



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:08 PM GMT

PDB ID : 1CLI  
Title : X-RAY CRYSTAL STRUCTURE OF AMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE (PURM), FROM THE E. COLI PURINE BIOSYNTHETIC PATHWAY, AT 2.5 Å RESOLUTION  
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Deposited on : 1999-04-28  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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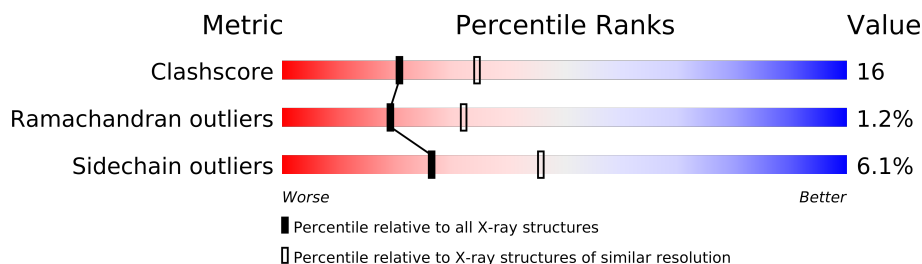
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	
1	B	345	
1	C	345	
1	D	345	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	D	3350	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10513 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOL ESYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2554	1612	431	497	14			
1	B	325	Total	C	N	O	S	0	0	0
			2441	1544	413	470	14			
1	C	341	Total	C	N	O	S	0	0	0
			2554	1612	431	497	14			
1	D	325	Total	C	N	O	S	0	0	0
			2441	1544	413	470	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	MET	conflict	UNP P08178
B	1001	VAL	MET	conflict	UNP P08178
C	2001	VAL	MET	conflict	UNP P08178
D	3001	VAL	MET	conflict	UNP P08178

- 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	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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total	O	0	0
			118	118		
3	B	126	Total	O	0	0
			126	126		
3	C	133	Total	O	0	0
			133	133		
3	D	126	Total	O	0	0
			126	126		

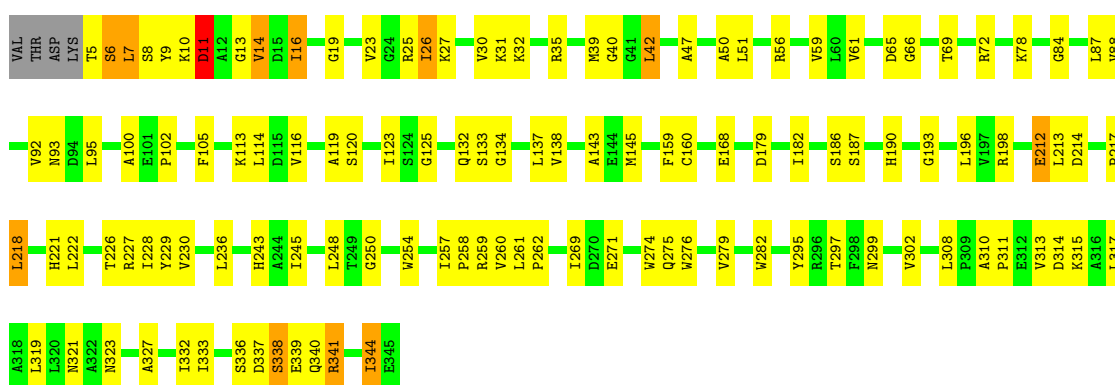
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

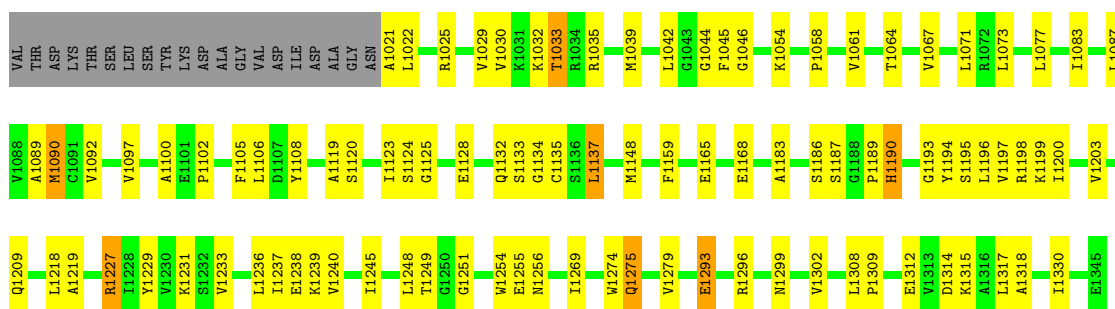
#### • Molecule 1: PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOLESYNTHETASE)

Chain A:



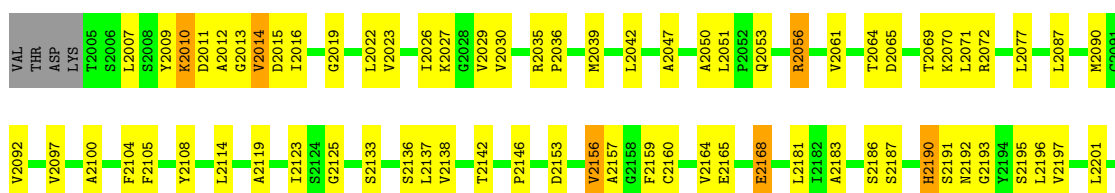
#### • Molecule 1: PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOLESYNTHETASE)

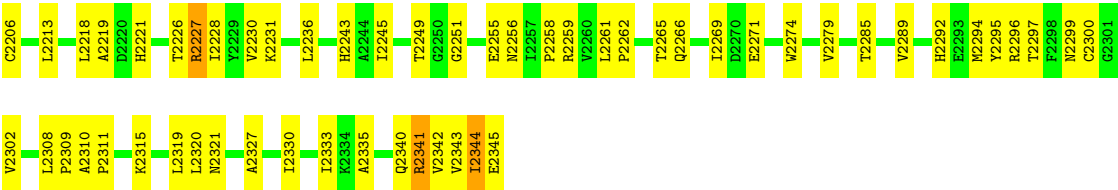
Chain B:



#### • Molecule 1: PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOLESYNTHETASE)

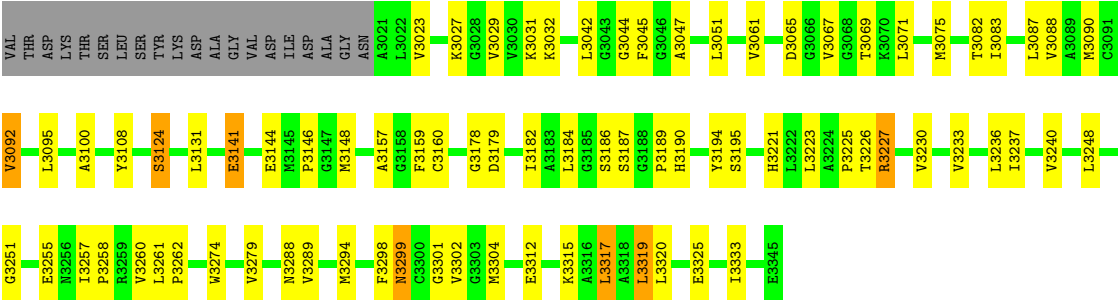
Chain C:





● Molecule 1: PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOLESYNTHETASE)

Chain D:



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.17Å 211.68Å 94.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	86.6 (20.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	4.70	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.192 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10513	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	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

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	0.33	0/2601	0.63	0/3531
1	B	0.32	0/2487	0.61	0/3376
1	C	0.33	0/2601	0.61	0/3531
1	D	0.32	0/2487	0.62	1/3376 (0.0%)
All	All	0.33	0/10176	0.62	1/13814 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3319	LEU	CA-CB-CG	5.21	127.27	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2554	0	2538	102	0
1	B	2441	0	2434	72	0
1	C	2554	0	2538	98	0
1	D	2441	0	2434	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	1	0
2	B	5	0	0	2	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	118	0	0	21	0
3	B	126	0	0	14	0
3	C	133	0	0	16	0
3	D	126	0	0	18	0
All	All	10513	0	9944	311	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (311) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:259:ARG:HH21	1:B:1044:GLY:HA2	1.40	0.85
1:D:3299:ASN:HD22	1:D:3301:GLY:H	1.25	0.84
1:A:92:VAL:HG12	1:A:230:VAL:HG21	1.61	0.83
1:C:2051:LEU:HD11	1:D:3051:LEU:HD11	1.61	0.82
1:A:16:ILE:H	1:A:16:ILE:HD13	1.45	0.82
1:B:1073:LEU:HB2	3:B:423:HOH:O	1.81	0.79
1:D:3131:LEU:HD21	3:D:308:HOH:O	1.84	0.77
1:C:2138:VAL:HG22	3:C:354:HOH:O	1.85	0.77
1:C:2133:SER:HA	1:C:2230:VAL:HG11	1.67	0.75
1:D:3289:VAL:HG11	1:D:3294:MET:HE3	1.69	0.75
1:A:341:ARG:HB3	3:A:4380:HOH:O	1.85	0.75
1:B:1197:VAL:HB	3:B:443:HOH:O	1.87	0.74
1:A:92:VAL:CG1	1:A:230:VAL:HG21	2.17	0.74
1:A:78:LYS:HA	3:A:4405:HOH:O	1.86	0.74
3:B:442:HOH:O	1:D:3319:LEU:HD23	1.88	0.74
1:C:2090:MET:SD	3:C:64:HOH:O	2.46	0.74
1:A:341:ARG:HD3	1:A:341:ARG:N	2.03	0.73
1:B:1033:THR:HG21	1:B:1137:LEU:H	1.54	0.72
1:A:72:ARG:NH2	1:B:1148:MET:HB2	2.03	0.72
1:A:341:ARG:HB2	3:A:4463:HOH:O	1.91	0.70
1:C:2077:LEU:HD21	1:C:2219:ALA:HB1	1.74	0.69
1:C:2092:VAL:HG12	3:C:289:HOH:O	1.92	0.69
1:B:1064:THR:HB	3:B:323:HOH:O	1.92	0.69
1:A:92:VAL:HG12	1:A:230:VAL:CG2	2.23	0.68
1:D:3186:SER:HB2	1:D:3190:HIS:CE1	2.29	0.68
1:C:2104:PHE:HB2	3:C:354:HOH:O	1.94	0.67
1:D:3299:ASN:ND2	1:D:3301:GLY:H	1.93	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2072:ARG:HD2	3:D:332:HOH:O	1.96	0.66
1:A:321:ASN:HD21	1:A:327:ALA:H	1.44	0.66
1:A:56:ARG:HG3	3:A:4387:HOH:O	1.96	0.66
1:A:72:ARG:HH22	1:B:1148:MET:HB2	1.59	0.65
1:C:2051:LEU:HG	3:D:291:HOH:O	1.97	0.65
1:A:257:ILE:HB	3:A:4380:HOH:O	1.96	0.65
1:B:1249:THR:H	1:B:1256:ASN:ND2	1.94	0.65
1:A:254:TRP:CE3	1:A:341:ARG:HG2	2.33	0.64
1:A:145:MET:HG2	3:A:4465:HOH:O	1.97	0.64
1:A:93:ASN:HD21	1:A:229:TYR:H	1.46	0.63
1:D:3187:SER:HB3	1:D:3227:ARG:HG3	1.80	0.63
1:A:92:VAL:HG13	1:A:102:PRO:HG2	1.81	0.62
1:B:1033:THR:CG2	1:B:1137:LEU:H	2.10	0.62
1:D:3031:LYS:HE2	3:D:463:HOH:O	1.99	0.62
1:C:2165:GLU:HB3	1:C:2168:GLU:HB2	1.82	0.62
1:A:315:LYS:O	1:A:319:LEU:HD13	2.00	0.61
1:B:1071:LEU:HD21	3:B:503:HOH:O	1.98	0.61
1:C:2335:ALA:HB1	3:C:479:HOH:O	2.01	0.61
1:D:3095:LEU:HD11	1:D:3160:CYS:SG	2.41	0.61
1:A:245:ILE:O	1:A:260:VAL:HG11	2.01	0.60
1:A:30:VAL:HG22	1:A:137:LEU:HD13	1.81	0.60
1:C:2051:LEU:HD11	1:D:3051:LEU:CD1	2.32	0.60
1:A:271:GLU:H	1:A:344:ILE:CG1	2.14	0.60
1:B:1092:VAL:HG21	1:B:1133:SER:HB3	1.84	0.60
1:D:3092:VAL:HG13	1:D:3230:VAL:CG2	2.31	0.60
1:A:340:GLN:HB2	1:A:341:ARG:HH11	1.67	0.60
1:C:2181:LEU:HD21	1:C:2333:ILE:HD11	1.83	0.59
1:A:92:VAL:HG11	1:A:133:SER:HB2	1.83	0.59
1:B:1183:ALA:HB1	1:B:1302:VAL:HG13	1.85	0.59
1:D:3251:GLY:HA3	1:D:3255:GLU:HB3	1.85	0.58
1:A:299:ASN:HB2	1:A:302:VAL:O	2.03	0.58
1:D:3233:VAL:O	1:D:3237:ILE:HG12	2.03	0.58
1:B:1165:GLU:HB3	1:B:1168:GLU:HG2	1.86	0.57
1:A:35:ARG:HD2	1:A:134:GLY:O	2.04	0.57
1:A:187:SER:H	1:A:190:HIS:HE1	1.52	0.57
1:B:1227:ARG:HD2	1:B:1229:TYR:CE1	2.40	0.57
1:D:3075:MET:SD	3:D:437:HOH:O	2.58	0.57
1:A:119:ALA:O	1:A:123:ILE:HG12	2.04	0.57
1:D:3182:ILE:HD12	1:D:3317:LEU:HD13	1.86	0.57
1:C:2271:GLU:HB2	1:C:2343:VAL:HG12	1.86	0.57
1:A:27:LYS:HA	3:A:4391:HOH:O	2.03	0.57
1:A:51:LEU:HD12	1:B:1058:PRO:HG2	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:254:TRP:HE3	1:A:341:ARG:HG2	1.69	0.56
1:D:3090:MET:SD	3:D:101:HOH:O	2.58	0.56
1:C:2308:LEU:HB2	1:C:2309:PRO:HD2	1.87	0.56
1:A:182:ILE:HD12	1:A:308:LEU:HD21	1.88	0.56
1:C:2013:GLY:HA3	1:C:2146:PRO:HG3	1.86	0.56
1:A:321:ASN:ND2	1:A:327:ALA:H	2.03	0.56
1:A:137:LEU:HG	3:A:4462:HOH:O	2.05	0.56
1:D:3187:SER:H	1:D:3190:HIS:HE1	1.52	0.56
1:A:187:SER:H	1:A:190:HIS:CE1	2.24	0.55
1:A:190:HIS:CG	1:A:226:THR:HG23	2.41	0.55
1:C:2193:GLY:HA2	1:C:2297:THR:HG22	1.88	0.55
1:A:92:VAL:HG13	1:A:102:PRO:CG	2.36	0.55
1:A:193:GLY:N	2:A:4350:SO4:O1	2.36	0.55
1:B:1119:ALA:O	1:B:1123:ILE:HD13	2.07	0.55
1:A:59:VAL:HG13	1:B:1039:MET:HE3	1.89	0.55
1:C:2193:GLY:CA	1:C:2297:THR:HG22	2.37	0.54
1:C:2061:VAL:HG21	1:C:2100:ALA:HB2	1.88	0.54
1:D:3182:ILE:HD12	1:D:3317:LEU:CD1	2.38	0.54
1:A:259:ARG:NH2	1:B:1044:GLY:HA2	2.17	0.53
1:C:2105:PHE:N	3:C:354:HOH:O	2.41	0.53
1:D:3289:VAL:CG1	1:D:3294:MET:HE3	2.38	0.53
1:B:1195:SER:N	2:B:1350:SO4:O4	2.40	0.53
1:D:3304:MET:SD	3:D:95:HOH:O	2.59	0.53
1:D:3067:VAL:HG11	1:D:3083:ILE:HG13	1.90	0.53
1:C:2294:MET:O	1:C:2300:CYS:SG	2.67	0.53
1:C:2007:LEU:H	1:C:2010:LYS:HB2	1.74	0.53
1:C:2321:ASN:HB2	3:C:531:HOH:O	2.09	0.53
1:C:2072:ARG:HH12	1:D:3148:MET:HB2	1.73	0.52
1:B:1022:LEU:HA	3:B:328:HOH:O	2.10	0.52
1:B:1035:ARG:HD2	1:B:1134:GLY:O	2.09	0.52
1:B:1092:VAL:HG23	1:B:1102:PRO:HB3	1.90	0.52
1:C:2258:PRO:HG2	3:C:237:HOH:O	2.09	0.52
1:C:2011:ASP:HB3	1:C:2014:VAL:CG2	2.39	0.52
1:B:1233:VAL:O	1:B:1237:ILE:HG13	2.09	0.52
1:D:3333:ILE:HB	3:D:311:HOH:O	2.09	0.52
1:B:1269:ILE:HG23	1:B:1330:ILE:HG12	1.91	0.52
1:D:3071:LEU:HD23	1:D:3083:ILE:HG12	1.90	0.52
1:C:2056:ARG:HE	1:C:2056:ARG:HA	1.75	0.52
1:B:1120:SER:O	1:B:1124:SER:HB2	2.10	0.52
1:A:10:LYS:O	1:B:1199:LYS:HG2	2.09	0.52
1:C:2011:ASP:HB3	1:C:2014:VAL:HG21	1.92	0.52
1:C:2030:VAL:HG12	1:C:2137:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2256:ASN:HD22	1:C:2259:ARG:HH21	1.58	0.52
1:D:3082:THR:HB	1:D:3225:PRO:HG3	1.92	0.51
1:C:2035:ARG:HG3	1:C:2136:SER:OG	2.10	0.51
1:C:2195:SER:HB2	2:C:2350:SO4:O4	2.11	0.51
1:C:2228:ILE:HG22	1:C:2230:VAL:HG12	1.93	0.51
1:C:2289:VAL:HG23	3:C:415:HOH:O	2.11	0.51
1:C:2266:GLN:HE21	1:C:2340:GLN:N	2.08	0.51
1:C:2299:ASN:HB2	1:C:2302:VAL:O	2.11	0.51
1:C:2064:THR:HG23	1:D:3141:GLU:HB2	1.93	0.51
1:C:2310:ALA:N	1:C:2311:PRO:HD2	2.26	0.51
1:A:72:ARG:HD2	1:A:198:ARG:NH1	2.26	0.51
1:D:3189:PRO:HB2	1:D:3194:TYR:OH	2.11	0.51
1:B:1029:VAL:HA	1:B:1032:LYS:HE2	1.93	0.50
1:C:2119:ALA:O	1:C:2123:ILE:HG12	2.11	0.50
1:A:25:ARG:HG2	1:A:120:SER:OG	2.11	0.50
1:C:2251:GLY:HA3	1:C:2255:GLU:HB3	1.93	0.50
1:A:6:SER:OG	1:A:7:LEU:N	2.43	0.50
1:B:1025:ARG:HB2	3:B:328:HOH:O	2.11	0.50
1:C:2047:ALA:HB1	1:C:2138:VAL:HB	1.94	0.50
1:C:2315:LYS:O	1:C:2319:LEU:HG	2.11	0.50
1:D:3248:LEU:HD12	1:D:3302:VAL:O	2.13	0.49
1:A:275:GLN:HG3	3:A:4375:HOH:O	2.12	0.49
1:C:2133:SER:HA	1:C:2230:VAL:CG1	2.39	0.49
1:A:257:ILE:N	1:A:258:PRO:HD2	2.28	0.49
1:A:218:LEU:HD11	1:A:282:TRP:CH2	2.47	0.49
1:C:2192:ASN:ND2	3:C:241:HOH:O	2.45	0.49
1:C:2007:LEU:HD23	1:C:2009:TYR:HB3	1.94	0.49
1:D:3029:VAL:HA	1:D:3032:LYS:HE2	1.93	0.49
1:A:258:PRO:HD3	3:A:4380:HOH:O	2.12	0.49
1:C:2097:VAL:HG13	1:C:2245:ILE:O	2.12	0.49
1:D:3146:PRO:HA	3:D:364:HOH:O	2.12	0.49
1:B:1089:ALA:HA	1:B:1092:VAL:HG12	1.95	0.48
1:B:1090:MET:CE	1:B:1090:MET:HA	2.43	0.48
1:C:2197:VAL:O	1:C:2201:LEU:HG	2.13	0.48
1:A:213:LEU:HD12	3:A:4427:HOH:O	2.12	0.48
1:B:1186:SER:HB2	1:B:1190:HIS:CE1	2.48	0.48
1:C:2256:ASN:HD22	1:C:2259:ARG:NH2	2.11	0.48
1:C:2183:ALA:HB1	1:C:2302:VAL:HG13	1.95	0.48
1:D:3240:VAL:HG13	1:D:3312:GLU:HB3	1.96	0.48
1:B:1240:VAL:HG13	1:B:1312:GLU:HB3	1.96	0.48
1:A:6:SER:O	1:A:10:LYS:HB2	2.14	0.48
1:C:2108:TYR:HB3	1:C:2157:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2016:ILE:HD12	3:C:318:HOH:O	2.14	0.48
1:B:1299:ASN:HB2	1:B:1302:VAL:O	2.14	0.47
1:A:59:VAL:HG22	1:B:1039:MET:HE1	1.95	0.47
1:A:125:GLY:HA3	3:A:4372:HOH:O	2.14	0.47
1:A:227:ARG:HH11	1:A:227:ARG:HG2	1.78	0.47
1:C:2183:ALA:O	1:C:2327:ALA:HA	2.14	0.47
1:A:218:LEU:HD11	1:A:282:TRP:CZ3	2.49	0.47
1:D:3032:LYS:HG3	3:D:308:HOH:O	2.14	0.47
1:A:105:PHE:HD1	3:A:4462:HOH:O	1.98	0.47
1:A:19:GLY:O	1:A:23:VAL:HG23	2.14	0.47
1:B:1021:ALA:HB3	3:B:292:HOH:O	2.15	0.47
1:A:14:VAL:HG22	1:B:1195:SER:OG	2.15	0.47
1:C:2258:PRO:HA	1:C:2261:LEU:HD12	1.95	0.47
1:C:2039:MET:HE2	1:C:2050:ALA:HB2	1.97	0.47
1:A:143:ALA:HA	3:A:4397:HOH:O	2.13	0.47
1:C:2292:HIS:CE1	1:C:2296:ARG:HH21	2.33	0.47
1:D:3108:TYR:HB3	1:D:3157:ALA:HB3	1.95	0.47
1:A:92:VAL:HG11	1:A:133:SER:CB	2.45	0.47
1:C:2190:HIS:CG	1:C:2226:THR:HG23	2.48	0.47
1:A:47:ALA:HB1	1:A:138:VAL:HB	1.96	0.47
1:C:2343:VAL:O	1:C:2344:ILE:HB	2.15	0.47
1:C:2047:ALA:CB	1:C:2138:VAL:HB	2.45	0.46
1:C:2061:VAL:HA	1:D:3047:ALA:O	2.16	0.46
1:A:190:HIS:HD2	3:A:4356:HOH:O	1.97	0.46
1:C:2187:SER:HB3	1:C:2227:ARG:HG3	1.98	0.46
1:C:2019:GLY:O	1:C:2023:VAL:HG23	2.15	0.46
1:A:31:LYS:O	1:A:31:LYS:HD3	2.15	0.46
1:B:1251:GLY:HA3	1:B:1255:GLU:HB3	1.97	0.46
1:B:1030:VAL:HG11	1:B:1042:LEU:HD11	1.96	0.46
1:A:11:ASP:HA	1:B:1199:LYS:HD3	1.98	0.46
1:D:3146:PRO:HD2	3:D:332:HOH:O	2.15	0.46
1:A:310:ALA:N	1:A:311:PRO:HD2	2.31	0.46
1:A:16:ILE:CD1	1:A:16:ILE:H	2.22	0.46
1:C:2271:GLU:H	1:C:2344:ILE:HG13	1.81	0.46
1:D:3221:HIS:ND1	1:D:3279:VAL:HG22	2.31	0.46
1:A:132:GLN:OE1	1:A:228:ILE:HD12	2.16	0.46
1:B:1248:LEU:HD12	1:B:1302:VAL:O	2.16	0.45
1:D:3061:VAL:HG21	1:D:3100:ALA:HB2	1.97	0.45
1:C:2221:HIS:HB3	1:C:2279:VAL:HG22	1.98	0.45
1:D:3261:LEU:HA	1:D:3262:PRO:HD3	1.85	0.45
1:B:1067:VAL:HB	1:B:1071:LEU:HG	1.98	0.45
1:C:2266:GLN:NE2	1:C:2340:GLN:H	2.13	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2159:PHE:CE1	1:D:3159:PHE:HB2	2.52	0.45
1:B:1128:GLU:O	1:B:1132:GLN:HG3	2.16	0.45
1:A:338:SER:O	1:A:339:GLU:HB2	2.15	0.45
1:B:1097:VAL:HG13	1:B:1245:ILE:O	2.16	0.45
1:B:1275:GLN:CD	1:B:1275:GLN:H	2.19	0.45
1:C:2036:PRO:HD2	3:C:44:HOH:O	2.15	0.45
1:C:2236:LEU:HD22	1:C:2320:LEU:HD21	1.98	0.45
1:C:2269:ILE:O	1:C:2344:ILE:N	2.47	0.45
1:B:1054:LYS:HE3	3:B:273:HOH:O	2.16	0.45
1:A:5:THR:O	1:A:6:SER:HB3	2.17	0.45
1:C:2159:PHE:CD1	1:D:3159:PHE:HB2	2.52	0.45
1:C:2125:GLY:HA3	3:C:75:HOH:O	2.16	0.45
1:B:1199:LYS:O	1:B:1203:VAL:HG22	2.17	0.44
1:C:2026:ILE:O	1:C:2029:VAL:HG22	2.17	0.44
1:C:2226:THR:HG21	3:C:64:HOH:O	2.16	0.44
1:D:3257:ILE:HB	1:D:3258:PRO:HD3	1.99	0.44
1:A:276:TRP:HZ2	1:A:295:TYR:CE2	2.36	0.44
1:B:1105:PHE:O	1:B:1106:LEU:HD12	2.17	0.44
1:D:3144:GLU:O	1:D:3146:PRO:HD3	2.17	0.44
1:C:2258:PRO:HD3	1:C:2341:ARG:HG2	2.00	0.44
1:B:1240:VAL:HG11	1:B:1308:LEU:HD12	1.98	0.44
1:D:3023:VAL:O	1:D:3027:LYS:HB2	2.16	0.44
1:A:95:LEU:HD11	1:A:160:CYS:SG	2.57	0.44
1:C:2007:LEU:HD23	1:C:2009:TYR:CB	2.48	0.44
1:A:61:VAL:HG21	1:A:100:ALA:HB2	2.00	0.44
1:A:32:LYS:HE2	1:A:32:LYS:HB3	1.81	0.44
1:A:179:ASP:OD2	1:A:243:HIS:HD2	2.00	0.44
1:A:168:GLU:HG3	3:A:4443:HOH:O	2.18	0.44
1:A:26:ILE:N	3:A:4411:HOH:O	2.51	0.43
1:A:11:ASP:OD1	1:A:14:VAL:HG23	2.18	0.43
1:C:2070:LYS:HG2	1:C:2070:LYS:O	2.18	0.43
1:B:1196:LEU:O	1:B:1200:ILE:HG13	2.18	0.43
1:C:2042:LEU:N	1:C:2042:LEU:HD22	2.33	0.43
1:A:42:LEU:HD11	3:A:4391:HOH:O	2.16	0.43
1:B:1061:VAL:HG21	1:B:1100:ALA:HB2	2.01	0.43
1:C:2186:SER:HB2	1:C:2190:HIS:CE1	2.53	0.43
1:D:3178:GLY:N	3:D:311:HOH:O	2.50	0.43
1:B:1125:GLY:HA3	3:B:94:HOH:O	2.18	0.43
1:C:2342:VAL:HG21	1:C:2345:GLU:OE2	2.19	0.43
1:C:2269:ILE:HG23	1:C:2330:ILE:HG12	2.00	0.43
1:D:3298:PHE:HA	3:D:10:HOH:O	2.18	0.43
1:D:3317:LEU:HD12	1:D:3317:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1132:GLN:O	1:B:1231:LYS:HE2	2.18	0.43
1:B:1198:ARG:HG2	3:B:423:HOH:O	2.18	0.43
1:B:1077:LEU:HD13	1:B:1219:ALA:HB1	2.00	0.43
1:A:92:VAL:CG1	1:A:102:PRO:HG2	2.49	0.42
1:C:2285:THR:HB	3:C:234:HOH:O	2.19	0.42
1:A:69:THR:HG22	1:A:69:THR:O	2.19	0.42
1:A:159:PHE:CD1	1:B:1159:PHE:HB2	2.53	0.42
1:B:1239:LYS:HD3	3:D:41:HOH:O	2.18	0.42
1:C:2077:LEU:CD2	1:C:2219:ALA:HB1	2.47	0.42
1:A:27:LYS:N	3:A:4411:HOH:O	2.52	0.42
1:C:2153:ASP:HB3	1:D:3148:MET:CE	2.49	0.42
1:B:1042:LEU:HA	3:B:141:HOH:O	2.20	0.42
1:C:2262:PRO:HG2	1:C:2265:THR:OG1	2.20	0.42
1:A:196:LEU:HD23	1:A:297:THR:HG21	2.00	0.42
1:C:2153:ASP:HB3	1:D:3148:MET:HE2	2.01	0.42
1:D:3184:LEU:HD12	1:D:3304:MET:HE2	2.01	0.42
1:A:221:HIS:HB3	1:A:279:VAL:HG22	2.00	0.42
1:A:39:MET:CE	1:A:50:ALA:HB2	2.50	0.42
1:A:84:GLY:O	1:A:88:VAL:HG23	2.19	0.42
1:D:3044:GLY:O	1:D:3045:PHE:HB2	2.20	0.42
1:A:186:SER:HB2	1:A:190:HIS:CE1	2.55	0.42
1:D:3289:VAL:CB	1:D:3294:MET:HE3	2.49	0.42
1:B:1240:VAL:HG22	1:B:1315:LYS:HE3	2.01	0.42
1:C:2221:HIS:ND1	1:C:2279:VAL:HG22	2.35	0.42
1:B:1198:ARG:CG	3:B:423:HOH:O	2.67	0.41
1:C:2271:GLU:HB2	1:C:2343:VAL:CG1	2.50	0.41
1:B:1102:PRO:HB2	1:B:1135:CYS:HB3	2.02	0.41
1:C:2243:HIS:CE1	1:C:2309:PRO:HD3	2.55	0.41
1:A:8:SER:HB2	1:A:14:VAL:HG11	2.02	0.41
1:C:2114:LEU:HD22	1:C:2142:THR:HG21	2.02	0.41
1:A:269:ILE:O	1:A:344:ILE:N	2.51	0.41
1:C:2344:ILE:O	1:C:2345:GLU:HB2	2.20	0.41
1:A:7:LEU:HG	1:B:1293:GLU:CG	2.51	0.41
1:A:332:ILE:HG12	1:A:333:ILE:N	2.35	0.41
1:D:3088:VAL:O	1:D:3092:VAL:HB	2.19	0.41
1:A:248:LEU:HD12	1:A:302:VAL:O	2.20	0.41
1:C:2010:LYS:HA	1:C:2010:LYS:HD3	1.88	0.41
1:C:2014:VAL:HG12	1:C:2015:ASP:N	2.34	0.41
1:D:3124:SER:HB3	3:D:370:HOH:O	2.20	0.41
1:A:313:VAL:HG13	1:A:314:ASP:N	2.35	0.41
1:B:1314:ASP:HB2	3:B:26:HOH:O	2.20	0.41
1:A:271:GLU:H	1:A:344:ILE:HG12	1.82	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:3257:ILE:O	1:D:3260:VAL:HG22	2.19	0.41
1:A:66:GLY:HA3	1:B:1108:TYR:OH	2.20	0.41
1:D:3320:LEU:O	1:D:3325:GLU:HB2	2.21	0.41
1:D:3095:LEU:CD1	1:D:3160:CYS:SG	3.09	0.41
1:C:2271:GLU:HG3	1:C:2295:TYR:OH	2.20	0.41
1:A:261:LEU:HA	1:A:262:PRO:HD3	1.90	0.41
1:D:3069:THR:HG21	1:D:3195:SER:HA	2.02	0.41
1:D:3179:ASP:N	3:D:311:HOH:O	2.45	0.41
1:C:2023:VAL:O	1:C:2027:LYS:HB2	2.21	0.41
1:A:160:CYS:HB3	3:A:4445:HOH:O	2.21	0.41
1:B:1254:TRP:HD1	1:B:1296:ARG:HB2	1.85	0.41
1:A:212:GLU:HA	1:A:217:PRO:HA	2.02	0.41
3:A:4448:HOH:O	1:B:1045:PHE:HD1	2.03	0.41
1:A:254:TRP:HA	1:A:341:ARG:HG3	2.02	0.41
1:B:1193:GLY:N	2:B:1350:SO4:O1	2.54	0.41
1:B:1309:PRO:HG2	1:B:1312:GLU:CG	2.51	0.41
1:C:2108:TYR:O	1:C:2156:VAL:HA	2.21	0.41
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.36	0.41
1:A:221:HIS:HB3	1:A:279:VAL:CG2	2.51	0.41
1:C:2007:LEU:HB3	1:C:2010:LYS:HE3	2.03	0.40
1:C:2192:ASN:ND2	1:C:2249:THR:HA	2.36	0.40
1:B:1187:SER:H	1:B:1190:HIS:HE1	1.69	0.40
1:C:2022:LEU:O	1:C:2026:ILE:HG13	2.21	0.40
1:D:3315:LYS:HB2	1:D:3315:LYS:HE3	1.94	0.40
1:C:2160:CYS:HB3	3:C:243:HOH:O	2.20	0.40
1:A:7:LEU:HG	1:B:1293:GLU:HG3	2.04	0.40
1:B:1249:THR:H	1:B:1256:ASN:HD21	1.68	0.40
1:D:3226:THR:HG21	3:D:101:HOH:O	2.21	0.40
1:B:1318:ALA:HB1	1:D:3131:LEU:HD11	2.02	0.40
1:D:3279:VAL:HG23	3:D:38:HOH:O	2.22	0.40
1:B:1189:PRO:HB2	1:B:1194:TYR:OH	2.22	0.40
1:A:336:SER:OG	1:A:337:ASP:N	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	339/345 (98%)	316 (93%)	12 (4%)	11 (3%)	6	8
1	B	323/345 (94%)	309 (96%)	13 (4%)	1 (0%)	50	73
1	C	339/345 (98%)	318 (94%)	18 (5%)	3 (1%)	25	42
1	D	323/345 (94%)	303 (94%)	19 (6%)	1 (0%)	50	73
All	All	1324/1380 (96%)	1246 (94%)	62 (5%)	16 (1%)	19	32

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	7	LEU
1	A	13	GLY
1	A	40	GLY
1	A	42	LEU
1	A	250	GLY
1	A	338	SER
1	A	11	ASP
1	C	2014	VAL
1	C	2344	ILE
1	A	344	ILE
1	C	2012	ALA
1	D	3042	LEU
1	A	26	ILE
1	B	1046	GLY
1	A	14	VAL

### 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	274/278 (99%)	257 (94%)	17 (6%)	26	45
1	B	262/278 (94%)	246 (94%)	16 (6%)	26	46
1	C	274/278 (99%)	254 (93%)	20 (7%)	20	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	262/278 (94%)	250 (95%)	12 (5%)	37 62
All	All	1072/1112 (96%)	1007 (94%)	65 (6%)	26 46

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	11	ASP
1	A	16	ILE
1	A	65	ASP
1	A	87	LEU
1	A	113	LYS
1	A	114	LEU
1	A	116	VAL
1	A	212	GLU
1	A	214	ASP
1	A	218	LEU
1	A	222	LEU
1	A	236	LEU
1	A	274	TRP
1	A	317	LEU
1	A	323	ASN
1	A	341	ARG
1	B	1033	THR
1	B	1083	ILE
1	B	1087	LEU
1	B	1090	MET
1	B	1137	LEU
1	B	1190	HIS
1	B	1209	GLN
1	B	1218	LEU
1	B	1227	ARG
1	B	1236	LEU
1	B	1238	GLU
1	B	1274	TRP
1	B	1275	GLN
1	B	1279	VAL
1	B	1293	GLU
1	B	1317	LEU
1	C	2010	LYS
1	C	2053	GLN
1	C	2056	ARG

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Mol	Chain	Res	Type
1	C	2065	ASP
1	C	2069	THR
1	C	2071	LEU
1	C	2087	LEU
1	C	2156	VAL
1	C	2164	VAL
1	C	2168	GLU
1	C	2190	HIS
1	C	2191	SER
1	C	2196	LEU
1	C	2206	CYS
1	C	2213	LEU
1	C	2218	LEU
1	C	2227	ARG
1	C	2231	LYS
1	C	2274	TRP
1	C	2341	ARG
1	D	3065	ASP
1	D	3087	LEU
1	D	3092	VAL
1	D	3124	SER
1	D	3141	GLU
1	D	3223	LEU
1	D	3227	ARG
1	D	3236	LEU
1	D	3274	TRP
1	D	3288	ASN
1	D	3299	ASN
1	D	3317	LEU

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

Mol	Chain	Res	Type
1	A	93	ASN
1	A	190	HIS
1	A	192	ASN
1	A	243	HIS
1	A	247	HIS
1	A	321	ASN
1	A	323	ASN
1	B	1190	HIS
1	B	1256	ASN

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Mol	Chain	Res	Type
1	B	1281	ASN
1	B	1284	GLN
1	C	2190	HIS
1	C	2192	ASN
1	C	2247	HIS
1	C	2256	ASN
1	C	2266	GLN
1	C	2323	ASN
1	D	3190	HIS
1	D	3299	ASN
1	D	3323	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	A	4350	-	4,4,4	3.08	4 (100%)	6,6,6	0.70	0
2	SO4	B	1350	-	4,4,4	2.76	4 (100%)	6,6,6	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	C	2350	-	4,4,4	4.45	4 (100%)	6,6,6	0.76	0
2	SO4	D	3350	-	4,4,4	2.75	4 (100%)	6,6,6	0.98	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	4350	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1350	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2350	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3350	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2350	SO4	O2-S	5.22	1.64	1.47
2	C	2350	SO4	O4-S	4.38	1.62	1.47
2	C	2350	SO4	O3-S	4.07	1.61	1.47
2	C	2350	SO4	O1-S	4.03	1.60	1.47
2	B	1350	SO4	O4-S	3.60	1.59	1.47
2	A	4350	SO4	O4-S	3.46	1.59	1.47
2	A	4350	SO4	O1-S	3.41	1.58	1.47
2	D	3350	SO4	O3-S	3.08	1.57	1.47
2	D	3350	SO4	O2-S	2.88	1.56	1.47
2	D	3350	SO4	O4-S	2.73	1.56	1.47
2	A	4350	SO4	O2-S	2.71	1.55	1.47
2	A	4350	SO4	O3-S	2.63	1.56	1.47
2	B	1350	SO4	O3-S	2.61	1.56	1.47
2	B	1350	SO4	O2-S	2.48	1.55	1.47
2	D	3350	SO4	O1-S	2.23	1.54	1.47
2	B	1350	SO4	O1-S	2.12	1.53	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3350	SO4	O4-S-O3	2.02	117.60	109.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.