



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:57 PM UTC

PDB ID : 6KKV / pdb_00006kkv
Title : Structural basis for domain rotation during adenylation of active site K123 and fragment library screening against NAD⁺ -dependent DNA ligase from *Mycobacterium tuberculosis*
Authors : Ramachandran, R.; Shukla, A.; Afsar, M.
Deposited on : 2019-07-27
Resolution : 2.56 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

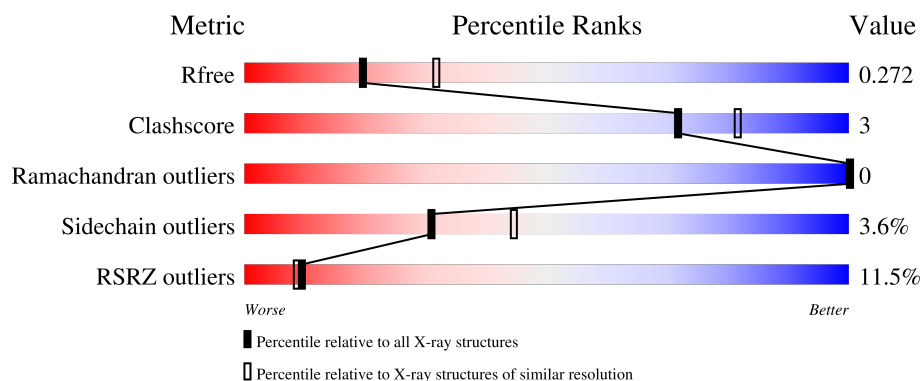
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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))
R_{free}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	11% 16% 76% 7%

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	DKR	A	401	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4940 atoms, of which 2391 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.

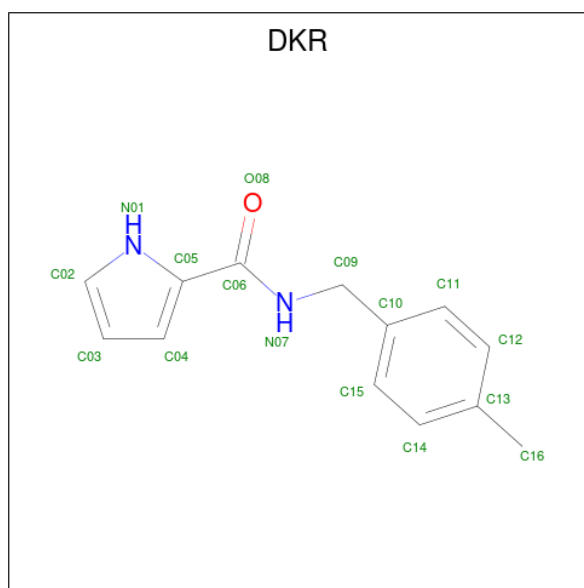
- Molecule 1 is a protein called DNA ligase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	321	4869	1563	2378	453	471	4	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

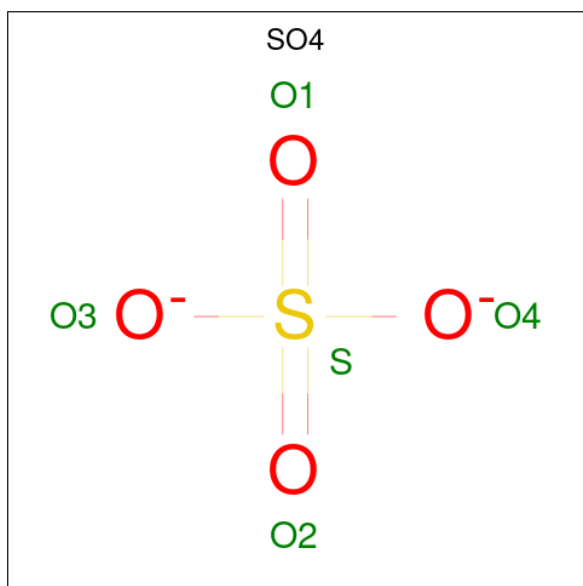
Chain	Residue	Modelled	Actual	Comment	Reference
A	329	HIS	-	expression tag	UNP P9WNV1
A	330	HIS	-	expression tag	UNP P9WNV1
A	331	HIS	-	expression tag	UNP P9WNV1
A	332	HIS	-	expression tag	UNP P9WNV1
A	333	HIS	-	expression tag	UNP P9WNV1
A	334	HIS	-	expression tag	UNP P9WNV1

- Molecule 2 is N-[(4-methylphenyl)methyl]-1H-pyrrole-2-carboxamide (CCD ID: DKR) (formula: C₁₃H₁₄N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			29	13	13	2	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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

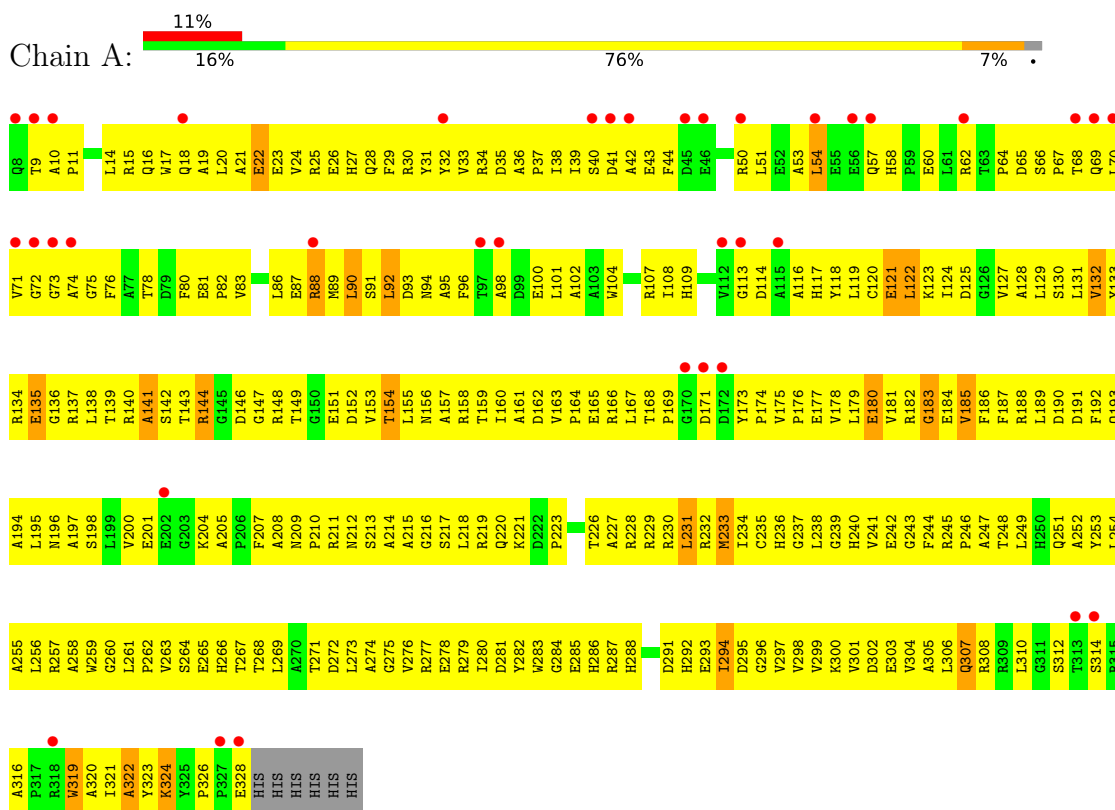
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		

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 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.

• Molecule 1: DNA ligase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	95.40Å 95.40Å 201.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.10 – 2.56 43.10 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.10-2.56) 99.9 (43.10-2.56)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.232 , 0.278 0.249 , 0.272	Depositor DCC
R_{free} test set	872 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4940	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, DKR

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	3.28	311/2549 (12.2%)	1.55	41/3474 (1.2%)

All (311) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	ASP	C-O	-14.44	1.07	1.24
1	A	53	ALA	CA-C	-11.23	1.38	1.52
1	A	179	LEU	C-O	-10.98	1.11	1.23
1	A	132	VAL	C-O	-10.96	1.12	1.24
1	A	326	PRO	N-CD	-10.76	1.32	1.47
1	A	209	ASN	C-O	-10.47	1.14	1.24
1	A	66	SER	C-O	-10.25	1.10	1.23
1	A	130	SER	C-O	-10.04	1.12	1.24
1	A	269	LEU	C-O	-9.70	1.12	1.24
1	A	187	PHE	C-O	-9.58	1.12	1.23
1	A	298	VAL	C-O	-9.51	1.13	1.24
1	A	263	VAL	C-O	-9.44	1.14	1.24
1	A	285	GLU	C-O	-9.31	1.12	1.24
1	A	226	THR	C-O	-9.23	1.13	1.24
1	A	134	ARG	C-O	-9.09	1.13	1.24
1	A	234	ILE	C-O	-9.06	1.14	1.24
1	A	182	ARG	C-O	-9.05	1.13	1.23
1	A	241	VAL	C-O	-9.04	1.14	1.23
1	A	300	LYS	C-O	-9.04	1.12	1.23
1	A	237	GLY	C-O	-8.88	1.14	1.24
1	A	299	VAL	C-O	-8.88	1.14	1.24
1	A	165	GLU	C-O	-8.72	1.13	1.24
1	A	18	GLN	C-O	-8.67	1.14	1.24
1	A	161	ALA	C-O	-8.59	1.14	1.24
1	A	149	THR	C-O	-8.54	1.13	1.23
1	A	153	VAL	C-O	-8.51	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	VAL	C-O	-8.45	1.15	1.24
1	A	131	LEU	C-O	-8.45	1.13	1.23
1	A	120	CYS	C-O	-8.40	1.14	1.24
1	A	154	THR	C-O	-8.37	1.14	1.24
1	A	233	MET	C-O	-8.33	1.13	1.23
1	A	10	ALA	C-O	-8.31	1.16	1.24
1	A	211	ARG	C-O	-8.31	1.14	1.24
1	A	266	HIS	C-O	-8.28	1.12	1.24
1	A	207	PHE	C-O	-8.21	1.13	1.23
1	A	95	ALA	C-O	-8.17	1.14	1.24
1	A	279	ARG	C-O	-8.16	1.14	1.24
1	A	242	GLU	C-O	-8.13	1.14	1.24
1	A	118	TYR	C-O	-8.11	1.14	1.24
1	A	178	VAL	C-O	-8.06	1.15	1.24
1	A	255	ALA	C-O	-8.06	1.14	1.24
1	A	232	ARG	C-O	-8.05	1.13	1.23
1	A	142	SER	C-O	-8.04	1.14	1.23
1	A	160	ILE	C-O	-8.03	1.15	1.24
1	A	301	VAL	C-O	-8.02	1.14	1.24
1	A	194	ALA	C-O	-8.02	1.14	1.24
1	A	217	SER	C-O	-8.02	1.14	1.24
1	A	218	LEU	C-O	-7.99	1.14	1.24
1	A	185	VAL	C-O	-7.97	1.15	1.24
1	A	76	PHE	C-O	-7.96	1.14	1.23
1	A	86	LEU	C-O	-7.96	1.14	1.24
1	A	221	LYS	C-O	-7.96	1.14	1.24
1	A	253	TYR	C-O	-7.95	1.14	1.24
1	A	256	LEU	C-O	-7.94	1.15	1.24
1	A	176	PRO	C-O	-7.93	1.14	1.23
1	A	159	THR	C-O	-7.88	1.13	1.24
1	A	183	GLY	C-O	-7.87	1.15	1.23
1	A	296	GLY	C-O	-7.85	1.13	1.23
1	A	164	PRO	C-O	-7.80	1.15	1.23
1	A	27	HIS	C-O	-7.79	1.13	1.24
1	A	119	LEU	C-O	-7.79	1.14	1.24
1	A	281	ASP	C-O	-7.79	1.14	1.24
1	A	92	LEU	C-O	-7.76	1.14	1.23
1	A	155	LEU	C-O	-7.74	1.15	1.24
1	A	247	ALA	C-O	-7.67	1.14	1.24
1	A	24	VAL	C-O	-7.66	1.15	1.24
1	A	22	GLU	C-O	-7.63	1.15	1.24
1	A	156	ASN	C-O	-7.62	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	LEU	C-O	-7.59	1.14	1.23
1	A	151	GLU	C-O	-7.58	1.15	1.23
1	A	214	ALA	C-O	-7.54	1.15	1.24
1	A	108	ILE	C-O	-7.52	1.15	1.24
1	A	274	ALA	C-O	-7.47	1.15	1.24
1	A	53	ALA	C-O	-7.46	1.15	1.24
1	A	140	ARG	C-O	-7.43	1.14	1.23
1	A	51	LEU	C-O	-7.42	1.15	1.24
1	A	138	LEU	C-O	-7.36	1.15	1.24
1	A	124	ILE	C-O	-7.35	1.15	1.24
1	A	216	GLY	C-O	-7.33	1.15	1.23
1	A	208	ALA	C-O	-7.31	1.14	1.24
1	A	246	PRO	C-O	-7.31	1.16	1.23
1	A	20	LEU	C-O	-7.26	1.15	1.24
1	A	265	GLU	C-O	-7.24	1.14	1.24
1	A	231	LEU	C-O	-7.21	1.14	1.23
1	A	189	LEU	C-O	-7.21	1.15	1.24
1	A	175	VAL	C-O	-7.18	1.15	1.24
1	A	252	ALA	C-O	-7.17	1.15	1.24
1	A	141	ALA	C-O	-7.13	1.15	1.23
1	A	70	LEU	CA-C	-7.12	1.42	1.52
1	A	294	ILE	C-O	-7.11	1.16	1.24
1	A	213	SER	C-O	-7.10	1.15	1.24
1	A	272	ASP	C-O	-7.10	1.15	1.23
1	A	197	ALA	C-O	-7.09	1.15	1.24
1	A	295	ASP	C-O	-7.08	1.14	1.24
1	A	51	LEU	CA-C	-7.08	1.43	1.52
1	A	81	GLU	C-O	-7.05	1.14	1.23
1	A	83	VAL	C-O	-7.05	1.16	1.24
1	A	245	ARG	C-O	-7.04	1.16	1.24
1	A	146	ASP	C-O	-7.03	1.14	1.24
1	A	16	GLN	C-O	-7.03	1.15	1.24
1	A	23	GLU	C-O	-7.02	1.15	1.24
1	A	210	PRO	C-O	-7.02	1.15	1.24
1	A	275	GLY	C-O	-7.01	1.15	1.23
1	A	147	GLY	C-O	-6.99	1.14	1.24
1	A	219	ARG	C-O	-6.97	1.16	1.23
1	A	57	GLN	CA-C	-6.96	1.44	1.52
1	A	262	PRO	C-O	-6.95	1.16	1.23
1	A	229	ARG	C-O	-6.95	1.15	1.24
1	A	75	GLY	C-O	-6.94	1.15	1.24
1	A	181	VAL	C-O	-6.92	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	GLU	C-O	-6.88	1.15	1.24
1	A	71	VAL	C-O	-6.86	1.16	1.24
1	A	321	ILE	C-O	-6.85	1.16	1.23
1	A	136	GLY	C-O	-6.84	1.15	1.24
1	A	121	GLU	C-O	-6.83	1.15	1.23
1	A	60	GLU	C-O	-6.82	1.15	1.24
1	A	163	VAL	C-O	-6.82	1.15	1.24
1	A	324	LYS	C-O	-6.82	1.15	1.24
1	A	291	ASP	C-O	-6.79	1.15	1.24
1	A	62	ARG	C-O	-6.79	1.16	1.24
1	A	186	PHE	C-O	-6.78	1.15	1.23
1	A	215	ALA	C-O	-6.78	1.16	1.24
1	A	191	ASP	C-O	-6.78	1.15	1.24
1	A	144	ARG	C-O	-6.72	1.16	1.24
1	A	29	PHE	C-O	-6.71	1.16	1.24
1	A	243	GLY	C-O	-6.70	1.15	1.24
1	A	129	LEU	C-O	-6.69	1.15	1.23
1	A	260	GLY	C-O	-6.68	1.15	1.24
1	A	127	VAL	C-O	-6.68	1.16	1.24
1	A	143	THR	C-O	-6.68	1.15	1.23
1	A	144	ARG	CZ-NH1	-6.68	1.23	1.32
1	A	123	LYS	C-O	-6.66	1.15	1.24
1	A	180	GLU	C-O	-6.66	1.16	1.24
1	A	100	GLU	N-CA	-6.65	1.38	1.46
1	A	258	ALA	C-O	-6.64	1.16	1.24
1	A	26	GLU	C-O	-6.63	1.15	1.24
1	A	158	ARG	C-O	-6.62	1.15	1.24
1	A	173	TYR	C-O	-6.60	1.18	1.24
1	A	188	ARG	C-O	-6.58	1.15	1.23
1	A	277	ARG	C-O	-6.58	1.15	1.24
1	A	323	TYR	C-O	-6.58	1.15	1.24
1	A	163	VAL	N-CA	-6.56	1.41	1.46
1	A	166	ARG	N-CA	-6.55	1.37	1.45
1	A	18	GLN	CA-C	-6.54	1.44	1.52
1	A	137	ARG	C-O	-6.50	1.15	1.24
1	A	200	VAL	C-O	-6.48	1.15	1.24
1	A	236	HIS	C-O	-6.47	1.15	1.24
1	A	181	VAL	N-CA	-6.44	1.38	1.46
1	A	244	PHE	C-O	-6.44	1.16	1.24
1	A	50	ARG	CA-C	-6.43	1.44	1.52
1	A	34	ARG	CZ-NH2	-6.43	1.25	1.33
1	A	73	GLY	C-O	-6.43	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	SER	CA-C	-6.41	1.44	1.53
1	A	316	ALA	C-O	-6.38	1.15	1.24
1	A	319	TRP	C-O	-6.37	1.15	1.24
1	A	177	GLU	C-O	-6.37	1.16	1.24
1	A	239	GLY	C-O	-6.37	1.15	1.23
1	A	282	TYR	C-O	-6.37	1.16	1.24
1	A	89	MET	C-O	-6.36	1.15	1.23
1	A	94	ASN	C-O	-6.35	1.16	1.23
1	A	303	GLU	C-O	-6.34	1.16	1.24
1	A	276	VAL	C-O	-6.33	1.16	1.24
1	A	35	ASP	CA-C	-6.33	1.44	1.52
1	A	266	HIS	CA-C	-6.32	1.44	1.52
1	A	257	ARG	C-O	-6.30	1.16	1.24
1	A	152	ASP	C-O	-6.29	1.16	1.24
1	A	25	ARG	C-O	-6.27	1.16	1.24
1	A	278	GLU	C-O	-6.26	1.16	1.24
1	A	14	LEU	C-O	-6.26	1.16	1.24
1	A	196	ASN	C-O	-6.25	1.16	1.24
1	A	37	PRO	C-O	-6.24	1.16	1.23
1	A	287	ARG	C-O	-6.24	1.16	1.24
1	A	249	LEU	C-O	-6.22	1.16	1.24
1	A	93	ASP	C-O	-6.17	1.16	1.23
1	A	90	LEU	C-O	-6.15	1.15	1.23
1	A	220	GLN	C-O	-6.14	1.16	1.24
1	A	88	ARG	C-O	-6.14	1.16	1.23
1	A	82	PRO	C-O	-6.12	1.16	1.23
1	A	238	LEU	C-O	-6.10	1.16	1.23
1	A	50	ARG	C-O	-6.09	1.17	1.24
1	A	307	GLN	C-O	-6.09	1.16	1.24
1	A	19	ALA	C-O	-6.06	1.16	1.24
1	A	198	SER	C-O	-6.06	1.17	1.24
1	A	41	ASP	N-CA	-6.06	1.39	1.46
1	A	165	GLU	CA-C	-6.06	1.45	1.52
1	A	125	ASP	C-O	-6.06	1.15	1.23
1	A	15	ARG	C-O	-6.05	1.17	1.24
1	A	33	VAL	C-O	-6.04	1.17	1.24
1	A	235	CYS	C-O	-6.04	1.16	1.23
1	A	223	PRO	C-O	-6.04	1.16	1.24
1	A	122	LEU	C-O	-6.04	1.16	1.24
1	A	123	LYS	N-CA	-6.04	1.38	1.46
1	A	30	ARG	C-O	-6.02	1.17	1.24
1	A	17	TRP	C-O	-6.00	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	ASP	N-CA	-6.00	1.38	1.46
1	A	247	ALA	CA-C	-6.00	1.44	1.52
1	A	283	TRP	C-O	-5.99	1.16	1.24
1	A	251	GLN	C-O	-5.97	1.16	1.24
1	A	254	LEU	C-O	-5.96	1.17	1.24
1	A	96	PHE	C-O	-5.89	1.15	1.24
1	A	142	SER	N-CA	-5.88	1.38	1.45
1	A	91	SER	C-O	-5.83	1.16	1.23
1	A	264	SER	C-O	-5.83	1.16	1.23
1	A	196	ASN	CG-ND2	-5.80	1.21	1.33
1	A	116	ALA	C-O	-5.80	1.17	1.24
1	A	139	THR	C-O	-5.80	1.15	1.23
1	A	38	ILE	C-O	-5.79	1.15	1.24
1	A	213	SER	N-CA	-5.79	1.39	1.46
1	A	268	THR	C-O	-5.79	1.16	1.23
1	A	304	VAL	C-O	-5.79	1.17	1.24
1	A	316	ALA	CA-C	-5.76	1.45	1.52
1	A	295	ASP	CA-C	-5.75	1.45	1.52
1	A	133	TYR	C-O	-5.73	1.17	1.24
1	A	11	PRO	C-O	-5.72	1.16	1.24
1	A	259	TRP	C-O	-5.71	1.16	1.24
1	A	78	THR	C-O	-5.70	1.17	1.24
1	A	190	ASP	C-O	-5.69	1.17	1.24
1	A	148	ARG	N-CA	-5.69	1.39	1.46
1	A	195	LEU	C-O	-5.69	1.17	1.24
1	A	135	GLU	C-O	-5.68	1.16	1.23
1	A	64	PRO	C-O	-5.64	1.16	1.24
1	A	104	TRP	C-O	-5.63	1.17	1.24
1	A	121	GLU	CA-C	-5.62	1.45	1.52
1	A	273	LEU	C-O	-5.62	1.17	1.24
1	A	194	ALA	N-CA	-5.61	1.39	1.46
1	A	322	ALA	C-O	-5.60	1.17	1.24
1	A	204	LYS	C-O	-5.59	1.16	1.23
1	A	238	LEU	CA-C	-5.59	1.45	1.52
1	A	69	GLN	CA-C	-5.58	1.45	1.52
1	A	65	ASP	C-O	-5.58	1.16	1.24
1	A	134	ARG	CZ-NH1	-5.57	1.25	1.32
1	A	229	ARG	CZ-NH2	-5.57	1.26	1.33
1	A	28	GLN	C-O	-5.56	1.17	1.24
1	A	69	GLN	C-O	-5.56	1.17	1.24
1	A	58	HIS	C-O	-5.55	1.17	1.24
1	A	166	ARG	C-O	-5.53	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	ALA	C-O	-5.53	1.17	1.24
1	A	144	ARG	CZ-NH2	-5.52	1.26	1.33
1	A	312	SER	C-O	-5.50	1.17	1.23
1	A	284	GLY	C-O	-5.49	1.17	1.23
1	A	168	THR	C-O	-5.47	1.16	1.24
1	A	107	ARG	C-O	-5.46	1.17	1.24
1	A	157	ALA	C-O	-5.45	1.17	1.24
1	A	16	GLN	N-CA	-5.45	1.39	1.46
1	A	226	THR	CB-CG2	-5.45	1.34	1.52
1	A	117	HIS	C-O	-5.44	1.16	1.23
1	A	212	ASN	C-O	-5.44	1.17	1.24
1	A	128	ALA	N-CA	-5.42	1.39	1.46
1	A	198	SER	N-CA	-5.42	1.39	1.46
1	A	229	ARG	N-CA	-5.39	1.39	1.46
1	A	267	THR	C-O	-5.39	1.17	1.23
1	A	209	ASN	CG-OD1	-5.38	1.13	1.23
1	A	201	GLU	N-CA	-5.36	1.39	1.46
1	A	233	MET	CG-SD	-5.36	1.67	1.80
1	A	98	ALA	C-O	-5.35	1.17	1.24
1	A	193	GLN	C-O	-5.35	1.17	1.24
1	A	205	ALA	C-O	-5.35	1.17	1.23
1	A	80	PHE	C-O	-5.34	1.16	1.23
1	A	44	PHE	C-O	-5.33	1.17	1.24
1	A	314	SER	C-O	-5.33	1.17	1.24
1	A	305	ALA	C-O	-5.32	1.17	1.24
1	A	295	ASP	N-CA	-5.32	1.39	1.46
1	A	288	HIS	C-O	-5.32	1.17	1.24
1	A	32	TYR	C-O	-5.31	1.17	1.23
1	A	66	SER	CA-C	-5.30	1.46	1.53
1	A	184	GLU	C-O	-5.29	1.17	1.24
1	A	67	PRO	C-O	-5.29	1.17	1.24
1	A	269	LEU	N-CA	-5.28	1.39	1.46
1	A	314	SER	CA-C	-5.28	1.45	1.52
1	A	320	ALA	C-O	-5.28	1.17	1.23
1	A	96	PHE	CA-C	-5.27	1.45	1.52
1	A	292	HIS	C-O	-5.27	1.17	1.23
1	A	162	ASP	C-O	-5.25	1.17	1.24
1	A	34	ARG	CZ-NH1	-5.23	1.25	1.32
1	A	175	VAL	N-CA	-5.23	1.40	1.47
1	A	169	PRO	CA-CB	-5.23	1.46	1.53
1	A	240	HIS	C-O	-5.22	1.17	1.23
1	A	247	ALA	N-CA	-5.21	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	ARG	CZ-NH2	-5.21	1.26	1.33
1	A	244	PHE	N-CA	-5.21	1.40	1.46
1	A	217	SER	N-CA	-5.20	1.39	1.46
1	A	87	GLU	C-O	-5.20	1.17	1.23
1	A	86	LEU	CA-C	-5.19	1.46	1.52
1	A	142	SER	CA-C	-5.19	1.46	1.52
1	A	230	ARG	C-O	-5.18	1.17	1.23
1	A	322	ALA	CA-C	-5.17	1.46	1.52
1	A	196	ASN	CG-OD1	-5.16	1.13	1.23
1	A	146	ASP	CA-C	-5.15	1.45	1.52
1	A	324	LYS	N-CA	-5.15	1.39	1.46
1	A	286	HIS	C-O	-5.13	1.17	1.24
1	A	174	PRO	C-O	-5.13	1.18	1.23
1	A	266	HIS	N-CA	-5.12	1.40	1.46
1	A	31	TYR	C-O	-5.11	1.18	1.24
1	A	36	ALA	C-O	-5.10	1.18	1.24
1	A	180	GLU	CD-OE1	-5.10	1.15	1.25
1	A	192	PHE	C-O	-5.09	1.18	1.24
1	A	143	THR	CB-CG2	-5.08	1.35	1.52
1	A	302	ASP	CG-OD1	-5.07	1.15	1.25
1	A	43	GLU	C-O	-5.06	1.18	1.24
1	A	271	THR	C-O	-5.06	1.17	1.24
1	A	102	ALA	C-O	-5.06	1.18	1.24
1	A	248	THR	C-O	-5.05	1.17	1.23
1	A	68	THR	C-O	-5.05	1.17	1.24
1	A	280	ILE	N-CA	-5.05	1.40	1.46
1	A	262	PRO	CA-CB	-5.04	1.47	1.53
1	A	228	ARG	C-O	-5.03	1.17	1.24
1	A	261	LEU	C-O	-5.02	1.17	1.24
1	A	140	ARG	CD-NE	-5.01	1.39	1.46
1	A	151	GLU	CA-C	-5.01	1.46	1.52
1	A	74	ALA	C-O	-5.00	1.17	1.24
1	A	25	ARG	CA-C	-5.00	1.46	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ALA	CA-C-O	-15.41	104.41	120.90
1	A	41	ASP	CA-C-O	-15.18	104.46	120.55
1	A	53	ALA	CA-C-N	13.92	138.94	120.28
1	A	53	ALA	C-N-CA	13.92	138.94	120.28
1	A	53	ALA	O-C-N	12.56	135.15	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ASP	CA-C-N	9.53	134.79	120.31
1	A	41	ASP	C-N-CA	9.53	134.79	120.31
1	A	42	ALA	N-CA-C	9.17	122.45	111.82
1	A	328	GLU	N-CA-C	-9.06	85.63	111.00
1	A	171	ASP	N-CA-C	-7.31	101.66	111.96
1	A	42	ALA	CA-C-N	7.22	130.54	120.29
1	A	42	ALA	C-N-CA	7.22	130.54	120.29
1	A	72	GLY	O-C-N	-6.90	118.24	123.35
1	A	41	ASP	O-C-N	6.76	129.29	122.12
1	A	302	ASP	N-CA-C	6.75	119.65	111.82
1	A	53	ALA	N-CA-C	-6.67	103.10	111.11
1	A	54	LEU	N-CA-C	6.55	118.42	111.28
1	A	71	VAL	N-CA-C	6.34	122.52	109.34
1	A	328	GLU	CA-C-O	6.33	131.56	120.80
1	A	189	LEU	N-CA-C	6.12	118.45	111.11
1	A	144	ARG	N-CA-C	6.05	117.88	111.28
1	A	74	ALA	N-CA-C	6.04	123.67	110.80
1	A	237	GLY	O-C-N	-5.91	117.90	123.87
1	A	114	ASP	N-CA-C	-5.89	105.67	112.92
1	A	230	ARG	N-CA-C	5.89	119.82	110.70
1	A	118	TYR	N-CA-C	5.85	118.06	108.52
1	A	54	LEU	N-CA-CB	5.84	118.71	110.12
1	A	163	VAL	N-CA-C	5.80	113.62	107.76
1	A	70	LEU	CB-CA-C	-5.72	99.43	110.35
1	A	316	ALA	N-CA-C	5.70	113.35	108.22
1	A	257	ARG	CB-CA-C	-5.42	102.38	110.88
1	A	9	THR	N-CA-C	-5.41	98.74	108.48
1	A	35	ASP	N-CA-C	-5.38	103.61	111.30
1	A	219	ARG	N-CA-C	5.37	117.93	109.39
1	A	228	ARG	CG-CD-NE	-5.24	100.48	112.00
1	A	72	GLY	N-CA-C	-5.19	101.19	111.31
1	A	142	SER	N-CA-CB	-5.12	101.99	111.52
1	A	171	ASP	CB-CA-C	5.11	119.93	110.88
1	A	227	ALA	N-CA-C	5.07	117.54	111.71
1	A	74	ALA	N-CA-CB	-5.05	101.96	110.49
1	A	293	GLU	N-CA-C	5.01	117.72	109.76

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	2491	2378	2379	15	0
2	A	16	13	0	1	0
3	A	10	0	0	1	0
4	A	32	0	0	0	0
All	All	2549	2391	2379	16	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 3.

All (16) 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:306:LEU:O	1:A:310:LEU:HD12	1.92	0.69
1:A:88:ARG:CD	1:A:90:LEU:HD21	2.30	0.61
1:A:183:GLY:HA3	1:A:233:MET:HE3	1.86	0.57
1:A:307:GLN:HB2	1:A:319:TRP:CG	2.40	0.55
1:A:109:HIS:O	1:A:109:HIS:CG	2.61	0.53
1:A:141:ALA:HB3	1:A:154:THR:HA	1.89	0.52
1:A:88:ARG:HD2	1:A:90:LEU:HD21	1.93	0.50
1:A:307:GLN:HB2	1:A:319:TRP:CD2	2.50	0.47
2:A:401:DKR:O08	2:A:401:DKR:C11	2.64	0.46
1:A:144:ARG:NH1	3:A:403:SO4:O1	2.49	0.45
1:A:109:HIS:ND1	1:A:113:GLY:O	2.40	0.43
1:A:122:LEU:HB3	1:A:294:ILE:HD12	2.02	0.42
1:A:307:GLN:HB2	1:A:319:TRP:CD1	2.54	0.42
1:A:92:LEU:HD13	1:A:322:ALA:HB2	2.03	0.41
1:A:132:VAL:HG22	1:A:180:GLU:HG3	2.04	0.40
1:A:54:LEU:O	1:A:54:LEU:HG	2.21	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	319/327 (98%)	309 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	249/267 (93%)	240 (96%)	9 (4%)	31	44

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	39	ILE
1	A	101	LEU
1	A	121	GLU
1	A	135	GLU
1	A	185	VAL
1	A	231	LEU
1	A	308	ARG
1	A	324	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

3 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	$\# Z > 2$
3	SO4	A	403	-	4,4,4	0.42	0	6,6,6	0.08	0
2	DKR	A	401	-	17,17,17	3.36	10 (58%)	22,22,22	4.42	6 (27%)
3	SO4	A	402	-	4,4,4	0.38	0	6,6,6	0.69	0

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	DKR	A	401	-	-	5/9/9/9	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	DKR	O08-C06	-7.87	1.08	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	DKR	C06-N07	5.75	1.43	1.33
2	A	401	DKR	C05-N01	-5.23	1.30	1.37
2	A	401	DKR	C02-N01	-3.68	1.27	1.37
2	A	401	DKR	C12-C11	-3.17	1.33	1.38
2	A	401	DKR	C11-C10	-3.16	1.32	1.38
2	A	401	DKR	C14-C15	-2.90	1.34	1.38
2	A	401	DKR	C15-C10	-2.79	1.33	1.38
2	A	401	DKR	C12-C13	-2.52	1.32	1.38
2	A	401	DKR	C04-C05	-2.33	1.35	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	DKR	C05-C06-N07	12.88	134.51	116.80
2	A	401	DKR	O08-C06-C05	-12.80	104.60	121.09
2	A	401	DKR	C09-N07-C06	6.46	131.29	122.07
2	A	401	DKR	C10-C09-N07	5.69	125.08	113.07
2	A	401	DKR	C04-C05-N01	2.41	109.30	106.95
2	A	401	DKR	C03-C04-C05	-2.04	105.83	107.72

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	DKR	C04-C05-C06-N07
2	A	401	DKR	N01-C05-C06-N07
2	A	401	DKR	N01-C05-C06-O08
2	A	401	DKR	C10-C09-N07-C06
2	A	401	DKR	C04-C05-C06-O08

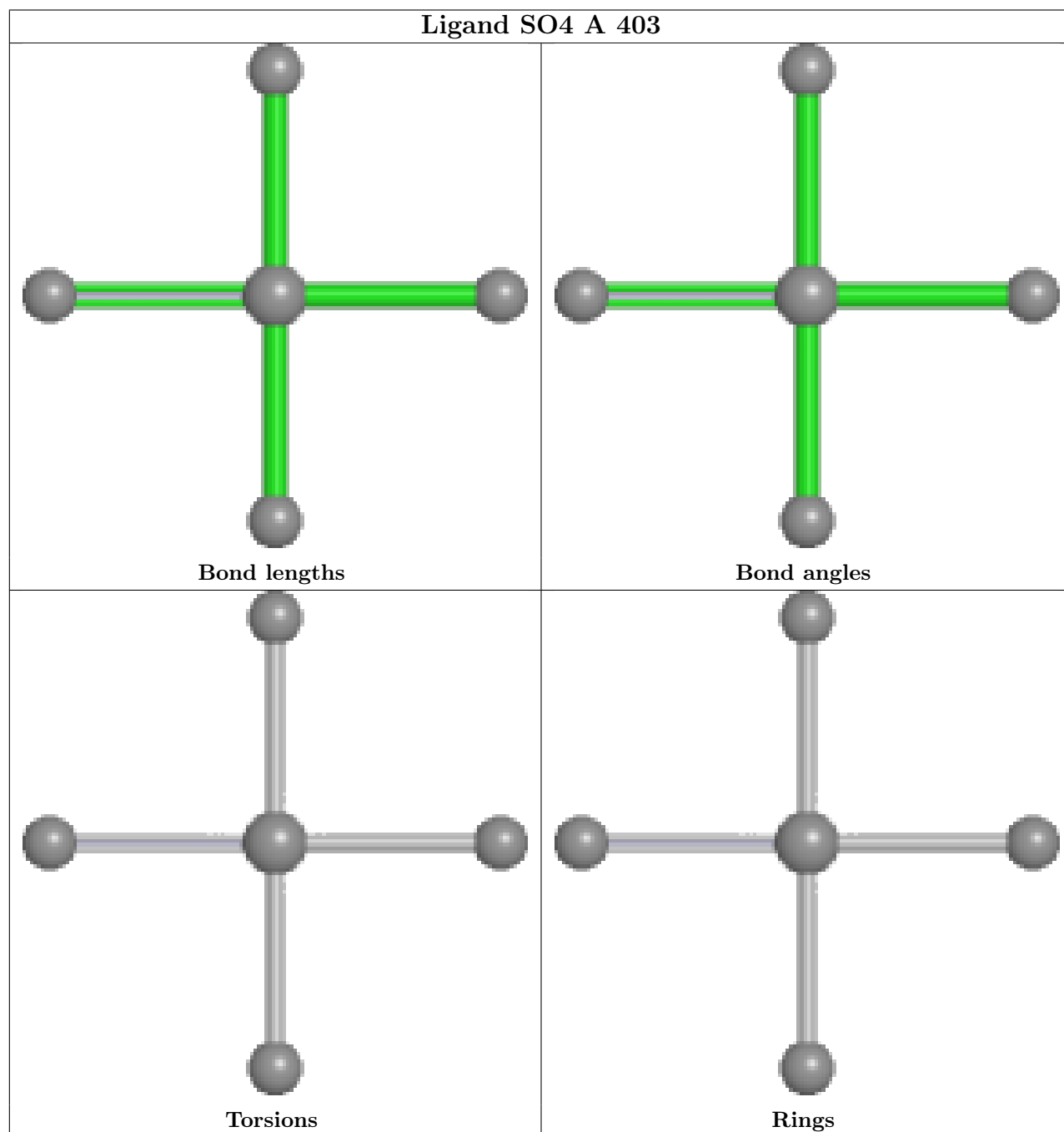
There are no ring outliers.

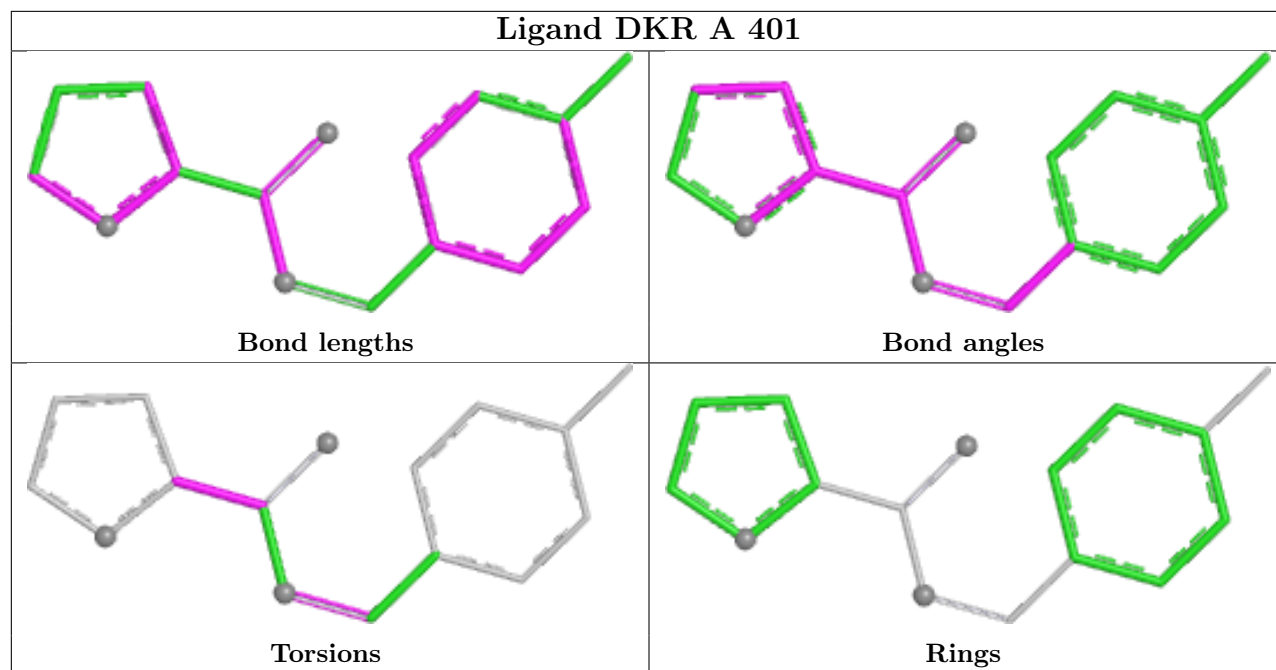
2 monomers are involved in 2 short contacts:

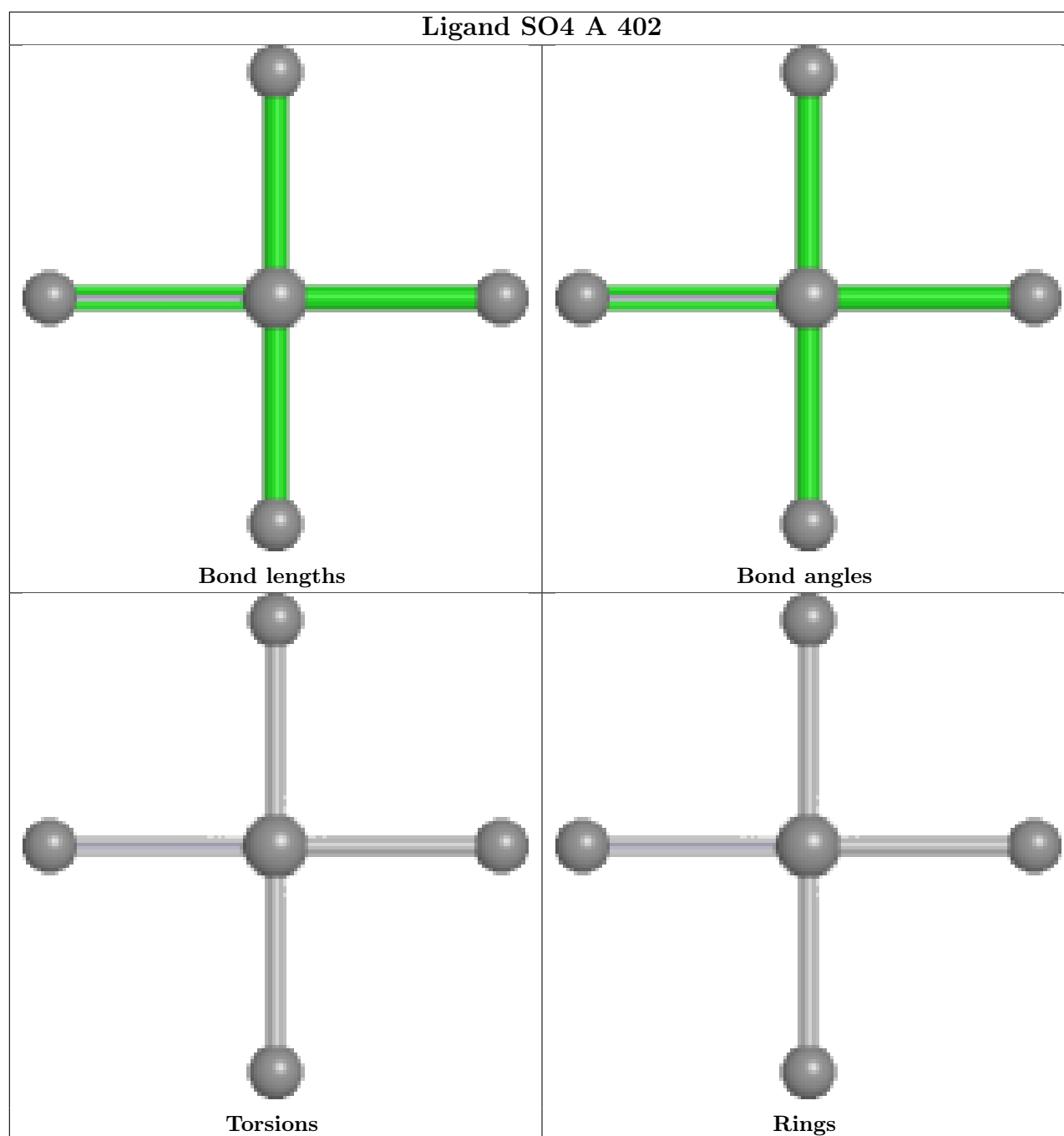
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	SO4	1	0
2	A	401	DKR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	321/327 (98%)	0.77	37 (11%) 9 9	27, 48, 80, 149	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	LEU	10.1
1	A	9	THR	9.3
1	A	8	GLN	8.7
1	A	41	ASP	7.8
1	A	170	GLY	6.4
1	A	328	GLU	6.2
1	A	73	GLY	6.0
1	A	327	PRO	5.7
1	A	69	GLN	5.5
1	A	10	ALA	5.0
1	A	71	VAL	5.0
1	A	57	GLN	4.9
1	A	18	GLN	4.7
1	A	40	SER	4.4
1	A	113	GLY	4.1
1	A	56	GLU	4.0
1	A	171	ASP	3.9
1	A	54	LEU	3.9
1	A	72	GLY	3.6
1	A	202	GLU	3.5
1	A	45	ASP	3.5
1	A	97	THR	3.5
1	A	74	ALA	3.5
1	A	318	ARG	3.4
1	A	112	VAL	3.3
1	A	42	ALA	2.9
1	A	172	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	88	ARG	2.8
1	A	32	TYR	2.7
1	A	68	THR	2.7
1	A	46	GLU	2.7
1	A	115	ALA	2.4
1	A	313	THR	2.3
1	A	314	SER	2.3
1	A	62	ARG	2.3
1	A	50	ARG	2.1
1	A	98	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

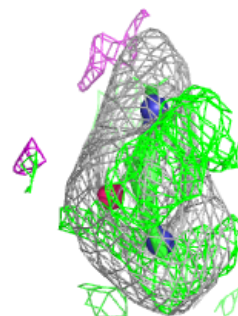
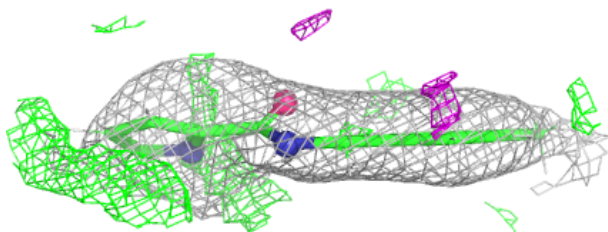
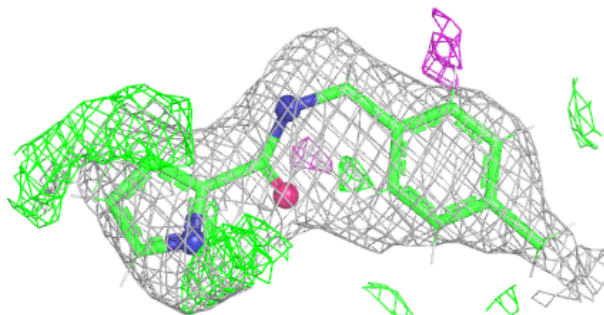
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DKR	A	401	16/16	0.76	0.28	49,66,90,99	0
3	SO4	A	403	5/5	0.97	0.09	40,42,51,52	0
3	SO4	A	402	5/5	0.98	0.08	37,40,45,55	0

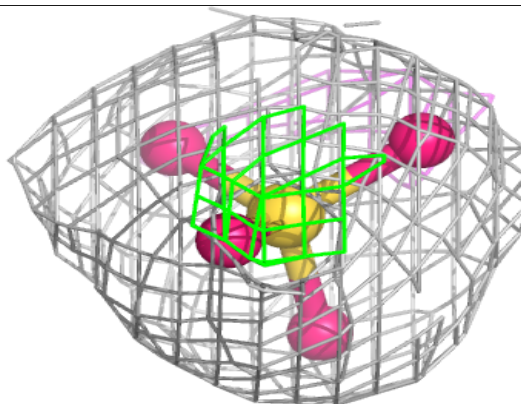
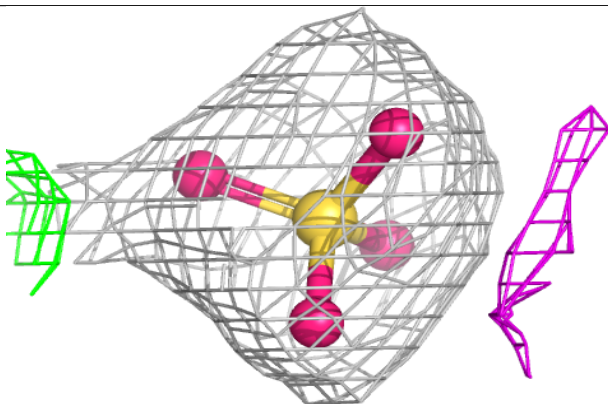
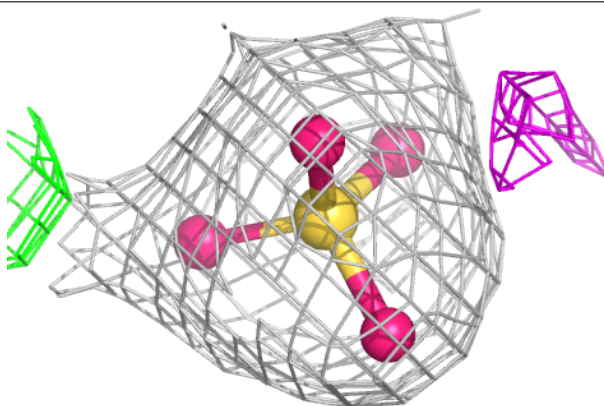
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DKR A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

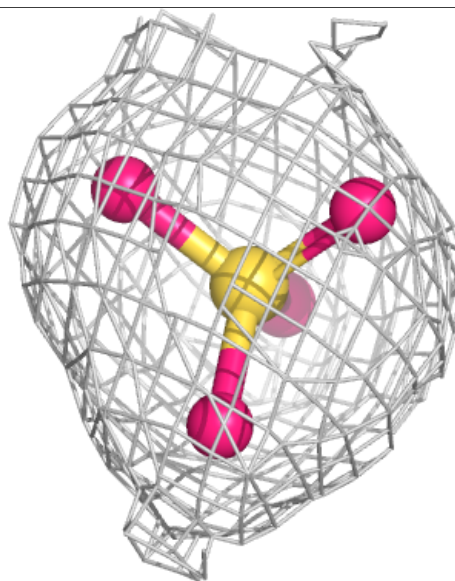
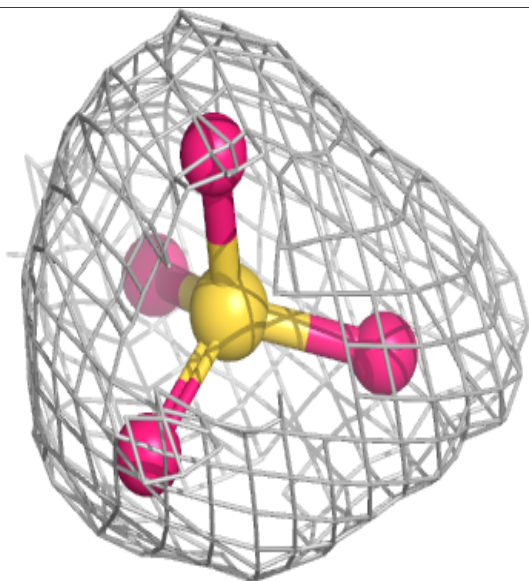
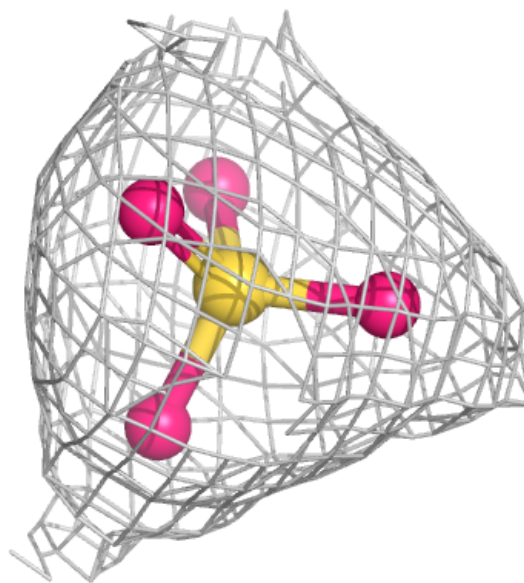
**Electron density around SO4 A 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SO4 A 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.