



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:05 AM UTC

PDB ID : 1CLI / pdb\_00001cli  
Title : X-RAY CRYSTAL STRUCTURE OF AMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE (PURM), FROM THE E. COLI PURINE BIOSYNTHETIC PATHWAY, AT 2.5 Å RESOLUTION  
Authors : Li, C.; Kappock, T.J.; Stubbe, J.; Weaver, T.M.; Ealick, S.E.  
Deposited on : 1999-04-28  
Resolution : 2.50 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

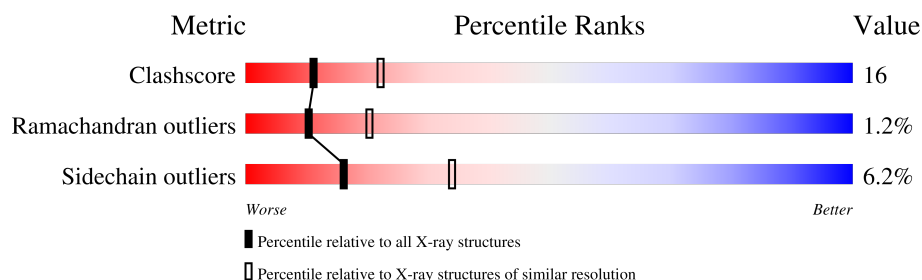
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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	345	
1	B	345	
1	C	345	
1	D	345	

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	B	1350	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10513 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 PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOLE SYNTHETASE).

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 (CCD ID: 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		

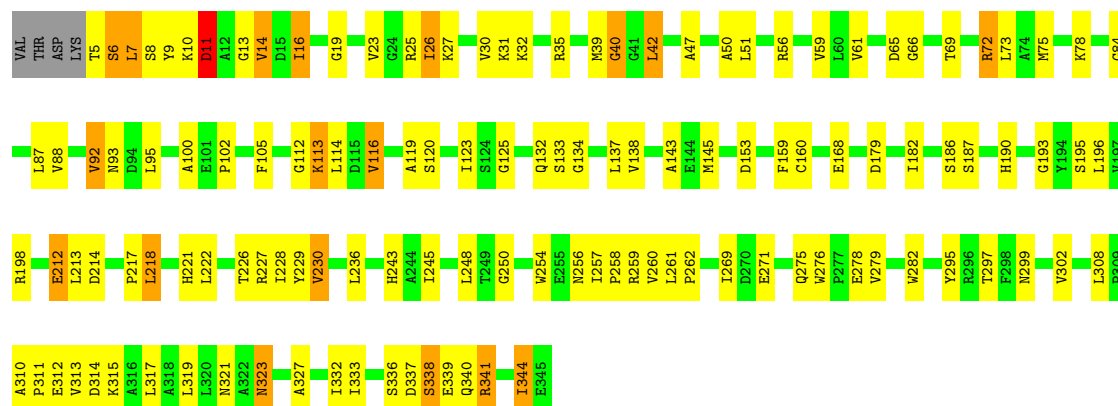
### 3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

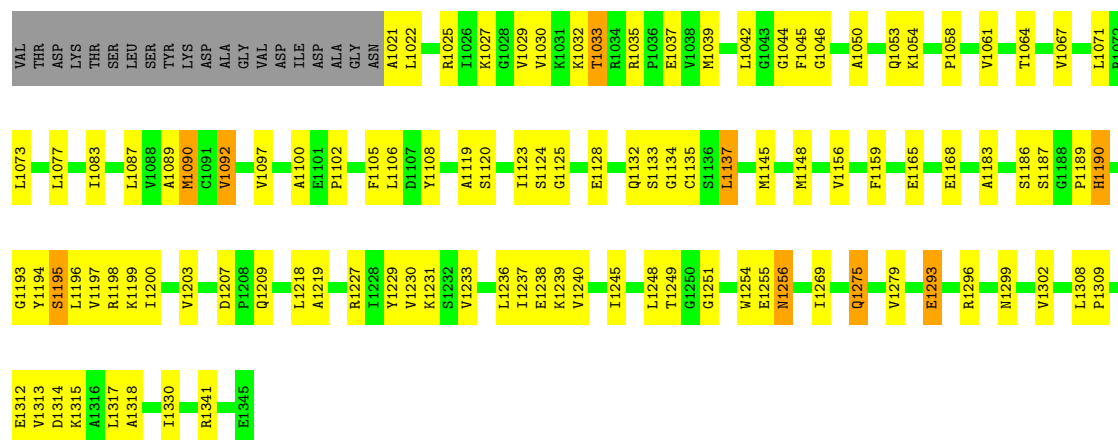
#### • Molecule 1: PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOLE SYNTHETASE)

Chain A: 



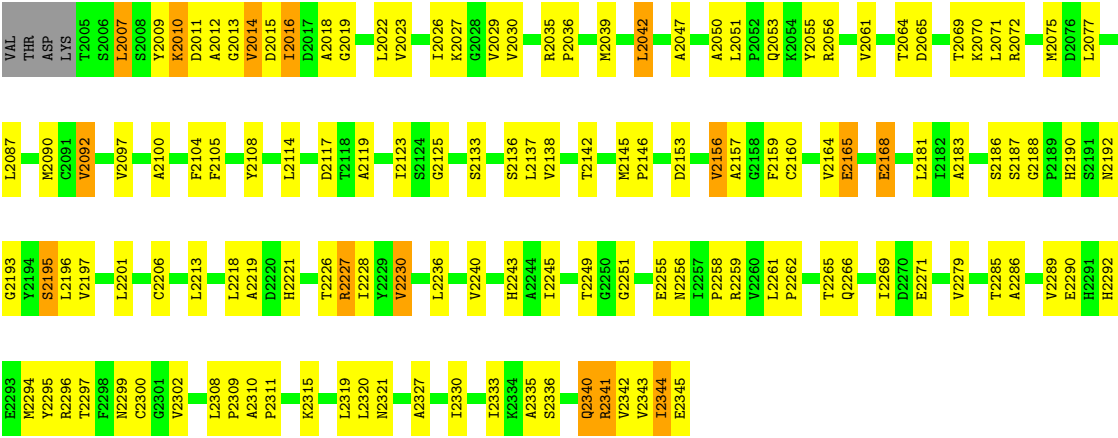
#### • Molecule 1: PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOLE SYNTHETASE)

Chain B: 



#### • Molecule 1: PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOLE SYNTHETASE)

Chain C: 



• Molecule 1: PROTEIN (PHOSPHORIBOSYL-AMINOIMIDAZOLE SYNTHETASE)



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	0.45	0/2601	0.96	7/3531 (0.2%)
1	B	0.44	0/2487	0.97	10/3376 (0.3%)
1	C	0.44	0/2601	0.96	13/3531 (0.4%)
1	D	0.45	1/2487 (0.0%)	0.95	11/3376 (0.3%)
All	All	0.45	1/10176 (0.0%)	0.96	41/13814 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3294	MET	SD-CE	-7.52	1.60	1.79

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1230	VAL	N-CA-C	8.27	118.83	110.23
1	A	230	VAL	N-CA-C	7.81	118.56	110.36
1	B	1145	MET	CA-C-N	7.28	127.92	119.47
1	B	1145	MET	C-N-CA	7.28	127.92	119.47
1	A	92	VAL	N-CA-C	6.91	117.67	110.62
1	B	1313	VAL	N-CA-C	6.87	117.58	110.36
1	D	3195	SER	N-CA-C	-6.66	103.28	111.40
1	C	2336	SER	N-CA-C	6.58	117.14	108.07
1	C	2195	SER	N-CA-C	-6.57	104.20	111.36
1	B	1256	ASN	N-CA-C	6.48	120.93	112.89
1	C	2055	TYR	N-CA-C	6.39	119.02	109.25
1	A	256	ASN	N-CA-C	6.34	121.26	112.45
1	B	1207	ASP	CA-C-N	6.32	125.81	119.24
1	B	1207	ASP	C-N-CA	6.32	125.81	119.24
1	B	1195	SER	N-CA-C	-6.27	103.98	111.69
1	D	3313	VAL	N-CA-C	6.13	116.88	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2145	MET	CA-C-N	6.06	126.22	119.32
1	C	2145	MET	C-N-CA	6.06	126.22	119.32
1	D	3145	MET	CA-C-N	6.01	127.36	119.84
1	D	3145	MET	C-N-CA	6.01	127.36	119.84
1	D	3256	ASN	N-CA-C	5.90	120.62	112.90
1	D	3057	GLU	CA-C-N	5.87	125.81	119.76
1	D	3057	GLU	C-N-CA	5.87	125.81	119.76
1	B	1053	GLN	N-CA-C	5.76	118.33	111.71
1	C	2230	VAL	N-CA-C	5.69	116.34	110.36
1	C	2092	VAL	N-CA-C	5.61	116.34	110.62
1	C	2188	GLY	CA-C-N	5.47	125.18	119.82
1	C	2188	GLY	C-N-CA	5.47	125.18	119.82
1	A	195	SER	N-CA-C	-5.29	105.68	111.82
1	D	3279	VAL	CB-CA-C	-5.28	105.21	111.97
1	A	116	VAL	N-CA-C	5.24	116.59	110.62
1	A	278	GLU	N-CA-C	5.21	118.74	112.38
1	D	3034	ARG	N-CA-C	5.20	117.85	110.10
1	C	2165	GLU	N-CA-C	-5.20	101.49	109.76
1	A	153	ASP	N-CA-C	5.19	117.56	110.24
1	D	3137	LEU	N-CA-C	-5.18	99.31	108.23
1	B	1341	ARG	N-CA-C	5.09	118.59	112.38
1	C	2286	ALA	N-CA-C	5.06	116.48	111.07
1	C	2117	ASP	N-CA-C	5.05	116.86	111.36
1	C	2340	GLN	N-CA-C	5.04	121.20	113.28
1	D	3324	GLY	N-CA-C	5.01	122.21	115.59

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	2554	0	2538	109	0
1	B	2441	0	2434	76	0
1	C	2554	0	2538	100	0
1	D	2441	0	2434	66	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	22	0
3	B	126	0	0	14	0
3	C	133	0	0	17	0
3	D	126	0	0	18	0
All	All	10513	0	9944	326	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (326) 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:A:75:MET:HE3	3:A:4405:HOH:O	1.73	0.87
1:A:259:ARG:HH21	1:B:1044:GLY:HA2	1.40	0.85
1:C:2153:ASP:HB3	1:D:3148:MET:HE2	1.59	0.84
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:HD13	1:A:16:ILE:H	1.45	0.82
1:B:1073:LEU:HB2	3:B:423:HOH:O	1.81	0.79
1:D:3184:LEU:HD12	1:D:3304:MET:HE2	1.65	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: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:A:59:VAL:HG22	1:B:1039:MET:HE1	1.69	0.74
1:C:2090:MET:SD	3:C:64:HOH:O	2.46	0.74
1:A:341:ARG:N	1:A:341:ARG:HD3	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:D:3289:VAL:HG11	1:D:3294:MET:HE3	1.74	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:3233:VAL:HG21	1:D:3304:MET:HE1	1.79	0.63
1:A:72:ARG:HH22	1:B:1148:MET:HE3	1.63	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:A:271:GLU:H	1:A:344:ILE:CG1	2.14	0.60
1:C:2051:LEU:HD11	1:D:3051:LEU:CD1	2.32	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:D:3233:VAL:CG2	1:D:3304:MET:HE1	2.32	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:B:1090:MET:HA	1:B:1090:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:VAL:CG2	1:B:1039:MET:HE1	2.34	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:C:2271:GLU:HB2	1:C:2343:VAL:HG12	1.86	0.57
1:D:3182:ILE:HD12	1:D:3317:LEU:HD13	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
1:C:2039:MET:HE2	1:C:2050:ALA:HB2	1.86	0.57
1:A:254:TRP:HE3	1:A:341:ARG:HG2	1.69	0.56
1:C:2308:LEU:HB2	1:C:2309:PRO:HD2	1.87	0.56
1:D:3090:MET:SD	3:D:101:HOH:O	2.58	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:137:LEU:HG	3:A:4462:HOH:O	2.05	0.56
1:A:321:ASN:ND2	1:A:327:ALA:H	2.03	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:B:1039:MET:HE2	1:B:1050:ALA:HB2	1.89	0.54
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:B:1195:SER:N	2:B:1350:SO4:O4	2.40	0.53
1:C:2105:PHE:N	3:C:354:HOH:O	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1233:VAL:O	1:B:1237:ILE:HG13	2.09	0.52
1:C:2011:ASP:HB3	1:C:2014:VAL:CG2	2.39	0.52
1:B:1269:ILE:HG23	1:B:1330:ILE:HG12	1.91	0.52
1:D:3333:ILE:HB	3:D:311:HOH:O	2.09	0.52
1:D:3071:LEU:HD23	1:D:3083:ILE:HG12	1.90	0.52
1:B:1120:SER:O	1:B:1124:SER:HB2	2.10	0.52
1:C:2056:ARG:HE	1:C:2056:ARG:HA	1.75	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
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:2266:GLN:HE21	1:C:2340:GLN:N	2.08	0.51
1:C:2289:VAL:HG23	3:C:415:HOH:O	2.11	0.51
1:C:2064:THR:HG23	1:D:3141:GLU:HB2	1.93	0.51
1:C:2299:ASN:HB2	1:C:2302:VAL:O	2.11	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:A:25:ARG:HG2	1:A:120:SER:OG	2.11	0.50
1:C:2119:ALA:O	1:C:2123:ILE:HG12	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:B:1275:GLN:CD	1:B:1275:GLN:H	2.19	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:218:LEU:HD11	1:A:282:TRP:CH2	2.47	0.49
1:A:257:ILE:N	1:A:258:PRO:HD2	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3289:VAL:CG1	1:D:3294:MET:HE3	2.42	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:3029:VAL:HA	1:D:3032:LYS:HE2	1.93	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:HA	1:B:1090:MET:CE	2.43	0.48
1:A:213:LEU:HD12	3:A:4427:HOH:O	2.12	0.48
1:C:2197:VAL:O	1:C:2201:LEU:HG	2.13	0.48
1:B:1186:SER:HB2	1:B:1190:HIS:CE1	2.48	0.48
1:C:2183:ALA:HB1	1:C:2302:VAL:HG13	1.95	0.48
1:C:2256:ASN:HD22	1:C:2259:ARG:NH2	2.11	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
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: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:A:218:LEU:HD11	1:A:282:TRP:CZ3	2.49	0.47
1:C:2183:ALA:O	1:C:2327:ALA:HA	2.14	0.47
1:A:72:ARG:NH2	1:B:1148:MET:HE3	2.29	0.47
1:D:3032:LYS:HG3	3:D:308:HOH:O	2.14	0.47
1:A:19:GLY:O	1:A:23:VAL:HG23	2.14	0.47
1:A:105:PHE:HD1	3:A:4462:HOH:O	1.98	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:A:143:ALA:HA	3:A:4397:HOH:O	2.13	0.47
1:C:2258:PRO:HA	1:C:2261:LEU:HD12	1.95	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:47:ALA:HB1	1:A:138:VAL:HB	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LYS:O	1:A:31:LYS:HD3	2.15	0.46
1:B:1030:VAL:HG11	1:B:1042:LEU:HD11	1.96	0.46
1:B:1251:GLY:HA3	1:B:1255:GLU:HB3	1.97	0.46
1:A:11:ASP:HA	1:B:1199:LYS:HD3	1.98	0.46
1:A:310:ALA:N	1:A:311:PRO:HD2	2.31	0.46
1:D:3146:PRO:HD2	3:D:332:HOH:O	2.15	0.46
1:A:16:ILE:H	1:A:16:ILE:CD1	2.22	0.46
1:A:132:GLN:OE1	1:A:228:ILE:HD12	2.16	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: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:2159:PHE:CE1	1:D:3159:PHE:HB2	2.52	0.45
1:C:2266:GLN:NE2	1:C:2340:GLN:H	2.13	0.45
1:A:338:SER:O	1:A:339:GLU:HB2	2.15	0.45
1:B:1128:GLU:O	1:B:1132:GLN:HG3	2.16	0.45
1:B:1097:VAL:HG13	1:B:1245:ILE:O	2.16	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:2125:GLY:HA3	3:C:75:HOH:O	2.16	0.45
1:C:2159:PHE:CD1	1:D:3159:PHE:HB2	2.52	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:A:95:LEU:HD11	1:A:160:CYS:SG	2.57	0.44
1:B:1240:VAL:HG11	1:B:1308:LEU:HD12	1.98	0.44
1:C:2258:PRO:HD3	1:C:2341:ARG:HG2	2.00	0.44
1:D:3023:VAL:O	1:D:3027:LYS:HB2	2.16	0.44
1:D:3144:GLU:O	1:D:3146:PRO:HD3	2.17	0.44
1:A:32:LYS:HE2	1:A:32:LYS:HB3	1.81	0.44
1:A:61:VAL:HG21	1:A:100:ALA:HB2	2.00	0.44
1:A:179:ASP:OD2	1:A:243:HIS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2007:LEU:HD23	1:C:2009:TYR:CB	2.48	0.44
1:A:112:GLY:C	1:A:113:LYS:HD3	2.42	0.44
1:D:3221:HIS:HD1	1:D:3279:VAL:HG22	1.82	0.44
1:A:168:GLU:HG3	3:A:4443:HOH:O	2.18	0.44
1:A:11:ASP:OD1	1:A:14:VAL:HG23	2.18	0.43
1:A:26:ILE:N	3:A:4411:HOH:O	2.51	0.43
1:C:2070:LYS:O	1:C:2070:LYS:HG2	2.18	0.43
1:A:39:MET:O	1:A:40:GLY:C	2.61	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:B:1132:GLN:O	1:B:1231:LYS:HE2	2.18	0.43
1:D:3317:LEU:HD12	1:D:3317:LEU:HA	1.83	0.43
1:A:321:ASN:C	1:A:323:ASN:H	2.25	0.43
1:B:1077:LEU:HD13	1:B:1219:ALA:HB1	2.00	0.43
1:B:1198:ARG:HG2	3:B:423:HOH:O	2.18	0.43
1:A:92:VAL:CG1	1:A:102:PRO:HG2	2.49	0.42
1:A:69:THR:O	1:A:69:THR:HG22	2.19	0.42
1:C:2016:ILE:C	1:C:2018:ALA:H	2.27	0.42
1:C:2285:THR:HB	3:C:234:HOH: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:A:196:LEU:HD23	1:A:297:THR:HG21	2.00	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: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:A:221:HIS:HB3	1:A:279:VAL:HG22	2.00	0.42
1:D:3044:GLY:O	1:D:3045:PHE:HB2	2.20	0.42
1:D:3304:MET:HE3	1:D:3304:MET:HB3	1.85	0.42
1:A:186:SER:HB2	1:A:190:HIS:CE1	2.55	0.42
1:C:2290:GLU:H	1:C:2290:GLU:CD	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:2243:HIS:CE1	1:C:2309:PRO:HD3	2.55	0.41
1:D:3289:VAL:CB	1:D:3294:MET:HE3	2.49	0.41
1:A:7:LEU:HG	1:B:1293:GLU:CG	2.51	0.41
1:A:269:ILE:O	1:A:344:ILE:N	2.51	0.41
1:A:332:ILE:HG12	1:A:333:ILE:N	2.35	0.41
1:C:2344:ILE:O	1:C:2345:GLU:HB2	2.20	0.41
1:A:248:LEU:HD12	1:A:302:VAL: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: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:3088:VAL:O	1:D:3092:VAL:HB	2.19	0.41
1:D:3124:SER:HB3	3:D:370:HOH:O	2.20	0.41
1:A:66:GLY:HA3	1:B:1108:TYR:OH	2.20	0.41
1:A:271:GLU:H	1:A:344:ILE:HG12	1.82	0.41
1:D:3257:ILE:O	1:D:3260:VAL:HG22	2.19	0.41
1:D:3320:LEU:O	1:D:3325:GLU:HB2	2.21	0.41
1:A:261:LEU:HA	1:A:262:PRO:HD3	1.90	0.41
1:C:2271:GLU:HG3	1:C:2295:TYR:OH	2.20	0.41
1:D:3095:LEU:CD1	1:D:3160:CYS:SG	3.09	0.41
1:D:3069:THR:HG21	1:D:3195:SER:HA	2.02	0.41
1:A:160:CYS:HB3	3:A:4445:HOH:O	2.21	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:B:1254:TRP:HD1	1:B:1296:ARG:HB2	1.85	0.41
1:C:2023:VAL:O	1:C:2027:LYS:HB2	2.21	0.41
1:D:3179:ASP:N	3:D:311:HOH:O	2.45	0.41
1:A:221:HIS:HB3	1:A:279:VAL:CG2	2.51	0.41
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.36	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:B:1187:SER:H	1:B:1190:HIS:HE1	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2007:LEU:HB3	1:C:2010:LYS:HE3	2.03	0.40
1:C:2022:LEU:O	1:C:2026:ILE:HG13	2.21	0.40
1:C:2160:CYS:HB3	3:C:243:HOH:O	2.20	0.40
1:C:2192:ASN:ND2	1:C:2249:THR:HA	2.36	0.40
1:D:3315:LYS:HE3	1:D:3315:LYS:HB2	1.94	0.40
1:A:7:LEU:HG	1:B:1293:GLU:HG3	2.04	0.40
1:A:310:ALA:C	1:A:312:GLU:H	2.29	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:C:2075:MET:HE2	3:C:331:HOH:O	2.21	0.40
1:A:336:SER:OG	1:A:337:ASP:N	2.55	0.40
1:B:1189:PRO:HB2	1:B:1194:TYR:OH	2.22	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

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/345 (98%)	316 (93%)	12 (4%)	11 (3%)	3	4
1	B	323/345 (94%)	309 (96%)	13 (4%)	1 (0%)	36	55
1	C	339/345 (98%)	318 (94%)	18 (5%)	3 (1%)	14	27
1	D	323/345 (94%)	303 (94%)	19 (6%)	1 (0%)	36	55
All	All	1324/1380 (96%)	1246 (94%)	62 (5%)	16 (1%)	10	20

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	SER

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Mol	Chain	Res	Type
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%)	256 (93%)	18 (7%)	15	32
1	B	262/278 (94%)	244 (93%)	18 (7%)	14	30
1	C	274/278 (99%)	255 (93%)	19 (7%)	14	30
1	D	262/278 (94%)	250 (95%)	12 (5%)	24	48
All	All	1072/1112 (96%)	1005 (94%)	67 (6%)	16	34

All (67) 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	72	ARG
1	A	73	LEU

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Mol	Chain	Res	Type
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	317	LEU
1	A	323	ASN
1	A	341	ARG
1	B	1027	LYS
1	B	1033	THR
1	B	1037	GLU
1	B	1083	ILE
1	B	1087	LEU
1	B	1090	MET
1	B	1092	VAL
1	B	1137	LEU
1	B	1156	VAL
1	B	1190	HIS
1	B	1209	GLN
1	B	1218	LEU
1	B	1236	LEU
1	B	1238	GLU
1	B	1275	GLN
1	B	1279	VAL
1	B	1293	GLU
1	B	1317	LEU
1	C	2007	LEU
1	C	2010	LYS
1	C	2016	ILE
1	C	2042	LEU
1	C	2053	GLN
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

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Mol	Chain	Res	Type
1	C	2196	LEU
1	C	2206	CYS
1	C	2213	LEU
1	C	2218	LEU
1	C	2227	ARG
1	C	2240	VAL
1	C	2341	ARG
1	D	3083	ILE
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	3279	VAL
1	D	3288	ASN
1	D	3299	ASN
1	D	3317	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) 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	264	ASN
1	A	292	HIS
1	A	321	ASN
1	A	323	ASN
1	B	1190	HIS
1	B	1256	ASN
1	B	1264	ASN
1	B	1284	GLN
1	B	1323	ASN
1	C	2080	HIS
1	C	2150	HIS
1	C	2190	HIS
1	C	2192	ASN
1	C	2247	HIS
1	C	2256	ASN

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Mol	Chain	Res	Type
1	C	2266	GLN
1	C	2291	HIS
1	C	2323	ASN
1	D	3190	HIS
1	D	3264	ASN
1	D	3292	HIS
1	D	3299	ASN
1	D	3323	ASN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	1.68	1 (25%)	6,6,6	0.73	0
2	SO4	C	2350	-	4,4,4	2.38	2 (50%)	6,6,6	1.06	0
2	SO4	B	1350	-	4,4,4	1.43	0	6,6,6	0.82	0
2	SO4	D	3350	-	4,4,4	1.48	0	6,6,6	0.98	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2350	SO4	O2-S	3.24	1.64	1.44
2	C	2350	SO4	O1-S	2.58	1.60	1.44
2	A	4350	SO4	O1-S	2.24	1.58	1.44

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4350	SO4	1	0
2	C	2350	SO4	1	0
2	B	1350	SO4	2	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.