



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 01:41 am BST

PDB ID : 6K8W
Title : Crystal structure of N-domain with NADP of bacterial malonyl-CoA reductase
Authors : Kim, S.; Kim, K.-J.
Deposited on : 2019-06-13
Resolution : 3.17 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

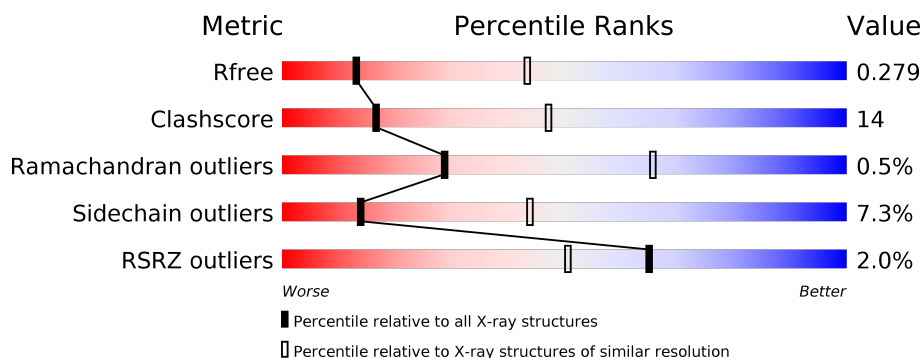
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	575	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>• 5%</div> </div> </div>
1	B	575	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8282 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.

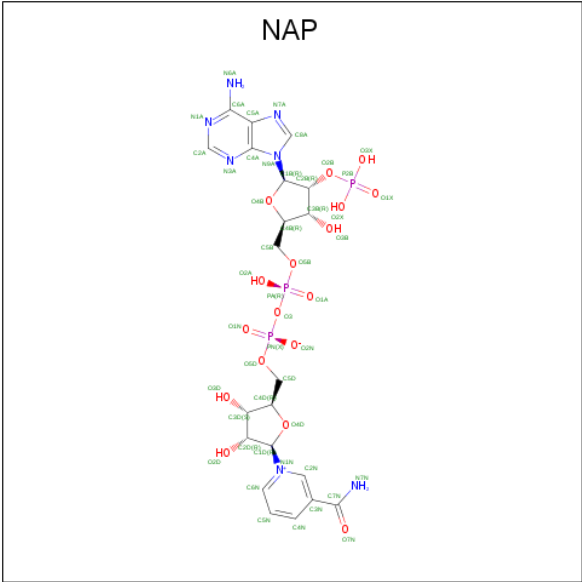
- Molecule 1 is a protein called NAD-dependent epimerase/dehydratase:Short-chain dehydrogenase/reductase SDR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4074	2541	733	784	16			
1	B	545	Total	C	N	O	S	0	1	0
			4082	2545	734	787	16			

There are 16 discrepancies between the modelled and reference sequences:

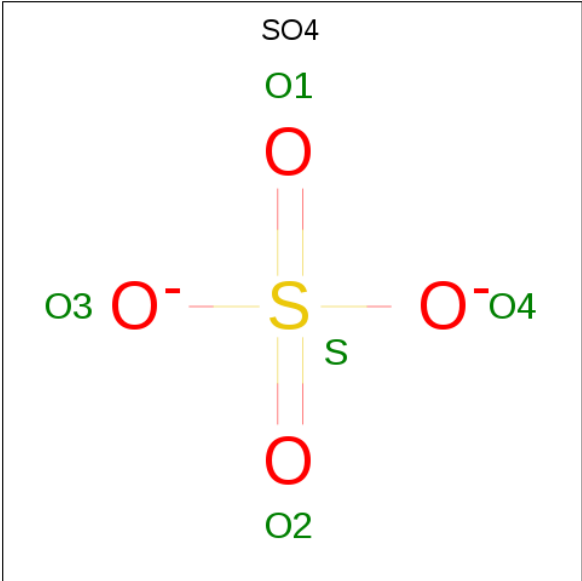
Chain	Residue	Modelled	Actual	Comment	Reference
A	568	LEU	-	expression tag	UNP A0A1A7BFR5
A	569	GLU	-	expression tag	UNP A0A1A7BFR5
A	570	HIS	-	expression tag	UNP A0A1A7BFR5
A	571	HIS	-	expression tag	UNP A0A1A7BFR5
A	572	HIS	-	expression tag	UNP A0A1A7BFR5
A	573	HIS	-	expression tag	UNP A0A1A7BFR5
A	574	HIS	-	expression tag	UNP A0A1A7BFR5
A	575	HIS	-	expression tag	UNP A0A1A7BFR5
B	568	LEU	-	expression tag	UNP A0A1A7BFR5
B	569	GLU	-	expression tag	UNP A0A1A7BFR5
B	570	HIS	-	expression tag	UNP A0A1A7BFR5
B	571	HIS	-	expression tag	UNP A0A1A7BFR5
B	572	HIS	-	expression tag	UNP A0A1A7BFR5
B	573	HIS	-	expression tag	UNP A0A1A7BFR5
B	574	HIS	-	expression tag	UNP A0A1A7BFR5
B	575	HIS	-	expression tag	UNP A0A1A7BFR5

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

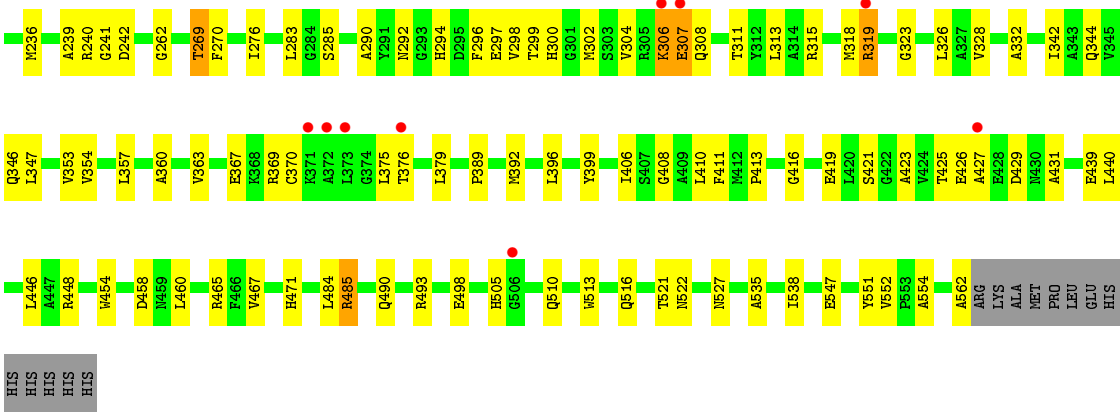
- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by author).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	15	Total 15	O 15	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.87Å 109.11Å 130.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.76 – 3.17 33.74 – 3.17	Depositor EDS
% Data completeness (in resolution range)	96.8 (33.76-3.17) 96.9 (33.74-3.17)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.35 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.209 , 0.278 0.210 , 0.279	Depositor DCC
R_{free} test set	1019 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	1.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8282	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: NAP, 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	0.69	0/4145	0.87	0/5623
1	B	0.68	0/4153	0.86	0/5634
All	All	0.69	0/8298	0.86	0/11257

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

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	4074	0	4059	120	0
1	B	4082	0	4062	125	0
2	A	48	0	25	6	0
2	B	48	0	25	3	0
3	B	5	0	0	0	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
All	All	8282	0	8171	234	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 14.

All (234) 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:40:VAL:HG13	1:A:50:VAL:HG11	1.46	0.94
1:A:53:THR:HG23	1:A:83:LEU:CD2	1.98	0.93
1:B:223:PRO:HD3	1:B:302:MET:HE1	1.54	0.88
1:A:458:ASP:O	1:A:510:GLN:HG3	1.77	0.84
1:A:223:PRO:O	1:A:271:PRO:HD2	1.80	0.82
1:A:88:ILE:O	1:A:92:ARG:HG2	1.79	0.82
1:A:229:ILE:HD11	1:A:270:PHE:CD2	2.16	0.79
1:A:53:THR:HG23	1:A:83:LEU:HD22	1.61	0.79
1:A:185:TYR:H	1:A:494:ILE:HD11	1.47	0.78
1:A:36:GLY:O	1:A:40:VAL:HG23	1.83	0.78
1:A:294:HIS:CE1	1:B:297:GLU:H	2.01	0.77
1:B:195:LYS:HE3	2:B:1301:NAP:O2D	1.83	0.77
1:A:294:HIS:HE1	1:B:297:GLU:H	1.33	0.76
1:A:545:LEU:HD23	1:A:545:LEU:N	2.01	0.76
1:A:208:GLU:OE2	1:A:425:THR:HB	1.84	0.75
1:A:185:TYR:H	1:A:494:ILE:CD1	2.00	0.75
1:B:19:GLY:HA3	1:B:46:GLU:O	1.87	0.74
1:A:258:GLU:HG3	1:A:268:LYS:NZ	2.03	0.73
1:A:88:ILE:HG13	1:A:92:ARG:HH21	1.54	0.72
1:A:149:LEU:HD23	1:A:194:PRO:HG3	1.70	0.72
1:A:85:GLY:HA3	1:A:155:VAL:CG1	2.20	0.71
1:B:423:ALA:HB3	1:B:426:GLU:HB2	1.72	0.70
1:A:185:TYR:O	1:A:494:ILE:HD12	1.92	0.69
1:B:223:PRO:CD	1:B:302:MET:HE1	2.23	0.69
1:A:272:THR:HB	1:A:274:GLU:OE1	1.93	0.68
1:A:120:PRO:HA	1:A:187:ALA:HA	1.75	0.68
1:A:294:HIS:HE1	1:B:297:GLU:N	1.91	0.68
1:A:258:GLU:CG	1:A:268:LYS:NZ	2.57	0.67
1:B:411:PHE:CD1	1:B:446:LEU:HD13	2.29	0.67
1:A:306:LYS:HE2	1:B:306:LYS:HD2	1.75	0.66
1:A:420:LEU:HD13	1:A:435:LEU:HB2	1.78	0.65
1:A:85:GLY:HA3	1:A:155:VAL:HG12	1.78	0.65
1:B:117:PRO:HD2	1:B:190:ALA:HB1	1.78	0.65
1:B:56:THR:HB	1:B:59:ARG:HG2	1.78	0.64
1:B:306:LYS:CE	1:B:307:GLU:OE1	2.46	0.64
1:B:161:ARG:HB2	1:B:425:THR:HA	1.79	0.64
1:A:164:ALA:HB3	1:A:165:PRO:HD3	1.80	0.64
1:B:306:LYS:HE3	1:B:307:GLU:OE1	1.98	0.63
1:B:83:LEU:HD11	1:B:159:VAL:HG22	1.78	0.63
1:A:53:THR:CG2	1:A:83:LEU:CD2	2.75	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:VAL:HG21	1:B:490:GLN:HE21	1.64	0.63
1:B:193:VAL:HG22	1:B:194:PRO:HD3	1.81	0.63
1:B:439:GLU:HB3	1:B:484:LEU:HD21	1.81	0.62
1:B:130:GLU:OE1	1:B:448:ARG:NH2	2.31	0.62
1:A:398:GLU:O	1:A:401:ARG:HG2	2.00	0.62
1:A:177:SER:O	1:A:221:PRO:HD2	1.99	0.61
1:A:178:THR:HB	2:A:1301:NAP:H6N	1.82	0.61
1:A:369:ARG:HH21	1:A:369:ARG:HG3	1.66	0.61
1:A:193:VAL:HB	1:A:194:PRO:HD3	1.83	0.61
1:A:397:GLU:OE1	1:A:397:GLU:HA	2.01	0.61
1:B:460:LEU:N	1:B:510:GLN:HE22	1.99	0.60
1:B:161:ARG:CB	1:B:425:THR:HA	2.32	0.60
1:B:146:ALA:HB1	1:B:150:ARG:HH21	1.65	0.60
1:A:229:ILE:CD1	1:A:270:PHE:CD2	2.84	0.60
1:A:29:THR:O	1:A:111:ASN:HB3	2.02	0.59
1:B:276:ILE:HD13	1:B:298:VAL:HG11	1.83	0.59
1:B:86:GLY:HA3	1:B:150:ARG:CG	2.32	0.59
1:A:229:ILE:HD11	1:A:270:PHE:HD2	1.67	0.59
1:A:400:THR:HG21	1:A:457:HIS:CE1	2.37	0.59
1:A:93:ALA:O	1:A:96:ALA:HB3	2.03	0.59
1:B:236:MET:O	1:B:239:ALA:HB3	2.03	0.59
1:B:182:ARG:HB3	1:B:304:VAL:HG11	1.84	0.59
1:A:490:GLN:OE1	1:A:493:ARG:NH1	2.35	0.59
1:A:439:GLU:HB3	1:A:484:LEU:HD11	1.84	0.59
1:B:547:GLU:CD	1:B:547:GLU:H	2.06	0.58
1:A:405:PRO:HB2	1:A:460:LEU:HD21	1.85	0.58
1:B:161:ARG:HA	1:B:425:THR:HG22	1.86	0.58
1:B:354:VAL:HG22	1:B:399:TYR:CE1	2.39	0.58
1:A:258:GLU:HG3	1:A:268:LYS:HZ2	1.68	0.58
1:A:439:GLU:HB3	1:A:484:LEU:CD1	2.34	0.57
1:A:203:ARG:O	1:A:206:SER:HB3	2.04	0.56
1:A:229:ILE:CD1	1:A:270:PHE:CE2	2.88	0.56
1:B:117:PRO:HD2	1:B:190:ALA:CB	2.35	0.56
1:A:35:LEU:HD12	2:A:1301:NAP:H52N	1.86	0.56
1:A:458:ASP:O	1:A:510:GLN:CG	2.52	0.56
1:A:519:ARG:HG2	1:A:531:THR:HG21	1.86	0.56
1:A:396:LEU:HD22	1:A:406:ILE:CD1	2.36	0.56
1:B:149:LEU:HD22	1:B:440:LEU:HD12	1.88	0.56
1:B:146:ALA:HB1	1:B:150:ARG:NH2	2.21	0.55
1:B:115:ALA:O	1:B:188:ARG:NH2	2.34	0.55
1:B:29:THR:HA	1:B:53:THR:HB	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LEU:HD23	1:B:83:LEU:C	2.27	0.55
1:A:550:LEU:HD22	1:B:313:LEU:CD1	2.37	0.54
1:A:258:GLU:CG	1:A:268:LYS:HZ2	2.20	0.54
1:B:465:ARG:HA	1:B:513:TRP:O	2.08	0.54
1:A:256:SER:OG	1:B:292:ASN:ND2	2.38	0.54
1:B:439:GLU:HB3	1:B:484:LEU:CD2	2.37	0.53
1:A:264:ASN:HD22	1:A:264:ASN:N	2.06	0.53
1:A:53:THR:CG2	1:A:83:LEU:HD21	2.38	0.53
1:A:83:LEU:O	1:A:83:LEU:HD23	2.09	0.53
1:A:88:ILE:CG1	1:A:92:ARG:HH21	2.21	0.53
1:B:52:MET:SD	1:B:78:LEU:HD11	2.48	0.53
1:A:119:GLN:HG3	1:A:123:ASN:HB3	1.90	0.53
1:B:19:GLY:O	1:B:22:ALA:N	2.34	0.53
1:B:299:THR:O	1:B:300:HIS:HB2	2.09	0.53
1:B:396:LEU:HD22	1:B:406:ILE:HD13	1.91	0.52
1:A:85:GLY:HA3	1:A:155:VAL:HG13	1.92	0.52
1:A:522:ASN:OD1	1:A:527:ASN:ND2	2.39	0.52
1:B:454:TRP:CD1	1:B:460:LEU:HD11	2.45	0.52
1:B:315:ARG:NE	1:B:562:ALA:HB3	2.25	0.52
1:B:427:ALA:HB1	1:B:431:ALA:CB	2.40	0.51
1:A:193:VAL:HB	1:A:444:MET:HE1	1.92	0.51
2:A:1301:NAP:H4B	2:A:1301:NAP:O1A	2.10	0.51
1:B:53:THR:HG23	1:B:83:LEU:HB3	1.91	0.51
1:B:306:LYS:HE2	1:B:307:GLU:OE1	2.09	0.51
1:B:342:ILE:O	1:B:346:GLN:HG2	2.11	0.51
1:B:241:GLY:O	1:B:505:HIS:NE2	2.42	0.51
1:A:170:GLY:O	1:A:215:ARG:NH1	2.43	0.51
1:B:144:THR:HG22	1:B:147:ASP:H	1.75	0.51
1:B:467:VAL:HG22	1:B:538:ILE:HG21	1.93	0.51
1:B:308:GLN:CD	1:B:493:ARG:NH1	2.65	0.50
1:B:521:THR:OG1	1:B:552:VAL:O	2.27	0.50
1:B:56:THR:HG22	1:B:58:ASP:H	1.75	0.50
1:A:398:GLU:HA	1:A:401:ARG:HG2	1.93	0.50
1:B:396:LEU:HD22	1:B:406:ILE:CD1	2.42	0.50
1:B:269:THR:OG1	1:B:270:PHE:N	2.45	0.49
1:B:86:GLY:HA3	1:B:150:ARG:HG2	1.93	0.49
1:A:134:LEU:O	1:A:137:THR:HB	2.11	0.49
1:B:363:VAL:O	1:B:367:GLU:HB2	2.12	0.49
1:A:384:PHE:CE2	1:A:392:MET:SD	3.06	0.49
1:B:19:GLY:CA	1:B:46:GLU:O	2.58	0.49
1:A:119:GLN:HG2	1:A:123:ASN:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:PRO:CB	1:B:471:HIS:CE1	2.96	0.49
1:A:405:PRO:HB2	1:A:460:LEU:CD2	2.43	0.48
1:B:410:LEU:HD12	1:B:535:ALA:HB1	1.95	0.48
1:A:215:ARG:NH2	1:A:285:SER:O	2.45	0.48
1:B:86:GLY:HA3	1:B:150:ARG:HG3	1.95	0.48
1:B:485:ARG:HD3	1:B:551:TYR:OH	2.13	0.48
1:B:308:GLN:OE1	1:B:493:ARG:NH1	2.47	0.48
1:A:208:GLU:CD	1:A:423:ALA:HB1	2.35	0.47
1:A:462:GLN:O	1:A:463:PRO:C	2.50	0.47
1:B:360:ALA:HA	1:B:363:VAL:HG23	1.95	0.47
1:B:97:GLU:O	1:B:101:LYS:HB2	2.14	0.47
1:A:148:ALA:O	1:A:152:ILE:HD12	2.14	0.47
1:B:86:GLY:CA	1:B:150:ARG:HG3	2.45	0.47
1:B:522:ASN:ND2	1:B:554:ALA:O	2.48	0.47
1:B:193:VAL:CG2	1:B:194:PRO:HD3	2.45	0.46
1:A:297:GLU:H	1:B:294:HIS:CE1	2.33	0.46
1:B:48:ALA:O	1:B:77:ARG:NH2	2.49	0.46
1:B:208:GLU:OE2	1:B:425:THR:OG1	2.31	0.46
1:A:258:GLU:CG	1:A:268:LYS:HZ3	2.26	0.46
1:B:332:ALA:HB3	1:B:357:LEU:HD23	1.96	0.46
1:A:206:SER:HA	1:A:216:VAL:HB	1.98	0.46
1:B:283:LEU:HD21	1:B:296:PHE:CZ	2.50	0.46
1:B:315:ARG:HE	1:B:562:ALA:HB3	1.79	0.46
1:A:344:GLN:HG2	1:A:375:LEU:HD21	1.98	0.46
1:B:57:PRO:HA	1:B:60:THR:HG22	1.96	0.46
1:B:53:THR:HG21	1:B:83:LEU:HD22	1.98	0.46
1:A:495:TRP:HD1	1:A:495:TRP:O	1.99	0.45
1:B:323:GLY:HA2	1:B:326:LEU:HD12	1.98	0.45
1:B:413:PRO:HB2	1:B:471:HIS:CE1	2.52	0.45
1:A:209:LEU:O	1:A:212:LYS:N	2.35	0.45
1:A:272:THR:OG1	1:A:275:ASP:OD1	2.34	0.45
1:A:526:GLU:O	1:A:529:ARG:N	2.47	0.45
1:B:223:PRO:HD3	1:B:302:MET:CE	2.34	0.45
1:B:396:LEU:CD2	1:B:406:ILE:HD13	2.47	0.45
1:B:157:TRP:CE3	1:B:201:TRP:CD1	3.05	0.45
1:B:396:LEU:CD2	1:B:406:ILE:CD1	2.95	0.45
1:A:120:PRO:O	1:A:121:ILE:C	2.55	0.45
1:A:411:PHE:CD2	1:A:468:PHE:CE1	3.04	0.45
1:A:535:ALA:O	1:A:539:LEU:HG	2.17	0.45
1:B:55:ARG:HG3	2:B:1301:NAP:C2A	2.47	0.45
1:B:454:TRP:O	1:B:458:ASP:OD1	2.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ILE:HG12	1:A:299:THR:HG21	1.99	0.44
1:A:29:THR:HA	1:A:53:THR:CG2	2.47	0.44
1:B:99:VAL:HG21	1:B:166:HIS:CD2	2.52	0.44
1:A:369:ARG:O	1:A:373:LEU:HB2	2.17	0.44
1:A:547:GLU:OE2	1:B:311:THR:OG1	2.30	0.44
1:A:204:GLU:OE1	1:A:479:ILE:HD13	2.17	0.44
1:A:522:ASN:ND2	1:A:524:GLU:OE1	2.50	0.44
1:A:35:LEU:HD23	1:A:273:PRO:HB3	1.99	0.44
1:A:157:TRP:CE2	1:A:432:VAL:HB	2.53	0.44
1:B:344:GLN:HG2	1:B:375:LEU:HD11	1.99	0.44
1:A:104:ARG:HH21	1:A:104:ARG:HG2	1.83	0.44
1:B:19:GLY:C	1:B:21:LEU:N	2.71	0.44
1:B:410:LEU:CD1	1:B:535:ALA:HB1	2.48	0.44
1:A:178:THR:HB	2:A:1301:NAP:C6N	2.46	0.44
1:B:347:LEU:HD11	1:B:379:LEU:HB2	1.99	0.44
1:A:466:PHE:CD1	1:A:514:GLY:HA3	2.53	0.44
1:B:29:THR:HB	1:B:112:ALA:HB2	2.00	0.43
1:B:179:ILE:HG21	1:B:302:MET:HE3	2.01	0.43
1:B:311:THR:HG22	1:B:551:TYR:HB2	1.99	0.43
1:A:178:THR:OG1	2:A:1301:NAP:H5N	2.18	0.43
1:A:280:CYS:O	1:A:281:VAL:C	2.57	0.43
1:B:85:GLY:HA3	1:B:155:VAL:HA	1.99	0.43
1:A:104:ARG:NH2	1:A:104:ARG:HG2	2.32	0.43
1:B:113:GLY:O	2:B:1301:NAP:H8A	2.18	0.43
1:B:319:ARG:N	1:B:319:ARG:HD3	2.33	0.43
1:A:240:ARG:O	1:A:507:ARG:NH1	2.48	0.43
1:B:19:GLY:O	1:B:21:LEU:N	2.52	0.43
1:B:416:GLY:O	1:B:419:GLU:HB3	2.19	0.43
1:B:219:VAL:O	1:B:221:PRO:HD3	2.18	0.43
1:A:298:VAL:HG13	1:B:290:ALA:HB3	2.00	0.43
1:A:113:GLY:O	2:A:1301:NAP:H52A	2.18	0.43
1:A:221:PRO:HB3	1:A:276:ILE:CD1	2.48	0.43
1:A:272:THR:CB	1:A:274:GLU:OE1	2.63	0.43
1:B:283:LEU:HD21	1:B:296:PHE:CE1	2.54	0.43
1:B:411:PHE:CG	1:B:446:LEU:HD13	2.53	0.43
1:B:186:TYR:CD2	1:B:498:GLU:HA	2.54	0.43
1:B:192:VAL:CG2	1:B:490:GLN:HE21	2.28	0.43
1:A:107:ILE:HA	1:A:172:SER:O	2.19	0.42
1:B:21:LEU:HA	1:B:21:LEU:HD12	1.86	0.42
1:A:306:LYS:HE2	1:B:306:LYS:CD	2.46	0.42
1:A:420:LEU:CD1	1:A:435:LEU:HB2	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD21	1:A:296:PHE:CZ	2.54	0.42
1:B:328:VAL:HA	1:B:408:GLY:O	2.20	0.42
1:A:485:ARG:HA	1:A:516:GLN:HE22	1.84	0.42
1:B:193:VAL:N	1:B:194:PRO:CD	2.83	0.42
1:A:298:VAL:HG13	1:B:290:ALA:CB	2.50	0.42
1:B:347:LEU:HG	1:B:353:VAL:HG21	2.02	0.42
1:B:99:VAL:O	1:B:103:GLY:N	2.52	0.42
1:B:439:GLU:HG3	1:B:484:LEU:HD11	2.01	0.41
1:A:333:GLY:HA3	1:A:413:PRO:O	2.20	0.41
1:A:462:GLN:O	1:A:463:PRO:O	2.38	0.41
1:B:175:ASN:O	1:B:218:LEU:HD12	2.20	0.41
1:B:179:ILE:O	1:B:183:THR:HG23	2.20	0.41
1:A:83:LEU:HD11	1:A:159:VAL:HG22	2.02	0.41
1:B:179:ILE:HG21	1:B:302:MET:CE	2.50	0.41
1:A:233:PHE:O	1:A:237:ASP:OD2	2.39	0.41
1:A:258:GLU:HG2	1:A:268:LYS:NZ	2.34	0.41
1:B:118:LYS:HG2	1:B:188:ARG:HD3	2.02	0.41
1:B:19:GLY:C	1:B:21:LEU:H	2.23	0.41
1:A:503:THR:HA	1:A:508:ARG:O	2.20	0.41
1:A:247:THR:O	1:A:250:GLN:HB2	2.21	0.41
1:B:105:ILE:O	1:B:167:ILE:HG12	2.20	0.41
1:A:144:THR:HG22	1:A:147:ASP:H	1.86	0.41
1:B:485:ARG:HA	1:B:516:GLN:HE22	1.85	0.41
1:A:178:THR:HG21	1:A:191:TYR:CE2	2.56	0.41
1:A:208:GLU:OE2	1:A:425:THR:CB	2.63	0.41
1:A:294:HIS:CE1	1:B:297:GLU:HB2	2.56	0.41
1:B:389:PRO:O	1:B:392:MET:HB2	2.21	0.40
1:B:410:LEU:HA	1:B:467:VAL:O	2.21	0.40
1:A:408:GLY:HA2	1:A:465:ARG:O	2.21	0.40
1:A:345:VAL:HG21	1:A:532:ALA:CB	2.52	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	543/575 (94%)	498 (92%)	42 (8%)	3 (1%)	25	63
1	B	544/575 (95%)	504 (93%)	38 (7%)	2 (0%)	34	69
All	All	1087/1150 (94%)	1002 (92%)	80 (7%)	5 (0%)	29	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	ARG
1	A	463	PRO
1	B	262	GLY
1	A	121	ILE
1	A	561	GLY

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	410/431 (95%)	375 (92%)	35 (8%)	10	36
1	B	411/431 (95%)	386 (94%)	25 (6%)	18	51
All	All	821/862 (95%)	761 (93%)	60 (7%)	14	44

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	83	LEU
1	A	90	SER
1	A	100	GLN
1	A	122	GLU
1	A	123	ASN
1	A	137	THR
1	A	144	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	155	VAL
1	A	161	ARG
1	A	183	THR
1	A	185	TYR
1	A	227	GLU
1	A	231	SER
1	A	232	VAL
1	A	236	MET
1	A	240	ARG
1	A	264	ASN
1	A	265	GLU
1	A	305	ARG
1	A	317	THR
1	A	318	MET
1	A	334	ASP
1	A	338	GLU
1	A	371	LYS
1	A	373	LEU
1	A	375	LEU
1	A	380	SER
1	A	387	LYS
1	A	400	THR
1	A	432	VAL
1	A	451	SER
1	A	461	LEU
1	A	522	ASN
1	A	545	LEU
1	B	21	LEU
1	B	59	ARG
1	B	83	LEU
1	B	129	GLU
1	B	137	THR
1	B	144	THR
1	B	150	ARG
1	B	182	ARG
1	B	185	TYR
1	B	203	ARG
1	B	240	ARG
1	B	242	ASP
1	B	269	THR
1	B	285	SER
1	B	306	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	307	GLU
1	B	318	MET
1	B	319	ARG
1	B	369	ARG
1	B	370	CYS
1	B	376	THR
1	B	421	SER
1	B	429	ASP
1	B	485	ARG
1	B	527	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	111	ASN
1	A	175	ASN
1	A	264	ASN
1	A	294	HIS
1	A	344	GLN
1	A	352	GLN
1	A	457	HIS
1	A	515	ASN
1	A	516	GLN
1	B	110	ASN
1	B	166	HIS
1	B	294	HIS
1	B	344	GLN
1	B	457	HIS
1	B	471	HIS
1	B	510	GLN
1	B	516	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	B	1302	-	4,4,4	0.39	0	6,6,6	0.08	0
2	NAP	B	1301	-	45,52,52	0.91	3 (6%)	56,80,80	1.37	8 (14%)
2	NAP	A	1301	-	45,52,52	1.04	3 (6%)	56,80,80	1.76	12 (21%)

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	NAP	B	1301	-	-	12/31/67/67	0/5/5/5
2	NAP	A	1301	-	-	8/31/67/67	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	NAP	O4D-C1D	2.98	1.45	1.41
2	B	1301	NAP	C5A-C4A	2.68	1.48	1.40
2	A	1301	NAP	C5A-C4A	2.27	1.46	1.40
2	B	1301	NAP	C2A-N3A	2.26	1.35	1.32
2	A	1301	NAP	C2N-C3N	2.02	1.42	1.39
2	B	1301	NAP	O4D-C1D	2.01	1.43	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	NAP	C6N-N1N-C2N	-5.03	117.39	121.97
2	A	1301	NAP	PN-O3-PA	-4.40	117.72	132.83
2	A	1301	NAP	N3A-C2A-N1A	-4.12	122.24	128.68
2	B	1301	NAP	N3A-C2A-N1A	-3.88	122.62	128.68
2	A	1301	NAP	C2N-N1N-C1D	3.87	127.77	119.14
2	B	1301	NAP	PN-O3-PA	-3.52	120.74	132.83
2	A	1301	NAP	C1B-N9A-C4A	-2.91	121.52	126.64
2	B	1301	NAP	C3D-C2D-C1D	2.49	104.73	100.98
2	A	1301	NAP	C2A-N1A-C6A	2.42	122.90	118.75
2	B	1301	NAP	N6A-C6A-N1A	2.38	123.50	118.57
2	B	1301	NAP	C6N-N1N-C2N	-2.37	119.82	121.97
2	A	1301	NAP	N6A-C6A-N1A	2.24	123.23	118.57
2	A	1301	NAP	O2N-PN-O1N	2.21	123.18	112.24
2	A	1301	NAP	C5N-C6N-N1N	2.21	123.57	120.40
2	A	1301	NAP	O4D-C4D-C5D	-2.17	102.24	109.37
2	A	1301	NAP	O5D-C5D-C4D	2.17	116.44	108.99
2	A	1301	NAP	C4N-C3N-C7N	-2.13	115.33	121.04
2	B	1301	NAP	C2A-N1A-C6A	2.12	122.37	118.75
2	B	1301	NAP	C2B-C3B-C4B	2.09	106.53	101.99
2	B	1301	NAP	O2A-PA-O1A	2.03	122.29	112.24

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1301	NAP	C5B-O5B-PA-O1A
2	B	1301	NAP	C5B-O5B-PA-O3
2	B	1301	NAP	C4B-C5B-O5B-PA
2	B	1301	NAP	C2B-O2B-P2B-O2X
2	B	1301	NAP	C5D-O5D-PN-O3
2	B	1301	NAP	C5D-O5D-PN-O1N
2	B	1301	NAP	C5D-O5D-PN-O2N
2	A	1301	NAP	C4B-C5B-O5B-PA
2	A	1301	NAP	C3B-C4B-C5B-O5B
2	A	1301	NAP	C2B-O2B-P2B-O1X
2	A	1301	NAP	O4D-C4D-C5D-O5D
2	A	1301	NAP	C3D-C4D-C5D-O5D
2	A	1301	NAP	O4B-C4B-C5B-O5B
2	B	1301	NAP	C3D-C4D-C5D-O5D
2	B	1301	NAP	O4D-C4D-C5D-O5D
2	B	1301	NAP	C3B-C4B-C5B-O5B
2	A	1301	NAP	C2B-O2B-P2B-O3X
2	B	1301	NAP	C4N-C3N-C7N-N7N

Continued on next page...

Continued from previous page...

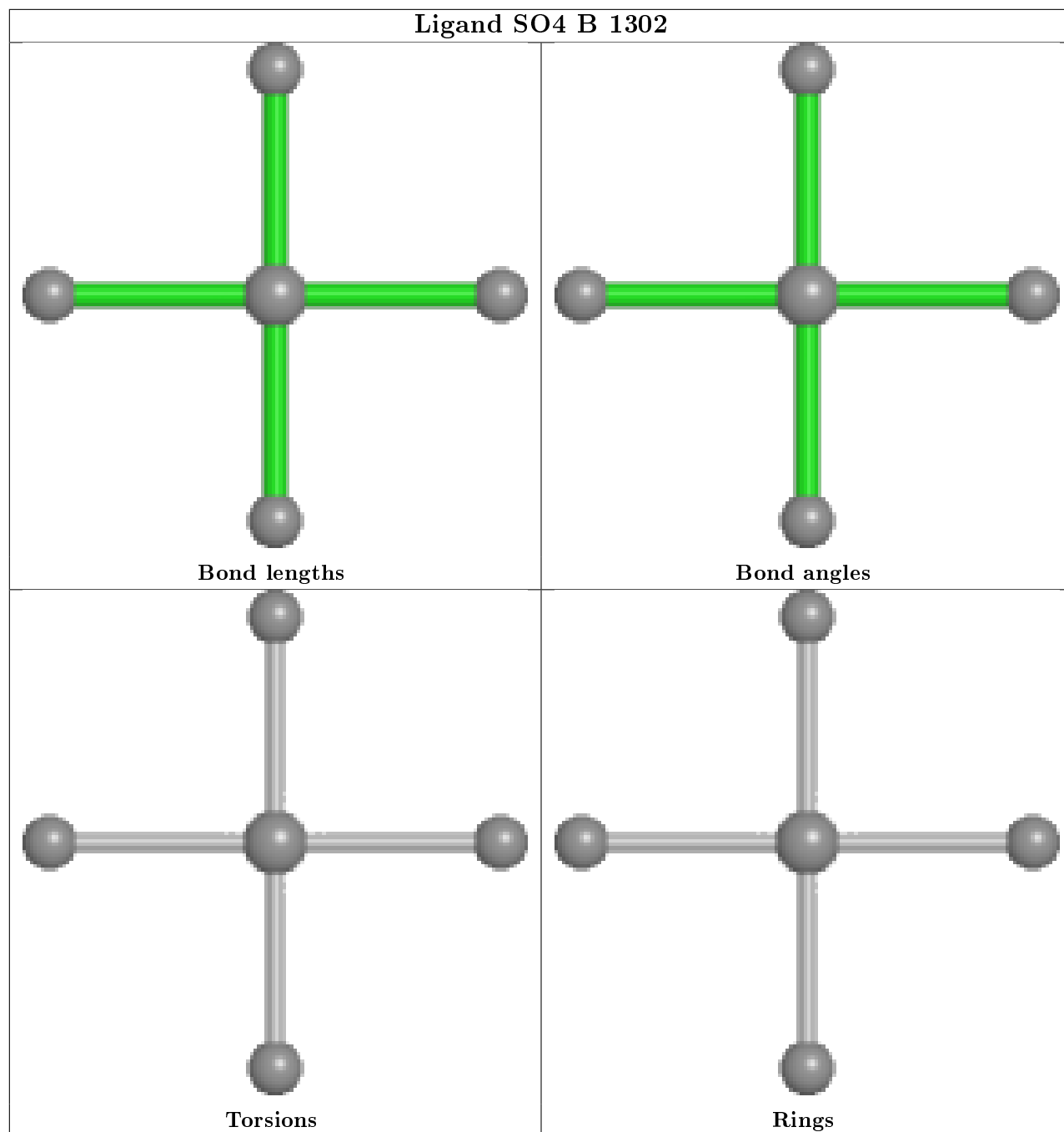
Mol	Chain	Res	Type	Atoms
2	B	1301	NAP	C4N-C3N-C7N-O7N
2	A	1301	NAP	C5B-O5B-PA-O1A

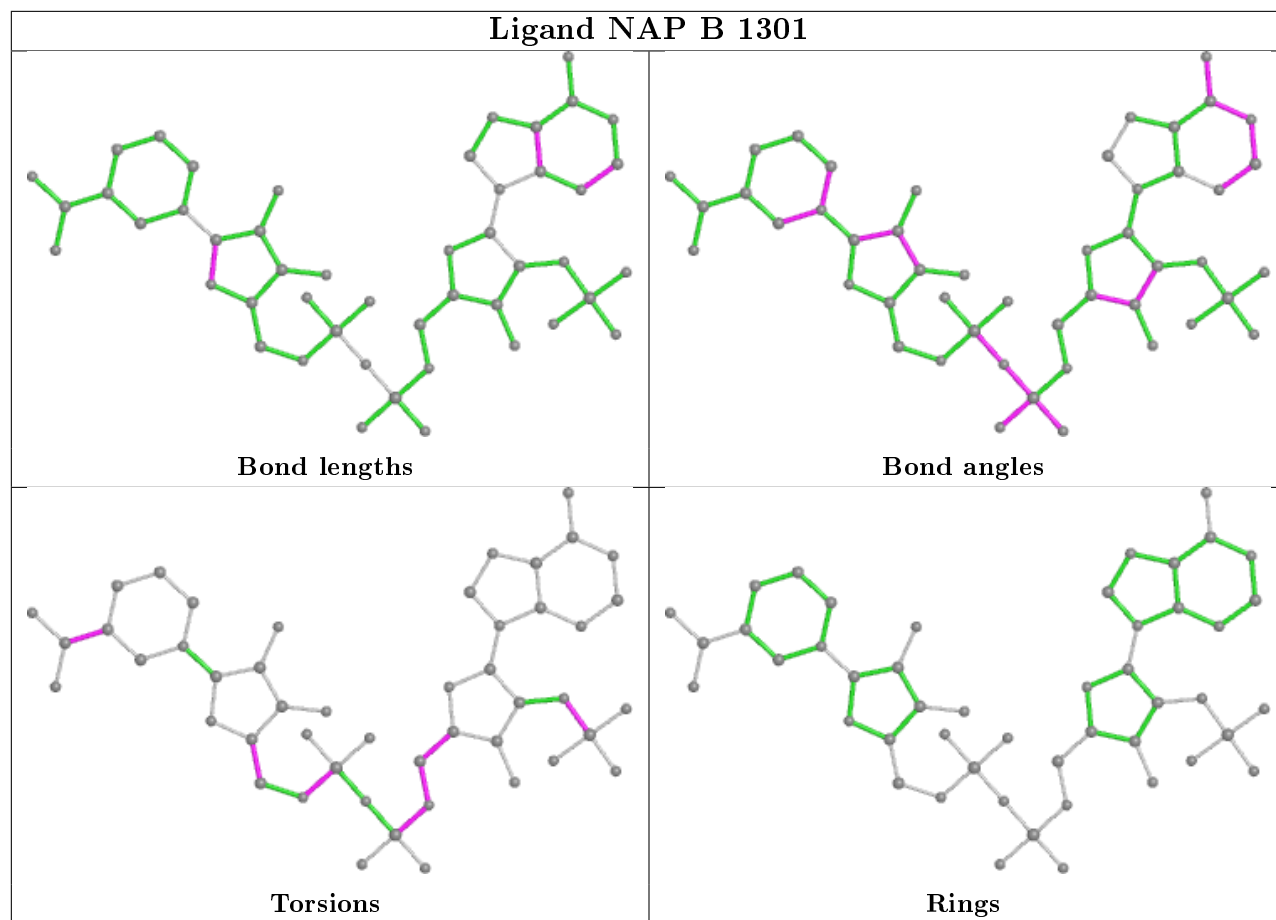
There are no ring outliers.

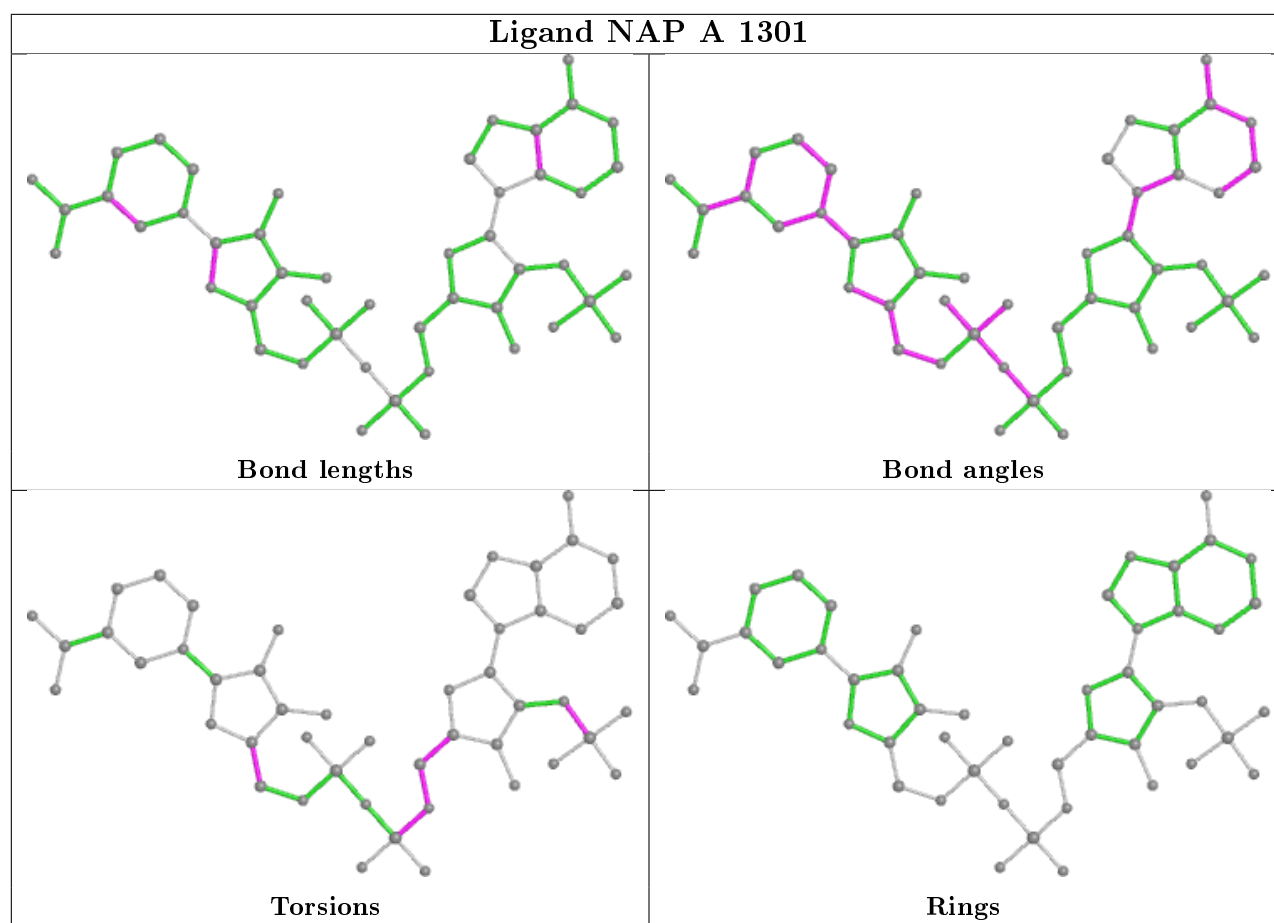
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1301	NAP	3	0
2	A	1301	NAP	6	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	545/575 (94%)	-0.08	11 (2%)	65 50	21, 43, 80, 131	0
1	B	545/575 (94%)	-0.07	11 (2%)	65 50	19, 41, 76, 119	0
All	All	1090/1150 (94%)	-0.08	22 (2%)	65 50	19, 42, 79, 131	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	561	GLY	3.8
1	B	18	PRO	3.4
1	A	458	ASP	3.0
1	B	319	ARG	2.9
1	B	372	ALA	2.7
1	A	320	SER	2.7
1	B	307	GLU	2.6
1	B	376	THR	2.6
1	A	376	THR	2.5
1	A	430	ASN	2.5
1	A	18	PRO	2.3
1	A	562	ALA	2.3
1	A	370	CYS	2.2
1	B	427	ALA	2.2
1	B	371	LYS	2.2
1	A	321	MET	2.1
1	B	58	ASP	2.1
1	B	373	LEU	2.1
1	B	306	LYS	2.1
1	A	361	ALA	2.0
1	B	506	GLY	2.0
1	A	313	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

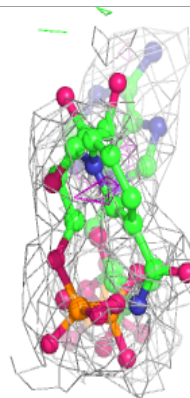
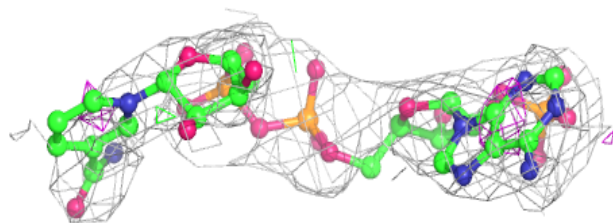
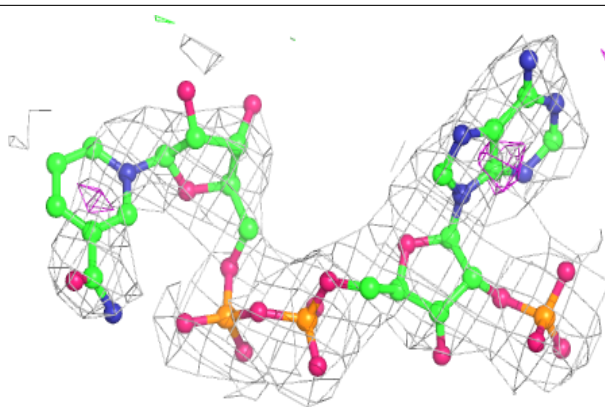
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAP	B	1301	48/48	0.92	0.20	58,70,77,78	0
3	SO4	B	1302	5/5	0.94	0.18	82,82,83,85	0
2	NAP	A	1301	48/48	0.95	0.17	34,45,59,67	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.

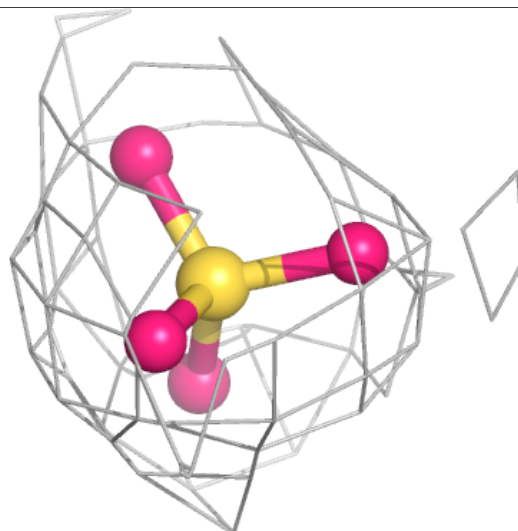
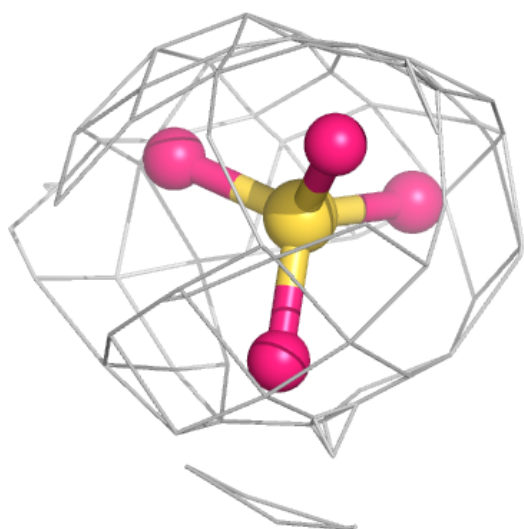
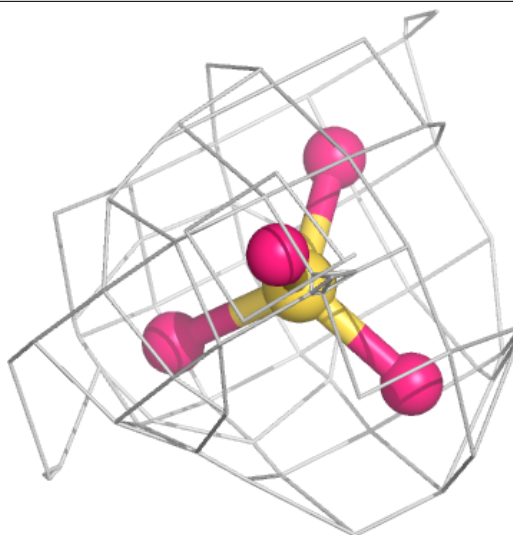
Electron density around NAP B 1301:

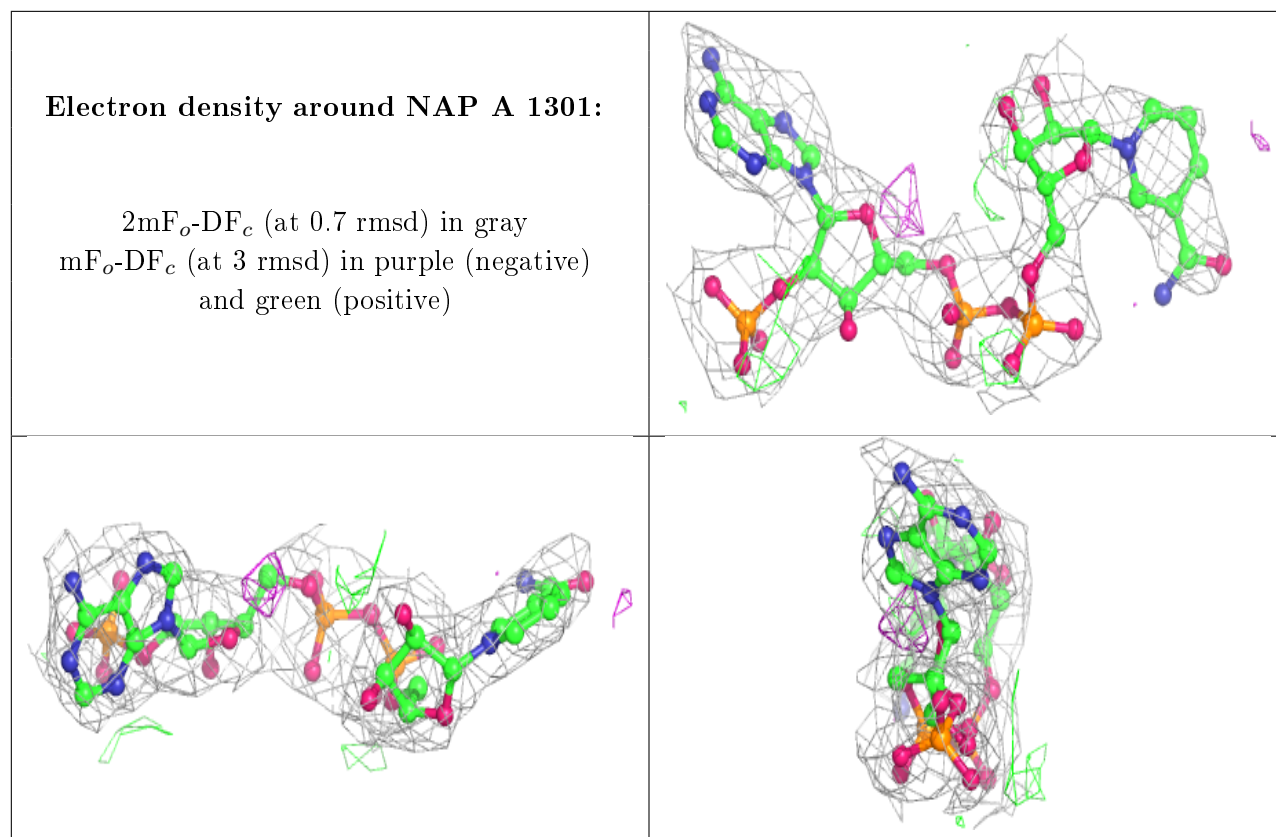
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SO4 B 1302:

$2mF_o-DF_c$ (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.