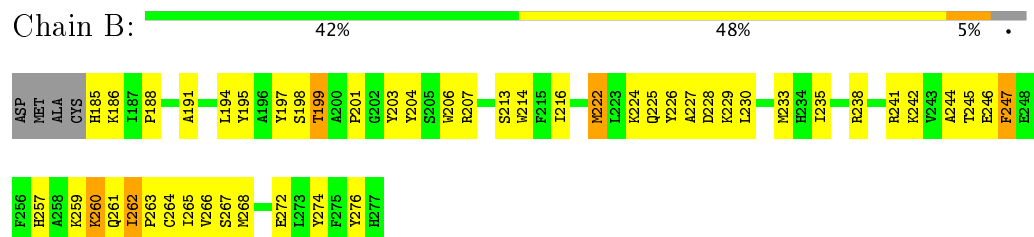
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: CASPASE-3 (APOPAIN, P20)



- Molecule 2: CASPASE-3 (APOPAIN, P10)



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	67.20Å 83.30Å 96.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80	Depositor
% Data completeness (in resolution range)	92.3 (40.00-2.80)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851 & CNS, CNS	Depositor
R, R_{free}	0.200 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1995	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.59	0/1160	0.81	1/1553 (0.1%)
2	B	0.65	0/802	0.80	0/1082
All	All	0.61	0/1962	0.81	1/2635 (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	A	129	GLY	N-CA-C	-6.06	97.94	113.10

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	A	1145	0	1141	50	0
2	B	777	0	752	43	0
3	A	28	0	20	3	0
4	A	28	0	0	0	0
4	B	17	0	0	4	0
All	All	1995	0	1913	85	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 23.

All (85) 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)
1:A:123:GLU:HB2	1:A:126:ILE:HD11	1.47	0.93
1:A:51:ASN:ND2	1:A:67:THR:OG1	2.10	0.83
1:A:123:GLU:CB	1:A:126:ILE:HD11	2.15	0.77
1:A:42:PRO:HG2	1:A:110:LYS:HB3	1.71	0.70
1:A:136:LEU:O	1:A:140:THR:HG23	1.92	0.69
1:A:123:GLU:HB2	1:A:126:ILE:CD1	2.20	0.69
2:B:241:ARG:O	2:B:245:THR:OG1	2.11	0.64
2:B:199:THR:HG21	2:B:204:TYR:O	1.98	0.63
2:B:207:ARG:HA	2:B:213:SER:HA	1.80	0.62
2:B:197:TYR:HB2	2:B:264:CYS:HB3	1.83	0.60
2:B:195:TYR:HB2	2:B:266:VAL:HB	1.83	0.60
1:A:38:LYS:HE2	1:A:40:ASP:OD1	2.03	0.59
1:A:38:LYS:HD3	1:A:41:TYR:CE1	2.38	0.58
2:B:222:MET:CE	2:B:225:GLN:HE21	2.16	0.58
1:A:120:SER:OG	1:A:121:HIS:N	2.37	0.58
3:A:1:MSI:H111	2:B:204:TYR:CD1	2.39	0.57
2:B:246:GLU:HG3	4:B:21:HOH:O	2.06	0.56
1:A:91:LEU:O	1:A:130:THR:HG23	2.06	0.56
2:B:225:GLN:HG2	2:B:226:TYR:CE2	2.42	0.55
2:B:242:LYS:HA	4:B:21:HOH:O	2.06	0.54
2:B:199:THR:HG23	2:B:261:GLN:HG3	1.88	0.54
1:A:143:PHE:HA	1:A:148:CYS:HB2	1.89	0.53
1:A:76:GLU:CD	1:A:79:ARG:HH21	2.12	0.53
1:A:56:HIS:O	1:A:58:SER:N	2.42	0.52
1:A:129:GLY:N	1:A:132:GLY:O	2.37	0.52
1:A:163:CYS:HB2	3:A:1:MSI:O2	2.10	0.52
2:B:233:MET:CE	2:B:265:ILE:HG21	2.38	0.52
1:A:35:ASN:N	1:A:35:ASN:ND2	2.58	0.51
1:A:167:GLU:HB2	2:B:203:TYR:HA	1.91	0.51
1:A:115:VAL:HG12	1:A:116:CYS:N	2.26	0.51
1:A:46:LEU:HD13	1:A:48:ILE:CD1	2.40	0.51
1:A:148:CYS:SG	1:A:151:LEU:HD12	2.51	0.50
2:B:222:MET:HE2	2:B:222:MET:HA	1.93	0.50
1:A:35:ASN:N	1:A:35:ASN:HD22	2.09	0.49
2:B:185:HIS:CE1	4:B:1:HOH:O	2.66	0.49
2:B:214:TRP:N	2:B:214:TRP:CD1	2.79	0.49
2:B:245:THR:OG1	4:B:21:HOH:O	2.19	0.49
2:B:262:ILE:HG22	2:B:262:ILE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:HIS:O	1:A:57:LYS:C	2.51	0.49
2:B:250:PHE:CD1	2:B:257:HIS:HE1	2.31	0.48
1:A:53:LYS:HD2	1:A:68:ASP:OD2	2.13	0.48
1:A:46:LEU:HD13	1:A:48:ILE:HD11	1.93	0.48
1:A:105:LYS:HE2	1:A:105:LYS:HA	1.95	0.48
1:A:127:ILE:HD12	1:A:127:ILE:O	2.13	0.48
1:A:99:LEU:HG	1:A:100:MET:HE3	1.96	0.48
1:A:64:ARG:HA	2:B:207:ARG:NH2	2.29	0.47
1:A:39:MET:HG3	2:B:274:TYR:O	2.14	0.47
2:B:262:ILE:CG2	2:B:262:ILE:O	2.63	0.47
1:A:92:THR:HB	1:A:131:ASN:OD1	2.15	0.46
1:A:53:LYS:HG3	1:A:64:ARG:O	2.17	0.45
1:A:81:LEU:HD21	2:B:227:ALA:CB	2.46	0.45
2:B:233:MET:HE1	2:B:267:SER:HB2	1.99	0.45
1:A:96:ILE:O	1:A:100:MET:HG2	2.17	0.45
1:A:172:ILE:HG23	1:A:172:ILE:O	2.16	0.45
2:B:214:TRP:HH2	2:B:249:SER:N	2.15	0.44
2:B:230:LEU:HB2	2:B:235:ILE:HG13	2.00	0.44
1:A:108:HIS:HA	1:A:111:ARG:HD2	1.99	0.44
2:B:247:PHE:N	2:B:247:PHE:CD2	2.85	0.44
2:B:244:ALA:O	2:B:260:LYS:NZ	2.31	0.43
1:A:55:PHE:N	1:A:55:PHE:CD1	2.85	0.43
1:A:110:LYS:HD3	1:A:110:LYS:HA	1.91	0.43
2:B:198:SER:O	2:B:263:PRO:HA	2.19	0.43
1:A:138:LYS:HG3	1:A:138:LYS:O	2.17	0.43
1:A:46:LEU:HD22	1:A:86:ARG:NH2	2.33	0.43
2:B:228:ASP:OD1	2:B:229:LYS:HG3	2.18	0.43
2:B:254:ALA:O	2:B:255:THR:C	2.56	0.43
1:A:159:ILE:C	1:A:160:ILE:HG13	2.39	0.43
2:B:188:PRO:HB2	2:B:191:ALA:HB2	2.02	0.42
1:A:74:LEU:HD21	2:B:216:ILE:HG23	2.01	0.42
1:A:35:ASN:O	2:B:272:GLU:HG3	2.20	0.42
1:A:100:MET:HA	1:A:100:MET:CE	2.50	0.42
2:B:255:THR:O	2:B:259:LYS:HE3	2.20	0.42
1:A:38:LYS:CE	1:A:40:ASP:OD1	2.68	0.41
3:A:1:MSI:H121	2:B:206:TRP:CE3	2.55	0.41
2:B:222:MET:CE	2:B:222:MET:HA	2.50	0.41
1:A:75:ARG:HG3	1:A:75:ARG:HH11	1.85	0.41
2:B:222:MET:HG2	2:B:238:ARG:HB2	2.02	0.41
2:B:276:TYR:CD1	2:B:276:TYR:C	2.93	0.41
1:A:82:LYS:HA	1:A:82:LYS:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD21	2:B:227:ALA:HB1	2.02	0.41
2:B:198:SER:C	2:B:263:PRO:HA	2.41	0.41
2:B:233:MET:HE1	2:B:265:ILE:CG2	2.50	0.40
1:A:48:ILE:HG21	1:A:100:MET:HE1	2.03	0.40
1:A:127:ILE:HD12	1:A:127:ILE:C	2.42	0.40
1:A:164:ARG:NH2	2:B:201:PRO:HB3	2.37	0.40

There are no symmetry-related clashes.

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	
1	A	143/147 (97%)	131 (92%)	9 (6%)	3 (2%)	8	27
2	B	91/97 (94%)	82 (90%)	9 (10%)	0	100	100
All	All	234/244 (96%)	213 (91%)	18 (8%)	3 (1%)	14	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	57	LYS
1	A	145	GLY

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
1	A	130/132 (98%)	124 (95%)	6 (5%)	31 65
2	B	83/86 (96%)	74 (89%)	9 (11%)	7 22
All	All	213/218 (98%)	198 (93%)	15 (7%)	18 45

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	82	LYS
1	A	93	ARG
1	A	126	ILE
1	A	133	PRO
1	A	138	LYS
2	B	186	LYS
2	B	194	LEU
2	B	199	THR
2	B	222	MET
2	B	224	LYS
2	B	247	PHE
2	B	260	LYS
2	B	262	ILE
2	B	268	MET

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

Mol	Chain	Res	Type
1	A	35	ASN
1	A	51	ASN
2	B	217	GLN
2	B	225	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MSI	A	1	1	31,31,31	3.08	17 (54%)	42,46,46	3.95	13 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MSI	A	1	1	-	0/17/43/43	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	MSI	C2-C3	-2.09	1.51	1.55
3	A	1	MSI	O1-C14	2.15	1.42	1.37
3	A	1	MSI	C18-C19	2.19	1.43	1.38
3	A	1	MSI	C19-C14	2.24	1.43	1.38
3	A	1	MSI	C7-C6	2.25	1.42	1.38
3	A	1	MSI	C4-C9	2.31	1.43	1.39
3	A	1	MSI	C16-C15	2.34	1.43	1.38
3	A	1	MSI	C18-C17	2.43	1.43	1.38
3	A	1	MSI	C15-C14	2.63	1.44	1.38
3	A	1	MSI	C4-C5	2.71	1.44	1.39
3	A	1	MSI	C2-N1	2.72	1.40	1.37
3	A	1	MSI	C13-C20	2.79	1.58	1.52
3	A	1	MSI	C8-N1	3.29	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	MSI	C6-C5	3.42	1.44	1.38
3	A	1	MSI	C5-S1	3.93	1.82	1.76
3	A	1	MSI	S1-N2	8.80	1.76	1.63
3	A	1	MSI	O3-C3	9.71	1.44	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	MSI	O3-C3-C2	-13.78	111.46	123.73
3	A	1	MSI	C9-C3-C2	-13.72	100.03	105.19
3	A	1	MSI	O3-C3-C9	-6.88	109.43	126.90
3	A	1	MSI	C8-N1-C2	-6.54	106.54	110.92
3	A	1	MSI	O2-C2-C3	-6.36	122.27	126.71
3	A	1	MSI	C4-C9-C3	-4.41	123.26	130.29
3	A	1	MSI	O5-S1-N2	-3.88	99.54	106.97
3	A	1	MSI	C12-N2-C20	-3.20	104.85	109.97
3	A	1	MSI	C9-C8-N1	-2.15	106.48	108.68
3	A	1	MSI	O4-S1-C5	2.10	110.74	108.00
3	A	1	MSI	C1-N1-C2	2.12	126.41	123.82
3	A	1	MSI	C11-C12-N2	3.35	109.80	103.28
3	A	1	MSI	C8-C9-C3	6.94	114.19	107.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	MSI	3	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.