



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 08:14 PM EDT

PDB ID : 2F03
Title : Crystal structure of tetrameric restriction endonuclease SfiI in complex with cognate DNA (partial bound form)
Authors : Aggarwal, A.K.; Vanamee, E.S.; Viadiu, H
Deposited on : 2005-11-11
Resolution : 3.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

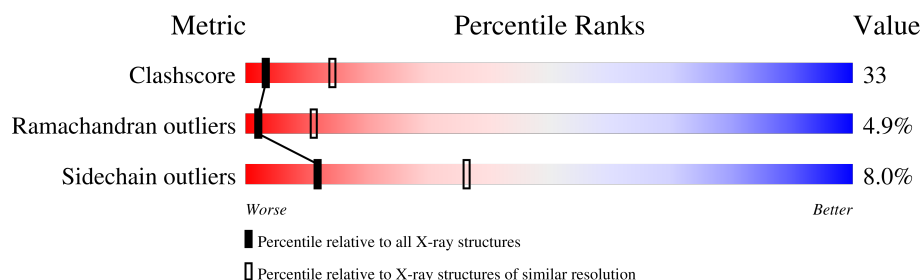
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)




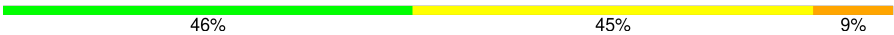
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1-E	21	24% 14% 62%
1	1-G	21	24% 76%
1	2-E	21	5% 14% 14% 67%
1	2-G	21	24% 76%
2	1-F	21	5% 10% 19% 67%
2	1-H	21	5% 19% 76%
2	2-F	21	14% 24% 62%
2	2-H	21	5% 19% 76%

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Mol	Chain	Length	Quality of chain
3	1-A	269	 44% 48% 7% •
3	1-C	269	 45% 46% 9%
3	2-A	269	 46% 46% 7% •
3	2-C	269	 46% 45% 9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9827 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 DNA chain called DNA (5'-D(*AP*TP*G*TP*GP*GP*CP*CP*AP*AP*CP*AP*AP*GP*GP*CP*CP*TP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-E	8	Total	C	N	O	P	0	8	0
			160	77	31	45	7			
1	2-E	7	Total	C	N	O	P	0	7	0
			144	68	28	41	7			
1	1-G	5	Total	C	N	O	P	0	5	0
			99	48	18	29	4			
1	2-G	5	Total	C	N	O	P	0	5	0
			99	48	18	29	4			

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*TP*AP*GP*GP*CP*CP*TP*TP*GP*TP*TP*GP*GP*CP*CP*AP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-F	7	Total	C	N	O	P	0	7	0
			143	68	25	43	7			
2	2-F	8	Total	C	N	O	P	0	8	0
			162	78	30	47	7			
2	1-H	5	Total	C	N	O	P	0	5	0
			100	48	21	27	4			
2	2-H	5	Total	C	N	O	P	0	5	0
			100	48	21	27	4			

- Molecule 3 is a protein called Type II restriction enzyme SfiI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	1-A	269	Total	C	N	O	S	Se	0	269	0
			2155	1366	380	404	1	4			
3	2-A	269	Total	C	N	O	S	Se	0	269	0
			2155	1366	380	404	1	4			
3	1-C	269	Total	C	N	O	S	Se	0	269	0
			2142	1359	377	401	1	4			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	2-C	269	Total	C	N	O	S	Se	0	269	0
			2142	1359	377	401	1	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP O52512
A	119	MSE	MET	MODIFIED RESIDUE	UNP O52512
A	134	MSE	MET	MODIFIED RESIDUE	UNP O52512
A	143	MSE	MET	MODIFIED RESIDUE	UNP O52512
C	1	MSE	MET	MODIFIED RESIDUE	UNP O52512
C	119	MSE	MET	MODIFIED RESIDUE	UNP O52512
C	134	MSE	MET	MODIFIED RESIDUE	UNP O52512
C	143	MSE	MET	MODIFIED RESIDUE	UNP O52512

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	1	Total	Ca	0	1
			1	1		
4	2-A	1	Total	Ca	0	1
			1	1		
4	1-C	1	Total	Ca	0	1
			1	1		
4	2-C	1	Total	Ca	0	1
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-E	5	Total	O	0	5
			5	5		
5	2-E	93	Total	O	0	93
			93	93		
5	1-F	3	Total	O	0	3
			3	3		
5	2-F	18	Total	O	0	18
			18	18		
5	1-G	3	Total	O	0	3
			3	3		
5	1-A	55	Total	O	0	55
			55	55		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-C	45	Total	O	0	45
			45	45		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

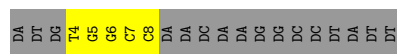
- Molecule 1: DNA (5'-D(*AP*TP*G*TP*GP*GP*CP*CP*AP*AP*CP*AP*AP*GP*GP*CP*CP*TP*AP*TP*T)-3')

Chain 1-E: 



- Molecule 1: DNA (5'-D(*AP*TP*G*TP*GP*GP*CP*CP*AP*AP*CP*AP*AP*GP*GP*CP*CP*TP*AP*TP*T)-3')

Chain 1-G: 



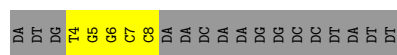
- Molecule 1: DNA (5'-D(*AP*TP*G*TP*GP*GP*CP*CP*AP*AP*CP*AP*AP*GP*GP*CP*CP*TP*AP*TP*T)-3')

Chain 2-E: 



- Molecule 1: DNA (5'-D(*AP*TP*G*TP*GP*GP*CP*CP*AP*AP*CP*AP*AP*GP*GP*CP*CP*TP*AP*TP*T)-3')

Chain 2-G: 



- Molecule 2: DNA (5'-D(*AP*AP*TP*AP*GP*GP*CP*CP*TP*TP*GP*TP*TP*GP*GP*CP*CP*AP*CP*AP*T)-3')

Chain 1-F: 



- Molecule 2: DNA (5'-D(*AP*AP*TP*AP*GP*GP*CP*CP*TP*TP*GP*TP*TP*GP*GP*CP*CP*AP*CP*AP*T)-3')

Chain 1-H:  5% 19% 76%

DA DA DA DA DG DG DC DT DT DT DT DT G14 G15 G16 G17 A18 DC DA DT

- Molecule 2: DNA (5'-D(*AP*AP*TP*AP*GP*GP*CP*CP*TP*TP*GP*TP*TP*GP*GP*CP*CP*AP*CP*AP*T)-3')

Chain 2-F:  14% 24% 62%

DA DA DA DT A4 G5 G6 C7 C8 T9 T10 G11 DT DT DT DG DG DC DC DC DC DA DA DA DT

- Molecule 2: DNA (5'-D(*AP*AP*TP*AP*GP*GP*CP*CP*TP*TP*GP*TP*TP*GP*GP*CP*CP*AP*CP*AP*T)-3')

Chain 2-H:  5% 19% 76%

DA DA DA DT G14 G15 G16 G17 A18 DC DA DT

- Molecule 3: Type II restriction enzyme SfiI

Chain 1-A:  44% 48% 7%

M1 H2 Y5 R6 E7 L8 S9 L10 E12 S15 L21 R22 T23 I24 V25 Q26 Q29 Q30 Y31 S32 K33 T41 T42 D45 S46 S47 G48 E49 L53 I57 T58 Q59 L62 E63 V64 Y68 P69 I70 N71 R72 R73 F74 I78 D79 Y80 K81 V83

R84 W85 L86 P87 S88 R89 H90 G91 L92 P94 Q95 Q96 L97 L98 V99 D100 A101 K102 A103 S104 T105 M108 R109 D110 T111 L112 Q113 R114 S115 Q116 L117 P118 M119 D120 Q121 M122 D123 S127 S128 E130 V131 V132 T133 M134 E135 A136 G137 V138 T139 P140 H141 L142 S146 A147 M148 D149

G150 V151 L152 V155 T156 V161 H162 F163 Y164 R165 R166 E167 L168 D169 D170 Y171 E172 R176 L178 S180 S185 L186 P187 H188 A189 R190 L191 Q192 Q193 R194 Y195 N196 F197 P199 S202 F203 F204 K208 H209 S210 P211 A212 R213 G214 E215 V216 A217 R218 I219 R220 M221

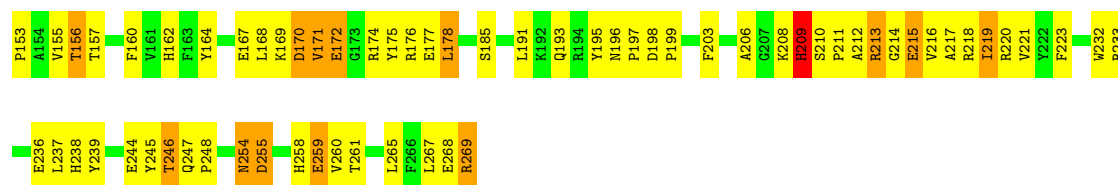
Y222 F223 D224 R225 L226 K227 C230 R233 H238 Y239 S240 A241 E244 T245 Q247 P248 R251 D252 L253 R254 D255 H258 E263 F266 L267 E268 R269

- Molecule 3: Type II restriction enzyme SfiI

Chain 1-C:  45% 46% 9%

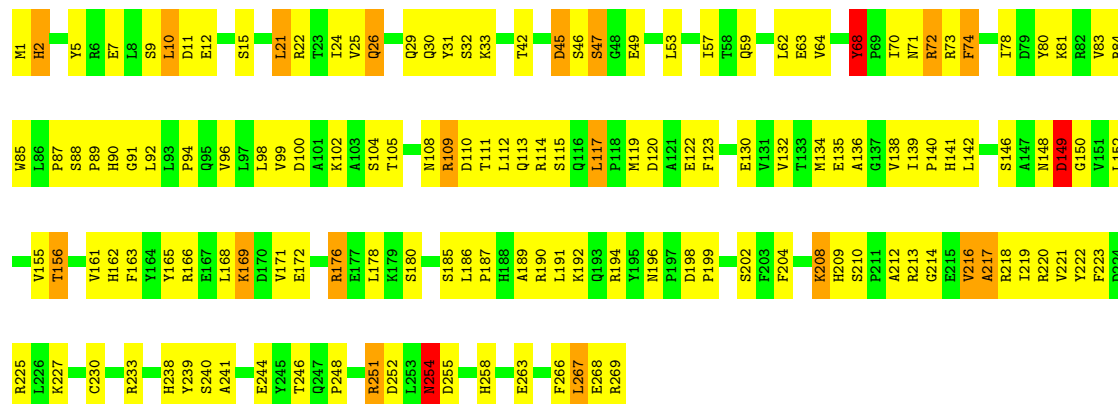
M1 D4 Y5 R6 S9 L10 D11 E12 L13 E14 K18 L21 R22 T23 T24 V25 Q26 A27 Q30 Y31 S32 K33 K36 F39 E40 T41 T42 A43 F123 A44 S47 G48 E49 L53 T58 Q59 Y60 A61 E63 V64 A65 E66 T67 Y68 R72 R73 F74 A75 G76

F77 I78 D79 Y80 K81 W85 G91 L92 L98 V99 K102 A103 S104 T105 E106 K107 N108 R109 D110 T111 L112 Q113 S114 S115 Q116 L117 P118 M119 D120 Q121 M122 D123 R124 N125 T126 S127 S128 T133 M134 E135 A136 T139 P140 H141 L142 M143 L144 Q145 N148 D149 G150 V151 L152



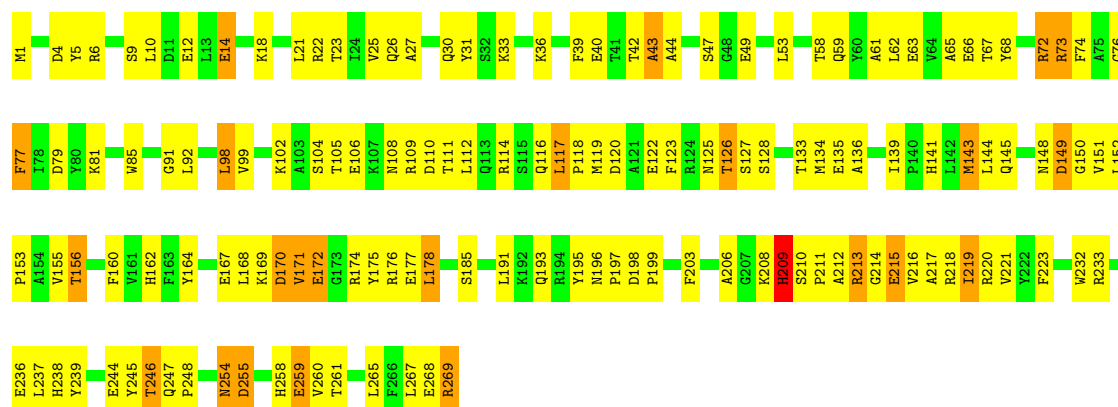
• Molecule 3: Type II restriction enzyme SfiI

Chain 2-A: 46% 46% 7% .



• Molecule 3: Type II restriction enzyme SfiI

Chain 2-C: 46% 45% 9%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.60Å 85.60Å 418.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.05	Depositor
% Data completeness (in resolution range)	95.8 (50.00-3.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9827	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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:
CA

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	1-E	0.63	0/179	1.68	7/274 (2.6%)
1	1-G	0.69	0/110	1.31	0/168
1	2-E	0.47	0/161	1.66	10/246 (4.1%)
1	2-G	0.69	0/110	1.31	0/168
2	1-F	0.55	0/159	1.66	8/243 (3.3%)
2	1-H	0.75	0/112	1.04	0/171
2	2-F	0.78	0/181	1.83	13/278 (4.7%)
2	2-H	0.75	0/112	1.04	0/171
3	1-A	0.45	0/2202	0.69	0/2984
3	1-C	0.50	2/2189 (0.1%)	0.68	0/2968
3	2-A	0.45	0/2202	0.69	0/2984
3	2-C	0.50	2/2189 (0.1%)	0.68	0/2968
All	All	0.50	4/9906 (0.0%)	0.84	38/13623 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	1-C	0	1
3	2-C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-C	143[A]	MSE	CG-SE	-5.50	1.76	1.95
3	2-C	143[B]	MSE	CG-SE	-5.50	1.76	1.95
3	1-C	255[A]	ASP	C-N	5.36	1.46	1.34
3	2-C	255[B]	ASP	C-N	5.36	1.46	1.34

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-F	11[A]	DG	O4'-C1'-C2'	8.45	112.66	105.90
2	2-F	11[A]	DG	O4'-C1'-N9	7.69	113.38	108.00
2	1-F	14[A]	DG	O4'-C1'-C2'	6.38	111.00	105.90
2	1-F	13[A]	DT	O4'-C1'-N1	6.31	112.42	108.00
2	2-F	10[A]	DT	O4'-C1'-N1	6.23	112.36	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	1-C	255[A]	ASP	Mainchain
3	2-C	255[B]	ASP	Mainchain

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	1-E	160	0	90	13	0
1	1-G	99	0	58	11	0
1	2-E	144	0	79	4	0
1	2-G	99	0	58	12	0
2	1-F	143	0	80	9	0
2	1-H	100	0	57	12	0
2	2-F	162	0	91	6	0
2	2-H	100	0	57	13	0
3	1-A	2155	0	2096	167	0
3	1-C	2142	0	2071	134	0
3	2-A	2155	0	2096	146	0
3	2-C	2142	0	2071	127	0
4	1-A	1	0	0	0	0
4	1-C	1	0	0	0	0
4	2-A	1	0	0	0	0
4	2-C	1	0	0	0	0
5	1-A	55	0	0	10	0
5	1-C	45	0	0	6	0
5	1-E	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1-F	3	0	0	0	0
5	1-G	3	0	0	0	0
5	2-E	93	0	0	0	0
5	2-F	18	0	0	1	0
All	All	9827	0	8904	607	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 33.

The worst 5 of 607 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)
2:F:12[A]:DT:H4'	2:F:13[A]:DT:H5'	1.23	1.13
3:A:22[A]:ARG:HH12	3:A:26[A]:GLN:HG2	1.17	1.06
3:A:22[B]:ARG:HH12	3:A:26[B]:GLN:HG2	1.17	1.06
3:A:45[A]:ASP:H	3:A:49[A]:GLU:HG3	1.19	1.04
3:A:45[B]:ASP:H	3:A:49[B]:GLU:HG3	1.19	1.04

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	
3	1-A	267/269 (99%)	232 (87%)	23 (9%)	12 (4%)	2	12
3	1-C	267/269 (99%)	226 (85%)	27 (10%)	14 (5%)	2	10
3	2-A	267/269 (99%)	232 (87%)	23 (9%)	12 (4%)	2	12
3	2-C	267/269 (99%)	226 (85%)	27 (10%)	14 (5%)	2	10
All	All	1068/1076 (99%)	916 (86%)	100 (9%)	52 (5%)	2	11

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1-A	47[A]	SER
3	1-A	130[A]	GLU
3	1-A	149[A]	ASP
3	1-A	254[A]	ASN
3	1-C	43[A]	ALA

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	
3	1-A	228/233 (98%)	210 (92%)	18 (8%)	12	36
3	1-C	224/233 (96%)	206 (92%)	18 (8%)	12	36
3	2-A	228/233 (98%)	210 (92%)	18 (8%)	12	36
3	2-C	224/233 (96%)	206 (92%)	18 (8%)	12	36
All	All	904/932 (97%)	832 (92%)	72 (8%)	12	36

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2-C	77[B]	PHE
3	2-C	269[B]	ARG
3	2-C	99[B]	VAL
3	2-C	209[B]	HIS
3	1-C	105[A]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
3	2-A	26[B]	GLN
3	2-A	59[B]	GLN
3	2-C	141[B]	HIS
3	2-A	30[B]	GLN
3	2-A	141[B]	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.