



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:48 AM UTC

PDB ID : 2CRK / pdb_00002crk
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

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>.

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

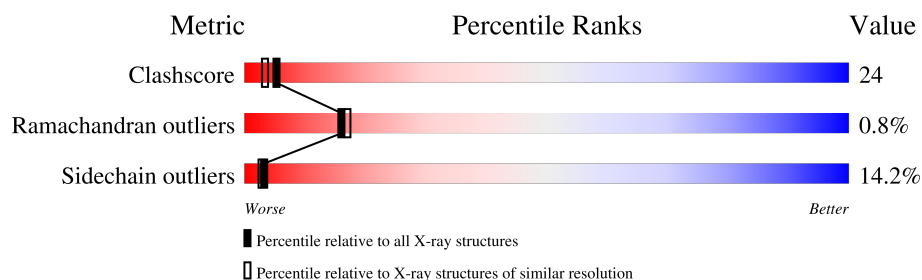
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 49% 35% 10% . .

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
1	A	365	Total	C	N	O	S	0	0	0
			2928	1849	516	549	14			

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 (CCD ID: SO4) (formula: O₄S).



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.

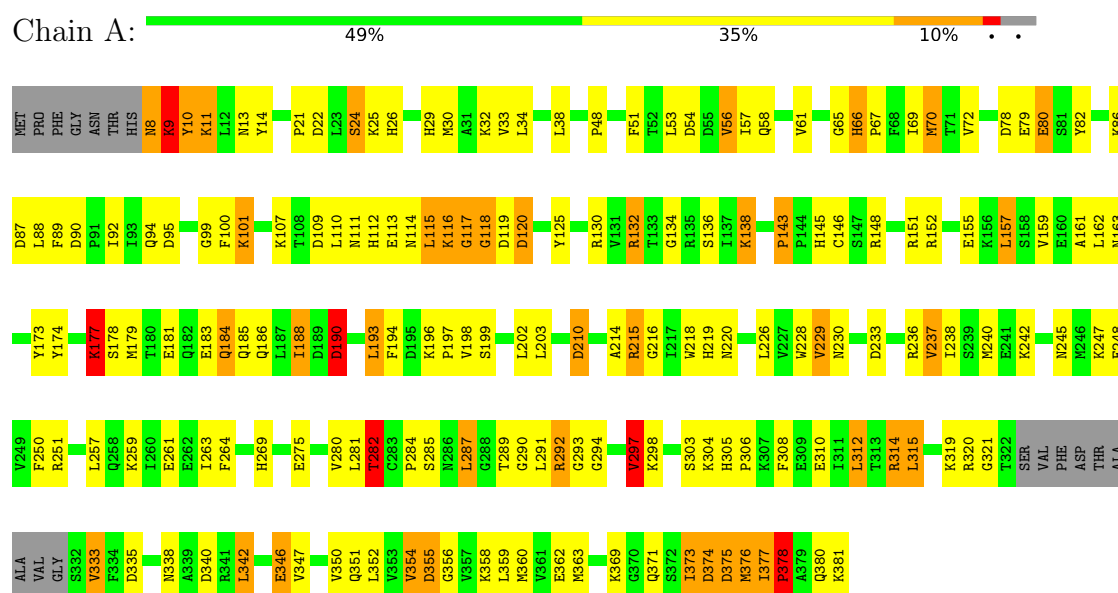
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	431	Total	O	0	0
			431	431		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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 (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, α , β , γ	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 ²)	27.0	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	0.86	1/2993 (0.0%)	1.28	45/4029 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	VAL	CA-CB	5.12	1.61	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	PRO	N-CA-C	9.26	122.00	110.70
1	A	377	ILE	CA-C-N	8.05	129.90	119.84
1	A	377	ILE	C-N-CA	8.05	129.90	119.84
1	A	374	ASP	N-CA-C	7.83	121.71	108.02
1	A	199	SER	CA-C-N	7.76	127.39	119.56
1	A	199	SER	C-N-CA	7.76	127.39	119.56
1	A	13	ASN	N-CA-C	-7.69	103.36	112.89
1	A	193	LEU	N-CA-C	7.25	121.21	110.48
1	A	117	GLY	N-CA-C	-6.92	96.77	113.18
1	A	119	ASP	N-CA-C	6.64	124.95	110.80
1	A	130	ARG	N-CA-C	6.62	119.28	108.55
1	A	101	LYS	CA-C-N	6.62	126.25	119.56
1	A	101	LYS	C-N-CA	6.62	126.25	119.56
1	A	177	LYS	N-CA-C	6.56	119.27	111.33
1	A	115	LEU	N-CA-C	-6.48	105.24	113.01
1	A	315	LEU	N-CA-C	-6.32	105.57	113.28
1	A	143	PRO	CA-C-N	-6.19	113.25	120.12
1	A	143	PRO	C-N-CA	-6.19	113.25	120.12
1	A	282	THR	N-CA-C	6.14	118.94	111.82
1	A	242	LYS	N-CA-C	-6.06	100.62	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	HIS	CA-C-N	5.95	125.63	119.56
1	A	66	HIS	C-N-CA	5.95	125.63	119.56
1	A	355	ASP	N-CA-C	5.95	117.44	111.07
1	A	190	ASP	N-CA-C	-5.90	105.92	114.12
1	A	118	GLY	N-CA-C	-5.58	99.96	113.18
1	A	358	LYS	N-CA-C	-5.40	105.30	111.14
1	A	321	GLY	CA-C-N	5.39	131.40	121.70
1	A	321	GLY	C-N-CA	5.39	131.40	121.70
1	A	120	ASP	CA-C-N	5.36	128.85	120.75
1	A	120	ASP	C-N-CA	5.36	128.85	120.75
1	A	101	LYS	N-CA-C	5.34	117.75	110.01
1	A	297	VAL	N-CA-C	5.28	116.08	108.48
1	A	290	GLY	N-CA-C	-5.26	108.58	115.47
1	A	228	TRP	CA-C-N	-5.22	116.72	123.19
1	A	228	TRP	C-N-CA	-5.22	116.72	123.19
1	A	146	CYS	N-CA-C	5.21	117.59	110.24
1	A	79	GLU	N-CA-C	-5.19	105.80	111.82
1	A	373	ILE	N-CA-C	5.15	117.02	108.99
1	A	33	VAL	N-CA-C	5.12	117.01	111.58
1	A	65	GLY	N-CA-C	5.08	121.46	112.02
1	A	229	VAL	N-CA-C	5.07	115.27	108.17
1	A	378	PRO	N-CA-C	5.01	122.80	112.47
1	A	196	LYS	CA-C-N	5.01	125.24	119.83
1	A	196	LYS	C-N-CA	5.01	125.24	119.83
1	A	210	ASP	N-CA-C	5.00	119.23	113.38

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	2928	0	2902	142	0
2	A	20	0	0	1	0
3	A	431	0	0	28	0
All	All	3379	0	2902	142	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 24.

All (142) 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:HH11	1:A:292:ARG:HG2	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: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:174:TYR:HB3	1:A:179:MET:HE1	1.70	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:9:LYS:HA	3:A:405:HOH:O	1.92	0.69
1:A:174:TYR:HB3	1:A:179:MET:CE	2.23	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
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:HG2	1:A:292:ARG:NH1	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:HE3	1:A:95:ASP:OD2	2.04	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:377:ILE:CG2	1:A:378:PRO:HD2	2.36	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:314:ARG:NH1	1:A:378:PRO:HD3	2.22	0.55
1:A:338:ASN:HD22	1:A:338:ASN:H	1.54	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:162:LEU:HD13	1:A:218:TRP:CG	2.43	0.54
1:A:173:TYR:OH	1:A:216:GLY:HA3	2.07	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:32:LYS:HE3	1:A:95:ASP:CG	2.33	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:118:GLY:CA	1:A:354:VAL:HG21	2.35	0.52
1:A:237:VAL:HG11	1:A:257:LEU:HD21	1.91	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:26:HIS:HE1	1:A:61:VAL:O	1.93	0.51
1:A:151:ARG:HD3	3:A:401:HOH:O	2.10	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
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:289:THR:C	1:A:291:LEU:H	2.19	0.49
1:A:115:LEU:O	1:A:116:LYS:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:86:LYS:O	1:A:90:ASP:HB2	2.15	0.47
1:A:292:ARG:NH2	1:A:335:ASP:OD1	2.46	0.47
1:A:155:GLU:O	1:A:159:VAL:HG23	2.15	0.47
1:A:359:LEU:HD21	1:A:363:MET:HE3	1.95	0.47
1:A:163:ASN:ND2	3:A:556:HOH:O	2.48	0.47
1:A:314:ARG:CD	1:A:376:MET:HE2	2.45	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: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:289:THR:C	1:A:291:LEU:N	2.74	0.45
1:A:375:ASP:N	1:A:375:ASP:OD1	2.50	0.45
1:A:177:LYS:HE3	1:A:177:LYS:HB3	1.79	0.45
1:A:369:LYS:HB2	1:A:371:GLN:HG3	1.98	0.45
1:A:30:MET:HE2	1:A:57:ILE:HB	1.99	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:289:THR:HG22	1:A:346:GLU:CD	2.44	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:132:ARG:O	1:A:291:LEU:HA	2.20	0.42
1:A:138:LYS:O	1:A:269:HIS:HD2	2.01	0.42
1:A:157:LEU:HG	3:A:707:HOH:O	2.19	0.42
1:A:245:ASN:C	1:A:245:ASN:HD22	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLN:O	1:A:354:VAL:HG13	2.20	0.42
1:A:21:PRO:HG3	1:A:57:ILE:HD12	2.01	0.42
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:161:ALA:HB2	1:A:264:PHE:HE1	1.85	0.42
1:A:261:GLU:HG2	3:A:486:HOH:O	2.20	0.42
1:A:53:LEU:HA	1:A:56:VAL:HG22	2.01	0.41
1:A:215:ARG:NH1	3:A:570:HOH:O	2.51	0.41
1:A:112:HIS:H	1:A:112:HIS:CD2	2.38	0.41
1:A:303:SER:HA	1:A:308:PHE:CD2	2.56	0.41
1:A:294:GLY:C	3:A:460:HOH:O	2.62	0.41
1:A:132:ARG:HG2	2:A:392:SO4:O4	2.21	0.41
1:A:315:LEU:O	1:A:381:LYS:OXT	2.38	0.41
1:A:371:GLN:HA	3:A:734:HOH:O	2.20	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:HD2	1:A:101:LYS:N	2.36	0.40
1:A:117:GLY:O	1:A:351:GLN:NE2	2.54	0.40
1:A:134:GLY:C	1:A:281:LEU:HD21	2.46	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%)	16 17

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%)	279 (86%)	46 (14%)	3 3

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	9	LYS
1	A	10	TYR
1	A	11	LYS
1	A	34	LEU
1	A	70	MET
1	A	78	ASP
1	A	80	GLU
1	A	88	LEU
1	A	120	ASP
1	A	132	ARG
1	A	136	SER
1	A	138	LYS
1	A	143	PRO
1	A	157	LEU
1	A	177	LYS
1	A	181	GLU
1	A	184	GLN
1	A	185	GLN
1	A	188	ILE
1	A	190	ASP
1	A	198	VAL
1	A	202	LEU
1	A	215	ARG

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Mol	Chain	Res	Type
1	A	226	LEU
1	A	229	VAL
1	A	236	ARG
1	A	237	VAL
1	A	238	ILE
1	A	240	MET
1	A	251	ARG
1	A	280	VAL
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	342	LEU
1	A	346	GLU
1	A	354	VAL
1	A	375	ASP
1	A	376	MET
1	A	378	PRO
1	A	380	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	26	HIS
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	185	GLN
1	A	219	HIS
1	A	245	ASN
1	A	269	HIS
1	A	286	ASN
1	A	301	HIS
1	A	318	GLN
1	A	338	ASN

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Mol	Chain	Res	Type
1	A	349	GLN
1	A	351	GLN
1	A	371	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 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	393	-	4,4,4	0.38	0	6,6,6	0.30	0
2	SO4	A	391	-	4,4,4	0.41	0	6,6,6	0.18	0
2	SO4	A	394	-	4,4,4	0.41	0	6,6,6	0.24	0
2	SO4	A	392	-	4,4,4	0.39	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 [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.