



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2018 – 05:39 pm GMT

PDB ID : 1A9U
Title : THE COMPLEX STRUCTURE OF THE MAP KINASE P38/SB203580
Authors : Wang, Z.; Canagarajah, B.; Boehm, J.C.; Kassis, S.; Cobb, M.H.; Young, P.R.;
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Deposited on : 1998-04-10
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

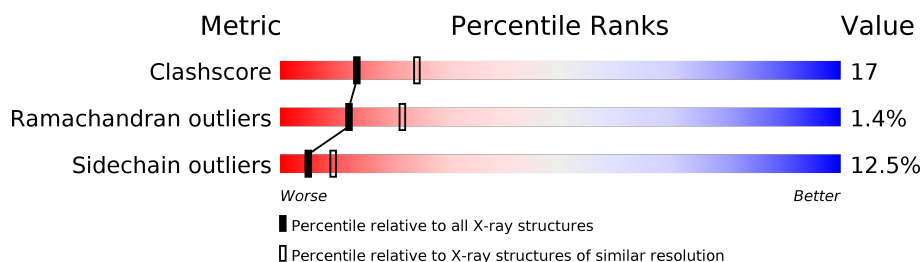
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	122078	4826 (2.50-2.50)
Ramachandran outliers	120005	4734 (2.50-2.50)
Sidechain outliers	119972	4736 (2.50-2.50)

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	379	<div>59% 28% 7%</div>

2 Entry composition [i](#)

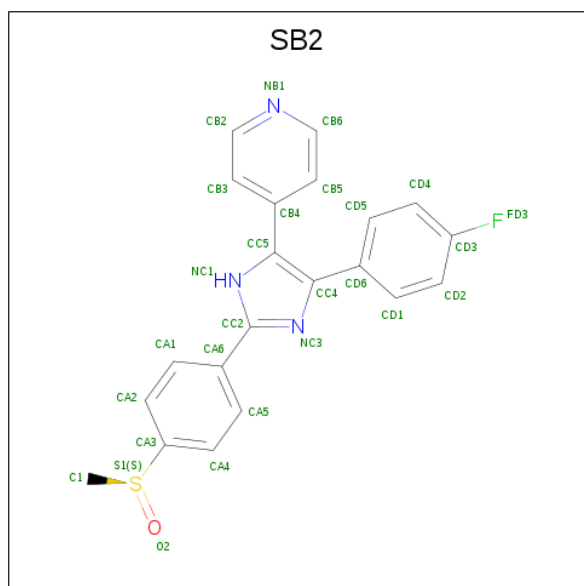
There are 3 unique types of molecules in this entry. The entry contains 2950 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MAP KINASE P38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	50	0	0
			2833	1813	483	524	13			

- Molecule 2 is 4-[5-(4-FLUORO-PHENYL)-2-(4-METHANESULFINYL-PHENYL)-3H-IMIDAZOL-4-YL]-PYRIDINE (three-letter code: SB2) (formula: C₂₁H₁₆FN₃OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			27	21	1	3	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	90	Total	O	0
			90	90	

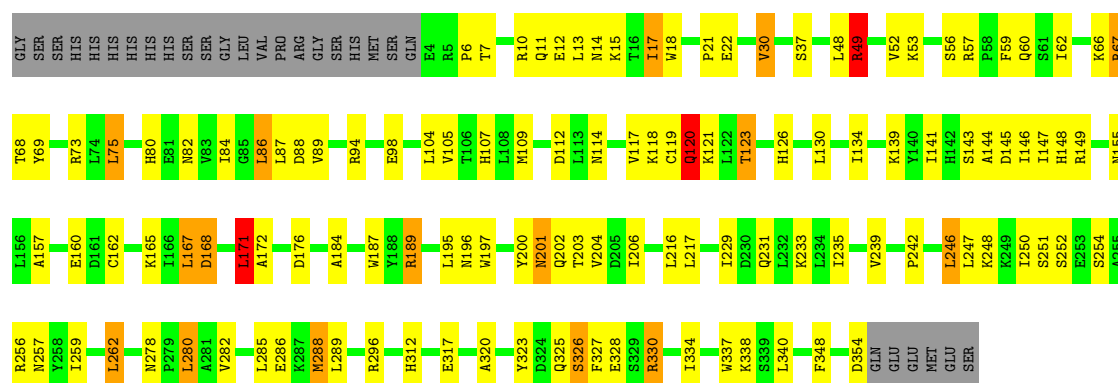
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: MAP KINASE P38

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.48Å 85.03Å 123.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2950	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SB2

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	0.46	0/2899	0.68	1/3937 (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	49	ARG	N-CA-C	-5.39	96.44	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2833	0	2821	96	0
2	A	27	0	16	1	0
3	A	90	0	0	2	0
All	All	2950	0	2837	96	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 17.

All (96) 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:201:ASN:HD22	1:A:201:ASN:H	1.20	0.90
1:A:149:ARG:NH2	1:A:171:LEU:HG	1.87	0.90
1:A:157:ALA:HB2	1:A:167:LEU:HD21	1.61	0.82
1:A:149:ARG:HH21	1:A:171:LEU:HG	1.46	0.81
1:A:86:LEU:HD11	1:A:89:VAL:CG2	2.12	0.80
1:A:200:TYR:HB2	1:A:204:VAL:HG11	1.67	0.76
1:A:80:HIS:HD2	1:A:82:ASN:H	1.34	0.76
1:A:117:VAL:HG21	1:A:216:LEU:HD21	1.75	0.69
1:A:86:LEU:HD11	1:A:89:VAL:HG23	1.74	0.68
1:A:117:VAL:HG21	1:A:216:LEU:CD2	2.25	0.67
1:A:84:ILE:HB	1:A:167:LEU:HD12	1.77	0.66
1:A:53:LYS:HE3	1:A:104:LEU:HD12	1.79	0.65
1:A:80:HIS:CD2	1:A:82:ASN:H	2.15	0.65
1:A:86:LEU:CD1	1:A:89:VAL:HG23	2.27	0.64
1:A:6:PRO:HG2	1:A:21:PRO:HB3	1.81	0.63
1:A:119:CYS:O	1:A:120:GLN:HB2	1.99	0.62
1:A:48:LEU:HD13	1:A:107:HIS:CD2	2.35	0.61
1:A:200:TYR:HB2	1:A:204:VAL:CG1	2.30	0.61
1:A:149:ARG:HH21	1:A:171:LEU:CG	2.14	0.60
1:A:326:SER:HB2	1:A:330:ARG:HH12	1.65	0.60
1:A:201:ASN:HD22	1:A:201:ASN:N	1.90	0.60
1:A:112:ASP:OD1	1:A:114:ASN:HB3	2.03	0.59
1:A:48:LEU:CD1	1:A:87:LEU:HD11	2.33	0.59
1:A:120:GLN:NE2	1:A:121:LYS:H	2.01	0.58
1:A:117:VAL:HG11	1:A:216:LEU:HD23	1.84	0.58
1:A:86:LEU:HD11	1:A:89:VAL:HG21	1.84	0.58
1:A:231:GLN:O	1:A:235:ILE:HG13	2.04	0.57
1:A:250:ILE:O	1:A:256:ARG:HD3	2.03	0.57
1:A:201:ASN:ND2	1:A:201:ASN:H	1.97	0.57
1:A:11:GLN:OE1	1:A:13:LEU:HD21	2.04	0.57
1:A:67:ARG:HG2	1:A:67:ARG:HH11	1.69	0.56
1:A:282:VAL:O	1:A:286:GLU:HG3	2.06	0.56
1:A:147:ILE:HG12	1:A:202:GLN:HG2	1.87	0.55
1:A:62:ILE:HG13	1:A:334:ILE:HG13	1.88	0.55
1:A:123:THR:HG23	1:A:126:HIS:HD2	1.72	0.54
1:A:130:LEU:O	1:A:134:ILE:HG13	2.07	0.54
1:A:326:SER:HB2	1:A:330:ARG:NH1	2.22	0.54
1:A:148:HIS:O	1:A:149:ARG:HB2	2.08	0.53
1:A:149:ARG:HD3	1:A:200:TYR:OH	2.08	0.53
1:A:52:VAL:HG22	1:A:105:VAL:HG22	1.91	0.52
1:A:109:MET:HG2	2:A:800:SB2:HB6	1.90	0.52
1:A:119:CYS:O	1:A:120:GLN:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TRP:CZ2	1:A:259:ILE:HD11	2.43	0.52
1:A:144:ALA:HB2	1:A:320:ALA:HB3	1.92	0.52
1:A:66:LYS:HG3	1:A:337:TRP:CE2	2.45	0.52
1:A:278:ASN:OD1	1:A:280:LEU:HB2	2.10	0.51
1:A:206:ILE:HG23	1:A:288:MET:HG2	1.92	0.50
1:A:155:ASN:ND2	1:A:168:ASP:HB2	2.27	0.49
1:A:66:LYS:HE3	1:A:337:TRP:CZ2	2.48	0.49
1:A:69:TYR:OH	1:A:73:ARG:HD3	2.12	0.49
1:A:323:TYR:CD2	1:A:325:GLN:HG2	2.47	0.49
1:A:49:ARG:NH2	3:A:506:HOH:O	2.44	0.49
1:A:67:ARG:HD3	1:A:68:THR:N	2.27	0.49
1:A:146:ILE:HG23	1:A:171:LEU:HD12	1.96	0.48
1:A:149:ARG:HD3	1:A:200:TYR:CZ	2.49	0.47
1:A:30:VAL:HG13	1:A:30:VAL:O	2.14	0.47
1:A:59:PHE:CD2	1:A:338:LYS:HD2	2.49	0.47
1:A:49:ARG:HB3	1:A:49:ARG:HE	1.52	0.47
1:A:7:THR:O	1:A:22:GLU:HG3	2.15	0.46
1:A:75:LEU:HB3	1:A:86:LEU:HG	1.97	0.46
1:A:12:GLU:HB2	1:A:17:ILE:CD1	2.46	0.46
1:A:88:ASP:HA	1:A:348:PHE:CE2	2.50	0.46
1:A:53:LYS:CE	1:A:104:LEU:HD12	2.46	0.46
1:A:109:MET:CE	1:A:165:LYS:HD2	2.45	0.46
1:A:167:LEU:HB3	1:A:168:ASP:H	1.60	0.45
1:A:201:ASN:ND2	1:A:201:ASN:N	2.60	0.45
1:A:312:HIS:HD2	1:A:317:GLU:OE2	1.99	0.45
1:A:18:TRP:HZ3	1:A:52:VAL:HG12	1.83	0.44
1:A:57:ARG:HA	1:A:57:ARG:HD3	1.67	0.44
1:A:48:LEU:HD13	1:A:87:LEU:HD11	1.99	0.44
1:A:242:PRO:HB3	1:A:246:LEU:HD12	2.00	0.44
1:A:48:LEU:HD12	1:A:87:LEU:HD11	1.99	0.43
1:A:48:LEU:HD13	1:A:107:HIS:HD2	1.80	0.43
1:A:259:ILE:O	1:A:262:LEU:HB2	2.19	0.43
1:A:184:ALA:HA	1:A:187:TRP:CE3	2.53	0.43
1:A:48:LEU:HD12	1:A:87:LEU:CD1	2.47	0.43
1:A:67:ARG:HG2	1:A:67:ARG:NH1	2.34	0.43
1:A:328:GLU:HA	1:A:328:GLU:OE1	2.19	0.43
1:A:167:LEU:O	1:A:168:ASP:C	2.58	0.43
1:A:206:ILE:CG2	1:A:288:MET:HG2	2.49	0.43
1:A:247:LEU:O	1:A:256:ARG:HD2	2.19	0.42
1:A:285:LEU:HD23	1:A:288:MET:CE	2.48	0.42
1:A:13:LEU:O	1:A:14:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HG13	1:A:334:ILE:CG1	2.50	0.42
1:A:155:ASN:HA	1:A:155:ASN:HD22	1.68	0.42
1:A:94:ARG:HB2	1:A:98:GLU:OE2	2.19	0.41
1:A:117:VAL:C	1:A:119:CYS:N	2.72	0.41
1:A:121:LYS:HG3	1:A:217:LEU:O	2.20	0.41
1:A:200:TYR:CD1	1:A:200:TYR:C	2.93	0.41
1:A:203:THR:HB	1:A:296:ARG:HD2	2.03	0.41
1:A:189:ARG:HH11	1:A:189:ARG:CG	2.34	0.41
1:A:327:PHE:HD2	3:A:511:HOH:O	2.03	0.41
1:A:139:LYS:O	1:A:143:SER:HB3	2.21	0.40
1:A:141:ILE:HG23	1:A:146:ILE:HB	2.04	0.40
1:A:144:ALA:O	1:A:145:ASP:HB2	2.22	0.40
1:A:201:ASN:ND2	1:A:203:THR:OG1	2.54	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	349/379 (92%)	322 (92%)	22 (6%)	5 (1%)	12	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	120	GLN
1	A	172	ALA
1	A	168	ASP
1	A	171	LEU

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	311/336 (93%)	272 (88%)	39 (12%)	5 9

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	15	LYS
1	A	17	ILE
1	A	30	VAL
1	A	37	SER
1	A	49	ARG
1	A	60	GLN
1	A	67	ARG
1	A	75	LEU
1	A	86	LEU
1	A	118	LYS
1	A	120	GLN
1	A	123	THR
1	A	160	GLU
1	A	162	CYS
1	A	167	LEU
1	A	171	LEU
1	A	176	ASP
1	A	189	ARG
1	A	195	LEU
1	A	196	ASN
1	A	201	ASN
1	A	229	ILE
1	A	233	LYS
1	A	239	VAL
1	A	246	LEU
1	A	248	LYS
1	A	251	SER
1	A	252	SER
1	A	254	SER

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Mol	Chain	Res	Type
1	A	257	ASN
1	A	262	LEU
1	A	280	LEU
1	A	288	MET
1	A	289	LEU
1	A	326	SER
1	A	330	ARG
1	A	340	LEU
1	A	354	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	107	HIS
1	A	120	GLN
1	A	126	HIS
1	A	155	ASN
1	A	201	ASN
1	A	202	GLN
1	A	272	ASN
1	A	312	HIS

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](#)

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	$\# Z > 2$
2	SB2	A	800	-	29,30,30	2.52	14 (48%)	35,42,42	1.46	5 (14%)

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
2	SB2	A	800	-	-	0/16/16/16	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	SB2	CD6-CC4	-6.16	1.41	1.49
2	A	800	SB2	CD1-CD6	2.05	1.43	1.39
2	A	800	SB2	CD2-CD3	2.58	1.42	1.37
2	A	800	SB2	CA4-CA3	2.62	1.42	1.38
2	A	800	SB2	CB3-CB2	2.62	1.43	1.38
2	A	800	SB2	CD5-CD6	2.68	1.45	1.39
2	A	800	SB2	CA2-CA3	2.71	1.42	1.38
2	A	800	SB2	CA1-CA6	2.81	1.45	1.39
2	A	800	SB2	CB3-CB4	2.99	1.45	1.39
2	A	800	SB2	CA5-CA6	3.05	1.45	1.39
2	A	800	SB2	CC2-NC1	3.18	1.39	1.35
2	A	800	SB2	CD4-CD3	3.41	1.43	1.37
2	A	800	SB2	CB5-CB4	3.66	1.47	1.39
2	A	800	SB2	O2-S1	4.08	1.61	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	SB2	CC4-CC5-NC1	-2.58	106.81	113.76
2	A	800	SB2	CA6-CC2-NC3	-2.42	120.83	123.75
2	A	800	SB2	CB6-NB1-CB2	2.48	122.80	116.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	SB2	O2-S1-C1	3.66	112.36	105.48
2	A	800	SB2	C1-S1-CA3	3.84	109.38	98.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	SB2	1	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.