



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 01:13 am BST

PDB ID : 1GJY  
Title : The X-ray structure of the Sorcin Calcium Binding Domain (SCBD) provides insight into the phosphorylation and calcium dependent processes  
Authors : Ilari, A.; Johnson, K.A.; Nastopoulos, V.; Tsernoglou, D.; Chiancone, E.  
Deposited on : 2001-08-06  
Resolution : 2.20 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.

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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)  
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

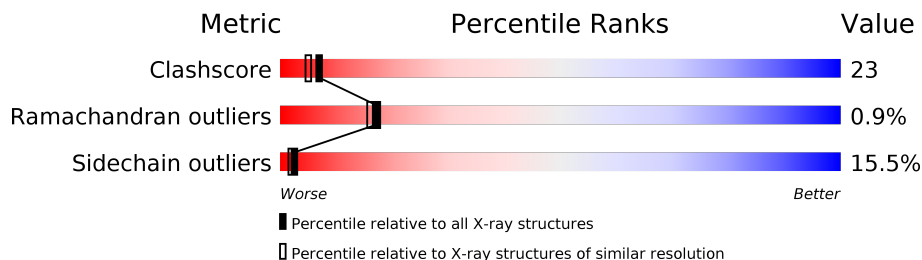
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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	167	
1	B	167	
1	C	167	
1	D	167	

## 2 Entry composition [i](#)

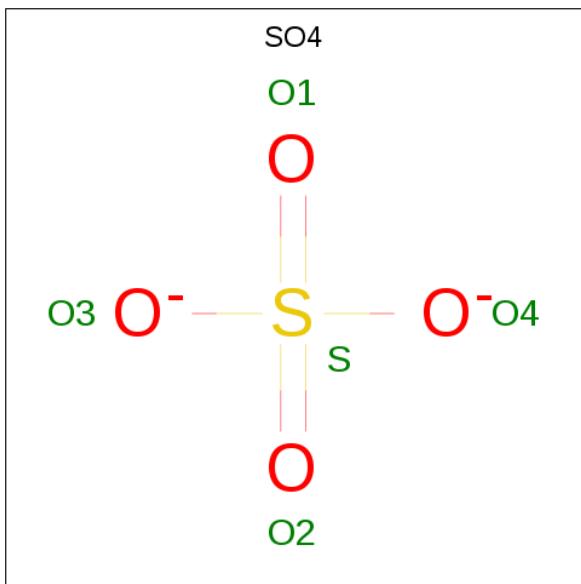
There are 3 unique types of molecules in this entry. The entry contains 5615 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SORCIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	167	Total 1321	C 826	N 227	O 255	S 13	0	0	0
1	B	167	Total 1321	C 826	N 227	O 255	S 13	0	0	0
1	C	167	Total 1321	C 826	N 227	O 255	S 13	0	0	0
1	D	167	Total 1321	C 826	N 227	O 255	S 13	0	0	0

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



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	62	Total	O	0	0
			62	62		
3	C	86	Total	O	0	0
			86	86		
3	D	97	Total	O	0	0
			97	97		

### 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.

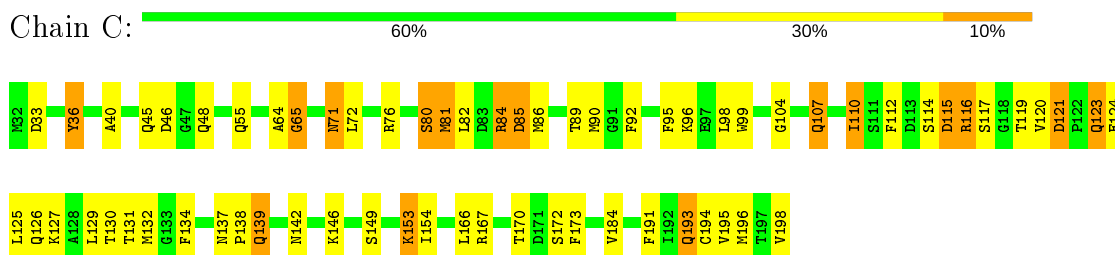
- Molecule 1: SORCIN



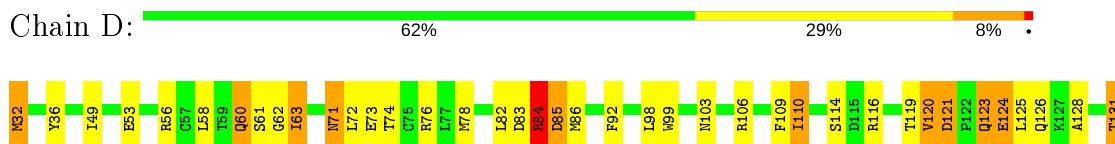
- Molecule 1: SORCIN



- Molecule 1: SORCIN



- Molecule 1: SORCIN





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.93Å 103.85Å 78.55Å 90.00° 117.96° 90.00°	Depositor
Resolution (Å)	14.00 – 2.20	Depositor
% Data completeness (in resolution range)	85.0 (14.00-2.20)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.232 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	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

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	0.63	0/1346	0.75	0/1812
1	B	0.71	0/1346	0.80	1/1812 (0.1%)
1	C	0.63	0/1346	0.76	0/1812
1	D	0.66	0/1346	0.77	0/1812
All	All	0.66	0/5384	0.77	1/7248 (0.0%)

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	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	187	SER	N-CA-C	-5.26	96.80	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	36	TYR	Sidechain
1	C	36	TYR	Sidechain



## 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	1321	0	1271	80	0
1	B	1321	0	1271	71	0
1	C	1321	0	1271	59	0
1	D	1321	0	1271	50	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	5	0	0	1	0
3	A	61	0	0	4	1
3	B	62	0	0	3	0
3	C	86	0	0	2	0
3	D	97	0	0	3	1
All	All	5615	0	5084	239	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 23.

All (239) 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:C:137:ASN:HB3	1:C:139:GLN:NE2	1.75	1.00
1:B:123:GLN:H	1:B:123:GLN:HE21	1.12	0.88
1:C:194:CYS:O	1:C:198:VAL:HG23	1.74	0.86
1:A:140:THR:HG23	1:B:193:GLN:HB2	1.59	0.83
1:A:129:LEU:HA	1:A:132:MET:HG3	1.58	0.83
1:A:45:GLN:HG2	1:A:46:ASP:N	1.94	0.83
1:C:137:ASN:HB3	1:C:139:GLN:HE22	1.43	0.82
1:A:126:GLN:HA	1:A:141:VAL:HG11	1.62	0.81
1:D:84:ARG:HB2	1:D:175:ARG:NH2	1.95	0.81
1:B:125:LEU:HD22	1:B:154:ILE:HD13	1.61	0.81
1:B:157:ASP:HB2	3:B:2022:HOH:O	1.78	0.81
1:D:60:GLN:HG3	3:D:2007:HOH:O	1.82	0.79
1:A:151:SER:HB2	1:A:153:LYS:NZ	1.99	0.76
1:C:92:PHE:CE1	1:C:96:LYS:HE2	2.22	0.74
1:D:56:ARG:O	1:D:60:GLN:HG2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ASP:HB3	1:C:123:GLN:OE1	1.89	0.73
1:A:70:PHE:CE1	1:A:160:ILE:HD13	2.24	0.72
1:B:120:VAL:HG13	1:B:124:GLU:HB2	1.70	0.72
1:C:45:GLN:HG2	1:C:46:ASP:N	2.04	0.72
1:A:70:PHE:HE1	1:A:160:ILE:HD13	1.54	0.72
1:A:146:LYS:HD2	1:B:86:MET:HG3	1.74	0.69
1:C:132:MET:CE	1:C:134:PHE:HE2	2.04	0.69
1:B:125:LEU:HD11	1:B:129:LEU:HD13	1.74	0.69
1:A:135:ARG:HD3	1:A:135:ARG:N	2.04	0.69
1:C:112:PHE:CE1	1:C:124:GLU:HG2	2.28	0.69
1:D:110:ILE:HG13	1:D:116:ARG:CZ	2.23	0.69
1:A:121:ASP:O	1:A:124:GLU:HG3	1.95	0.67
1:B:127:LYS:O	1:B:131:THR:HG23	1.95	0.67
1:B:125:LEU:HD23	1:B:145:ALA:HA	1.75	0.67
1:B:123:GLN:N	1:B:123:GLN:HE21	1.90	0.66
1:A:147:ARG:NH1	1:B:198:VAL:OXT	2.29	0.65
1:A:189:ASP:O	1:A:193:GLN:HB2	1.97	0.65
1:D:84:ARG:HG3	1:D:84:ARG:O	1.97	0.64
1:B:132:MET:HG3	1:B:132:MET:O	1.94	0.64
1:C:132:MET:CE	1:C:166:LEU:HD23	2.26	0.64
1:B:106:ARG:HG2	1:B:106:ARG:HH11	1.63	0.63
1:A:128:ALA:O	1:A:132:MET:HG2	1.99	0.63
1:B:45:GLN:CD	1:B:45:GLN:H	1.98	0.63
1:C:138:PRO:HD2	1:C:139:GLN:HE21	1.64	0.63
1:C:112:PHE:CD1	1:C:124:GLU:HG2	2.33	0.62
1:D:175:ARG:NH1	2:D:200:SO4:O2	2.33	0.62
1:D:83:ASP:CG	1:D:83:ASP:O	2.37	0.62
1:D:82:LEU:CD1	1:D:98:LEU:HB2	2.30	0.61
1:A:110:ILE:HG12	1:A:116:ARG:CZ	2.31	0.61
1:A:151:SER:HB2	1:A:153:LYS:HZ1	1.63	0.61
1:C:123:GLN:CD	1:C:123:GLN:H	2.02	0.61
1:A:183:MET:CE	1:B:187:SER:HB2	2.31	0.61
1:B:126:GLN:HA	1:B:141:VAL:CG1	2.31	0.60
1:D:84:ARG:HD2	1:D:175:ARG:HH21	1.66	0.60
1:D:83:ASP:OD2	1:D:83:ASP:O	2.20	0.60
1:D:171:ASP:HB3	1:D:175:ARG:NH2	2.17	0.60
1:D:86:MET:SD	1:D:193:GLN:NE2	2.75	0.60
1:A:77:LEU:HD23	1:B:147:ARG:HH12	1.67	0.59
1:C:132:MET:HE2	1:C:166:LEU:HD23	1.84	0.59
1:B:55:GLN:HB2	1:B:75:CYS:SG	2.42	0.59
1:C:129:LEU:HD22	1:C:166:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ILE:HD11	1:C:116:ARG:HH11	1.68	0.59
1:B:189:ASP:HB2	3:B:2059:HOH:O	2.02	0.58
1:B:36:TYR:HA	1:B:92:PHE:CE2	2.37	0.58
1:A:151:SER:HB2	1:A:153:LYS:HZ3	1.65	0.58
1:A:156:PHE:O	1:A:159:TYR:HB3	2.03	0.58
1:A:169:LEU:HD13	1:B:195:VAL:HG21	1.85	0.58
1:C:90:MET:CE	1:C:95:PHE:HA	2.33	0.58
1:C:112:PHE:CZ	1:C:124:GLU:HG2	2.39	0.58
1:A:33:ASP:OD1	1:A:35:LEU:HB2	2.04	0.57
1:C:132:MET:HE3	1:C:134:PHE:HE2	1.68	0.57
1:C:82:LEU:CD1	1:C:98:LEU:HB2	2.35	0.57
1:B:45:GLN:CD	1:B:45:GLN:N	2.57	0.57
1:B:126:GLN:HA	1:B:141:VAL:HG11	1.87	0.56
1:A:92:PHE:CE1	1:A:96:LYS:HE2	2.40	0.56
1:A:185:ASN:HA	1:B:185:ASN:HA	1.86	0.56
1:C:132:MET:HE2	1:C:134:PHE:HE2	1.70	0.56
1:C:48:GLN:HB3	1:C:89:THR:HB	1.86	0.56
1:A:198:VAL:O	1:B:147:ARG:NH1	2.39	0.56
1:B:120:VAL:CG1	1:B:124:GLU:HB2	2.34	0.56
1:D:84:ARG:CG	1:D:84:ARG:O	2.53	0.56
1:A:173:PHE:CZ	1:A:184:VAL:HG23	2.42	0.55
1:A:156:PHE:CZ	1:A:160:ILE:HD11	2.41	0.55
1:A:183:MET:HE2	1:B:187:SER:HB2	1.89	0.55
1:B:125:LEU:CD2	1:B:154:ILE:HD13	2.33	0.55
1:D:193:GLN:O	1:D:197:THR:HG23	2.07	0.55
1:A:45:GLN:HG2	1:A:46:ASP:H	1.70	0.54
1:C:125:LEU:HD23	1:C:154:ILE:HD12	1.90	0.54
1:C:138:PRO:HD2	1:C:139:GLN:NE2	2.22	0.54
1:B:126:GLN:O	1:B:130:THR:OG1	2.16	0.54
1:A:156:PHE:CE2	1:A:160:ILE:HD11	2.42	0.54
1:A:106:ARG:HH11	1:A:106:ARG:HG2	1.72	0.54
1:B:73:GLU:OE1	1:B:76:ARG:NH2	2.41	0.54
1:D:84:ARG:HD2	1:D:175:ARG:NH2	2.23	0.54
1:D:171:ASP:HB3	1:D:175:ARG:HH21	1.72	0.53
1:D:179:ALA:CB	1:D:181:GLN:HE21	2.20	0.53
1:B:106:ARG:NH1	1:B:106:ARG:HG2	2.23	0.53
1:D:83:ASP:O	1:D:85:ASP:N	2.41	0.53
1:A:90:MET:CE	1:A:95:PHE:HA	2.39	0.53
1:B:125:LEU:CD1	1:B:129:LEU:HD13	2.38	0.53
1:D:71:ASN:HD22	1:D:71:ASN:N	2.06	0.53
1:A:146:LYS:O	1:A:149:SER:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TYR:HA	1:A:92:PHE:CE2	2.44	0.52
1:A:169:LEU:HD13	1:B:195:VAL:CG2	2.39	0.52
1:B:82:LEU:CD1	1:B:98:LEU:HB2	2.39	0.52
1:D:63:ILE:O	1:D:63:ILE:HG13	2.10	0.52
1:D:85:ASP:O	1:D:86:MET:HB2	2.10	0.52
1:B:108:HIS:CE1	1:B:131:THR:O	2.62	0.52
1:A:32:MET:HE2	3:A:2004:HOH:O	2.09	0.52
1:A:136:LEU:HD21	1:B:192:ILE:HG21	1.92	0.52
1:D:49:ILE:HA	1:D:53:GLU:OE1	2.10	0.52
1:A:109:PHE:CE2	1:A:156:PHE:HA	2.45	0.52
1:B:125:LEU:O	1:B:129:LEU:HB2	2.10	0.52
1:C:80:SER:OG	1:C:198:VAL:HA	2.09	0.52
1:B:73:GLU:OE1	1:B:76:ARG:CZ	2.58	0.51
1:C:137:ASN:HB3	1:C:139:GLN:CD	2.30	0.51
1:C:191:PHE:O	1:C:195:VAL:HG23	2.11	0.51
1:A:38:TYR:O	1:A:41:SER:HB2	2.11	0.51
1:B:132:MET:CE	1:B:159:TYR:HH	2.23	0.50
1:C:120:VAL:HG13	1:C:124:GLU:HB2	1.93	0.50
1:A:121:ASP:OD1	1:A:121:ASP:C	2.50	0.50
1:B:67:TYR:OH	1:B:110:ILE:HG13	2.11	0.50
1:C:193:GLN:HB3	1:D:140:THR:HG23	1.93	0.50
1:A:170:THR:O	1:A:174:ARG:HG3	2.10	0.50
1:C:131:THR:HG22	1:C:131:THR:O	2.11	0.50
1:C:132:MET:HE1	1:C:166:LEU:HD23	1.93	0.50
1:B:32:MET:N	1:D:103:ASN:HD21	2.09	0.50
1:C:104:GLY:O	1:C:107:GLN:HB2	2.12	0.50
1:C:142:ASN:HB3	3:C:2058:HOH:O	2.12	0.49
1:D:128:ALA:O	1:D:131:THR:HG22	2.12	0.49
1:D:73:GLU:HA	1:D:76:ARG:HD2	1.93	0.49
1:B:132:MET:CE	1:B:159:TYR:OH	2.60	0.49
1:C:120:VAL:HG13	1:C:124:GLU:OE1	2.13	0.49
1:A:51:ALA:CB	1:A:76:ARG:HG2	2.42	0.49
1:C:132:MET:HE2	1:C:134:PHE:CE2	2.47	0.49
1:A:183:MET:HE1	1:B:187:SER:HB2	1.94	0.49
1:C:33:ASP:OD2	1:C:96:LYS:HD3	2.11	0.49
1:A:135:ARG:CD	1:A:135:ARG:N	2.75	0.49
1:B:101:VAL:HA	3:B:2042:HOH:O	2.12	0.49
1:D:131:THR:CG2	3:D:2072:HOH:O	2.60	0.49
1:A:45:GLN:CG	1:A:46:ASP:N	2.68	0.48
1:B:108:HIS:NE2	1:B:131:THR:OG1	2.42	0.48
1:D:71:ASN:H	1:D:71:ASN:HD22	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASP:OD1	1:A:86:MET:HA	2.13	0.48
1:A:150:THR:O	1:A:151:SER:HB2	2.14	0.48
1:C:85:ASP:O	1:C:86:MET:C	2.51	0.48
1:D:176:ARG:HH11	1:D:176:ARG:HG3	1.79	0.48
1:A:43:ALA:HA	1:A:49:ILE:HG22	1.95	0.48
1:B:108:HIS:HE1	1:B:131:THR:O	1.96	0.48
1:A:135:ARG:HD3	1:A:135:ARG:H	1.77	0.48
1:A:36:TYR:CZ	1:A:40:ALA:HB2	2.48	0.48
1:D:119:THR:HB	1:D:153:LYS:HB3	1.95	0.48
1:C:112:PHE:CG	1:C:124:GLU:HG2	2.49	0.48
1:A:136:LEU:CD2	1:B:192:ILE:HG21	2.44	0.47
1:C:173:PHE:CZ	1:C:184:VAL:HG23	2.50	0.47
1:D:121:ASP:HB3	1:D:123:GLN:OE1	2.14	0.47
1:D:36:TYR:HA	1:D:92:PHE:CE2	2.49	0.47
1:C:90:MET:HE3	1:C:95:PHE:HA	1.96	0.47
1:A:90:MET:HE2	1:A:95:PHE:HA	1.95	0.47
1:A:141:VAL:HG12	1:A:141:VAL:O	2.14	0.47
1:C:125:LEU:HD12	1:C:125:LEU:O	2.15	0.47
1:C:36:TYR:CE2	1:C:40:ALA:HB2	2.49	0.47
1:A:32:MET:HB3	3:A:2004:HOH:O	2.14	0.47
1:B:123:GLN:H	1:B:123:GLN:NE2	1.94	0.47
1:B:132:MET:CG	1:B:132:MET:O	2.62	0.47
1:A:112:PHE:HD1	1:A:124:GLU:HB3	1.80	0.47
1:C:81:MET:HG3	1:C:81:MET:O	2.14	0.47
1:D:120:VAL:HG13	1:D:124:GLU:HB2	1.97	0.47
1:C:112:PHE:HB3	1:C:120:VAL:HG22	1.97	0.47
1:D:126:GLN:HG2	1:D:142:ASN:HD22	1.80	0.47
1:B:116:ARG:HD2	1:B:116:ARG:HA	1.70	0.46
1:B:191:PHE:O	1:B:195:VAL:HG13	2.15	0.46
1:D:173:PHE:CZ	1:D:184:VAL:HG23	2.50	0.46
1:C:149:SER:HA	1:C:153:LYS:O	2.16	0.46
1:D:179:ALA:HB3	1:D:181:GLN:HE21	1.80	0.46
1:C:129:LEU:CD2	1:C:166:LEU:HD22	2.46	0.46
1:A:71:ASN:ND2	3:A:2019:HOH:O	2.48	0.46
1:A:121:ASP:HB2	1:A:122:PRO:HD2	1.98	0.46
1:A:140:THR:HG23	1:B:193:GLN:CB	2.39	0.46
1:A:50:ASP:OD1	1:A:50:ASP:C	2.54	0.46
1:D:109:PHE:CE1	1:D:156:PHE:HA	2.52	0.45
1:A:119:THR:HG22	1:A:155:THR:HA	1.98	0.45
1:C:72:LEU:O	1:C:76:ARG:HG3	2.15	0.45
1:B:120:VAL:HG13	1:B:124:GLU:CB	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:GLN:HA	1:C:126:GLN:OE1	2.16	0.45
1:B:136:LEU:HD22	1:B:140:THR:HG21	1.98	0.45
1:C:126:GLN:O	1:C:130:THR:OG1	2.32	0.44
1:C:45:GLN:OE1	1:C:45:GLN:N	2.50	0.44
1:A:52:ASP:O	1:A:56:ARG:HG3	2.18	0.44
1:B:121:ASP:H	1:B:124:GLU:HG3	1.83	0.44
1:C:71:ASN:N	1:C:71:ASN:HD22	2.14	0.44
1:B:32:MET:HB3	1:D:103:ASN:ND2	2.32	0.44
1:C:112:PHE:CE2	1:C:124:GLU:HG2	2.53	0.44
1:A:106:ARG:NH1	1:A:110:ILE:CD1	2.81	0.44
1:A:90:MET:CE	1:A:95:PHE:N	2.81	0.44
1:A:142:ASN:O	1:A:146:LYS:HG3	2.17	0.43
1:C:119:THR:HB	1:C:153:LYS:HB3	2.00	0.43
1:C:64:ALA:O	1:C:65:GLY:C	2.57	0.43
1:D:139:GLN:O	1:D:143:SER:HB2	2.18	0.43
1:B:32:MET:HE1	1:D:62:GLY:O	2.17	0.43
1:A:96:LYS:HE3	1:A:96:LYS:HB2	1.80	0.43
1:B:140:THR:O	1:B:144:ILE:HG13	2.19	0.43
1:D:137:ASN:HA	1:D:138:PRO:HD2	1.80	0.43
1:A:45:GLN:CG	1:A:46:ASP:H	2.31	0.43
1:B:38:TYR:CE2	1:B:61:SER:HA	2.53	0.43
1:B:108:HIS:CG	1:B:132:MET:HE3	2.54	0.43
1:C:137:ASN:N	1:C:137:ASN:ND2	2.66	0.43
1:C:71:ASN:HD22	1:C:71:ASN:H	1.65	0.43
1:D:78:MET:HG2	1:D:98:LEU:HD11	2.01	0.43
1:A:147:ARG:HD3	1:B:197:THR:O	2.18	0.42
3:C:2085:HOH:O	1:D:165:LYS:HE2	2.18	0.42
1:A:49:ILE:HA	1:A:53:GLU:OE1	2.19	0.42
1:A:90:MET:CE	1:A:95:PHE:CA	2.98	0.42
1:D:125:LEU:HD22	1:D:154:ILE:HG21	2.02	0.42
1:A:137:ASN:O	1:A:141:VAL:HG23	2.20	0.42
1:B:103:ASN:OD1	1:D:32:MET:HB2	2.20	0.42
1:B:82:LEU:HD11	1:B:98:LEU:HB2	2.00	0.42
1:A:174:ARG:O	1:A:175:ARG:C	2.57	0.41
1:B:70:PHE:HE2	1:B:160:ILE:HG13	1.85	0.41
1:A:124:GLU:O	1:A:127:LYS:N	2.52	0.41
1:C:115:ASP:OD2	1:C:117:SER:HB3	2.20	0.41
1:A:143:SER:O	1:B:86:MET:HE1	2.19	0.41
1:D:58:LEU:HD23	1:D:58:LEU:HA	1.94	0.41
1:A:192:ILE:HA	1:A:192:ILE:HD13	1.90	0.41
1:C:125:LEU:CD2	1:C:154:ILE:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ARG:HG3	1:C:85:ASP:H	1.84	0.41
1:D:71:ASN:ND2	1:D:74:THR:CB	2.83	0.41
1:B:194:CYS:O	1:B:198:VAL:HG23	2.21	0.41
1:B:84:ARG:HG3	1:B:84:ARG:O	2.20	0.41
1:D:131:THR:HG22	3:D:2072:HOH:O	2.21	0.41
1:A:106:ARG:HG2	1:A:106:ARG:NH1	2.36	0.41
1:D:82:LEU:HD11	1:D:98:LEU:HB2	2.02	0.41
1:A:70:PHE:HE1	1:A:160:ILE:CD1	2.29	0.41
1:B:137:ASN:HA	1:B:138:PRO:HD3	1.88	0.41
1:A:135:ARG:HD3	1:A:135:ARG:HA	1.47	0.40
1:C:134:PHE:CE1	1:C:170:THR:HG21	2.56	0.40
1:A:68:LYS:HA	1:A:69:PRO:HD3	1.93	0.40
1:D:194:CYS:O	1:D:198:VAL:HG23	2.21	0.40
1:B:38:TYR:CZ	1:B:61:SER:HA	2.57	0.40
1:A:106:ARG:NH1	1:A:110:ILE:HD12	2.36	0.40
1:A:167:ARG:NE	3:A:2045:HOH:O	2.54	0.40
1:A:90:MET:HB2	1:A:94:GLU:HB2	2.03	0.40
1:B:135:ARG:NH2	1:B:174:ARG:HG3	2.36	0.40
1:B:177:ASP:HB2	1:B:184:VAL:CG2	2.52	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)
3:A:2003:HOH:O	3:D:2092:HOH:O[4_546]	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	165/167 (99%)	151 (92%)	13 (8%)	1 (1%)	25 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	165/167 (99%)	149 (90%)	14 (8%)	2 (1%)	13	10
1	C	165/167 (99%)	157 (95%)	7 (4%)	1 (1%)	25	26
1	D	165/167 (99%)	158 (96%)	5 (3%)	2 (1%)	13	10
All	All	660/668 (99%)	615 (93%)	39 (6%)	6 (1%)	17	16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	179	ALA
1	D	84	ARG
1	A	85	ASP
1	D	85	ASP
1	C	65	GLY
1	B	122	PRO

### 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	144/144 (100%)	116 (81%)	28 (19%)	1	1
1	B	144/144 (100%)	126 (88%)	18 (12%)	4	4
1	C	144/144 (100%)	122 (85%)	22 (15%)	2	2
1	D	144/144 (100%)	123 (85%)	21 (15%)	3	2
All	All	576/576 (100%)	487 (84%)	89 (16%)	2	2

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	52	ASP
1	A	55	GLN
1	A	57	CYS
1	A	72	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	73	GLU
1	A	83	ASP
1	A	87	SER
1	A	110	ILE
1	A	114	SER
1	A	115	ASP
1	A	116	ARG
1	A	120	VAL
1	A	121	ASP
1	A	126	GLN
1	A	127	LYS
1	A	131	THR
1	A	135	ARG
1	A	137	ASN
1	A	139	GLN
1	A	143	SER
1	A	147	ARG
1	A	149	SER
1	A	153	LYS
1	A	174	ARG
1	A	185	ASN
1	A	189	ASP
1	A	193	GLN
1	B	41	SER
1	B	45	GLN
1	B	94	GLU
1	B	110	ILE
1	B	120	VAL
1	B	123	GLN
1	B	124	GLU
1	B	126	GLN
1	B	127	LYS
1	B	137	ASN
1	B	143	SER
1	B	147	ARG
1	B	167	ARG
1	B	172	SER
1	B	175	ARG
1	B	181	GLN
1	B	189	ASP
1	B	193	GLN
1	C	55	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	71	ASN
1	C	80	SER
1	C	81	MET
1	C	84	ARG
1	C	85	ASP
1	C	99	TRP
1	C	107	GLN
1	C	110	ILE
1	C	114	SER
1	C	115	ASP
1	C	116	ARG
1	C	121	ASP
1	C	123	GLN
1	C	127	LYS
1	C	139	GLN
1	C	146	LYS
1	C	153	LYS
1	C	167	ARG
1	C	172	SER
1	C	193	GLN
1	C	196	MET
1	D	32	MET
1	D	60	GLN
1	D	61	SER
1	D	63	ILE
1	D	71	ASN
1	D	72	LEU
1	D	84	ARG
1	D	99	TRP
1	D	106	ARG
1	D	110	ILE
1	D	114	SER
1	D	120	VAL
1	D	121	ASP
1	D	123	GLN
1	D	124	GLU
1	D	131	THR
1	D	132	MET
1	D	137	ASN
1	D	139	GLN
1	D	178	SER
1	D	183	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	71	ASN
1	A	126	GLN
1	A	137	ASN
1	A	142	ASN
1	A	185	ASN
1	B	45	GLN
1	B	103	ASN
1	B	123	GLN
1	B	142	ASN
1	B	181	GLN
1	C	71	ASN
1	C	137	ASN
1	C	139	GLN
1	C	193	GLN
1	D	48	GLN
1	D	60	GLN
1	D	71	ASN
1	D	93	ASN
1	D	103	ASN
1	D	126	GLN
1	D	142	ASN
1	D	181	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

5 ligands are modelled in this entry.

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	D	200	-	4,4,4	0.35	0	6,6,6	0.50	0
2	SO4	B	200	-	4,4,4	1.74	2 (50%)	6,6,6	1.50	1 (16%)
2	SO4	C	200	-	4,4,4	0.44	0	6,6,6	0.37	0
2	SO4	C	201	-	4,4,4	0.59	0	6,6,6	0.63	0
2	SO4	A	200	-	4,4,4	0.55	0	6,6,6	0.51	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	200	SO4	O1-S	2.66	1.60	1.46
2	B	200	SO4	O2-S	-2.07	1.34	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	200	SO4	O4-S-O2	2.67	123.27	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	200	SO4	1	0

## 5.7 Other polymers

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.