



wwPDB X-ray Structure Validation Summary Report

May 14, 2020 – 08:14 pm BST

PDB ID : 2IVB
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 : 2006-06-09
Resolution : 1.95 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 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)
Xtrriage (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

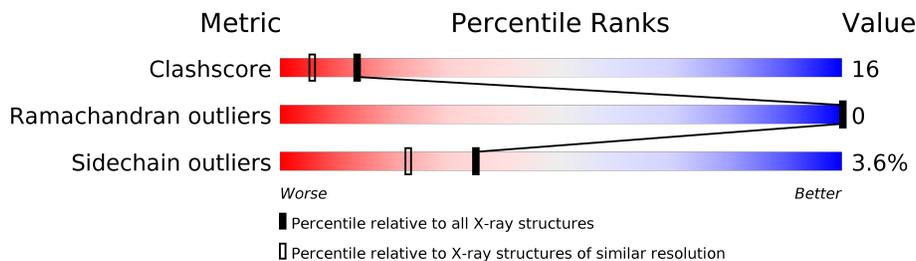
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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 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	81% 19% .
1	B	156	80% 19% .
1	C	156	80% 17% .
1	D	156	72% 25% ..
1	E	156	80% 19% .
1	F	156	81% 18% .
1	G	156	79% 19% ..
1	H	156	73% 25% .

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Mol	Chain	Length	Quality of chain
1	I	156	 81% 18% .
1	J	156	 76% 22% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14972 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
			Total	C	N	O	S			
1	A	156	1207	777	199	226	5	0	2	0
1	B	156	1212	782	199	226	5	0	3	0
1	C	156	1212	782	199	226	5	0	3	0
1	D	156	1220	788	200	227	5	0	4	0
1	E	156	1212	781	199	226	6	0	3	0
1	F	156	1212	782	199	226	5	0	3	0
1	G	156	1212	782	199	226	5	0	3	0
1	H	156	1212	782	199	226	5	0	3	0
1	I	156	1217	786	199	226	6	0	4	0
1	J	156	1223	790	199	228	6	0	5	0

There are 10 discrepancies between the modelled and reference sequences:

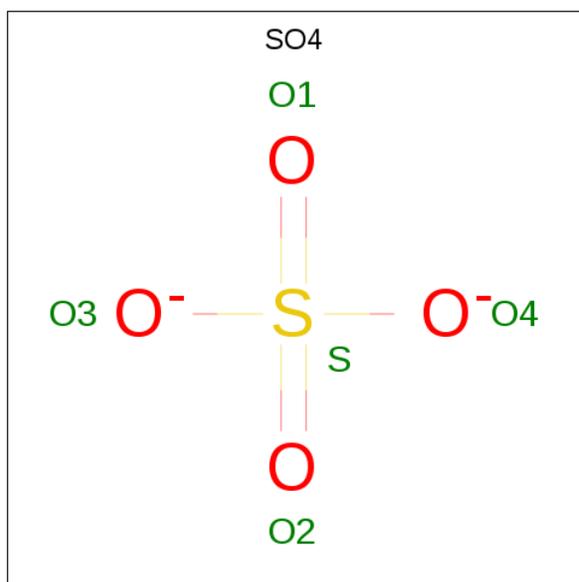
Chain	Residue	Modelled	Actual	Comment	Reference
A	122	ALA	SER	engineered mutation	UNP P00816
B	122	ALA	SER	engineered mutation	UNP P00816
C	122	ALA	SER	engineered mutation	UNP P00816
D	122	ALA	SER	engineered mutation	UNP P00816
E	122	ALA	SER	engineered mutation	UNP P00816
F	122	ALA	SER	engineered mutation	UNP P00816
G	122	ALA	SER	engineered mutation	UNP P00816
H	122	ALA	SER	engineered mutation	UNP P00816
I	122	ALA	SER	engineered mutation	UNP P00816

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Chain	Residue	Modelled	Actual	Comment	Reference
J	122	ALA	SER	engineered mutation	UNP P00816

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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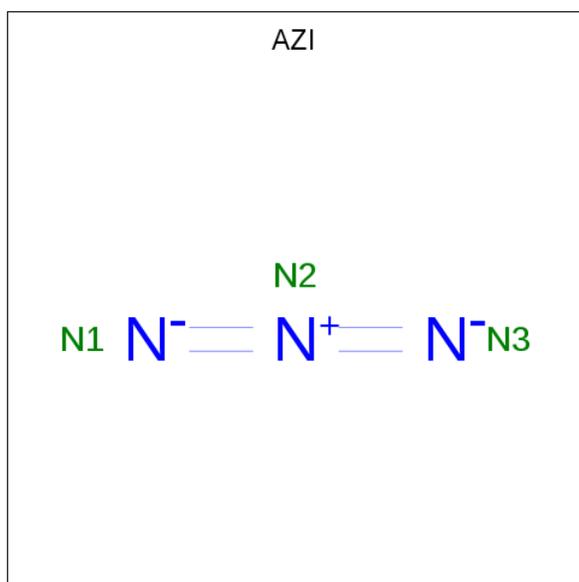
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

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

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

- Molecule 4 is AZIDE ION (three-letter code: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total N 3 3	0	0
4	D	1	Total N 3 3	0	0
4	E	1	Total N 3 3	0	0
4	F	1	Total N 3 3	0	0
4	G	1	Total N 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	241	Total O 241 241	0	0
5	B	284	Total O 284 284	0	0
5	C	256	Total O 256 256	0	0
5	D	252	Total O 252 252	0	0
5	E	275	Total O 275 275	0	0
5	F	289	Total O 289 289	0	0
5	G	280	Total O 280 280	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	277	Total 277	O 277	0	0
5	I	277	Total 277	O 277	0	0
5	J	297	Total 297	O 297	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: 



- Molecule 1: CYANATE HYDRATASE

Chain B: 



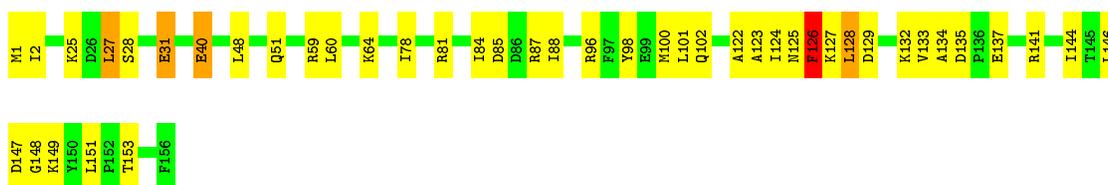
- Molecule 1: CYANATE HYDRATASE

Chain C: 



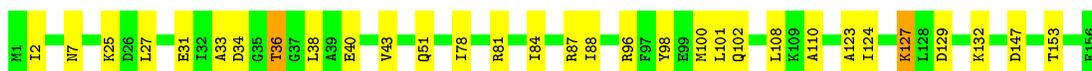
- Molecule 1: CYANATE HYDRATASE

Chain D: 



- Molecule 1: CYANATE HYDRATASE

Chain E: 



- Molecule 1: CYANATE HYDRATASE

Chain F:  81% 18%



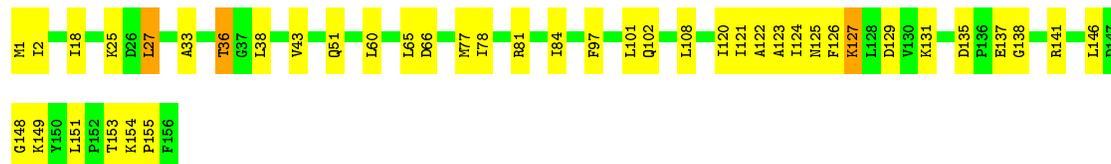
- Molecule 1: CYANATE HYDRATASE

Chain G:  79% 19%



- Molecule 1: CYANATE HYDRATASE

Chain H:  73% 25%



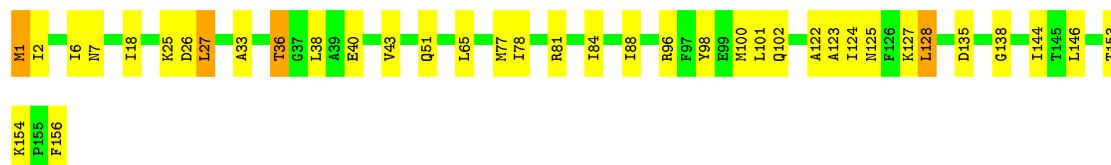
- Molecule 1: CYANATE HYDRATASE

Chain I:  81% 18%



- Molecule 1: CYANATE HYDRATASE

Chain J:  76% 22%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.50Å 80.60Å 82.11Å 69.86° 71.38° 66.43°	Depositor
Resolution (Å)	75.38 – 1.95	Depositor
% Data completeness (in resolution range)	96.2 (75.38-1.95)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.145 , 0.207	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14972	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: AZI, 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	0.83	1/1230 (0.1%)	0.81	1/1663 (0.1%)
1	B	0.91	2/1238 (0.2%)	0.87	3/1675 (0.2%)
1	C	0.84	0/1238	0.88	1/1675 (0.1%)
1	D	0.87	1/1246 (0.1%)	0.86	2/1686 (0.1%)
1	E	0.90	1/1238 (0.1%)	0.84	1/1673 (0.1%)
1	F	0.88	0/1238	0.87	2/1675 (0.1%)
1	G	0.83	0/1238	0.88	1/1675 (0.1%)
1	H	0.82	0/1238	0.87	0/1675
1	I	0.77	0/1246	0.80	0/1685
1	J	0.83	0/1255	0.82	2/1697 (0.1%)
All	All	0.85	5/12405 (0.0%)	0.85	13/16779 (0.1%)

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
1	D	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	40	GLU	CB-CG	-6.83	1.39	1.52
1	E	40	GLU	CB-CG	-5.97	1.40	1.52
1	B	69	GLU	CD-OE1	5.33	1.31	1.25
1	A	46	ALA	CA-CB	5.15	1.63	1.52
1	B	69	GLU	CG-CD	5.06	1.59	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	MET	CG-SD-CE	-8.89	85.97	100.20
1	G	1	MET	CG-SD-CE	6.87	111.19	100.20
1	B	87	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	B	147	ASP	CB-CG-OD2	6.05	123.74	118.30
1	B	1	MET	CG-SD-CE	6.00	109.80	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	126	PHE	Peptide

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	1207	0	1265	34	0
1	B	1212	0	1276	44	0
1	C	1212	0	1276	38	0
1	D	1220	0	1286	52	0
1	E	1212	0	1274	41	0
1	F	1212	0	1276	36	0
1	G	1212	0	1276	46	0
1	H	1212	0	1276	68	0
1	I	1217	0	1285	34	0
1	J	1223	0	1291	55	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	D	20	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	5	0	0	0	0
2	I	15	0	0	0	0
2	J	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	G	2	0	0	1	0
3	H	1	0	0	0	0
3	I	2	0	0	0	0
3	J	1	0	0	0	0
4	C	3	0	0	1	0
4	D	3	0	0	1	0
4	E	3	0	0	1	0
4	F	3	0	0	1	0
4	G	3	0	0	1	0
5	A	241	0	0	13	1
5	B	284	0	0	12	1
5	C	256	0	0	11	0
5	D	252	0	0	15	0
5	E	275	0	0	13	1
5	F	289	0	0	16	1
5	G	280	0	0	26	0
5	H	277	0	0	29	0
5	I	277	0	0	17	0
5	J	297	0	0	21	0
All	All	14972	0	12781	399	2

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 16.

The worst 5 of 399 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:J:1:MET:CE	1:J:2:ILE:HG22	1.52	1.39
1:A:1:MET:CE	1:A:2:ILE:HG22	1.54	1.34
1:E:78:ILE:HG12	5:E:2181:HOH:O	1.19	1.33
1:B:123:ALA:HB3	5:F:2219:HOH:O	1.23	1.32
1:H:101[B]:LEU:CD1	5:H:2211:HOH:O	1.64	1.31

All (2) 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)
5:A:2199:HOH:O	5:E:2250:HOH:O[1_565]	1.99	0.21
5:B:2099:HOH:O	5:F:2179:HOH:O[1_655]	2.16	0.04

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	156/156 (100%)	153 (98%)	3 (2%)	0	100	100
1	B	157/156 (101%)	153 (98%)	4 (2%)	0	100	100
1	C	157/156 (101%)	153 (98%)	4 (2%)	0	100	100
1	D	158/156 (101%)	153 (97%)	5 (3%)	0	100	100
1	E	157/156 (101%)	154 (98%)	3 (2%)	0	100	100
1	F	157/156 (101%)	154 (98%)	3 (2%)	0	100	100
1	G	157/156 (101%)	154 (98%)	3 (2%)	0	100	100
1	H	157/156 (101%)	152 (97%)	5 (3%)	0	100	100
1	I	158/156 (101%)	152 (96%)	6 (4%)	0	100	100
1	J	159/156 (102%)	154 (97%)	5 (3%)	0	100	100
All	All	1573/1560 (101%)	1532 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	128/126 (102%)	125 (98%)	3 (2%)	50	42
1	B	129/126 (102%)	126 (98%)	3 (2%)	50	42
1	C	129/126 (102%)	122 (95%)	7 (5%)	22	10
1	D	130/126 (103%)	123 (95%)	7 (5%)	22	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	129/126 (102%)	125 (97%)	4 (3%)	40	28
1	F	129/126 (102%)	124 (96%)	5 (4%)	32	19
1	G	129/126 (102%)	123 (95%)	6 (5%)	26	13
1	H	129/126 (102%)	125 (97%)	4 (3%)	40	28
1	I	130/126 (103%)	127 (98%)	3 (2%)	50	42
1	J	131/126 (104%)	127 (97%)	4 (3%)	40	28
All	All	1293/1260 (103%)	1247 (96%)	46 (4%)	35	23

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	36	THR
1	F	102	GLN
1	J	27	LEU
1	E	102	GLN
1	E	129	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	51	GLN
1	F	102	GLN
1	J	51	GLN
1	E	102	GLN
1	F	51	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 31 ligands modelled in this entry, 10 are monoatomic - leaving 21 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	1157	-	4,4,4	0.79	0	6,6,6	0.87	0
2	SO4	B	1157	-	4,4,4	0.15	0	6,6,6	0.29	0
4	AZI	D	1161	-	0,2,2	0.00	-	0,1,1	0.00	-
2	SO4	D	1157	-	4,4,4	0.34	0	6,6,6	0.31	0
2	SO4	I	1158	-	4,4,4	0.64	0	6,6,6	0.77	0
2	SO4	D	1160	-	4,4,4	0.16	0	6,6,6	0.31	0
2	SO4	G	1158	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	J	1157	-	4,4,4	0.19	0	6,6,6	0.41	0
2	SO4	G	1157	-	4,4,4	0.63	0	6,6,6	0.72	0
2	SO4	F	1158	-	4,4,4	0.24	0	6,6,6	0.33	0
2	SO4	F	1157	-	4,4,4	0.26	0	6,6,6	0.38	0
2	SO4	H	1157	-	4,4,4	0.18	0	6,6,6	0.42	0
2	SO4	E	1157	-	4,4,4	0.25	0	6,6,6	0.38	0
2	SO4	I	1159	-	4,4,4	0.16	0	6,6,6	0.23	0
4	AZI	G	1161	-	0,2,2	0.00	-	0,1,1	0.00	-
2	SO4	A	1157	-	4,4,4	0.16	0	6,6,6	0.43	0
4	AZI	E	1158	-	0,2,2	0.00	-	0,1,1	0.00	-
2	SO4	D	1158	-	4,4,4	0.80	0	6,6,6	0.60	0
4	AZI	C	1158	-	0,2,2	0.00	-	0,1,1	0.00	-
4	AZI	F	1160	-	0,2,2	0.00	-	0,1,1	0.00	-
2	SO4	D	1159	-	4,4,4	0.62	0	6,6,6	1.17	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 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1161	AZI	1	0
4	G	1161	AZI	1	0
2	A	1157	SO4	1	0
4	E	1158	AZI	1	0
4	C	1158	AZI	1	0
4	F	1160	AZI	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.