



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:18 PM UTC

PDB ID : 1FPM / pdb\_00001fpm  
Title : MONOVALENT CATION BINDING SITES IN N10-FORMYLTETRAHYDROFOLATE SYNTHETASE FROM MOORELLA THERMOACETICA  
Authors : Radfar, R.; Leaphart, A.; Brewer, J.M.; Minor, W.; Odom, J.D.  
Deposited on : 2000-08-31  
Resolution : 3.00 Å(reported)

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The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

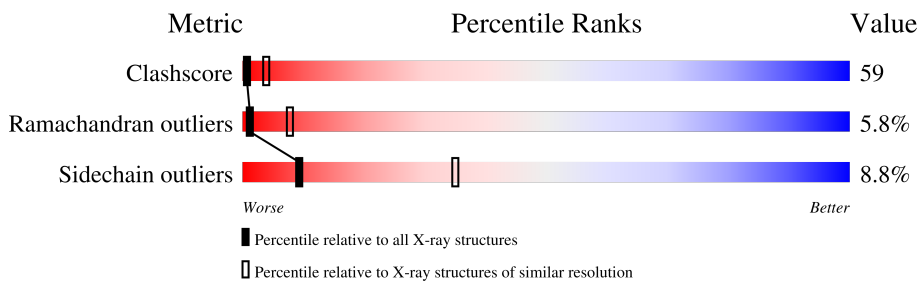
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	557	 35% 53% 10% ..
1	B	557	 22% 62% 13% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	561	-	-	X	-
2	SO4	A	565	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8585 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.

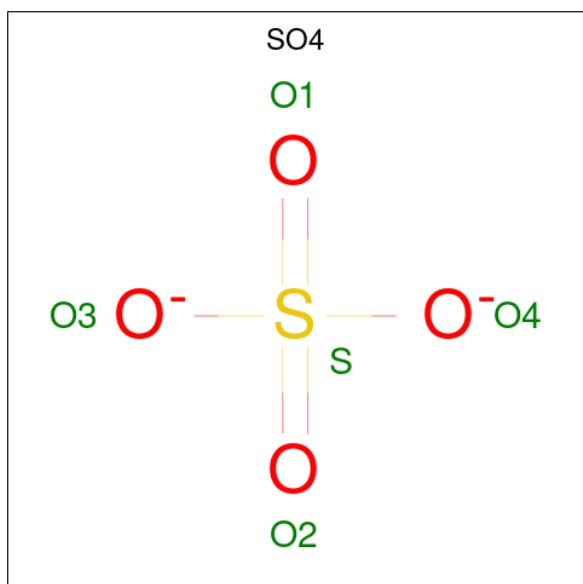
- Molecule 1 is a protein called FORMATE--TETRAHYDROFOLATE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	549	4133	2617	715	780	21	0	0	0
1	B	548	4125	2613	714	777	21	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P21164
A	?	-	VAL	deletion	UNP P21164
B	?	-	GLU	deletion	UNP P21164
B	?	-	VAL	deletion	UNP P21164

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is CESIUM ION (CCD ID: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cs 1 1	0	0
3	B	1	Total Cs 1 1	0	0

- Molecule 4 is water.

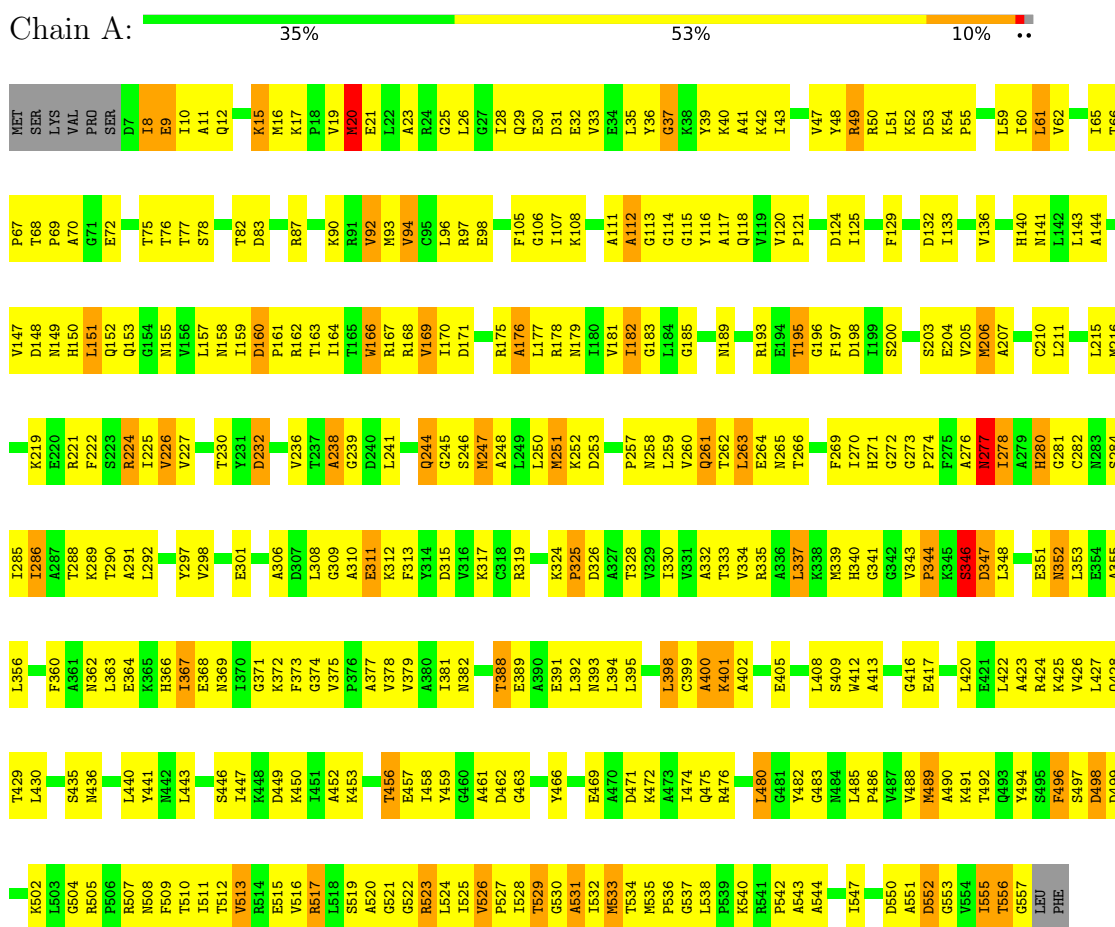
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	200	Total O 200 200	0	0
4	B	70	Total O 70 70	0	0

### 3 Residue-property plots

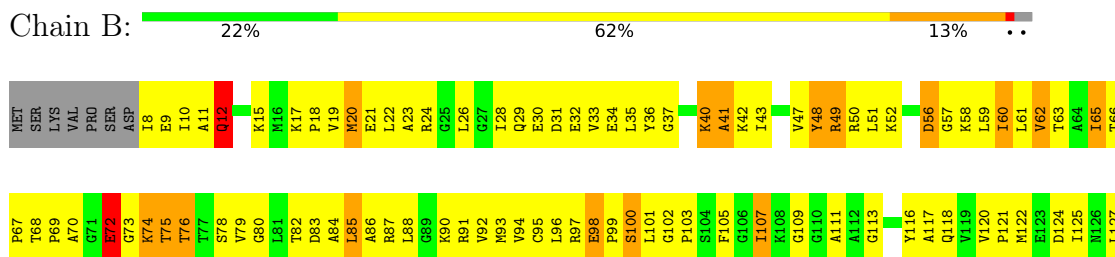
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: FORMATE--TETRAHYDROFOLATE LIGASE



- Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE



I511	V378	V316	K256	P192	H128
T512	V379	K317	P257	R193	F129
V513	A380	C318	N258	E194	T130
R514	I381	R319	L259	T195	G131
E515	N382	Y320	V260	G196	D132
V516	A383	A321	Q261	F197	I133
R517	F384	G322	T262	D198	H134
L518	P385	F323	L263	I199	A135
S519	T386	K324	E264	S200	V136
A520	D387	P325	N265	V201	
G521	T388	D326	T266	A202	H140
G522	E389	A327	P267	S203	N141
R523		T328	A268	E204	L142
L524	L392	V329	F269	V205	L143
I525	N393	I330	I270	M206	A144
V526	L394	V331	H271	A207	
P527	L395	A332	G272	C208	M146
I528	Y396	T333	G273	L209	V147
T529	E397	V334	P274	C210	D148
	L398	R335	F275	L211	M149
	C399	A336	A276	A212	H150
	A400	L337	N277	S213	L151
	K401	K338	I278	D214	Q152
	A402	M339	A279	L215	Q153
	G403	H340	H280	M216	G154
	A404	G341	G281	D217	M155
	E405	G342	C282	L218	V156
		V343	N283	K219	L157
	L408	P344	S284	E220	N158
	S409		I285	R221	I159
	W412		I286	F222	D160
	A413		A287	S223	P161
	K414		T288	K224	R162
	G415		K289	I225	T163
	G416		T290	V226	I164
	E417		A291	Y229	T165
	G418		L292	T230	M166
	G419		K293	G231	R167
	L420		L294	D232	R168
	E421		A295	V236	V169
	L422		D296		L172
	A423		Y297	G239	N173
	A490		V298	D240	D174
	K424		V299	L241	R175
	K425		T300	E242	A176
	V426		E301	A243	L177
			A302	R178	R178
	T429		G303	Q244	M179
	L430		F304	G245	I180
			K365	S246	V181
	R433		H366	M247	I182
	F434		I367	L248	G185
	S435		E368	A248	G186
	N436		L308	L249	K187
	F437		G309	A310	A188
			A310	M251	M189
	L440		E311	K252	G190
	Y441		K312	D253	V191
	M442		F313	A254	
	L443		Y314	I255	
	D444		A377		
L445	L445	V316	K256	P192	H128
S446	S446	K317	P257	R193	F129
I447	I447	C318	N258	E194	T130
K448	K448	R319	L259	T195	G131
D449	D449	Y320	V260	G196	D132
K450	K450	A321	Q261	F197	I133
I451	I451	G322	T262	D198	H134
A452	A452	F323	L263	I199	A135
K453	K453	K324	E264	S200	V136
I454	I454	P325	N265	V201	
A455	A455	D326	T266	A202	H140
T456	T456	A327	P267	S203	N141
E457	E457	T328	A268	E204	L142
I458	I458	V329	F269	V205	L143
Y459	Y459	I330	I270	M206	A144
G460	G460	V331	H271	A207	
A461	A461	A332	G272	C208	M146
D462	D462	T333	G273	L209	V147
G463	G463	V334	P274	C210	D148
Y466	Y466	R335	F275	L211	M149
A470	A470	A336	A276	A212	H150
D471	D471	L337	N277	S213	L151
K472	K472	K338	I278	D214	Q152
A473	A473	M339	A279	L215	Q153
I474	I474	H340	H280	M216	G154
Q475	Q475	G341	G281	D217	M155
R476	R476	G342	C282	L218	V156
Y477	Y477	V343	N283	K219	L157
E478	E478	P344	S284	E220	N158
S479	S479		I285	R221	I159
L480	L480		I286	F222	D160
G481	G481		A287	S223	P161
Y482	Y482		T288	K224	R162
A551	A551		K289	I225	T163
D552	D552		T290	V226	I164
G553	G553		A291	Y229	T165
V554	V554		L292	T230	M166
T555	T555		K293	G231	R167
G557	G557		L294	D232	R168
LEU	LEU		A295	V236	V169
PHE	PHE		D296		L172
			Y297	G239	N173
			V298	D240	D174
			K425	L241	R175
			V426	E242	A176
				A243	L177
				R178	R178
				Q244	M179
				G245	I180
				S246	V181
				M247	I182
				L248	G185
				A248	G186
				L249	K187
				A310	A188
				M251	M189
				K252	G190
				D253	V191
				A254	
				I255	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.88Å 160.88Å 256.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00	Depositor
% Data completeness (in resolution range)	84.0 (40.00-3.00)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.266 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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: SO4, CS

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	4/4201 (0.1%)	1.11	26/5690 (0.5%)
1	B	0.53	2/4193 (0.0%)	1.05	24/5679 (0.4%)
All	All	0.59	6/8394 (0.1%)	1.08	50/11369 (0.4%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	MET	SD-CE	-7.82	1.59	1.79
1	A	206	MET	SD-CE	-7.40	1.61	1.79
1	A	489	MET	SD-CE	-7.31	1.61	1.79
1	A	251	MET	SD-CE	-6.65	1.62	1.79
1	B	251	MET	SD-CE	-5.93	1.64	1.79

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	VAL	N-CA-C	9.62	117.07	107.55
1	B	263	LEU	N-CA-C	-9.22	101.13	111.82
1	B	324	LYS	CA-C-N	8.24	130.14	119.84
1	B	324	LYS	C-N-CA	8.24	130.14	119.84
1	A	8	ILE	N-CA-C	-7.78	101.41	110.21

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	4133	0	4219	411	0
1	B	4125	0	4215	580	1
2	A	35	0	0	10	0
2	B	20	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	200	0	0	27	0
4	B	70	0	0	14	1
All	All	8585	0	8434	991	1

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 59.

The worst 5 of 991 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:B:166:TRP:CZ3	1:B:225:ILE:HD11	1.30	1.59
1:A:166:TRP:CZ3	1:A:225:ILE:HD11	1.42	1.53
1:B:166:TRP:CH2	1:B:225:ILE:HD11	1.58	1.38
1:B:166:TRP:CH2	1:B:225:ILE:CD1	2.11	1.34
1:B:166:TRP:CZ3	1:B:225:ILE:CD1	2.10	1.33

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LYS:NZ	4:B:572:HOH:O[4_555]	2.02	0.18

## 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	547/557 (98%)	445 (81%)	84 (15%)	18 (3%)	3	17
1	B	546/557 (98%)	392 (72%)	109 (20%)	45 (8%)	0	3
All	All	1093/1114 (98%)	837 (77%)	193 (18%)	63 (6%)	1	8

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	52	LYS
1	A	352	ASN
1	A	556	THR
1	B	65	ILE

### 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	432/440 (98%)	398 (92%)	34 (8%)	11	39
1	B	431/440 (98%)	389 (90%)	42 (10%)	8	30
All	All	863/880 (98%)	787 (91%)	76 (9%)	9	35

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	290	THR
1	B	529	THR
1	B	313	PHE
1	B	480	LEU
1	B	556	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	150	HIS

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Mol	Chain	Res	Type
1	B	244	GLN
1	B	189	ASN
1	B	265	ASN
1	A	362	ASN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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	SO4	A	566	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	562	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	561	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	563	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	560	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	562	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	A	564	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	A	565	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	563	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	560	-	4,4,4	0.69	0	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	561	-	4,4,4	0.68	0	6,6,6	0.49	0

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.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	566	SO4	1	0
2	B	561	SO4	1	0
2	A	563	SO4	1	0
2	A	565	SO4	4	0
2	B	560	SO4	1	0
2	A	561	SO4	4	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.