



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 06:27 pm BST

PDB ID : 2IVQ  
Title : SITE DIRECTED MUTAGENESIS OF KEY RESIDUES INVOLVED IN  
THE CATALYTIC MECHANISM OF CYANASE  
Authors : Guilloton, M.; Walsh, M.A.; Joachimiak, A.; Anderson, P.M.  
Deposited on : 2006-06-14  
Resolution : 2.10 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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) : 2.11

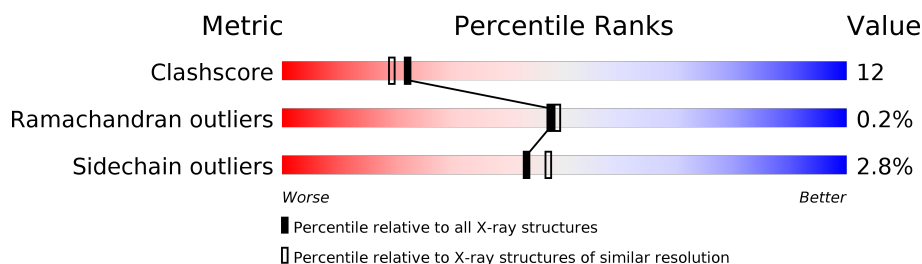
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)



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  $\geq 3$ , 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	156	
1	B	156	
1	C	156	
1	D	156	
1	E	156	
1	F	156	
1	G	156	
1	H	156	

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Mol	Chain	Length	Quality of chain
1	I	156	 81% 19%
1	J	156	 79% 19%

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	F	1158	-	-	X	-
2	SO4	I	1158	-	-	X	-
3	CL	C	1159	-	-	X	-
3	CL	I	1160	-	-	X	-
3	CL	J	1160	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13229 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 CYANATE HYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	B	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	C	156	Total	C	N	O	S	0	1	0
			1202	772	198	227	5			
1	D	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	E	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	F	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	G	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	H	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	I	156	Total	C	N	O	S	0	0	0
			1196	767	197	227	5			
1	J	156	Total	C	N	O	S	0	1	0
			1202	772	198	227	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	LYS	ARG	engineered mutation	UNP P00816
B	96	LYS	ARG	engineered mutation	UNP P00816
C	96	LYS	ARG	engineered mutation	UNP P00816
D	96	LYS	ARG	engineered mutation	UNP P00816
E	96	LYS	ARG	engineered mutation	UNP P00816
F	96	LYS	ARG	engineered mutation	UNP P00816
G	96	LYS	ARG	engineered mutation	UNP P00816
H	96	LYS	ARG	engineered mutation	UNP P00816
I	96	LYS	ARG	engineered mutation	UNP P00816

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Chain	Residue	Modelled	Actual	Comment	Reference
J	96	LYS	ARG	engineered mutation	UNP P00816

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Cl	0	0
			1	1		
3	J	2	Total	Cl	0	0
			2	2		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total 1	Cl 1	0	0
3	C	2	Total 2	Cl 2	0	0
3	A	1	Total 1	Cl 1	0	0
3	F	2	Total 2	Cl 2	0	0

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total 112	O 112	0	0
4	B	130	Total 130	O 130	0	0
4	C	107	Total 107	O 107	0	0
4	D	114	Total 114	O 114	0	0
4	E	131	Total 131	O 131	0	0
4	F	116	Total 116	O 116	0	0
4	G	98	Total 98	O 98	0	0
4	H	108	Total 108	O 108	0	0
4	I	91	Total 91	O 91	0	0
4	J	117	Total 117	O 117	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. 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: CYANATE HYDRATASE

Chain A:  81% 17%




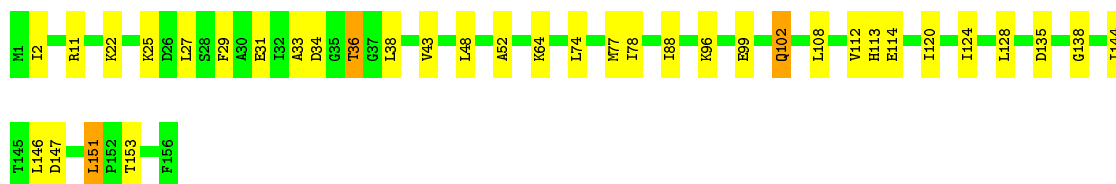
#### • Molecule 1: CYANATE HYDRATASE

Chain B:  83% 17%




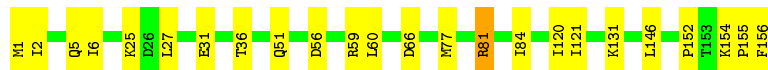
#### • Molecule 1: CYANATE HYDRATASE

Chain C:  77% 21%




#### • Molecule 1: CYANATE HYDRATASE

Chain D:  85% 15%




#### • Molecule 1: CYANATE HYDRATASE

Chain E:  80% 19%







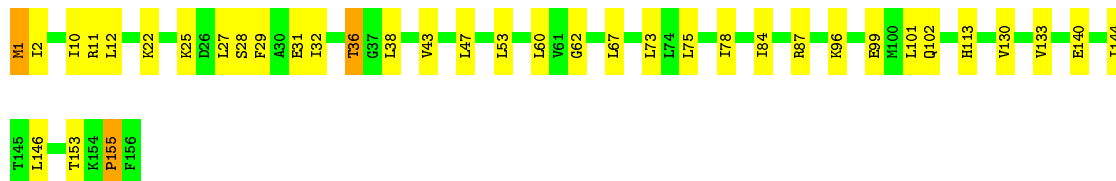
## • Molecule 1: CYANATE HYDRATASE

Chain F:  85% 15%


## • Molecule 1: CYANATE HYDRATASE

Chain G:  81% 18% •


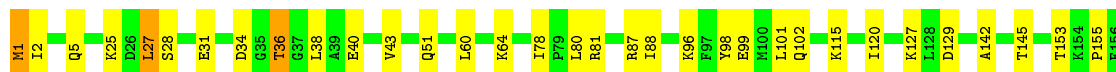
## • Molecule 1: CYANATE HYDRATASE

Chain H:  76% 22% •

## • Molecule 1: CYANATE HYDRATASE

Chain I:  81% 19%

## • Molecule 1: CYANATE HYDRATASE

Chain J:  79% 19% •

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.88 Å   80.84 Å   82.65 Å 69.99°   71.98°   66.17°	Depositor
Resolution (Å)	76.03 – 2.10	Depositor
% Data completeness (in resolution range)	95.7 (76.03-2.10)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.180 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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: SO4, CL

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	0.94	0/1213	0.94	3/1638 (0.2%)
1	B	0.99	2/1213 (0.2%)	0.90	0/1638
1	C	0.92	0/1222	0.93	3/1649 (0.2%)
1	D	0.99	1/1213 (0.1%)	0.94	2/1638 (0.1%)
1	E	0.93	0/1213	0.90	0/1638
1	F	0.90	0/1213	0.87	2/1638 (0.1%)
1	G	0.89	0/1213	0.87	2/1638 (0.1%)
1	H	0.94	0/1213	0.95	3/1638 (0.2%)
1	I	0.86	0/1213	0.85	0/1638
1	J	0.97	0/1222	0.91	1/1649 (0.1%)
All	All	0.93	3/12148 (0.0%)	0.90	16/16402 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	GLU	CG-CD	5.35	1.59	1.51
1	B	69	GLU	CB-CG	5.32	1.62	1.52
1	D	31	GLU	CG-CD	5.30	1.59	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	11	ARG	NE-CZ-NH2	8.33	124.46	120.30
1	A	11	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	D	66	ASP	CB-CG-OD1	6.38	124.05	118.30
1	A	1	MET	CG-SD-CE	6.27	110.23	100.20
1	C	11	ARG	NE-CZ-NH2	6.03	123.31	120.30

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	1196	0	1243	27	0
1	B	1196	0	1243	31	0
1	C	1202	0	1256	51	0
1	D	1196	0	1243	22	0
1	E	1196	0	1243	37	0
1	F	1196	0	1243	26	0
1	G	1196	0	1243	35	0
1	H	1196	0	1243	44	0
1	I	1196	0	1243	32	0
1	J	1202	0	1256	48	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	C	5	0	0	0	0
2	D	15	0	0	0	0
2	E	10	0	0	0	0
2	F	15	0	0	2	0
2	G	15	0	0	1	0
2	H	15	0	0	0	0
2	I	15	0	0	2	0
2	J	10	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	3	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	G	1	0	0	1	0
3	H	1	0	0	0	0
3	I	1	0	0	2	0
3	J	2	0	0	4	0
4	A	112	0	0	4	0
4	B	130	0	0	7	0
4	C	107	0	0	6	0
4	D	114	0	0	2	0
4	E	131	0	0	5	0
4	F	116	0	0	4	0
4	G	98	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	108	0	0	4	0
4	I	91	0	0	4	0
4	J	117	0	0	4	0
All	All	13229	0	12456	287	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 12.

The worst 5 of 287 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:D:1:MET:CE	1:D:2:ILE:HG22	1.62	1.29
1:J:1:MET:CE	1:J:2:ILE:HG22	1.62	1.29
3:I:1160:CL:CL	3:J:1160:CL:CL	1.29	1.28
1:A:1:MET:CE	1:A:2:ILE:HG22	1.64	1.26
1:J:2:ILE:HD11	1:J:78:ILE:HD11	1.29	1.13

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	154/156 (99%)	148 (96%)	5 (3%)	1 (1%)	25	21
1	B	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
1	C	155/156 (99%)	151 (97%)	4 (3%)	0	100	100
1	D	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
1	E	154/156 (99%)	149 (97%)	4 (3%)	1 (1%)	25	21
1	F	154/156 (99%)	151 (98%)	3 (2%)	0	100	100
1	G	154/156 (99%)	149 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	154/156 (99%)	149 (97%)	4 (3%)	1 (1%)	25	21
1	I	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
1	J	155/156 (99%)	150 (97%)	5 (3%)	0	100	100
All	All	1542/1560 (99%)	1493 (97%)	46 (3%)	3 (0%)	47	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	155	PRO
1	A	136	PRO
1	E	155	PRO

### 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	127/127 (100%)	123 (97%)	4 (3%)	40	43
1	B	127/127 (100%)	124 (98%)	3 (2%)	49	53
1	C	128/127 (101%)	124 (97%)	4 (3%)	40	43
1	D	127/127 (100%)	125 (98%)	2 (2%)	62	69
1	E	127/127 (100%)	122 (96%)	5 (4%)	32	33
1	F	127/127 (100%)	125 (98%)	2 (2%)	62	69
1	G	127/127 (100%)	123 (97%)	4 (3%)	40	43
1	H	127/127 (100%)	124 (98%)	3 (2%)	49	53
1	I	127/127 (100%)	124 (98%)	3 (2%)	49	53
1	J	128/127 (101%)	123 (96%)	5 (4%)	32	33
All	All	1272/1270 (100%)	1237 (97%)	35 (3%)	43	47

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	36	THR
1	F	128	LEU
1	J	102	GLN
1	E	127	LYS
1	E	129	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	5	GLN
1	F	102	GLN
1	J	5	GLN
1	F	51	GLN
1	F	76	GLN

### 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](#)

Of 37 ligands modelled in this entry, 13 are monoatomic - leaving 24 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	I	1158	-	4,4,4	0.37	0	6,6,6	1.96	2 (33%)
2	SO4	F	1158	-	4,4,4	0.62	0	6,6,6	1.51	2 (33%)
2	SO4	A	1158	-	4,4,4	0.15	0	6,6,6	0.23	0
2	SO4	A	1157	-	4,4,4	0.16	0	6,6,6	1.17	0
2	SO4	E	1158	-	4,4,4	0.18	0	6,6,6	0.39	0
2	SO4	I	1159	-	4,4,4	0.25	0	6,6,6	0.31	0
2	SO4	J	1157	-	4,4,4	0.44	0	6,6,6	0.58	0
2	SO4	F	1159	-	4,4,4	0.24	0	6,6,6	0.28	0
2	SO4	B	1158	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	G	1159	-	4,4,4	0.16	0	6,6,6	0.21	0
2	SO4	F	1157	-	4,4,4	0.14	0	6,6,6	0.40	0
2	SO4	G	1158	-	4,4,4	0.70	0	6,6,6	1.74	1 (16%)
2	SO4	H	1159	-	4,4,4	0.14	0	6,6,6	0.55	0
2	SO4	I	1157	-	4,4,4	0.12	0	6,6,6	0.32	0
2	SO4	D	1157	-	4,4,4	0.27	0	6,6,6	0.54	0
2	SO4	D	1159	-	4,4,4	0.20	0	6,6,6	0.35	0
2	SO4	J	1158	-	4,4,4	0.24	0	6,6,6	0.83	0
2	SO4	H	1158	-	4,4,4	0.41	0	6,6,6	1.40	1 (16%)
2	SO4	D	1158	-	4,4,4	0.48	0	6,6,6	1.14	1 (16%)
2	SO4	G	1157	-	4,4,4	0.19	0	6,6,6	0.58	0
2	SO4	B	1157	-	4,4,4	0.15	0	6,6,6	0.42	0
2	SO4	H	1157	-	4,4,4	0.21	0	6,6,6	0.49	0
2	SO4	E	1157	-	4,4,4	0.17	0	6,6,6	0.51	0
2	SO4	C	1157	-	4,4,4	0.23	0	6,6,6	0.50	0

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1158	SO4	O3-S-O1	-3.13	92.97	109.31
2	H	1158	SO4	O3-S-O2	-2.93	94.02	109.31
2	G	1158	SO4	O4-S-O3	2.68	120.52	109.06
2	F	1158	SO4	O4-S-O2	-2.51	96.23	109.31
2	I	1158	SO4	O4-S-O1	2.40	121.81	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1158	SO4	2	0
2	F	1158	SO4	2	0
2	J	1157	SO4	1	0
2	G	1158	SO4	1	0
2	B	1157	SO4	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.