



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:07 AM UTC

PDB ID : 8W50 / pdb_00008w50
Title : Crystal structure of DNA binding and cleavage core of human topoisomerase 2-alpha in a DNA binding-competent conformation
Authors : Chan, N.L.; Liu, K.T.; Chen, S.F.
Deposited on : 2023-08-25
Resolution : 2.67 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

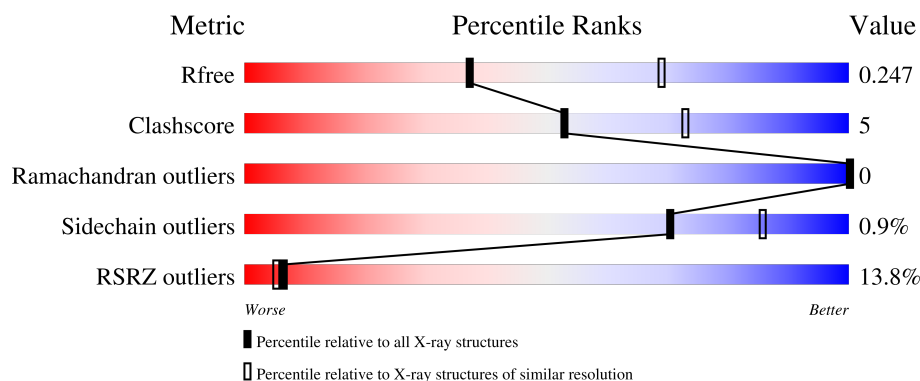
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	806	6% 78% 12% 10%
1	B	806	7% 77% 12% 11%
1	C	806	14% 70% 10% 20%
1	D	806	21% 72% 9% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20918 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 DNA topoisomerase 2-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	1	0
			5689	3662	932	1068	27			
1	B	716	Total	C	N	O	S	0	0	0
			5457	3500	906	1028	23			
1	C	644	Total	C	N	O	S	0	0	0
			4702	3006	788	888	20			
1	D	656	Total	C	N	O	S	0	0	0
			4673	2995	786	870	22			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	403	MET	-	expression tag	UNP P11388
A	404	ALA	-	expression tag	UNP P11388
A	405	SER	-	expression tag	UNP P11388
A	406	TRP	-	expression tag	UNP P11388
A	407	SER	-	expression tag	UNP P11388
A	408	HIS	-	expression tag	UNP P11388
A	409	PRO	-	expression tag	UNP P11388
A	410	GLN	-	expression tag	UNP P11388
A	411	PHE	-	expression tag	UNP P11388
A	412	GLU	-	expression tag	UNP P11388
A	413	LYS	-	expression tag	UNP P11388
A	414	GLY	-	expression tag	UNP P11388
A	415	ALA	-	expression tag	UNP P11388
A	416	ASP	-	expression tag	UNP P11388
A	417	ASP	-	expression tag	UNP P11388
A	418	ASP	-	expression tag	UNP P11388
A	419	ASP	-	expression tag	UNP P11388
A	420	LYS	-	expression tag	UNP P11388
A	421	VAL	-	expression tag	UNP P11388
A	422	PRO	-	expression tag	UNP P11388
A	423	ASP	-	expression tag	UNP P11388

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Chain	Residue	Modelled	Actual	Comment	Reference
A	424	PRO	-	expression tag	UNP P11388
A	425	THR	-	expression tag	UNP P11388
A	426	SER	-	expression tag	UNP P11388
A	427	VAL	-	expression tag	UNP P11388
A	428	ASP	-	expression tag	UNP P11388
A	1189	GLY	-	expression tag	UNP P11388
A	1190	ALA	-	expression tag	UNP P11388
A	1191	PRO	-	expression tag	UNP P11388
A	1192	GLY	-	expression tag	UNP P11388
A	1193	PHE	-	expression tag	UNP P11388
A	1194	SER	-	expression tag	UNP P11388
A	1195	SER	-	expression tag	UNP P11388
A	1196	ILE	-	expression tag	UNP P11388
A	1197	SER	-	expression tag	UNP P11388
A	1198	ALA	-	expression tag	UNP P11388
A	1199	HIS	-	expression tag	UNP P11388
A	1200	HIS	-	expression tag	UNP P11388
A	1201	HIS	-	expression tag	UNP P11388
A	1202	HIS	-	expression tag	UNP P11388
A	1203	HIS	-	expression tag	UNP P11388
A	1204	HIS	-	expression tag	UNP P11388
A	1205	HIS	-	expression tag	UNP P11388
A	1206	HIS	-	expression tag	UNP P11388
A	1207	HIS	-	expression tag	UNP P11388
A	1208	HIS	-	expression tag	UNP P11388
B	403	MET	-	expression tag	UNP P11388
B	404	ALA	-	expression tag	UNP P11388
B	405	SER	-	expression tag	UNP P11388
B	406	TRP	-	expression tag	UNP P11388
B	407	SER	-	expression tag	UNP P11388
B	408	HIS	-	expression tag	UNP P11388
B	409	PRO	-	expression tag	UNP P11388
B	410	GLN	-	expression tag	UNP P11388
B	411	PHE	-	expression tag	UNP P11388
B	412	GLU	-	expression tag	UNP P11388
B	413	LYS	-	expression tag	UNP P11388
B	414	GLY	-	expression tag	UNP P11388
B	415	ALA	-	expression tag	UNP P11388
B	416	ASP	-	expression tag	UNP P11388
B	417	ASP	-	expression tag	UNP P11388
B	418	ASP	-	expression tag	UNP P11388
B	419	ASP	-	expression tag	UNP P11388

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Chain	Residue	Modelled	Actual	Comment	Reference
B	420	LYS	-	expression tag	UNP P11388
B	421	VAL	-	expression tag	UNP P11388
B	422	PRO	-	expression tag	UNP P11388
B	423	ASP	-	expression tag	UNP P11388
B	424	PRO	-	expression tag	UNP P11388
B	425	THR	-	expression tag	UNP P11388
B	426	SER	-	expression tag	UNP P11388
B	427	VAL	-	expression tag	UNP P11388
B	428	ASP	-	expression tag	UNP P11388
B	1189	GLY	-	expression tag	UNP P11388
B	1190	ALA	-	expression tag	UNP P11388
B	1191	PRO	-	expression tag	UNP P11388
B	1192	GLY	-	expression tag	UNP P11388
B	1193	PHE	-	expression tag	UNP P11388
B	1194	SER	-	expression tag	UNP P11388
B	1195	SER	-	expression tag	UNP P11388
B	1196	ILE	-	expression tag	UNP P11388
B	1197	SER	-	expression tag	UNP P11388
B	1198	ALA	-	expression tag	UNP P11388
B	1199	HIS	-	expression tag	UNP P11388
B	1200	HIS	-	expression tag	UNP P11388
B	1201	HIS	-	expression tag	UNP P11388
B	1202	HIS	-	expression tag	UNP P11388
B	1203	HIS	-	expression tag	UNP P11388
B	1204	HIS	-	expression tag	UNP P11388
B	1205	HIS	-	expression tag	UNP P11388
B	1206	HIS	-	expression tag	UNP P11388
B	1207	HIS	-	expression tag	UNP P11388
B	1208	HIS	-	expression tag	UNP P11388
C	403	MET	-	expression tag	UNP P11388
C	404	ALA	-	expression tag	UNP P11388
C	405	SER	-	expression tag	UNP P11388
C	406	TRP	-	expression tag	UNP P11388
C	407	SER	-	expression tag	UNP P11388
C	408	HIS	-	expression tag	UNP P11388
C	409	PRO	-	expression tag	UNP P11388
C	410	GLN	-	expression tag	UNP P11388
C	411	PHE	-	expression tag	UNP P11388
C	412	GLU	-	expression tag	UNP P11388
C	413	LYS	-	expression tag	UNP P11388
C	414	GLY	-	expression tag	UNP P11388
C	415	ALA	-	expression tag	UNP P11388

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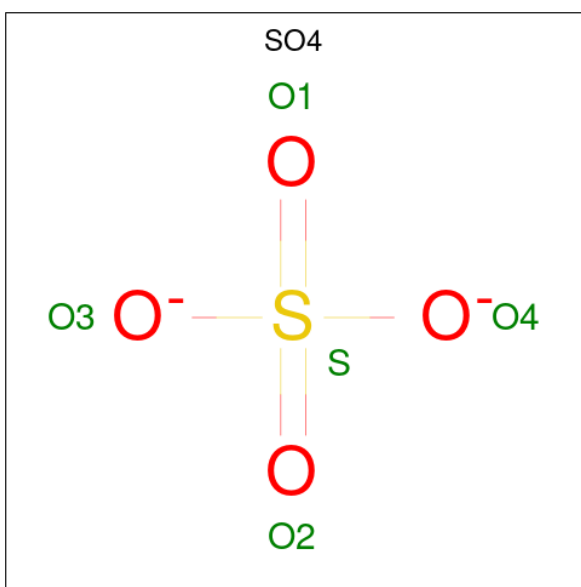
Chain	Residue	Modelled	Actual	Comment	Reference
C	416	ASP	-	expression tag	UNP P11388
C	417	ASP	-	expression tag	UNP P11388
C	418	ASP	-	expression tag	UNP P11388
C	419	ASP	-	expression tag	UNP P11388
C	420	LYS	-	expression tag	UNP P11388
C	421	VAL	-	expression tag	UNP P11388
C	422	PRO	-	expression tag	UNP P11388
C	423	ASP	-	expression tag	UNP P11388
C	424	PRO	-	expression tag	UNP P11388
C	425	THR	-	expression tag	UNP P11388
C	426	SER	-	expression tag	UNP P11388
C	427	VAL	-	expression tag	UNP P11388
C	428	ASP	-	expression tag	UNP P11388
C	1189	GLY	-	expression tag	UNP P11388
C	1190	ALA	-	expression tag	UNP P11388
C	1191	PRO	-	expression tag	UNP P11388
C	1192	GLY	-	expression tag	UNP P11388
C	1193	PHE	-	expression tag	UNP P11388
C	1194	SER	-	expression tag	UNP P11388
C	1195	SER	-	expression tag	UNP P11388
C	1196	ILE	-	expression tag	UNP P11388
C	1197	SER	-	expression tag	UNP P11388
C	1198	ALA	-	expression tag	UNP P11388
C	1199	HIS	-	expression tag	UNP P11388
C	1200	HIS	-	expression tag	UNP P11388
C	1201	HIS	-	expression tag	UNP P11388
C	1202	HIS	-	expression tag	UNP P11388
C	1203	HIS	-	expression tag	UNP P11388
C	1204	HIS	-	expression tag	UNP P11388
C	1205	HIS	-	expression tag	UNP P11388
C	1206	HIS	-	expression tag	UNP P11388
C	1207	HIS	-	expression tag	UNP P11388
C	1208	HIS	-	expression tag	UNP P11388
D	403	MET	-	expression tag	UNP P11388
D	404	ALA	-	expression tag	UNP P11388
D	405	SER	-	expression tag	UNP P11388
D	406	TRP	-	expression tag	UNP P11388
D	407	SER	-	expression tag	UNP P11388
D	408	HIS	-	expression tag	UNP P11388
D	409	PRO	-	expression tag	UNP P11388
D	410	GLN	-	expression tag	UNP P11388
D	411	PHE	-	expression tag	UNP P11388

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Chain	Residue	Modelled	Actual	Comment	Reference
D	412	GLU	-	expression tag	UNP P11388
D	413	LYS	-	expression tag	UNP P11388
D	414	GLY	-	expression tag	UNP P11388
D	415	ALA	-	expression tag	UNP P11388
D	416	ASP	-	expression tag	UNP P11388
D	417	ASP	-	expression tag	UNP P11388
D	418	ASP	-	expression tag	UNP P11388
D	419	ASP	-	expression tag	UNP P11388
D	420	LYS	-	expression tag	UNP P11388
D	421	VAL	-	expression tag	UNP P11388
D	422	PRO	-	expression tag	UNP P11388
D	423	ASP	-	expression tag	UNP P11388
D	424	PRO	-	expression tag	UNP P11388
D	425	THR	-	expression tag	UNP P11388
D	426	SER	-	expression tag	UNP P11388
D	427	VAL	-	expression tag	UNP P11388
D	428	ASP	-	expression tag	UNP P11388
D	1189	GLY	-	expression tag	UNP P11388
D	1190	ALA	-	expression tag	UNP P11388
D	1191	PRO	-	expression tag	UNP P11388
D	1192	GLY	-	expression tag	UNP P11388
D	1193	PHE	-	expression tag	UNP P11388
D	1194	SER	-	expression tag	UNP P11388
D	1195	SER	-	expression tag	UNP P11388
D	1196	ILE	-	expression tag	UNP P11388
D	1197	SER	-	expression tag	UNP P11388
D	1198	ALA	-	expression tag	UNP P11388
D	1199	HIS	-	expression tag	UNP P11388
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D	1202	HIS	-	expression tag	UNP P11388
D	1203	HIS	-	expression tag	UNP P11388
D	1204	HIS	-	expression tag	UNP P11388
D	1205	HIS	-	expression tag	UNP P11388
D	1206	HIS	-	expression tag	UNP P11388
D	1207	HIS	-	expression tag	UNP P11388
D	1208	HIS	-	expression tag	UNP P11388

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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		
2	B	1	Total	O	S	0	0
			5	4	1		

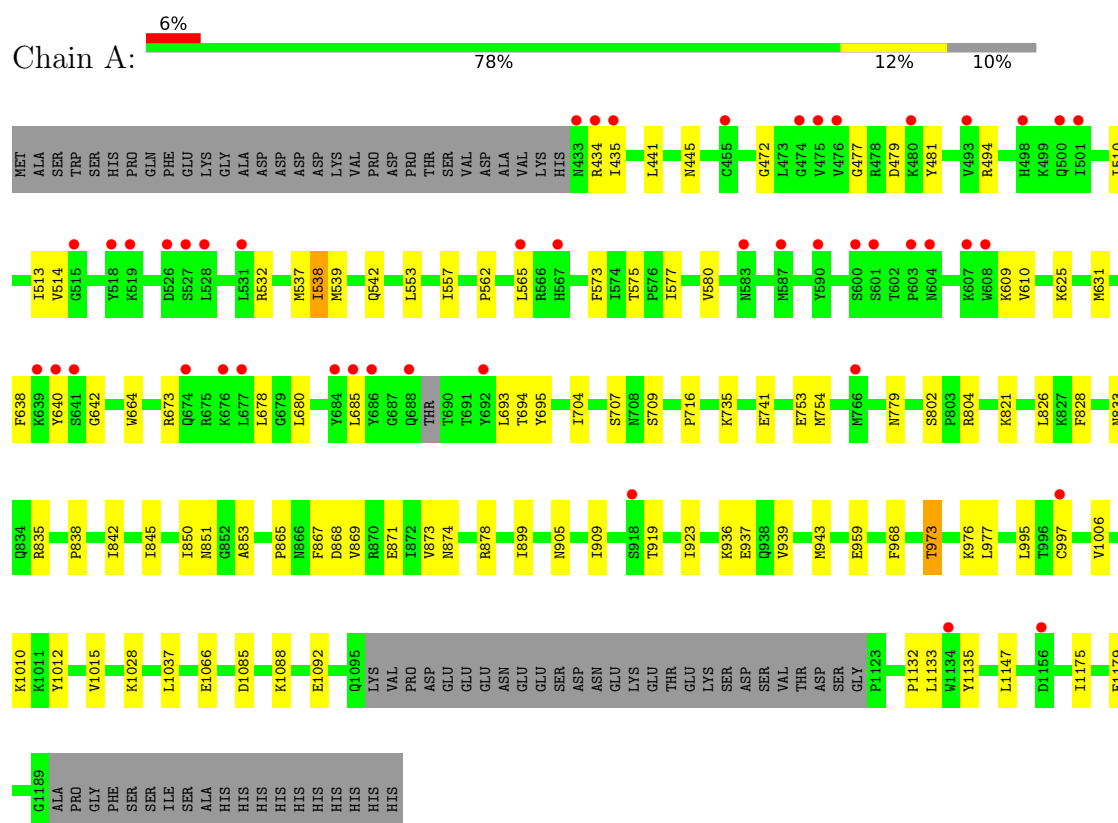
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	201	Total	O	0	0
			201	201		
3	B	120	Total	O	0	0
			120	120		
3	C	54	Total	O	0	0
			54	54		
3	D	7	Total	O	0	0
			7	7		

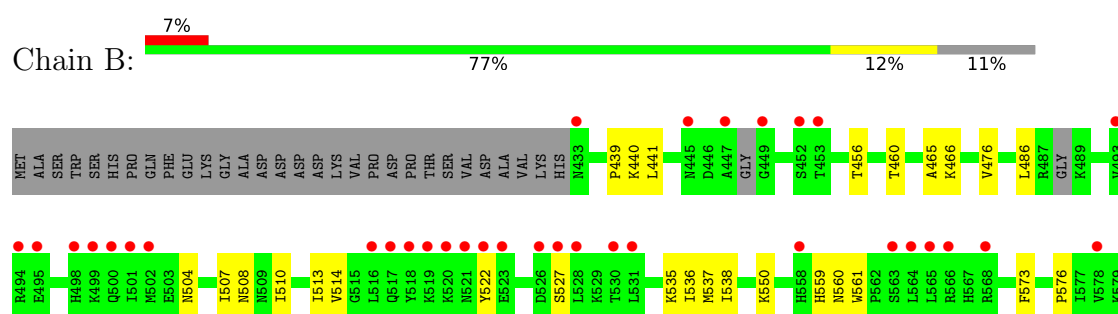
3 Residue-property plots [i](#)

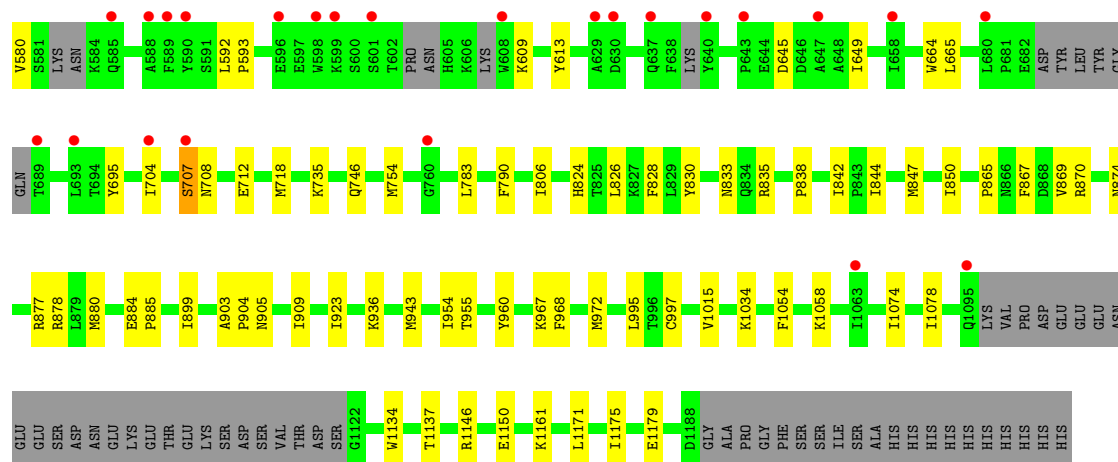
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 topoisomerase 2-alpha

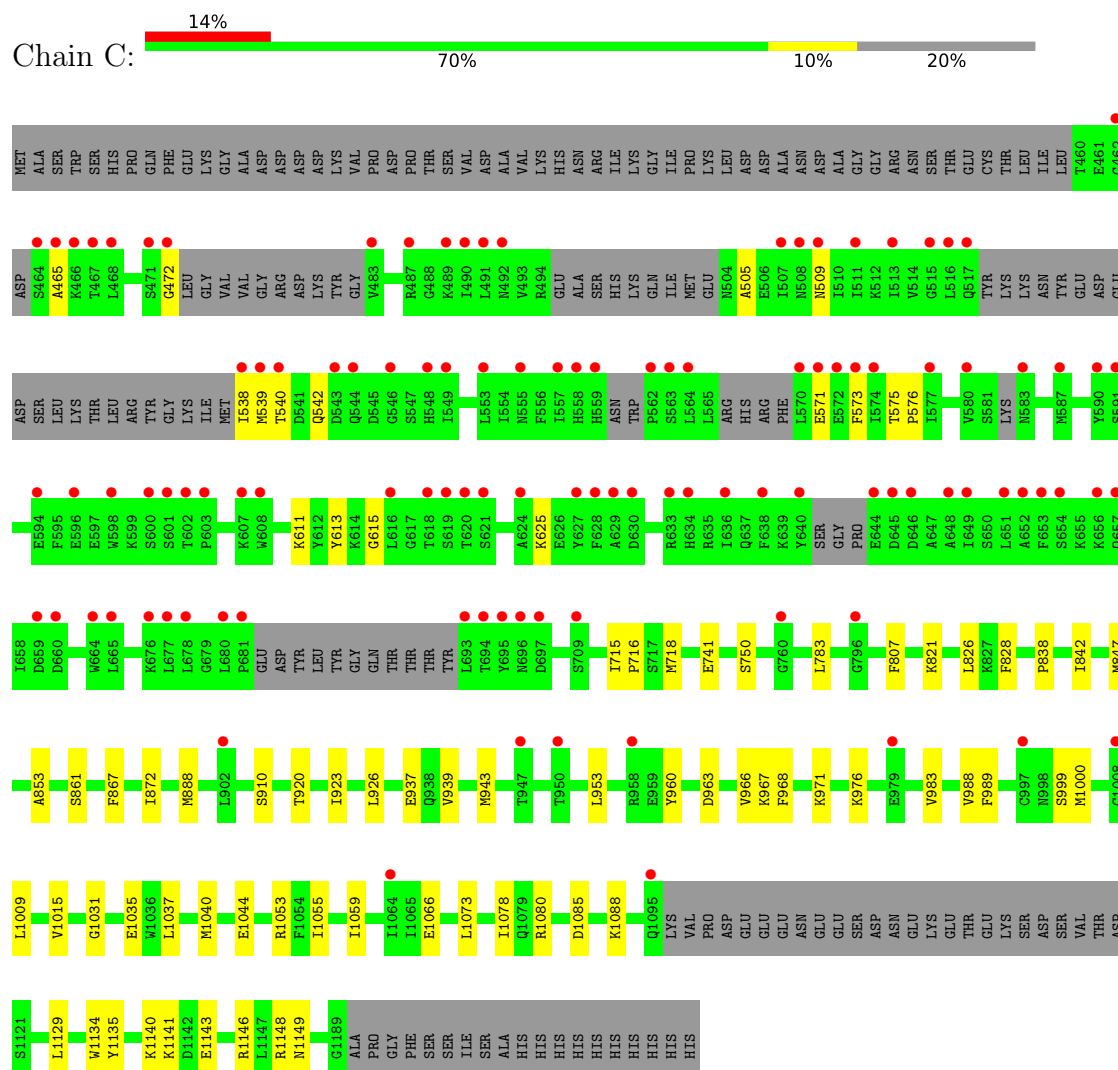


• Molecule 1: DNA topoisomerase 2-alpha

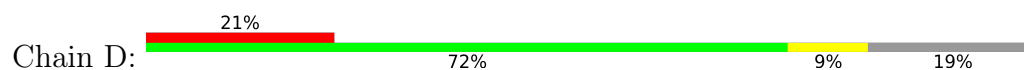


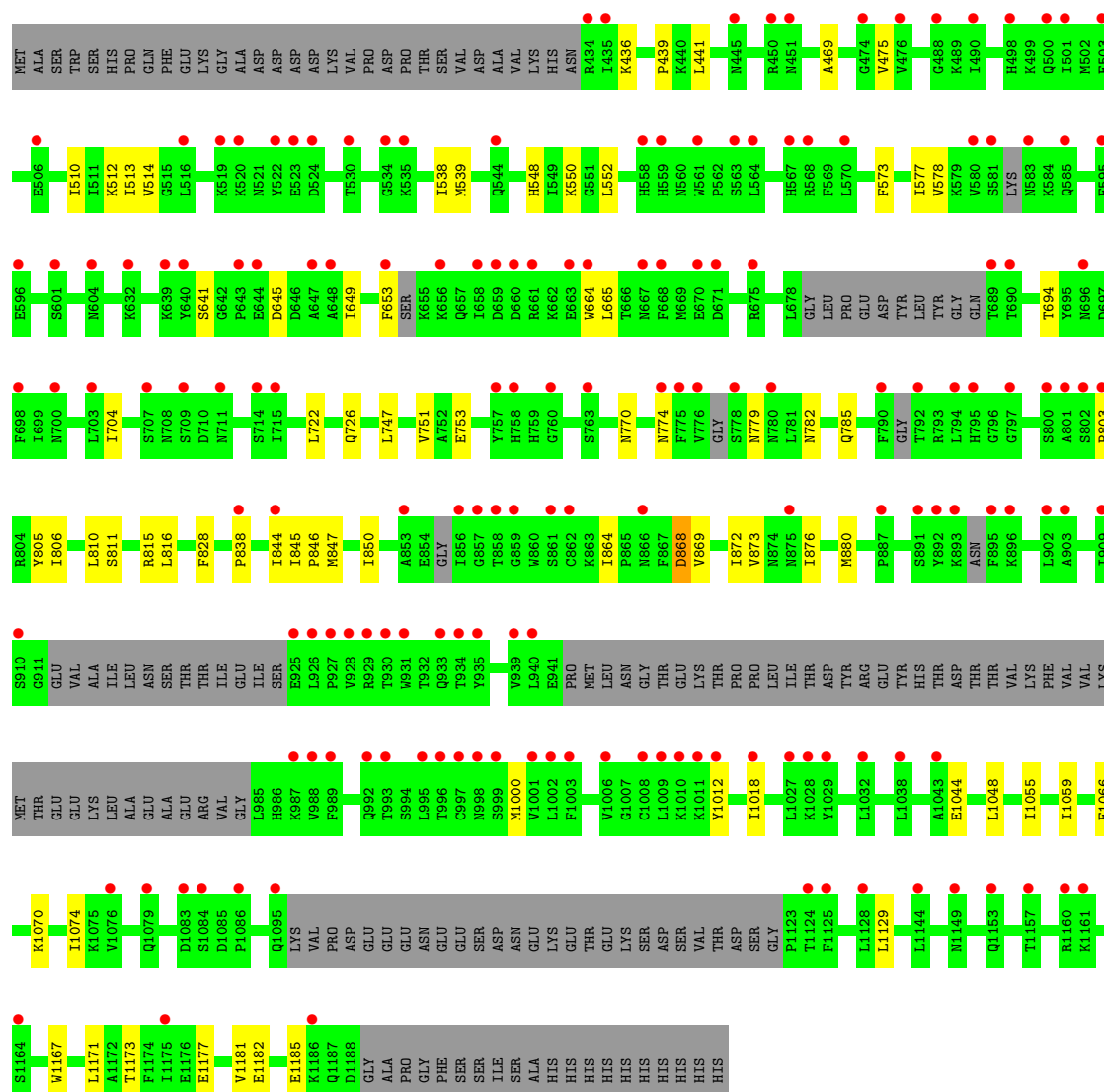


- Molecule 1: DNA topoisomerase 2-alpha



- Molecule 1: DNA topoisomerase 2-alpha





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	266.10Å 266.10Å 172.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.19 – 2.67 23.19 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.0 (23.19-2.67) 98.9 (23.19-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.67Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.222 , 0.248 0.222 , 0.247	Depositor DCC
R_{free} test set	2025 reflections (1.56%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20918	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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 [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	0.16	0/5810	0.34	0/7866
1	B	0.15	0/5561	0.33	0/7534
1	C	0.15	0/4786	0.30	0/6496
1	D	0.14	0/4767	0.30	0/6495
All	All	0.15	0/20924	0.32	0/28391

There are no bond length outliers.

There are no bond angle outliers.

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	5689	0	5467	58	0
1	B	5457	0	5129	57	0
1	C	4702	0	4204	49	0
1	D	4673	0	3960	46	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	201	0	0	3	0
3	B	120	0	0	1	0
3	C	54	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	7	0	0	0	0
All	All	20918	0	18760	197	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 5.

All (197) 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:D:577:ILE:HG23	1:D:578:VAL:HG23	1.62	0.81
1:C:542:GLN:HE21	1:C:575:THR:HG22	1.55	0.72
1:D:864:ILE:HG12	1:D:1000:MET:HG2	1.72	0.71
1:C:1059:ILE:HG23	1:D:1066:GLU:HB3	1.75	0.68
1:B:850:ILE:HD12	1:B:869:VAL:HG22	1.78	0.66
1:A:821:LYS:HD3	1:A:1037:LEU:HD11	1.78	0.66
1:C:923:ILE:HB	1:C:968:PHE:HB2	1.76	0.66
1:A:735:LYS:HD3	1:A:754:MET:HE3	1.77	0.65
1:D:645:ASP:O	1:D:649:ILE:HG13	1.97	0.65
1:C:1066:GLU:HB3	1:D:1059:ILE:HG23	1.77	0.65
1:D:641:SER:OG	1:D:645:ASP:OD2	2.11	0.64
1:B:522:TYR:HA	1:B:527:SER:HB3	1.80	0.63
1:A:939:VAL:O	1:A:943:MET:HG3	1.98	0.63
1:A:1088:LYS:O	1:A:1092:GLU:HG3	1.98	0.63
1:D:774:ASN:HB3	1:D:782:ASN:HD22	1.63	0.63
1:C:538:ILE:N	1:C:571:GLU:O	2.33	0.62
1:C:920:THR:HG23	1:C:971:LYS:HG2	1.81	0.62
1:A:1132:PRO:HD2	1:A:1135:TYR:CE1	2.35	0.61
1:A:1066:GLU:OE1	1:B:1058:LYS:NZ	2.32	0.60
1:C:943:MET:HE1	1:C:989:PHE:CE1	2.36	0.60
1:C:937:GLU:HG2	1:D:439:PRO:HB2	1.82	0.60
1:A:537:MET:HE1	1:A:631:MET:HE3	1.82	0.60
1:A:850:ILE:HD12	1:A:869:VAL:HG22	1.84	0.59
1:A:973:THR:HG22	1:A:976:LYS:H	1.68	0.59
1:A:542:GLN:HE22	1:A:575:THR:H	1.50	0.59
1:B:649:ILE:HD11	1:B:695:TYR:HB3	1.85	0.59
1:A:562:PRO:HA	1:A:565:LEU:HD13	1.83	0.58
1:A:441:LEU:HD22	1:A:513:ILE:HG12	1.84	0.58
1:A:735:LYS:HB3	1:A:754:MET:HE1	1.85	0.58
1:A:716:PRO:HG2	1:A:853:ALA:HB1	1.85	0.58
1:B:665:LEU:HD11	1:B:707:SER:HB3	1.86	0.57
1:C:939:VAL:O	1:C:943:MET:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:LEU:HD22	1:A:693:LEU:HD11	1.87	0.57
1:C:828:PHE:HA	1:C:838:PRO:HA	1.87	0.56
1:D:664:TRP:CE2	1:D:704:ILE:HD13	2.41	0.56
1:B:1074:ILE:O	1:B:1078:ILE:HG13	2.05	0.56
1:D:770:ASN:O	1:D:779:ASN:ND2	2.38	0.55
1:D:1044:GLU:O	1:D:1048:LEU:HD12	2.05	0.55
1:B:1146:ARG:NH2	1:B:1150:GLU:OE1	2.39	0.55
1:D:1055:ILE:O	1:D:1059:ILE:HG13	2.07	0.55
1:B:826:LEU:HD21	1:B:842:ILE:HG22	1.88	0.55
1:B:954:ILE:HG22	1:B:972:MET:HG2	1.89	0.54
1:A:835:ARG:NE	3:A:1406:HOH:O	2.40	0.54
1:B:735:LYS:HB3	1:B:754:MET:HE1	1.89	0.54
1:A:779:ASN:HD22	1:A:851:ASN:HB3	1.72	0.54
1:B:504:ASN:O	1:B:508:ASN:ND2	2.41	0.54
1:A:923:ILE:HB	1:A:968:PHE:HB2	1.89	0.54
1:B:708:ASN:ND2	1:B:712:GLU:OE2	2.41	0.54
1:A:680:LEU:HD21	1:C:988:VAL:HA	1.88	0.54
1:D:1070:LYS:O	1:D:1074:ILE:HG13	2.07	0.54
1:B:486:LEU:HD11	1:B:510:ILE:HD11	1.91	0.53
1:A:865:PRO:HB3	1:A:995:LEU:HD21	1.91	0.53
1:D:469:ALA:HB2	1:D:539:MET:HE1	1.91	0.53
1:A:867:PHE:CZ	1:A:1015:VAL:HG11	2.44	0.53
1:D:1177:GLU:O	1:D:1181:VAL:HG12	2.08	0.53
1:C:826:LEU:HD21	1:C:842:ILE:HG22	1.90	0.53
1:B:1034:LYS:NZ	1:B:1161:LYS:O	2.38	0.53
1:C:1085:ASP:HB3	1:C:1088:LYS:HB3	1.90	0.53
1:A:538:ILE:HD13	1:A:553:LEU:HD22	1.90	0.52
1:D:846:PRO:HD2	1:D:872:ILE:HG21	1.91	0.52
1:A:539:MET:HE2	1:A:573:PHE:CG	2.45	0.51
1:C:539:MET:HG3	1:C:573:PHE:HB3	1.92	0.51
1:B:1134:TRP:O	1:B:1137:THR:OG1	2.16	0.51
1:D:803:PRO:HA	1:D:806:ILE:HG12	1.91	0.51
1:B:865:PRO:HB3	1:B:995:LEU:HD21	1.91	0.51
1:C:472:GLY:HA2	1:C:625:LYS:HA	1.92	0.51
1:D:552:LEU:HD22	1:D:653:PHE:HE2	1.74	0.51
1:A:477:GLY:O	1:A:481:TYR:HB2	2.11	0.51
1:D:876:ILE:O	1:D:880:MET:HG3	2.10	0.51
1:B:441:LEU:HD22	1:B:513:ILE:HG12	1.92	0.50
1:B:537:MET:HE2	1:B:573:PHE:HB2	1.93	0.50
1:A:1028:LYS:NZ	3:A:1404:HOH:O	2.39	0.50
1:B:824:HIS:ND1	3:B:1401:HOH:O	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1055:ILE:O	1:C:1059:ILE:HG13	2.11	0.50
1:B:828:PHE:HA	1:B:838:PRO:HA	1.94	0.50
1:C:542:GLN:NE2	1:C:575:THR:H	2.09	0.50
1:B:903:ALA:HB1	1:B:904:PRO:HD2	1.94	0.49
1:A:936:LYS:HD2	1:A:959:GLU:OE2	2.12	0.49
1:C:1134:TRP:CH2	1:D:1129:LEU:HD12	2.47	0.49
1:A:664:TRP:CE2	1:A:704:ILE:HD12	2.48	0.49
1:D:539:MET:HG3	1:D:573:PHE:HB3	1.95	0.49
1:B:867:PHE:CZ	1:B:1015:VAL:HG11	2.47	0.49
1:B:943:MET:HB3	1:B:954:ILE:HG12	1.94	0.48
1:B:830:TYR:CZ	1:B:835:ARG:HG3	2.47	0.48
1:A:434:ARG:HH12	1:B:936:LYS:HE3	1.77	0.48
1:A:868:ASP:HB3	1:A:871:GLU:HB2	1.96	0.48
1:D:868:ASP:O	1:D:872:ILE:HD12	2.14	0.48
1:D:847:MET:HA	1:D:850:ILE:HD12	1.95	0.48
1:A:445:ASN:HB2	1:A:479:ASP:HA	1.94	0.48
1:D:828:PHE:HA	1:D:838:PRO:HA	1.95	0.48
1:A:1133:LEU:HD12	1:B:1054:PHE:HE2	1.78	0.48
1:B:664:TRP:CE2	1:B:704:ILE:HD12	2.49	0.48
1:D:844:ILE:HG13	1:D:845:ILE:HG23	1.96	0.48
1:D:1167:TRP:O	1:D:1171:LEU:HG	2.14	0.47
1:A:673:ARG:HG3	1:A:1006:VAL:HG11	1.96	0.47
1:D:785:GLN:NE2	1:D:810:LEU:O	2.47	0.47
1:B:456:THR:HG23	1:B:535:LYS:HB2	1.96	0.47
1:D:538:ILE:HG21	1:D:550:LYS:HG2	1.95	0.47
1:A:1085:ASP:HB3	1:A:1088:LYS:HB3	1.95	0.47
1:C:741:GLU:HG3	1:C:807:PHE:CD2	2.50	0.47
1:A:874:ASN:O	1:A:878:ARG:HG3	2.14	0.47
1:D:869:VAL:O	1:D:873:VAL:HG23	2.14	0.47
1:C:953:LEU:HD12	1:C:976:LYS:HD3	1.97	0.47
1:A:435:ILE:HD11	1:A:532:ARG:CZ	2.45	0.46
1:A:1010:LYS:HD3	1:A:1012:TYR:CZ	2.50	0.46
1:D:436:LYS:O	1:D:512:LYS:NZ	2.48	0.46
1:C:963:ASP:OD1	1:C:963:ASP:N	2.47	0.46
1:A:828:PHE:HA	1:A:838:PRO:HA	1.97	0.46
1:B:440:LYS:O	1:B:466:LYS:NZ	2.46	0.46
1:C:867:PHE:CZ	1:C:1015:VAL:HG11	2.50	0.46
1:B:504:ASN:CG	1:B:507:ILE:HG12	2.41	0.46
1:C:1000:MET:HE1	1:C:1015:VAL:HG13	1.98	0.46
1:A:919:THR:H	1:A:977:LEU:HD23	1.80	0.46
1:B:783:LEU:HD21	1:B:847:MET:HE2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:MET:HE3	1:C:888:MET:HB2	1.77	0.45
1:B:870:ARG:NH2	1:B:1179:GLU:OE1	2.46	0.45
1:C:960:TYR:HB3	1:D:475:VAL:HG13	1.99	0.45
1:A:580:VAL:HA	1:A:609:LYS:O	2.16	0.45
1:D:665:LEU:HD23	1:D:704:ILE:HD11	1.98	0.45
1:B:580:VAL:HA	1:B:609:LYS:O	2.16	0.45
1:A:937:GLU:HG2	1:B:439:PRO:HB2	1.98	0.45
1:D:722:LEU:HD12	1:D:726:GLN:HB3	1.97	0.45
1:C:1031:GLY:O	1:C:1035:GLU:HG3	2.17	0.44
1:C:1073:LEU:HD21	1:C:1129:LEU:HD21	1.98	0.44
1:A:565:LEU:H	1:A:565:LEU:HD12	1.82	0.44
1:B:510:ILE:O	1:B:514:VAL:HG22	2.18	0.44
1:B:538:ILE:HG21	1:B:550:LYS:HG2	1.99	0.44
1:C:539:MET:HE2	1:C:539:MET:HB3	1.80	0.44
1:C:1040:MET:HE3	1:C:1044:GLU:HG3	1.99	0.44
1:D:747:LEU:O	1:D:751:VAL:HG23	2.18	0.44
1:B:514:VAL:HG11	1:B:536:ILE:HD11	1.99	0.44
1:B:560:ASN:HB2	1:B:561:TRP:CE3	2.53	0.44
1:B:905:ASN:HB3	1:B:997:CYS:HB2	1.99	0.44
1:C:505:ALA:O	1:C:509:ASN:N	2.48	0.44
1:C:615:GLY:HA3	1:D:805:TYR:CG	2.53	0.44
1:D:548:HIS:O	1:D:552:LEU:HD23	2.18	0.44
1:D:1012:TYR:CD1	1:D:1018:ILE:HG12	2.52	0.44
1:A:802:SER:OG	1:A:804:ARG:HG2	2.18	0.43
1:C:465:ALA:O	1:C:539:MET:HE1	2.18	0.43
1:D:785:GLN:HE21	1:D:811:SER:HA	1.83	0.43
1:D:774:ASN:HB3	1:D:782:ASN:ND2	2.32	0.43
1:A:678:LEU:HD13	1:C:983:VAL:HG11	1.99	0.43
1:B:877:ARG:HA	1:B:880:MET:HE2	2.01	0.43
1:D:552:LEU:HD22	1:D:653:PHE:CE2	2.53	0.43
1:A:753:GLU:HG2	1:B:746:GLN:HG3	2.00	0.43
1:A:826:LEU:HD21	1:A:842:ILE:HG22	2.00	0.43
1:C:861:SER:O	1:C:999:SER:OG	2.35	0.43
1:C:960:TYR:HB2	1:C:967:LYS:HB3	2.01	0.43
1:B:560:ASN:HB2	1:B:561:TRP:CZ3	2.54	0.43
1:B:790:PHE:CZ	1:B:806:ILE:HD12	2.54	0.43
1:B:923:ILE:HB	1:B:968:PHE:HB2	2.01	0.43
1:C:715:ILE:HG21	1:C:1009:LEU:HD21	2.01	0.43
1:D:1182:GLU:HA	1:D:1185:GLU:HG3	2.01	0.43
1:B:576:PRO:O	1:B:613:TYR:HB2	2.19	0.43
1:C:1148:ARG:NH2	1:C:1149:ASN:OD1	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:ILE:HG12	1:A:909:ILE:HG12	2.01	0.42
1:B:960:TYR:HB2	1:B:967:LYS:HG2	2.00	0.42
1:C:1053:ARG:NH2	1:C:1080:ARG:O	2.44	0.42
1:D:815:ARG:HD3	1:D:815:ARG:HA	1.86	0.42
1:B:718:MET:HE2	1:B:718:MET:HB2	1.80	0.42
1:A:905:ASN:HB3	1:A:997:CYS:HB2	2.01	0.42
1:C:611:LYS:HB3	1:C:613:TYR:HE1	1.83	0.42
1:D:441:LEU:HD13	1:D:513:ILE:HD13	2.00	0.42
1:B:874:ASN:O	1:B:878:ARG:HG3	2.20	0.42
1:D:510:ILE:O	1:D:514:VAL:HG23	2.20	0.42
1:B:1175:ILE:O	1:B:1179:GLU:HG2	2.19	0.42
1:C:1141:LYS:HB3	1:C:1141:LYS:HE3	1.82	0.42
1:C:718:MET:HE2	1:C:718:MET:HB2	1.93	0.42
1:C:1135:TYR:HA	1:C:1140:LYS:HB3	2.01	0.42
1:A:557:ILE:HG22	1:A:565:LEU:HD11	2.02	0.42
1:B:592:LEU:HB2	1:B:593:PRO:HD3	2.01	0.42
1:C:926:LEU:HG	1:C:966:VAL:HG11	2.01	0.42
1:B:790:PHE:CE2	1:B:806:ILE:HB	2.55	0.41
1:B:884:GLU:HG3	1:B:885:PRO:HD2	2.01	0.41
1:C:716:PRO:HG2	1:C:853:ALA:HB1	2.02	0.41
1:C:1143:GLU:HG3	1:C:1146:ARG:HH21	1.84	0.41
1:A:577:ILE:H	1:A:577:ILE:HG12	1.71	0.41
1:A:638:PHE:HB3	1:A:695:TYR:CE1	2.56	0.41
1:B:645:ASP:HB3	1:B:695:TYR:HB2	2.02	0.41
1:D:816:LEU:HD13	1:D:1173:THR:HG22	2.02	0.41
1:D:1181:VAL:O	1:D:1185:GLU:HG3	2.21	0.41
1:A:1175:ILE:O	1:A:1179:GLU:HG2	2.20	0.41
1:C:576:PRO:O	1:C:613:TYR:HB2	2.21	0.41
1:C:783:LEU:HD21	1:C:847:MET:HE2	2.02	0.41
1:A:610:VAL:O	1:A:833:ASN:ND2	2.47	0.41
1:B:460:THR:HB	1:B:465:ALA:HB3	2.03	0.41
1:A:472:GLY:HA2	1:A:625:LYS:HA	2.03	0.41
1:B:844:ILE:HD12	1:B:1171:LEU:HD23	2.02	0.41
1:B:899:ILE:HG12	1:B:909:ILE:HG12	2.02	0.41
1:C:1078:ILE:HD13	1:C:1078:ILE:HA	1.93	0.41
1:A:640:TYR:HD1	1:A:642:GLY:H	1.67	0.40
1:B:559:HIS:C	1:B:559:HIS:HD1	2.29	0.40
1:A:494:ARG:NH1	3:A:1413:HOH:O	2.48	0.40
1:A:845:ILE:HG21	1:A:873:VAL:HG22	2.04	0.40
1:A:510:ILE:O	1:A:514:VAL:HG23	2.21	0.40
1:A:539:MET:HE2	1:A:573:PHE:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:821:LYS:HD3	1:C:1037:LEU:HD11	2.04	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	724/806 (90%)	711 (98%)	13 (2%)	0	100	100
1	B	698/806 (87%)	683 (98%)	15 (2%)	0	100	100
1	C	622/806 (77%)	609 (98%)	13 (2%)	0	100	100
1	D	634/806 (79%)	622 (98%)	12 (2%)	0	100	100
All	All	2678/3224 (83%)	2625 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	575/724 (79%)	568 (99%)	7 (1%)	63	82
1	B	535/724 (74%)	531 (99%)	4 (1%)	76	89
1	C	420/724 (58%)	416 (99%)	4 (1%)	68	84
1	D	382/724 (53%)	379 (99%)	3 (1%)	73	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1912/2896 (66%)	1894 (99%)	18 (1%)	70 86

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	538	ILE
1	A	694	THR
1	A	707	SER
1	A	709	SER
1	A	741	GLU
1	A	973	THR
1	A	1147	LEU
1	B	476	VAL
1	B	707	SER
1	B	833	ASN
1	B	955	THR
1	C	540	THR
1	C	750	SER
1	C	872	ILE
1	C	910	SER
1	D	694	THR
1	D	753	GLU
1	D	868	ASP

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	508	ASN
1	A	542	GLN
1	A	746	GLN
1	A	773	GLN
1	A	779	ASN
1	A	905	ASN
1	A	906	GLN
1	A	1005	HIS
1	A	1094	GLN
1	B	770	ASN
1	B	833	ASN
1	B	986	HIS
1	C	542	GLN
1	C	700	ASN

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Mol	Chain	Res	Type
1	C	746	GLN
1	C	905	ASN
1	C	986	HIS
1	C	1094	GLN
1	D	445	ASN
1	D	451	ASN
1	D	548	HIS
1	D	558	HIS
1	D	782	ASN
1	D	785	GLN
1	D	789	GLN
1	D	1051	GLN
1	D	1126	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](#)

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	$\# Z > 2$
2	SO4	B	1301	-	4,4,4	0.84	0	6,6,6	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	1301	-	4,4,4	0.84	0	6,6,6	0.57	0
2	SO4	A	1302	-	4,4,4	0.85	0	6,6,6	0.53	0

There are no bond length outliers.

There are no bond angle outliers.

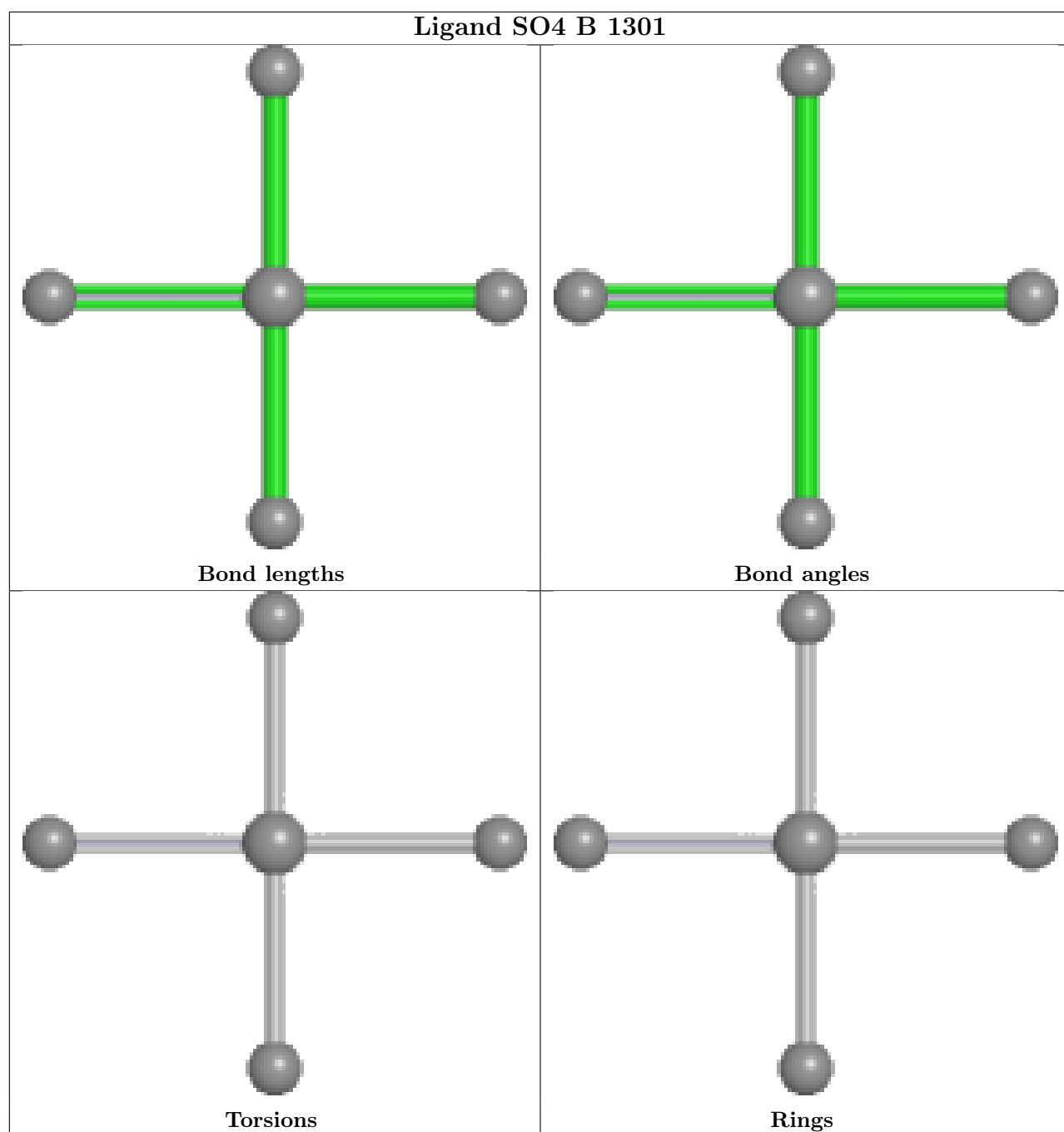
There are no chirality outliers.

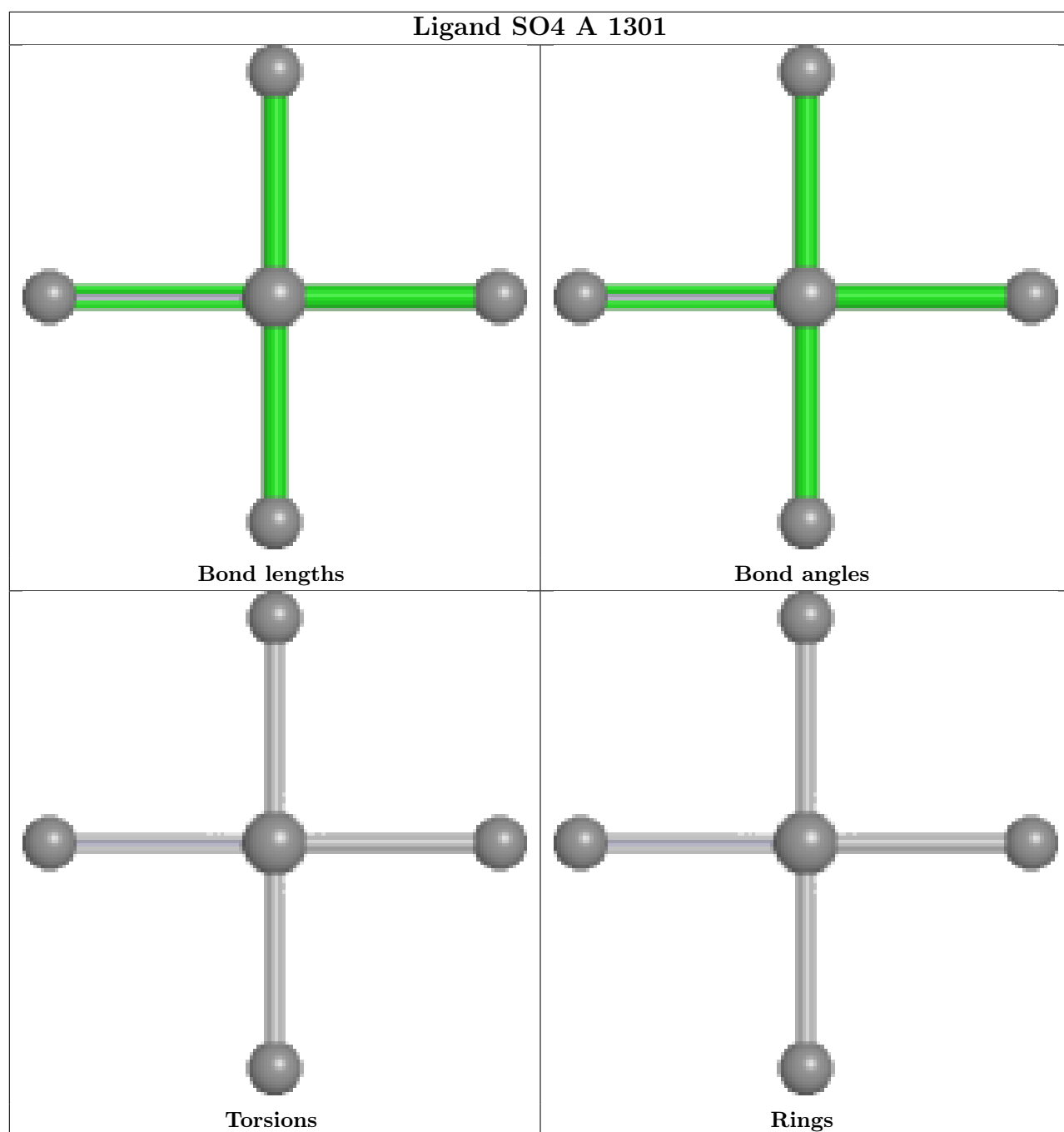
There are no torsion outliers.

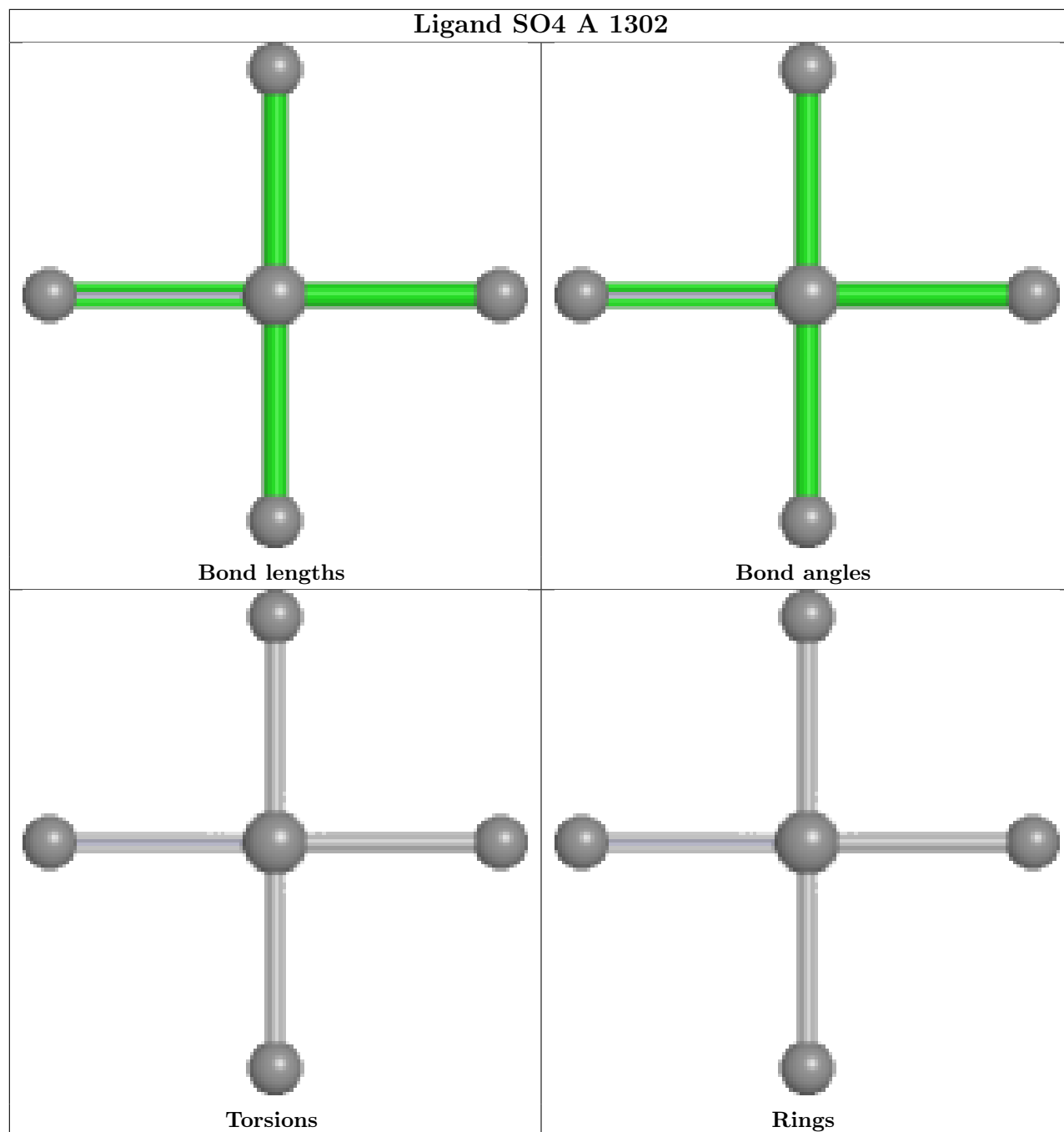
There are no ring outliers.

No monomer is involved in short contacts.

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	729/806 (90%)	0.26	46 (6%)	26 22	27, 51, 100, 151	1 (0%)
1	B	716/806 (88%)	0.36	58 (8%)	18 15	29, 56, 113, 167	0
1	C	644/806 (79%)	0.84	110 (17%)	4 3	41, 68, 127, 158	0
1	D	656/806 (81%)	1.46	166 (25%)	1 1	54, 91, 116, 142	0
All	All	2745/3224 (85%)	0.71	380 (13%)	6 5	27, 67, 118, 167	1 (0%)

All (380) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	562	PRO	7.6
1	D	902	LEU	6.2
1	B	433	ASN	6.1
1	C	538	ILE	6.0
1	D	559	HIS	5.3
1	C	621	SER	5.3
1	C	517	GLN	5.3
1	A	600	SER	5.2
1	B	494	ARG	5.1
1	C	627	TYR	5.1
1	B	498	HIS	5.0
1	C	598	TRP	5.0
1	C	570	LEU	4.9
1	A	527	SER	4.9
1	A	498	HIS	4.9
1	C	587	MET	4.9
1	D	926	LEU	4.9
1	C	697	ASP	4.9
1	C	571	GLU	4.9
1	B	453	THR	4.7
1	D	1095	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	563	SER	4.5
1	D	939	VAL	4.4
1	C	472	GLY	4.3
1	C	645	ASP	4.3
1	D	659	ASP	4.2
1	B	608	TRP	4.2
1	C	633	ARG	4.1
1	C	491	LEU	4.1
1	D	660	ASP	4.1
1	A	434	ARG	4.1
1	D	450	ARG	4.1
1	A	528	LEU	4.0
1	D	1001	VAL	4.0
1	A	567	HIS	4.0
1	C	630	ASP	4.0
1	A	475	VAL	4.0
1	D	644	GLU	4.0
1	C	648	ALA	4.0
1	C	664	TRP	3.9
1	D	775	PHE	3.9
1	A	433	ASN	3.9
1	B	445	ASN	3.9
1	D	925	GLU	3.9
1	D	903	ALA	3.8
1	B	526	ASP	3.8
1	D	1011	LYS	3.8
1	C	602	THR	3.8
1	D	998	ASN	3.7
1	D	794	LEU	3.7
1	C	507	ILE	3.7
1	C	558	HIS	3.7
1	D	1009	LEU	3.7
1	B	640	TYR	3.7
1	D	927	PRO	3.7
1	C	539	MET	3.6
1	B	522	TYR	3.6
1	D	776	VAL	3.6
1	D	802	SER	3.6
1	B	658	ILE	3.5
1	C	590	TYR	3.5
1	D	500	GLN	3.5
1	D	639	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	1010	LYS	3.5
1	D	520	LYS	3.5
1	D	999	SER	3.5
1	C	694	THR	3.5
1	D	667	ASN	3.5
1	C	680	LEU	3.5
1	B	558	HIS	3.5
1	C	489	LYS	3.5
1	B	531	LEU	3.5
1	B	585	GLN	3.5
1	C	573	PHE	3.5
1	A	518	TYR	3.4
1	D	604	ASN	3.4
1	D	928	VAL	3.4
1	A	684	TYR	3.4
1	B	563	SER	3.4
1	D	758	HIS	3.4
1	B	704	ILE	3.4
1	B	518	TYR	3.4
1	C	471	SER	3.4
1	A	501	ILE	3.4
1	D	760	GLY	3.4
1	B	501	ILE	3.3
1	C	468	LEU	3.3
1	C	997	CYS	3.3
1	D	653	PHE	3.3
1	D	1083	ASP	3.3
1	C	577	ILE	3.3
1	C	618	THR	3.3
1	C	634	HIS	3.3
1	D	1125	PHE	3.3
1	D	862	CYS	3.3
1	A	531	LEU	3.3
1	D	516	LEU	3.3
1	D	934	THR	3.3
1	D	1027	LEU	3.3
1	D	711	ASN	3.3
1	D	996	THR	3.2
1	B	1095	GLN	3.2
1	C	628	PHE	3.2
1	D	476	VAL	3.2
1	D	933	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	600	SER	3.2
1	C	490	ILE	3.2
1	A	604	ASN	3.2
1	B	521	ASN	3.2
1	D	993	THR	3.2
1	B	588	ALA	3.2
1	C	492	ASN	3.1
1	A	1156	ASP	3.1
1	A	997	CYS	3.1
1	C	515	GLY	3.1
1	D	853	ALA	3.1
1	C	513	ILE	3.1
1	D	803	PRO	3.1
1	A	515	GLY	3.1
1	D	778	SER	3.1
1	D	696	ASN	3.1
1	C	543	ASP	3.1
1	C	572	GLU	3.1
1	C	467	THR	3.1
1	D	601	SER	3.1
1	D	700	ASN	3.1
1	B	523	GLU	3.1
1	C	660	ASP	3.1
1	C	466	LYS	3.1
1	C	516	LEU	3.0
1	D	935	TYR	3.0
1	C	696	ASN	3.0
1	B	589	PHE	3.0
1	D	931	TRP	3.0
1	C	654	SER	3.0
1	D	1084	SER	3.0
1	B	566	ARG	3.0
1	D	861	SER	3.0
1	C	681	PRO	3.0
1	D	707	SER	2.9
1	D	1029	TYR	2.9
1	C	659	ASP	2.9
1	D	989	PHE	2.9
1	B	565	LEU	2.9
1	C	651	LEU	2.9
1	D	1002	LEU	2.9
1	A	607	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	866	ASN	2.9
1	C	695	TYR	2.9
1	B	530	THR	2.9
1	D	663	GLU	2.9
1	A	686	TYR	2.9
1	D	1012	TYR	2.9
1	B	449	GLY	2.9
1	D	859	GLY	2.9
1	B	495	GLU	2.9
1	C	1095	GLN	2.9
1	D	1153	GLN	2.9
1	D	671	ASP	2.9
1	C	620	THR	2.9
1	D	930	THR	2.9
1	A	476	VAL	2.9
1	C	678	LEU	2.9
1	A	603	PRO	2.8
1	D	501	ILE	2.8
1	D	909	ILE	2.8
1	A	676	LYS	2.8
1	D	857	GLY	2.8
1	A	565	LEU	2.8
1	C	653	PHE	2.8
1	D	474	GLY	2.8
1	A	641	SER	2.8
1	D	891	SER	2.8
1	C	462	GLY	2.8
1	B	578	VAL	2.8
1	D	670	GLU	2.8
1	D	800	SER	2.8
1	D	995	LEU	2.8
1	B	493	VAL	2.8
1	C	483	VAL	2.8
1	C	557	ILE	2.7
1	D	715	ILE	2.7
1	D	940	LEU	2.7
1	D	558	HIS	2.7
1	C	979	GLU	2.7
1	D	503	GLU	2.7
1	D	506	GLU	2.7
1	A	640	TYR	2.7
1	D	583	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	714	SER	2.7
1	B	447	ALA	2.7
1	B	689	THR	2.7
1	C	638	PHE	2.7
1	A	583	ASN	2.7
1	D	763	SER	2.7
1	D	580	VAL	2.7
1	D	668	PHE	2.7
1	B	517	GLN	2.7
1	D	581	SER	2.7
1	D	987	LYS	2.7
1	B	564	LEU	2.6
1	C	1008	CYS	2.6
1	D	1160	ARG	2.6
1	D	523	GLU	2.6
1	C	465	ALA	2.6
1	C	629	ALA	2.6
1	D	647	ALA	2.6
1	D	1164	SER	2.6
1	D	1124	THR	2.6
1	D	585	GLN	2.6
1	D	640	TYR	2.6
1	D	1175	ILE	2.6
1	D	703	LEU	2.6
1	B	599	LYS	2.6
1	C	594	GLU	2.6
1	C	601	SER	2.6
1	D	895	PHE	2.6
1	D	1043	ALA	2.6
1	D	1076	VAL	2.6
1	D	1018	ILE	2.6
1	D	1032	LEU	2.6
1	D	675	ARG	2.6
1	B	499	LYS	2.6
1	C	508	ASN	2.6
1	A	601	SER	2.6
1	D	664	TRP	2.6
1	C	549	ILE	2.6
1	C	640	TYR	2.6
1	D	519	LYS	2.6
1	D	892	TYR	2.5
1	D	648	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	445	ASN	2.5
1	D	792	THR	2.5
1	B	601	SER	2.5
1	C	616	LEU	2.5
1	D	535	LYS	2.5
1	C	574	ILE	2.5
1	B	760	GLY	2.5
1	D	1008	CYS	2.5
1	B	680	LEU	2.5
1	B	630	ASP	2.5
1	D	643	PRO	2.5
1	A	519	LYS	2.4
1	D	893	LYS	2.4
1	A	685	LEU	2.4
1	C	693	LEU	2.4
1	D	490	ILE	2.4
1	C	546	GLY	2.4
1	C	657	GLN	2.4
1	D	1079	GLN	2.4
1	B	516	LEU	2.4
1	B	707	SER	2.4
1	D	498	HIS	2.4
1	C	646	ASP	2.4
1	D	524	ASP	2.4
1	D	561	TRP	2.4
1	C	676	LYS	2.4
1	D	757	TYR	2.4
1	C	487	ARG	2.4
1	D	568	ARG	2.4
1	B	528	LEU	2.4
1	C	649	ILE	2.4
1	C	608	TRP	2.4
1	D	1161	LYS	2.4
1	B	590	TYR	2.4
1	C	902	LEU	2.4
1	D	435	ILE	2.4
1	D	564	LEU	2.4
1	D	570	LEU	2.4
1	D	1144	LEU	2.4
1	D	1157	THR	2.4
1	D	875	ASN	2.4
1	C	619	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	709	SER	2.4
1	D	780	ASN	2.3
1	B	500	GLN	2.3
1	C	958	ARG	2.3
1	A	692	TYR	2.3
1	D	689	THR	2.3
1	B	502	MET	2.3
1	C	644	GLU	2.3
1	A	526	ASP	2.3
1	C	760	GLY	2.3
1	D	797	GLY	2.3
1	D	801	ALA	2.3
1	D	434	ARG	2.3
1	D	661	ARG	2.3
1	A	474	GLY	2.3
1	D	1038	LEU	2.3
1	C	553	LEU	2.3
1	C	677	LEU	2.3
1	D	1003	PHE	2.3
1	C	559	HIS	2.2
1	D	567	HIS	2.2
1	B	596	GLU	2.2
1	A	590	TYR	2.2
1	D	910	SER	2.2
1	D	488	GLY	2.2
1	D	534	GLY	2.2
1	A	493	VAL	2.2
1	D	988	VAL	2.2
1	C	652	ALA	2.2
1	C	1064	ILE	2.2
1	D	795	HIS	2.2
1	D	856	ILE	2.2
1	D	774	ASN	2.2
1	B	693	LEU	2.2
1	B	1063	ILE	2.2
1	D	530	THR	2.2
1	A	500	GLN	2.2
1	B	519	LYS	2.2
1	C	796	GLY	2.2
1	B	527	SER	2.2
1	B	598	TRP	2.2
1	D	595	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	629	ALA	2.2
1	D	522	TYR	2.2
1	C	544	GLN	2.2
1	A	480	LYS	2.2
1	D	632	LYS	2.2
1	D	1028	LYS	2.2
1	D	709	SER	2.2
1	D	858	THR	2.1
1	A	455	CYS	2.1
1	D	997	CYS	2.1
1	A	639	LYS	2.1
1	D	544	GLN	2.1
1	D	992	GLN	2.1
1	A	587	MET	2.1
1	D	1128	LEU	2.1
1	A	918	SER	2.1
1	B	452	SER	2.1
1	C	511	ILE	2.1
1	D	790	PHE	2.1
1	B	647	ALA	2.1
1	C	540	THR	2.1
1	C	950	THR	2.1
1	B	643	PRO	2.1
1	B	637	GLN	2.1
1	A	677	LEU	2.1
1	C	509	ASN	2.1
1	D	1149	ASN	2.1
1	C	636	ILE	2.1
1	D	563	SER	2.1
1	D	698	PHE	2.1
1	C	947	THR	2.1
1	D	690	THR	2.1
1	B	520	LYS	2.1
1	D	656	LYS	2.1
1	D	1086	PRO	2.1
1	A	674	GLN	2.1
1	A	766[A]	MET	2.1
1	C	564	LEU	2.1
1	C	580	VAL	2.1
1	D	844	ILE	2.1
1	D	1006	VAL	2.1
1	C	464	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	591	SER	2.1
1	D	596	GLU	2.1
1	A	608	TRP	2.1
1	D	1186	LYS	2.1
1	D	887	PRO	2.1
1	A	688	GLN	2.1
1	C	665	LEU	2.1
1	C	583	ASN	2.1
1	C	548	HIS	2.1
1	A	435	ILE	2.1
1	B	568	ARG	2.0
1	C	656	LYS	2.0
1	D	896	LYS	2.0
1	C	603	PRO	2.0
1	D	838	PRO	2.0
1	D	451	ASN	2.0
1	C	596	GLU	2.0
1	C	607	LYS	2.0
1	C	624	ALA	2.0
1	A	1134	TRP	2.0
1	C	555	ASN	2.0
1	D	658	ILE	2.0
1	D	929	ARG	2.0

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.

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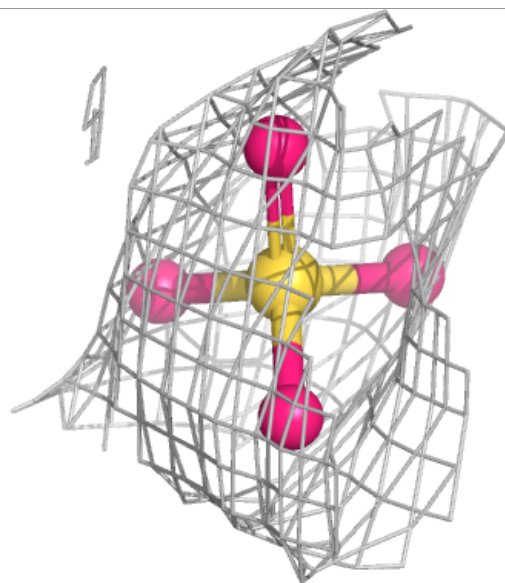
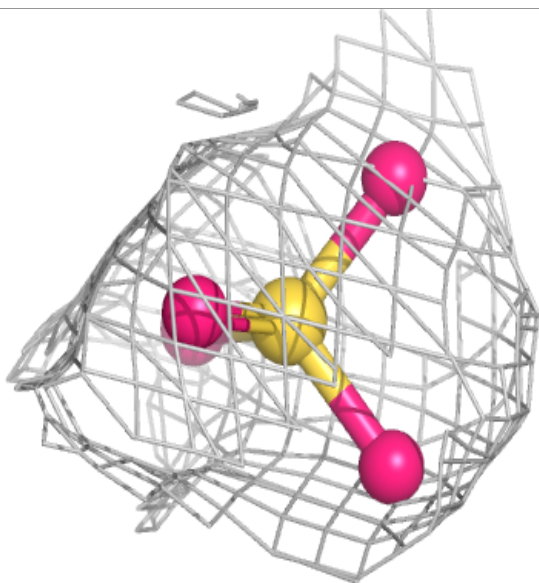
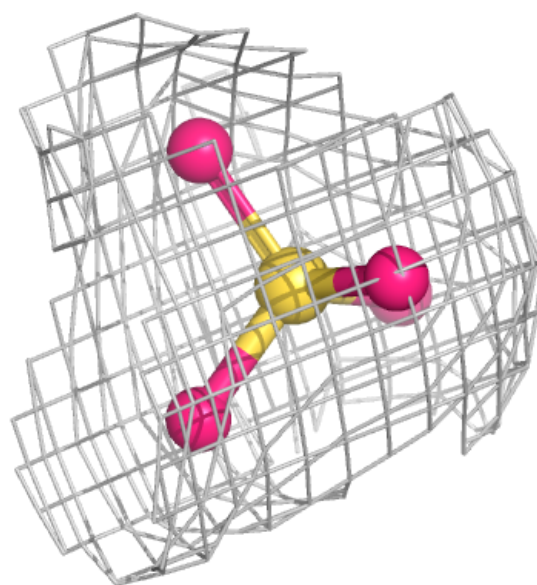
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1301	5/5	0.75	0.15	139,139,140,144	0
2	SO4	A	1302	5/5	0.82	0.15	95,96,97,104	0
2	SO4	B	1301	5/5	0.91	0.17	115,115,119,124	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.

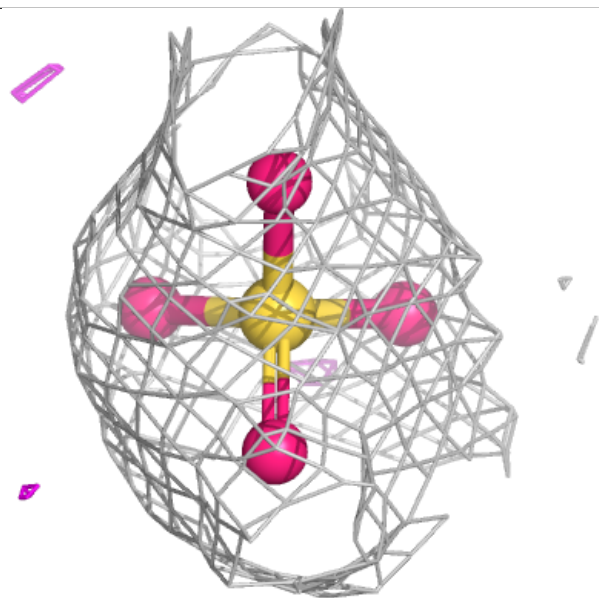
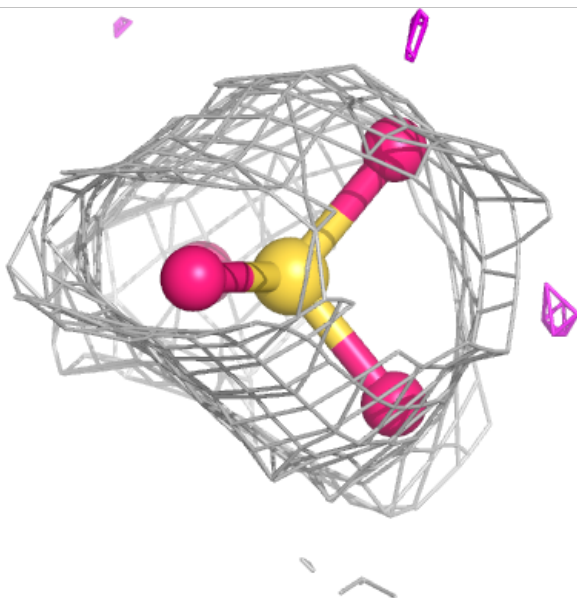
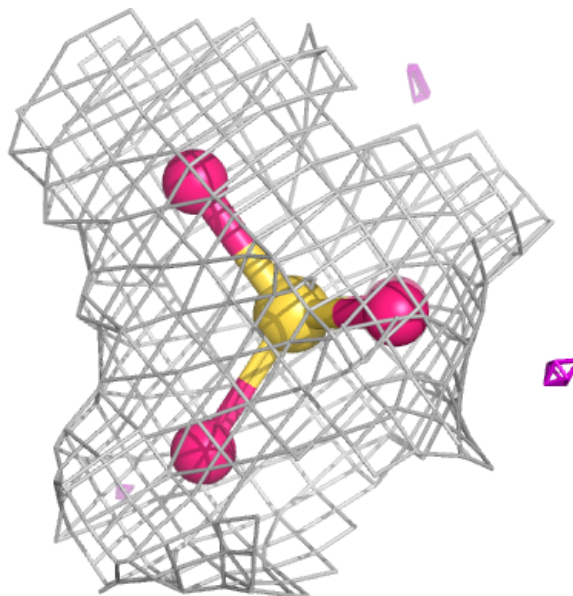
Electron density around SO4 A 1301:

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



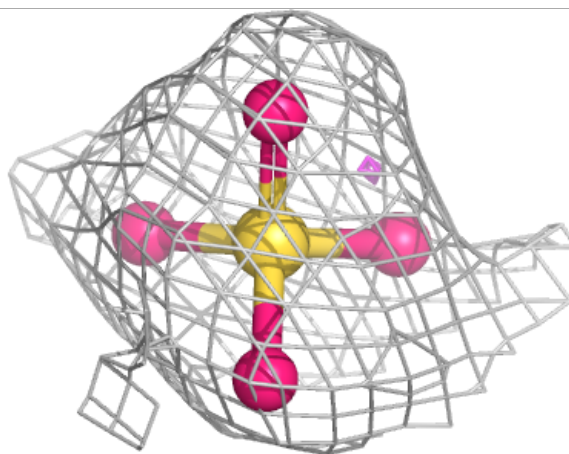
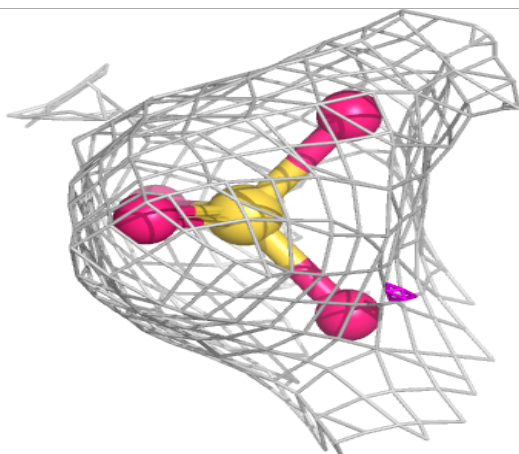
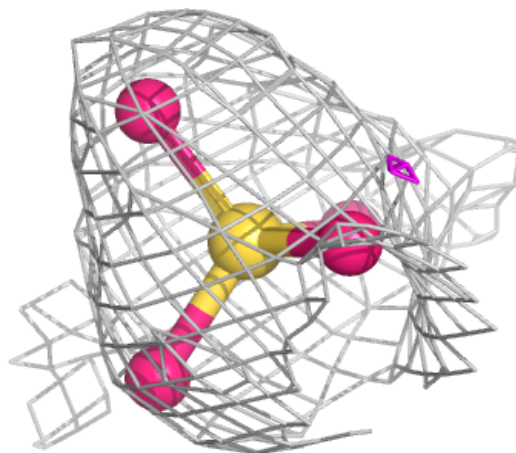
Electron density around SO4 A 1302:

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



Electron density around SO4 B 1301:

$2mF_o-DF_c$ (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.