



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 03:02 pm BST

PDB ID : 2CRK  
Title : MUSCLE CREATINE KINASE  
Authors : Rao, J.K.; Bujacz, G.; Wlodawer, A.  
Deposited on : 1998-09-28  
Resolution : 2.35 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)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

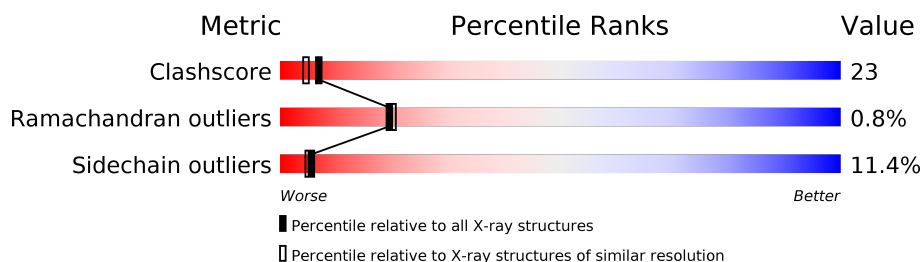
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

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	381	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3379 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 (CREATINE KINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	365	2928	1849	516	549	14	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	SER	GLY	CONFLICT	UNP P00563
A	324	VAL	GLY	CONFLICT	UNP P00563
A	325	PHE	VAL	CONFLICT	UNP P00563

- 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	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is water.

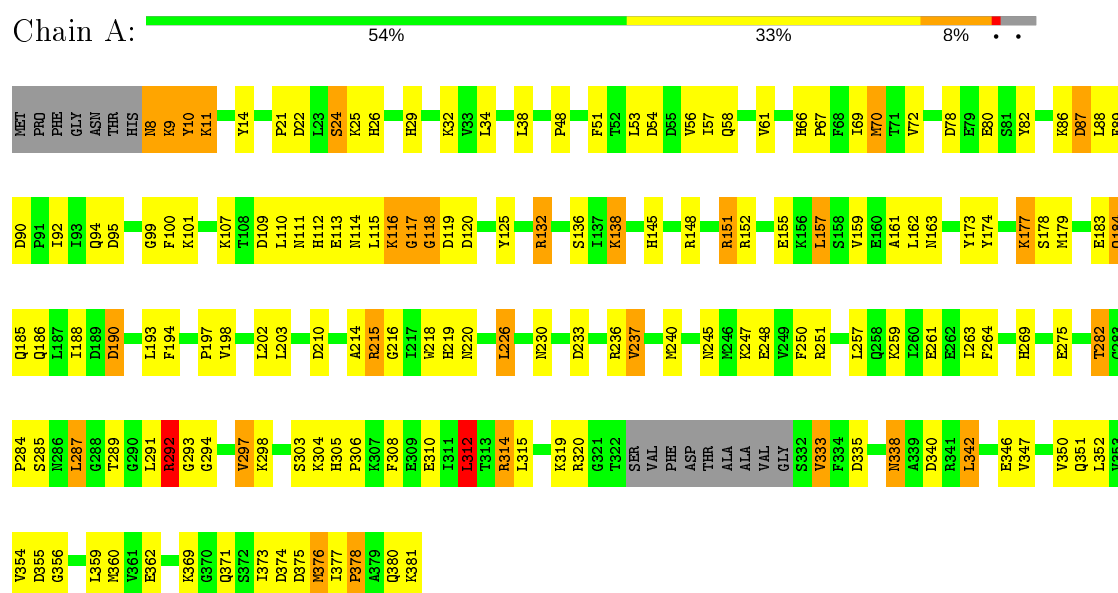
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	431	Total	O	0	0
			431	431		

### 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 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 (CREATINE KINASE)



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.60 Å   199.60 Å   71.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	7.00 – 2.35	Depositor
% Data completeness (in resolution range)	96.5 (7.00-2.35)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.195 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3379	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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	0.67	0/2993	0.92	9/4029 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	A	117	GLY	N-CA-C	-6.53	96.77	113.10
1	A	151	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	292	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	226	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	118	GLY	N-CA-C	-5.26	99.96	113.10
1	A	119	ASP	N-CA-C	5.17	124.95	111.00
1	A	87	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	312	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2928	0	2902	135	0
2	A	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	431	0	0	27	0
All	All	3379	0	2902	135	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 23.

All (135) 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:292:ARG:HG2	1:A:292:ARG:HH11	1.28	0.98
1:A:376:MET:SD	1:A:376:MET:N	2.40	0.94
1:A:118:GLY:HA2	1:A:354:VAL:HG21	1.58	0.85
1:A:66:HIS:ND1	1:A:67:PRO:HD2	1.99	0.76
1:A:174:TYR:HB3	1:A:179:MET:HE1	1.66	0.76
1:A:114:ASN:HA	1:A:116:LYS:HD2	1.67	0.73
1:A:233:ASP:OD1	1:A:282:THR:HG22	1.88	0.73
1:A:8:ASN:HA	1:A:58:GLN:OE1	1.89	0.72
1:A:292:ARG:HE	1:A:320:ARG:NH1	1.88	0.72
1:A:56:VAL:HG23	1:A:57:ILE:HG23	1.73	0.71
1:A:310:GLU:O	1:A:314:ARG:HG2	1.91	0.71
1:A:174:TYR:HB3	1:A:179:MET:CE	2.23	0.69
1:A:9:LYS:HA	3:A:405:HOH:O	1.92	0.69
1:A:151:ARG:HG2	1:A:214:ALA:HB3	1.75	0.68
1:A:248:GLU:HG2	3:A:593:HOH:O	1.92	0.68
1:A:148:ARG:O	1:A:152:ARG:HG3	1.94	0.68
1:A:48:PRO:CD	1:A:80:GLU:HG3	2.24	0.67
1:A:9:LYS:HB2	3:A:585:HOH:O	1.95	0.67
1:A:109:ASP:O	1:A:346:GLU:HG2	1.94	0.67
1:A:247:LYS:HD2	3:A:709:HOH:O	1.96	0.66
1:A:29:HIS:O	1:A:32:LYS:HG2	1.95	0.66
1:A:11:LYS:HE3	1:A:11:LYS:HA	1.79	0.65
1:A:352:LEU:HD22	1:A:381:LYS:OXT	1.95	0.65
1:A:184:GLN:O	1:A:188:ILE:HG13	1.96	0.65
1:A:259:LYS:HE3	3:A:744:HOH:O	1.95	0.64
1:A:215:ARG:HD2	1:A:230:ASN:O	1.98	0.64
1:A:219:HIS:HD2	1:A:220:ASN:O	1.81	0.63
1:A:377:ILE:HG23	1:A:378:PRO:HD2	1.81	0.62
1:A:10:TYR:HB3	1:A:54:ASP:OD2	1.99	0.62
1:A:32:LYS:HD2	3:A:491:HOH:O	1.99	0.62
1:A:314:ARG:HD3	1:A:376:MET:O	2.01	0.61
1:A:356:GLY:O	1:A:360:MET:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PRO:HD2	1:A:80:GLU:HG3	1.85	0.59
1:A:25:LYS:HE3	3:A:783:HOH:O	2.03	0.59
1:A:107:LYS:HG2	3:A:681:HOH:O	2.04	0.57
1:A:305:HIS:ND1	1:A:306:PRO:HD2	2.19	0.57
1:A:292:ARG:NH1	1:A:292:ARG:HG2	2.02	0.56
1:A:32:LYS:HE3	1:A:95:ASP:OD2	2.04	0.56
1:A:377:ILE:CG2	1:A:378:PRO:HD2	2.36	0.56
1:A:53:LEU:O	1:A:56:VAL:HG22	2.06	0.56
1:A:99:GLY:O	1:A:101:LYS:HD2	2.04	0.56
1:A:179:MET:HG2	1:A:184:GLN:HB2	1.87	0.55
1:A:315:LEU:HD22	1:A:381:LYS:HB2	1.88	0.55
1:A:10:TYR:H	1:A:10:TYR:HD1	1.53	0.55
1:A:292:ARG:HE	1:A:320:ARG:CZ	2.19	0.55
1:A:338:ASN:H	1:A:338:ASN:HD22	1.54	0.55
1:A:314:ARG:NH1	1:A:378:PRO:HD3	2.22	0.55
1:A:111:ASN:OD1	1:A:113:GLU:HB2	2.07	0.55
1:A:22:ASP:OD1	1:A:24:SER:HB2	2.07	0.54
1:A:340:ASP:HB3	3:A:469:HOH:O	2.06	0.54
1:A:173:TYR:OH	1:A:216:GLY:HA3	2.07	0.54
1:A:162:LEU:HD13	1:A:218:TRP:CG	2.43	0.54
1:A:115:LEU:HD23	1:A:247:LYS:HD3	1.88	0.54
1:A:275:GLU:HG2	3:A:676:HOH:O	2.08	0.54
1:A:110:LEU:HD23	1:A:346:GLU:HG3	1.89	0.53
1:A:193:LEU:HG	1:A:194:PHE:N	2.23	0.53
1:A:177:LYS:HD2	1:A:178:SER:N	2.24	0.53
1:A:284:PRO:HA	1:A:287:LEU:HD22	1.90	0.53
1:A:94:GLN:HG2	1:A:99:GLY:HA2	1.92	0.52
1:A:151:ARG:NH2	1:A:210:ASP:OD2	2.42	0.52
1:A:293:GLY:H	1:A:338:ASN:HD21	1.56	0.52
1:A:237:VAL:HG11	1:A:257:LEU:HD21	1.91	0.52
1:A:118:GLY:CA	1:A:354:VAL:HG21	2.35	0.52
1:A:264:PHE:HB3	1:A:269:HIS:O	2.10	0.52
1:A:110:LEU:CD2	1:A:346:GLU:HG3	2.40	0.51
1:A:293:GLY:H	1:A:338:ASN:ND2	2.08	0.51
1:A:291:LEU:HD13	1:A:346:GLU:HB3	1.93	0.51
1:A:51:PHE:HD1	1:A:145:HIS:CD2	2.29	0.51
1:A:151:ARG:HD3	3:A:401:HOH:O	2.10	0.51
1:A:26:HIS:HE1	1:A:61:VAL:O	1.93	0.51
1:A:312:LEU:HD21	1:A:319:LYS:HD3	1.93	0.50
1:A:292:ARG:HH21	1:A:320:ARG:HD2	1.76	0.50
1:A:359:LEU:O	1:A:362:GLU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PRO:O	1:A:203:LEU:HD21	2.11	0.50
1:A:304:LYS:HE2	3:A:793:HOH:O	2.11	0.50
1:A:32:LYS:HE3	1:A:95:ASP:CG	2.33	0.49
1:A:374:ASP:HA	3:A:700:HOH:O	2.14	0.48
1:A:250:PHE:HB3	3:A:709:HOH:O	2.13	0.48
1:A:292:ARG:NH2	1:A:335:ASP:OD1	2.46	0.47
1:A:86:LYS:O	1:A:90:ASP:HB2	2.15	0.47
1:A:155:GLU:O	1:A:159:VAL:HG23	2.15	0.47
1:A:163:ASN:ND2	3:A:556:HOH:O	2.48	0.47
1:A:305:HIS:CD2	1:A:373:ILE:HD11	2.49	0.46
1:A:29:HIS:HB3	1:A:92:ILE:HG23	1.97	0.46
1:A:289:THR:C	1:A:291:LEU:H	2.19	0.46
1:A:350:VAL:O	1:A:354:VAL:HG12	2.16	0.45
1:A:100:PHE:CD2	1:A:342:LEU:HD13	2.52	0.45
1:A:347:VAL:O	1:A:351:GLN:HB2	2.16	0.45
1:A:259:LYS:O	1:A:263:ILE:HG13	2.17	0.45
1:A:375:ASP:N	1:A:375:ASP:OD1	2.50	0.45
1:A:177:LYS:HB3	1:A:177:LYS:HE3	1.79	0.45
1:A:369:LYS:HB2	1:A:371:GLN:HG3	1.98	0.45
1:A:115:LEU:O	1:A:116:LYS:C	2.55	0.44
1:A:355:ASP:HB3	1:A:381:LYS:HG2	1.99	0.44
1:A:219:HIS:HE1	3:A:805:HOH:O	1.99	0.44
1:A:294:GLY:HA3	3:A:460:HOH:O	2.16	0.44
1:A:378:PRO:HB3	3:A:500:HOH:O	2.17	0.44
1:A:25:LYS:NZ	3:A:826:HOH:O	2.50	0.43
1:A:82:TYR:HA	1:A:89:PHE:CD2	2.53	0.43
1:A:56:VAL:HG23	1:A:57:ILE:N	2.33	0.43
1:A:305:HIS:ND1	1:A:306:PRO:CD	2.82	0.43
1:A:72:VAL:HG21	1:A:285:SER:HB3	2.00	0.43
1:A:66:HIS:ND1	1:A:67:PRO:CD	2.77	0.43
1:A:69:ILE:HD12	1:A:70:MET:H	1.84	0.43
1:A:298:LYS:HD2	1:A:333:VAL:HG12	2.00	0.43
1:A:183:GLU:HA	3:A:613:HOH:O	2.19	0.42
1:A:315:LEU:CD2	1:A:381:LYS:HB2	2.48	0.42
1:A:157:LEU:HG	3:A:707:HOH:O	2.19	0.42
1:A:138:LYS:O	1:A:269:HIS:HD2	2.01	0.42
1:A:132:ARG:O	1:A:291:LEU:HA	2.20	0.42
1:A:125:TYR:O	1:A:297:VAL:HA	2.20	0.42
1:A:304:LYS:HA	1:A:304:LYS:HD3	1.74	0.42
1:A:314:ARG:HA	3:A:500:HOH:O	2.19	0.42
1:A:351:GLN:O	1:A:354:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLN:O	1:A:190:ASP:HB2	2.20	0.42
1:A:219:HIS:CE1	3:A:805:HOH:O	2.73	0.42
1:A:21:PRO:HG3	1:A:57:ILE:HD12	2.01	0.42
1:A:261:GLU:HG2	3:A:486:HOH:O	2.20	0.42
1:A:161:ALA:HB2	1:A:264:PHE:HE1	1.85	0.42
1:A:215:ARG:NH1	3:A:570:HOH:O	2.51	0.41
1:A:53:LEU:HA	1:A:56:VAL:HG22	2.01	0.41
1:A:112:HIS:CD2	1:A:112:HIS:H	2.38	0.41
1:A:303:SER:HA	1:A:308:PHE:CD2	2.56	0.41
1:A:315:LEU:O	1:A:381:LYS:OXT	2.38	0.41
1:A:132:ARG:HG2	2:A:392:SO4:O4	2.21	0.41
1:A:371:GLN:HA	3:A:734:HOH:O	2.20	0.41
1:A:289:THR:C	1:A:291:LEU:N	2.74	0.41
1:A:38:LEU:HD11	1:A:87:ASP:HB3	2.02	0.41
1:A:319:LYS:HA	1:A:335:ASP:O	2.21	0.41
1:A:11:LYS:HG2	1:A:14:TYR:HD2	1.86	0.40
1:A:94:GLN:O	1:A:99:GLY:N	2.53	0.40
1:A:101:LYS:N	1:A:101:LYS:HD2	2.36	0.40
1:A:117:GLY:O	1:A:351:GLN:NE2	2.54	0.40
1:A:304:LYS:HA	3:A:753:HOH:O	2.21	0.40
1:A:376:MET:H	1:A:376:MET:CE	2.32	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	361/381 (95%)	339 (94%)	19 (5%)	3 (1%)	19	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	116	LYS
1	A	9	LYS

### 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	325/337 (96%)	288 (89%)	37 (11%)	<b>5</b> <b>5</b>

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	10	TYR
1	A	11	LYS
1	A	34	LEU
1	A	70	MET
1	A	78	ASP
1	A	88	LEU
1	A	120	ASP
1	A	132	ARG
1	A	136	SER
1	A	138	LYS
1	A	157	LEU
1	A	177	LYS
1	A	184	GLN
1	A	185	GLN
1	A	190	ASP
1	A	198	VAL
1	A	202	LEU
1	A	215	ARG
1	A	226	LEU
1	A	236	ARG
1	A	237	VAL
1	A	240	MET
1	A	245	ASN

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Mol	Chain	Res	Type
1	A	251	ARG
1	A	282	THR
1	A	287	LEU
1	A	292	ARG
1	A	297	VAL
1	A	312	LEU
1	A	314	ARG
1	A	333	VAL
1	A	338	ASN
1	A	342	LEU
1	A	376	MET
1	A	378	PRO
1	A	380	GLN

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	8	ASN
1	A	13	ASN
1	A	26	HIS
1	A	27	ASN
1	A	63	ASN
1	A	112	HIS
1	A	114	ASN
1	A	145	HIS
1	A	163	ASN
1	A	184	GLN
1	A	219	HIS
1	A	245	ASN
1	A	269	HIS
1	A	286	ASN
1	A	296	HIS
1	A	301	HIS
1	A	318	GLN
1	A	338	ASN
1	A	349	GLN
1	A	351	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 carbohydrates 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	394	-	4,4,4	0.47	0	6,6,6	0.22	0
2	SO4	A	392	-	4,4,4	0.45	0	6,6,6	0.18	0
2	SO4	A	393	-	4,4,4	0.43	0	6,6,6	0.29	0
2	SO4	A	391	-	4,4,4	0.48	0	6,6,6	0.20	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	392	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.