



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 05:34 am GMT

PDB ID : 2IVG  
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 : 2006-06-13  
Resolution : 1.87 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](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.

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 : 4.02b-467  
Mogul : 1.8.4, 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) : 2.36

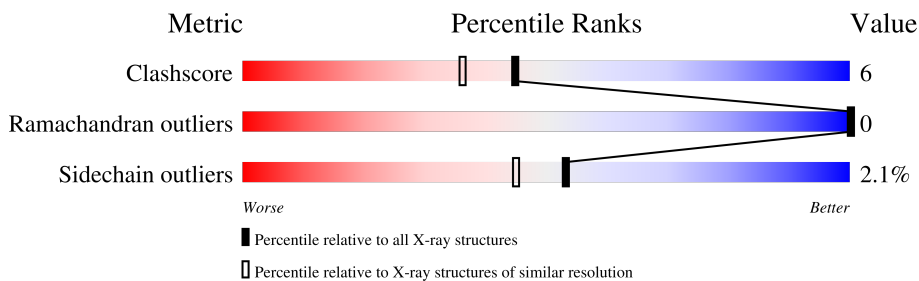
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 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	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)

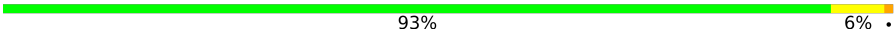

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	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	 93% 6%
1	J	156	 91% 8%

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	1159[A]	-	-	X	-
2	SO4	I	1160[A]	-	-	X	-
2	SO4	I	1161[B]	-	-	X	-
2	SO4	J	1160[B]	-	-	X	-
3	CL	F	1162[A]	-	-	X	-
3	CL	G	1160[A]	-	-	X	-
3	CL	I	1163	-	-	X	-
3	CL	I	1164	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13926 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 LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1199	768	199	227	5	0	1	0
1	B	156	1194	763	199	227	5	0	0	0
1	C	156	1199	768	199	227	5	0	1	0
1	D	156	1208	777	199	227	5	0	3	0
1	E	156	1199	768	199	227	5	0	1	0
1	F	156	1204	773	199	227	5	0	2	0
1	G	156	1199	768	199	227	5	0	1	0
1	H	156	1204	773	199	227	5	0	2	0
1	I	156	1199	768	199	227	5	0	1	0
1	J	156	1199	768	199	227	5	0	1	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	GLY	LEU	engineered mutation	UNP P00816
B	151	GLY	LEU	engineered mutation	UNP P00816
C	151	GLY	LEU	engineered mutation	UNP P00816
D	151	GLY	LEU	engineered mutation	UNP P00816
E	151	GLY	LEU	engineered mutation	UNP P00816
F	151	GLY	LEU	engineered mutation	UNP P00816
G	151	GLY	LEU	engineered mutation	UNP P00816
H	151	GLY	LEU	engineered mutation	UNP P00816
I	151	GLY	LEU	engineered mutation	UNP P00816

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Chain	Residue	Modelled	Actual	Comment	Reference
J	151	GLY	LEU	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
			Total	O	S		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	1
2	D	1	5	4	1	0	1
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0

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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	F	1	Total	O	S	0	1
			5	4	1		
2	F	1	Total	O	S	0	1
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	1
			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	1
			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	I	1	Total	O	S	0	1
			5	4	1		
2	I	1	Total	O	S	0	1
			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		
2	J	1	Total	O	S	0	1
			5	4	1		
2	J	1	Total	O	S	0	1
			5	4	1		

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

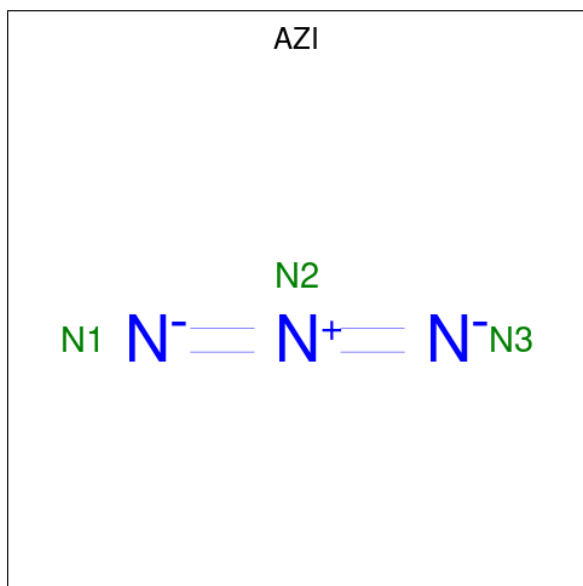
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

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

- Molecule 4 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 3	N 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	182	Total O 182 182	0	0
5	B	159	Total O 159 159	0	0
5	C	168	Total O 168 168	0	0
5	D	188	Total O 188 188	0	0
5	E	148	Total O 148 148	0	0
5	F	169	Total O 169 169	0	0
5	G	183	Total O 183 183	0	0
5	H	175	Total O 175 175	0	0
5	I	186	Total O 186 186	0	0
5	J	196	Total O 196 196	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: CYANATE LYASE

Chain A:  88% 10%




- Molecule 1: CYANATE LYASE

Chain B:  89% 10%



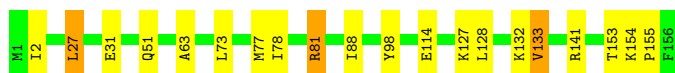
- Molecule 1: CYANATE LYASE

Chain C:  88% 11%




- Molecule 1: CYANATE LYASE

Chain D:  87% 11%



- Molecule 1: CYANATE LYASE

Chain E:  91% 8%

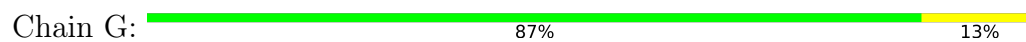


- Molecule 1: CYANATE LYASE

Chain F:  92% 8%



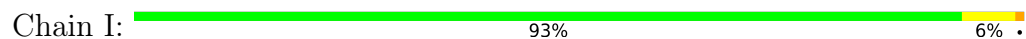
- Molecule 1: CYANATE LYASE



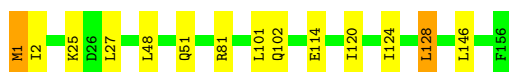
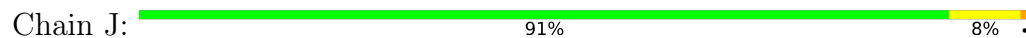
- Molecule 1: CYANATE LYASE



- Molecule 1: CYANATE LYASE



- Molecule 1: CYANATE LYASE



## 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, $\alpha$ , $\beta$ , $\gamma$	78.39Å 80.90Å 81.09Å 70.69° 75.98° 65.15°	Depositor
Resolution (Å)	76.70 – 1.87	Depositor
% Data completeness (in resolution range)	95.3 (76.70-1.87)	Depositor
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.145 , 0.188	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	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: 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	0.85	0/1219	0.81	0/1646
1	B	0.80	0/1211	0.83	2/1635 (0.1%)
1	C	0.81	0/1219	0.81	1/1646 (0.1%)
1	D	0.84	0/1234	0.85	1/1668 (0.1%)
1	E	0.79	0/1219	0.74	0/1647
1	F	0.80	0/1227	0.80	2/1658 (0.1%)
1	G	0.83	0/1219	0.79	0/1647
1	H	0.80	0/1227	0.80	0/1658
1	I	0.80	0/1219	0.80	1/1646 (0.1%)
1	J	0.82	0/1219	0.78	1/1646 (0.1%)
All	All	0.81	0/12213	0.80	8/16497 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	60	LEU	CA-CB-CG	5.99	129.07	115.30
1	B	60	LEU	CA-CB-CG	5.70	128.42	115.30
1	J	1	MET	CG-SD-CE	5.43	108.89	100.20
1	B	128	LEU	CA-CB-CG	5.32	127.54	115.30
1	F	128[A]	LEU	CA-CB-CG	5.22	127.30	115.30
1	F	128[B]	LEU	CA-CB-CG	5.22	127.30	115.30
1	D	81	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	11	ARG	NE-CZ-NH1	-5.12	117.74	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	1199	0	1246	21	0
1	B	1194	0	1235	20	0
1	C	1199	0	1246	14	0
1	D	1208	0	1266	19	0
1	E	1199	0	1246	14	0
1	F	1204	0	1257	16	0
1	G	1199	0	1246	27	0
1	H	1204	0	1257	19	0
1	I	1199	0	1246	8	0
1	J	1199	0	1246	14	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	1	0
2	D	25	0	0	1	0
2	E	10	0	0	0	0
2	F	20	0	0	4	0
2	G	10	0	0	1	0
2	H	15	0	0	1	0
2	I	25	0	0	11	0
2	J	20	0	0	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	3	0	0	1	0
3	E	2	0	0	0	0
3	F	2	0	0	4	0
3	G	2	0	0	2	0
3	H	2	0	0	0	0
3	I	3	0	0	10	0
3	J	3	0	0	1	0
4	C	3	0	0	0	0
5	A	182	0	0	3	1
5	B	159	0	0	5	0
5	C	168	0	0	2	0
5	D	188	0	0	5	0
5	E	148	0	0	3	0
5	F	169	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	183	0	0	6	0
5	H	175	0	0	1	0
5	I	186	0	0	3	0
5	J	196	0	0	4	1
All	All	13926	0	12491	159	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 6.

All (159) 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)
3:F:1162[A]:CL:CL	2:F:1159[A]:SO4:S	1.43	1.44
3:I:1163:CL:CL	2:I:1161[B]:SO4:S	1.28	1.29
3:I:1164:CL:CL	2:I:1160[A]:SO4:O3	1.95	1.21
3:I:1164:CL:CL	2:I:1160[A]:SO4:S	1.14	1.16
3:F:1162[A]:CL:CL	2:F:1159[A]:SO4:O2	2.03	1.13
1:D:2:ILE:HD11	1:D:78[A]:ILE:HD11	1.19	1.10
3:F:1162[A]:CL:CL	2:F:1159[A]:SO4:O3	0.74	1.09
1:F:2:ILE:HD11	1:F:78[A]:ILE:HD11	1.32	1.07
1:G:2:ILE:HD11	1:G:78[A]:ILE:HD11	1.15	1.06
3:I:1164:CL:CL	2:I:1160[A]:SO4:O1	2.10	1.06
3:I:1163:CL:CL	2:I:1161[B]:SO4:O2	2.11	1.05
1:E:2:ILE:HD11	1:E:78[A]:ILE:HD11	1.07	1.03
1:C:87:ARG:HD2	2:C:1158:SO4:O2	1.61	0.99
1:E:2:ILE:CD1	1:E:78[A]:ILE:HD11	1.94	0.98
3:I:1163:CL:CL	2:I:1161[B]:SO4:O1	2.18	0.98
1:B:1:MET:HE3	1:B:2:ILE:HG22	1.45	0.98
1:A:153:THR:HG22	1:J:124:ILE:HG23	1.48	0.95
1:F:1:MET:HE3	1:F:2:ILE:HG22	1.49	0.95
1:G:2:ILE:HD11	1:G:78[A]:ILE:CD1	1.95	0.94
1:A:153:THR:CG2	5:A:2144:HOH:O	2.14	0.94
1:A:153:THR:HG21	5:A:2144:HOH:O	1.68	0.94
1:A:114:GLU:HG3	1:J:1:MET:HE2	1.50	0.91
1:D:73:LEU:HD12	5:D:2102:HOH:O	1.69	0.90
1:D:2:ILE:CD1	1:D:78[A]:ILE:HD11	2.03	0.88
1:B:1:MET:CE	1:B:2:ILE:HG22	2.03	0.87
1:H:2:ILE:HD11	1:H:78[A]:ILE:HD11	1.59	0.85
1:F:1:MET:CE	1:F:2:ILE:HG22	2.05	0.85
1:G:114:GLU:HG3	1:H:1:MET:HE3	1.57	0.84
3:F:1162[A]:CL:CL	2:F:1159[A]:SO4:O4	2.29	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ILE:HD11	1:E:78[A]:ILE:CD1	2.01	0.84
3:I:1164:CL:CL	2:I:1160[A]:SO4:O4	2.32	0.84
1:G:122:SER:OG	2:G:1158[B]:SO4:O1	1.96	0.84
1:G:114:GLU:HG3	1:H:1:MET:CE	2.07	0.83
1:A:114:GLU:HG3	1:J:1:MET:CE	2.09	0.82
1:A:1:MET:HE1	1:J:114:GLU:HG3	1.62	0.81
1:F:2:ILE:HD11	1:F:78[A]:ILE:CD1	2.10	0.81
1:B:1:MET:HE3	1:B:2:ILE:CG2	2.10	0.81
1:I:154:LYS:O	5:I:2178:HOH:O	1.98	0.80
1:A:120:ILE:CD1	2:J:1160[B]:SO4:O1	2.35	0.75
1:I:87:ARG:HD2	2:I:1158:SO4:O4	1.88	0.74
1:A:114:GLU:CG	1:J:1:MET:HE2	2.18	0.73
1:C:36:THR:HG21	1:C:43:VAL:HG21	1.70	0.72
1:A:120:ILE:HD13	2:J:1160[B]:SO4:O1	1.90	0.72
1:F:1:MET:HE3	1:F:2:ILE:CG2	2.18	0.72
3:I:1163:CL:CL	2:I:1161[B]:SO4:O4	0.40	0.72
3:I:1164:CL:CL	2:I:1160[A]:SO4:O2	0.53	0.72
1:G:2:ILE:CD1	1:G:78[A]:ILE:HD11	2.09	0.67
1:J:1:MET:CE	1:J:2:ILE:HG22	2.24	0.67
3:G:1160[A]:CL:CL	5:G:2183:HOH:O	2.47	0.67
1:A:1:MET:CE	1:J:114:GLU:HG3	2.25	0.67
1:A:153:THR:HG23	5:A:2144:HOH:O	1.88	0.67
1:A:153:THR:HB	5:J:2160:HOH:O	1.94	0.66
1:I:40:GLU:OE1	5:I:2062:HOH:O	2.15	0.65
1:G:114:GLU:CG	1:H:1:MET:CE	2.75	0.64
1:D:127:LYS:HD2	5:D:2066:HOH:O	1.98	0.64
1:J:1:MET:HE3	1:J:2:ILE:HG22	1.79	0.63
1:B:34:ASP:HB2	5:B:2044:HOH:O	1.98	0.63
1:A:127:LYS:HD2	5:J:2095:HOH:O	1.98	0.62
1:H:88:ILE:HD12	1:H:98:TYR:CZ	2.35	0.62
1:G:114:GLU:CG	1:H:1:MET:HE3	2.30	0.61
1:G:114:GLU:CD	1:H:1:MET:HE1	2.21	0.60
1:G:155:PRO:HB3	1:H:38:LEU:HD22	1.84	0.60
1:G:114:GLU:CD	1:H:1:MET:CE	2.71	0.59
1:D:63:ALA:HB3	5:D:2092:HOH:O	2.03	0.59
3:G:1160[A]:CL:CL	2:H:1159[A]:SO4:O3	2.58	0.59
1:J:128[B]:LEU:HD23	1:J:146:LEU:HD23	1.84	0.59
1:C:36:THR:CG2	1:C:38:LEU:H	2.15	0.59
3:D:1163[B]:CL:CL	2:D:1161[B]:SO4:O3	2.58	0.58
1:J:51:GLN:NE2	1:J:81:ARG:HH21	2.00	0.58
1:A:128[A]:LEU:HD12	1:A:129:ASP:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ILE:HD11	2:J:1160[B]:SO4:O1	2.03	0.57
1:E:114:GLU:HG3	1:F:1:MET:CE	2.34	0.57
3:I:1163:CL:CL	2:I:1161[B]:SO4:O3	2.43	0.56
1:B:1:MET:CE	1:D:114:GLU:HG3	2.35	0.56
1:C:36:THR:HG22	1:C:38:LEU:H	1.70	0.56
1:G:131:LYS:NZ	5:G:2150:HOH:O	2.34	0.55
1:D:153:THR:O	1:D:153:THR:HG22	2.07	0.55
1:G:114:GLU:HG3	1:H:1:MET:HE1	1.86	0.54
1:E:24:LYS:NZ	5:E:2035:HOH:O	2.25	0.54
1:H:51:GLN:NE2	1:H:81:ARG:HH21	2.07	0.53
1:B:127:LYS:HD2	5:F:2065:HOH:O	2.08	0.52
1:F:1:MET:HE1	1:F:2:ILE:HG22	1.90	0.52
1:A:119:GLY:HA2	1:A:153:THR:HG23	1.92	0.52
1:G:114:GLU:CG	1:H:1:MET:HE1	2.40	0.51
1:G:2:ILE:CD1	1:G:78[A]:ILE:CD1	2.80	0.51
1:C:56:ASP:OD1	1:C:59:ARG:NH2	2.43	0.51
1:G:140:GLU:HG2	5:G:2153:HOH:O	2.11	0.51
1:C:88:ILE:HD11	1:H:87:ARG:HB3	1.95	0.49
1:E:51:GLN:NE2	1:E:81:ARG:HH21	2.11	0.49
1:G:114:GLU:OE1	1:H:1:MET:CE	2.61	0.49
1:D:27:LEU:HA	1:D:31:GLU:OE2	2.13	0.48
1:J:25:LYS:HE2	5:J:2048:HOH:O	2.13	0.48
1:B:1:MET:HE1	1:B:2:ILE:HG22	1.91	0.48
1:E:131:LYS:HE3	5:E:2120:HOH:O	2.12	0.48
1:E:114:GLU:HG3	1:F:1:MET:HE2	1.96	0.48
1:F:51:GLN:NE2	1:F:81:ARG:HH21	2.12	0.48
1:H:2:ILE:HD11	1:H:78[A]:ILE:CD1	2.36	0.48
1:A:51:GLN:NE2	1:A:81:ARG:HH21	2.11	0.48
1:E:88:ILE:HD12	1:E:98:TYR:CZ	2.49	0.48
1:J:1:MET:HE1	1:J:2:ILE:HG22	1.96	0.48
1:C:51:GLN:NE2	1:C:81:ARG:HH21	2.12	0.47
1:F:88:ILE:HD12	1:F:98:TYR:CZ	2.50	0.47
1:D:77:MET:HG2	5:D:2103:HOH:O	2.14	0.47
1:D:51:GLN:NE2	1:D:81:ARG:HH21	2.12	0.47
1:B:1:MET:HE1	1:D:114:GLU:HG3	1.97	0.47
1:I:88:ILE:HD12	1:I:98:TYR:CZ	2.50	0.47
5:B:2122:HOH:O	1:D:153:THR:HG23	2.16	0.46
1:B:51:GLN:NE2	1:B:81:ARG:HH21	2.12	0.46
1:I:51:GLN:NE2	1:I:81:ARG:HH21	2.14	0.46
1:G:88:ILE:HD12	1:G:98:TYR:CZ	2.50	0.46
1:G:74:LEU:HA	1:G:77:MET:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:LYS:N	5:G:2176:HOH:O	2.15	0.46
1:B:102:GLN:NE2	1:F:84:ILE:H	2.14	0.45
1:C:6:ILE:HD13	1:J:48:LEU:HD22	1.98	0.45
3:J:1163[B]:CL:CL	2:J:1160[B]:SO4:O2	2.71	0.45
1:G:127:LYS:HD2	5:G:2087:HOH:O	2.17	0.45
1:C:20:LEU:HG	1:C:24:LYS:HE3	1.99	0.45
1:C:63:ALA:HB3	5:C:2077:HOH:O	2.16	0.45
1:I:120:ILE:HD12	1:I:120:ILE:C	2.37	0.45
1:A:128[B]:LEU:HD23	1:A:146:LEU:HD23	1.99	0.45
1:B:88:ILE:HD12	1:B:98:TYR:CZ	2.52	0.44
1:E:38:LEU:HD22	1:F:155:PRO:HB3	1.98	0.44
1:B:1:MET:CE	1:B:2:ILE:CG2	2.79	0.44
1:B:18:ILE:HG23	1:B:65:LEU:HD13	2.00	0.44
1:D:128[A]:LEU:H	1:D:128[A]:LEU:HD23	1.83	0.44
1:B:140:GLU:HG2	5:B:2135:HOH:O	2.17	0.43
1:A:88:ILE:HD12	1:A:98:TYR:CZ	2.52	0.43
1:B:102:GLN:HE22	1:F:84:ILE:H	1.65	0.43
1:C:56:ASP:HB2	5:C:2075:HOH:O	2.18	0.43
1:D:154:LYS:HA	1:D:155:PRO:HD2	1.41	0.43
1:G:118:ASP:HB2	1:H:78[A]:ILE:CD1	2.48	0.43
1:B:1:MET:HE2	1:D:114:GLU:HG3	2.01	0.43
1:C:33:ALA:O	1:C:36:THR:HB	2.19	0.43
1:D:88:ILE:HD12	1:D:98:TYR:CZ	2.53	0.43
1:E:2:ILE:CD1	1:E:78[A]:ILE:CD1	2.80	0.42
1:D:133[A]:VAL:HG12	1:D:141:ARG:HB2	2.01	0.42
1:E:114:GLU:HG3	1:F:1:MET:HE1	2.01	0.42
1:G:18:ILE:HG23	1:G:65:LEU:HD13	2.01	0.42
1:B:77:MET:HG2	5:B:2082:HOH:O	2.19	0.42
1:G:40:GLU:OE2	5:G:2071:HOH:O	2.22	0.42
1:J:101:LEU:HD21	5:J:2143:HOH:O	2.20	0.42
1:G:118:ASP:CB	1:H:78[A]:ILE:HD13	2.50	0.41
1:G:153:THR:O	1:G:153:THR:HG22	2.19	0.41
1:H:77:MET:HG2	5:H:2105:HOH:O	2.20	0.41
1:E:102:GLN:HE22	1:G:84:ILE:H	1.68	0.41
1:D:154:LYS:NZ	5:D:2180:HOH:O	2.53	0.41
1:F:131:LYS:HE3	5:F:2135:HOH:O	2.20	0.41
1:E:77:MET:HG2	5:E:2074:HOH:O	2.21	0.41
1:I:80:LEU:C	1:I:80:LEU:HD13	2.41	0.41
1:B:63:ALA:HB3	5:B:2071:HOH:O	2.20	0.41
1:B:127:LYS:HE3	1:B:127:LYS:HB2	1.92	0.41
1:A:74:LEU:HA	1:A:77:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:THR:HG23	1:C:38:LEU:H	1.85	0.40
1:B:34:ASP:O	1:B:64:LYS:NZ	2.53	0.40
1:C:104:TYR:CD2	1:H:128[A]:LEU:HD21	2.56	0.40
1:I:131:LYS:HD2	5:I:2153:HOH:O	2.21	0.40
1:A:96:ARG:O	1:A:100:MET:HG3	2.21	0.40

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)
5:A:2160:HOH:O	5:J:2174:HOH:O[1_545]	1.56	0.64

## 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	155/156 (99%)	151 (97%)	4 (3%)	0	100	100
1	B	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
1	C	155/156 (99%)	151 (97%)	4 (3%)	0	100	100
1	D	157/156 (101%)	154 (98%)	3 (2%)	0	100	100
1	E	155/156 (99%)	151 (97%)	4 (3%)	0	100	100
1	F	156/156 (100%)	153 (98%)	3 (2%)	0	100	100
1	G	155/156 (99%)	152 (98%)	3 (2%)	0	100	100
1	H	156/156 (100%)	152 (97%)	4 (3%)	0	100	100
1	I	155/156 (99%)	151 (97%)	4 (3%)	0	100	100
1	J	155/156 (99%)	151 (97%)	4 (3%)	0	100	100
All	All	1553/1560 (100%)	1516 (98%)	37 (2%)	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	127/126 (101%)	123 (97%)	4 (3%)	40	29
1	B	126/126 (100%)	125 (99%)	1 (1%)	81	80
1	C	127/126 (101%)	124 (98%)	3 (2%)	49	39
1	D	129/126 (102%)	125 (97%)	4 (3%)	40	29
1	E	127/126 (101%)	124 (98%)	3 (2%)	49	39
1	F	128/126 (102%)	124 (97%)	4 (3%)	40	29
1	G	127/126 (101%)	125 (98%)	2 (2%)	62	56
1	H	128/126 (102%)	126 (98%)	2 (2%)	62	56
1	I	127/126 (101%)	126 (99%)	1 (1%)	81	80
1	J	127/126 (101%)	122 (96%)	5 (4%)	32	20
All	All	1273/1260 (101%)	1244 (98%)	29 (2%)	53	41

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	MET
1	A	102	GLN
1	A	127	LYS
1	A	153	THR
1	B	102	GLN
1	C	27	LEU
1	C	36	THR
1	C	129	ASP
1	D	27	LEU
1	D	132	LYS
1	D	133[A]	VAL
1	D	133[B]	VAL
1	E	27	LEU
1	E	102	GLN
1	E	128	LEU
1	F	27	LEU

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Mol	Chain	Res	Type
1	F	102	GLN
1	F	128[A]	LEU
1	F	128[B]	LEU
1	G	27	LEU
1	G	102	GLN
1	H	27	LEU
1	H	102	GLN
1	I	60	LEU
1	J	27	LEU
1	J	102	GLN
1	J	120	ILE
1	J	128[A]	LEU
1	J	128[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	102	GLN
1	B	51	GLN
1	B	102	GLN
1	C	51	GLN
1	C	102	GLN
1	D	51	GLN
1	D	102	GLN
1	E	51	GLN
1	E	102	GLN
1	F	51	GLN
1	F	102	GLN
1	G	51	GLN
1	G	102	GLN
1	H	51	GLN
1	H	102	GLN
1	I	51	GLN
1	I	102	GLN
1	J	51	GLN
1	J	102	GLN

### 5.3.3 RNA

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 50 ligands modelled in this entry, 20 are monoatomic - leaving 30 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	1157	-	4,4,4	0.17	0	6,6,6	0.60	0
2	SO4	F	1158	-	4,4,4	0.21	0	6,6,6	0.26	0
2	SO4	D	1160[A]	-	4,4,4	0.13	0	6,6,6	0.18	0
2	SO4	I	1157	-	4,4,4	0.14	0	6,6,6	0.32	0
2	SO4	B	1157	-	4,4,4	0.42	0	6,6,6	1.87	2 (33%)
2	SO4	F	1159[A]	-	4,4,4	0.14	0	6,6,6	0.69	0
2	SO4	C	1158	-	4,4,4	0.51	0	6,6,6	0.96	0
2	SO4	I	1158	-	4,4,4	0.39	0	6,6,6	1.83	2 (33%)
2	SO4	H	1159[A]	-	4,4,4	0.24	0	6,6,6	0.47	0
2	SO4	E	1157	-	4,4,4	0.42	0	6,6,6	1.42	1 (16%)
4	AZI	C	1160	-	0,2,2	-	-	0,1,1	-	-
2	SO4	D	1158	-	4,4,4	0.44	0	6,6,6	1.51	1 (16%)
2	SO4	G	1157	-	4,4,4	0.15	0	6,6,6	0.68	0
2	SO4	D	1159	-	4,4,4	0.18	0	6,6,6	0.18	0
2	SO4	I	1161[B]	-	4,4,4	0.25	0	6,6,6	0.22	0
2	SO4	F	1160[B]	-	4,4,4	0.34	0	6,6,6	0.35	0
2	SO4	I	1160[A]	-	4,4,4	0.28	0	6,6,6	0.36	0
2	SO4	J	1160[B]	-	4,4,4	0.09	0	6,6,6	0.75	0
2	SO4	D	1161[B]	-	4,4,4	0.23	0	6,6,6	0.34	0
2	SO4	H	1158	-	4,4,4	0.12	0	6,6,6	0.25	0
2	SO4	I	1159	-	4,4,4	0.11	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	E	1158	-	4,4,4	0.17	0	6,6,6	0.31	0
2	SO4	J	1157	-	4,4,4	0.14	0	6,6,6	0.27	0
2	SO4	C	1157	-	4,4,4	0.14	0	6,6,6	0.41	0
2	SO4	J	1159[A]	-	4,4,4	0.23	0	6,6,6	0.54	0
2	SO4	F	1157	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	H	1157	-	4,4,4	0.23	0	6,6,6	0.23	0
2	SO4	D	1157	-	4,4,4	0.15	0	6,6,6	0.37	0
2	SO4	G	1158[B]	-	4,4,4	0.20	0	6,6,6	0.90	0
2	SO4	J	1158	-	4,4,4	0.16	0	6,6,6	0.39	0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1158	SO4	O4-S-O2	-3.18	92.73	109.31
2	B	1157	SO4	O3-S-O2	-3.05	93.41	109.31
2	I	1158	SO4	O4-S-O3	2.47	119.60	109.06
2	B	1157	SO4	O4-S-O2	2.42	121.93	109.31
2	D	1158	SO4	O4-S-O2	-2.21	97.79	109.31
2	E	1157	SO4	O3-S-O2	-2.10	98.34	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1159[A]	SO4	4	0
2	C	1158	SO4	1	0
2	I	1158	SO4	1	0
2	H	1159[A]	SO4	1	0
2	I	1161[B]	SO4	5	0
2	I	1160[A]	SO4	5	0
2	J	1160[B]	SO4	4	0
2	D	1161[B]	SO4	1	0
2	G	1158[B]	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.