



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:59 PM EDT

PDB ID : 6K8W / pdb_00006k8w
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 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

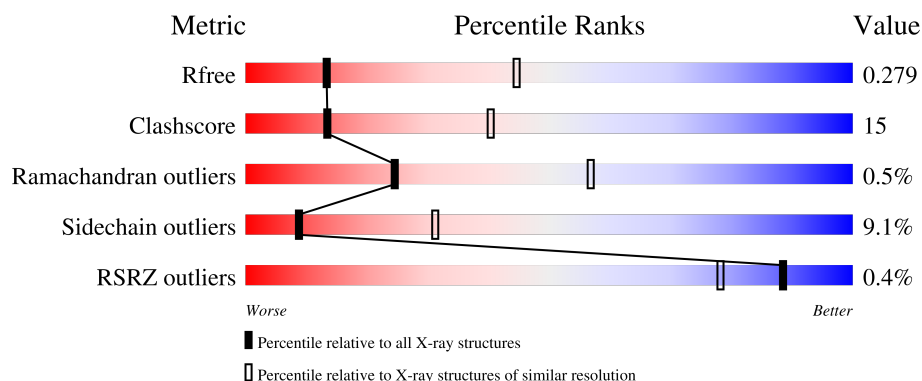
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

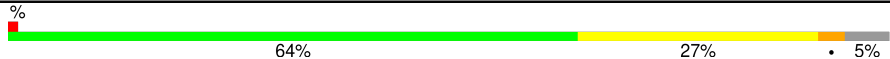
The reported resolution of this entry is 3.17 Å.

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}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (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 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	575	
1	B	575	

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.

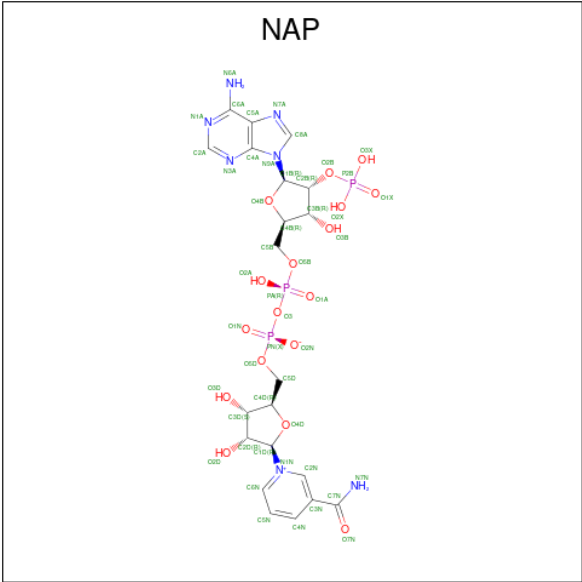
- Molecule 1 is a protein called NAD-dependent epimerase/dehydratase:Short-chain dehydrogenase/reductase SDR.

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:

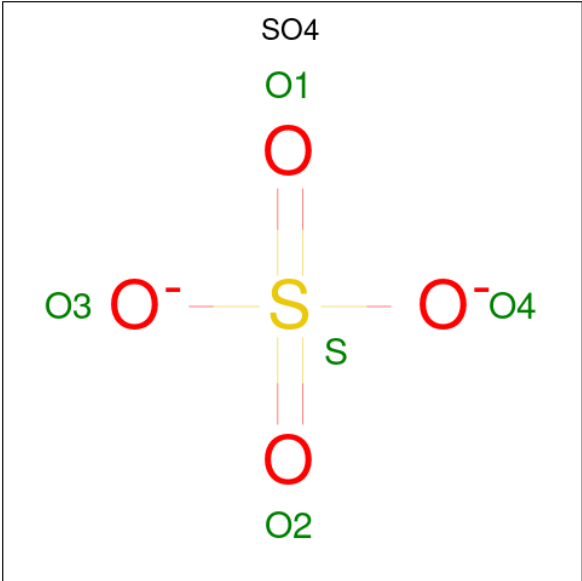
Chain	Residue	Modelled	Actual	Comment	Reference
A	568	LEU	-	expression tag	UNP A0A1A7BFR5
A	569	GLU	-	expression tag	UNP A0A1A7BFR5
A	570	HIS	-	expression tag	UNP A0A1A7BFR5
A	571	HIS	-	expression tag	UNP A0A1A7BFR5
A	572	HIS	-	expression tag	UNP A0A1A7BFR5
A	573	HIS	-	expression tag	UNP A0A1A7BFR5
A	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 (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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

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



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

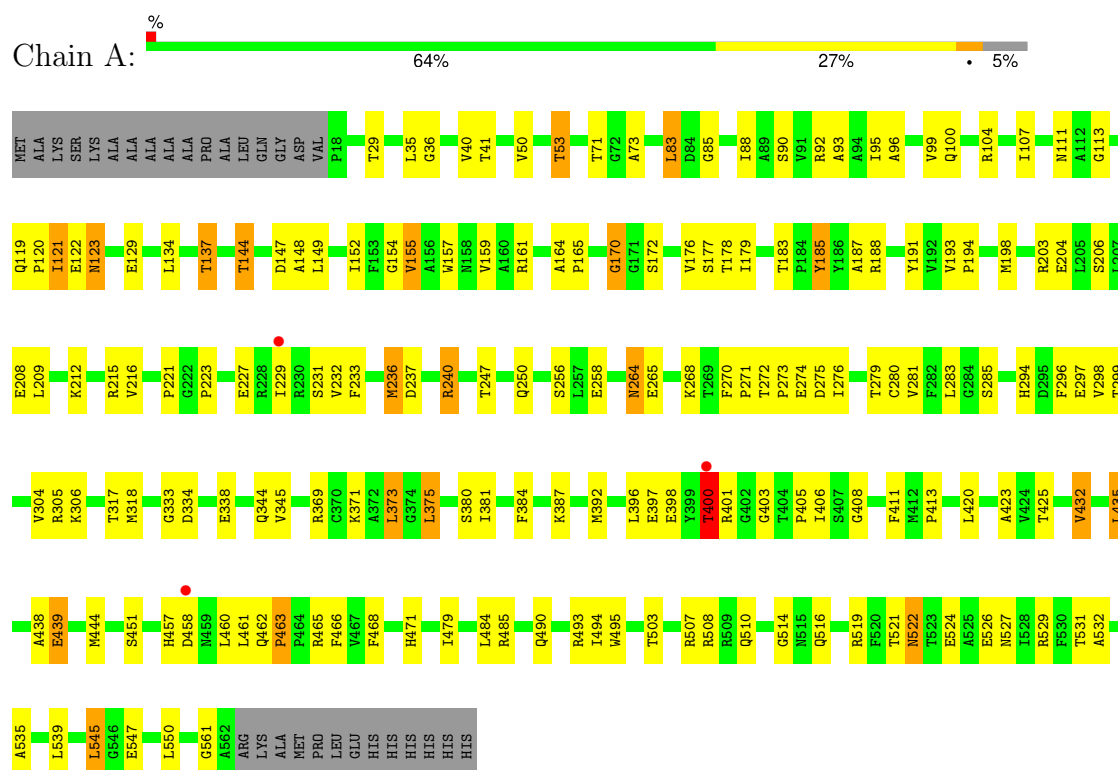
- Molecule 4 is water.

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

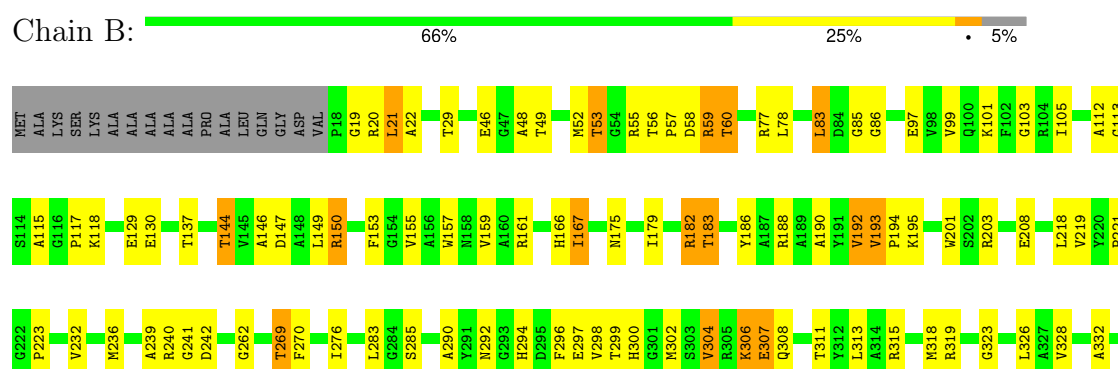
3 Residue-property plots

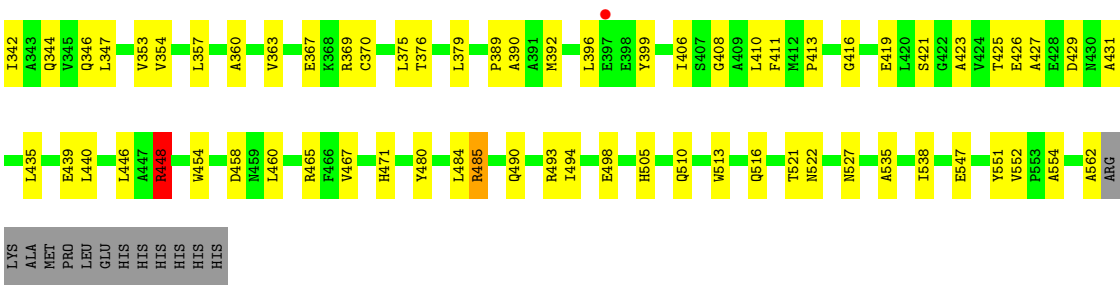
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NAD-dependent epimerase/dehydratase:Short-chain dehydrogenase/reductase SDR



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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 33.76 – 3.17	Depositor EDS
% Data completeness (in resolution range)	96.8 (33.76-3.17) 96.8 (33.76-3.17)	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 (4.76%)	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)	0.32 , 41.1	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 [i](#)

5.1 Standard geometry [i](#)

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	1.04	0/4145	1.58	11/5623 (0.2%)
1	B	1.04	1/4153 (0.0%)	1.56	13/5634 (0.2%)
All	All	1.04	1/8298 (0.0%)	1.57	24/11257 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	ILE	N-CA	5.77	1.50	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	VAL	N-CA-CB	6.25	114.44	110.50
1	A	154	GLY	CA-C-N	5.51	127.98	120.77
1	A	154	GLY	C-N-CA	5.51	127.98	120.77
1	B	494	ILE	CA-C-N	5.43	127.50	120.44
1	B	494	ILE	C-N-CA	5.43	127.50	120.44
1	A	170	GLY	CA-C-N	5.40	125.47	120.34
1	A	170	GLY	C-N-CA	5.40	125.47	120.34
1	A	439	GLU	CA-C-N	-5.36	111.41	120.58
1	A	439	GLU	C-N-CA	-5.36	111.41	120.58
1	B	192	VAL	N-CA-C	5.36	115.57	110.53
1	B	480	TYR	CA-C-N	5.28	125.80	119.94
1	B	480	TYR	C-N-CA	5.28	125.80	119.94
1	B	49	THR	CB-CA-C	5.27	119.02	110.22
1	A	400	THR	CB-CA-C	5.24	119.49	110.79
1	A	403	GLY	CA-C-N	5.20	131.28	122.65
1	A	403	GLY	C-N-CA	5.20	131.28	122.65
1	B	448	ARG	CA-C-N	5.19	127.19	120.44
1	B	448	ARG	C-N-CA	5.19	127.19	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	PHE	CA-C-N	5.19	125.70	120.00
1	B	153	PHE	C-N-CA	5.19	125.70	120.00
1	B	390	ALA	CA-C-N	5.17	127.64	120.29
1	B	390	ALA	C-N-CA	5.17	127.64	120.29
1	A	438	ALA	CA-C-N	-5.03	111.97	120.58
1	A	438	ALA	C-N-CA	-5.03	111.97	120.58

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	125	0
1	B	4082	0	4062	127	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	241	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 15.

All (241) 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:A:458:ASP:O	1:A:510:GLN:HG3	1.77	0.84
1:B:223:PRO:HD3	1:B:302:MET:HE1	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:545:LEU:HD23	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: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:176:VAL:O	1:A:198:MET:HE1	1.97	0.65
1:A:85:GLY:HA3	1:A:155:VAL:HG12	1.78	0.65
1:A:420:LEU:HD13	1:A:435:LEU:HB2	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:B:299:THR:HB	1:B:302:MET:HE3	1.80	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:547:GLU:CD	1:B:547:GLU:H	2.06	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:83:LEU:HD23	1:B:83:LEU:C	2.27	0.59
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:182:ARG:HB3	1:B:304:VAL:HG11	1.84	0.59
1:B:236:MET:O	1:B:239:ALA:HB3	2.03	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: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:B:179:ILE:HG21	1:B:302:MET:HE1	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:29:THR:HA	1:B:53:THR:HB	1.88	0.55
1:B:115:ALA:O	1:B:188:ARG:NH2	2.34	0.55
1:B:223:PRO:HD3	1:B:302:MET:CE	2.34	0.55
1:B:308:GLN:CD	1:B:493:ARG:NH1	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:462:GLN:O	1:A:463:PRO:C	2.50	0.52
1:A:208:GLU:CD	1:A:423:ALA:HB1	2.35	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
2:A:1301:NAP:O1A	2:A:1301:NAP:H4B	2.10	0.51
1:B:53:THR:HG23	1:B:83:LEU:HB3	1.91	0.51
1:B:241:GLY:O	1:B:505:HIS:NE2	2.42	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: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: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:A:120:PRO:O	1:A:121:ILE:C	2.55	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:GLY:HA3	1:B:150:ARG:HG3	1.95	0.48
1:A:280:CYS:O	1:A:281:VAL:C	2.57	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: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: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:193:VAL:CG2	1:B:194:PRO:HD3	2.45	0.46
1:B:19:GLY:C	1:B:21:LEU:N	2.71	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:53:THR:HG21	1:B:83:LEU:HD22	1.98	0.46
1:B:57:PRO:HA	1:B:60:THR:HG22	1.96	0.46
1:B:19:GLY:C	1:B:21:LEU:H	2.23	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:188:ARG:CG	1:A:236:MET:HE3	2.46	0.45
1:A:188:ARG:HG2	1:A:236:MET:HE3	1.99	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:396:LEU:CD2	1:B:406:ILE:HD13	2.47	0.45
1:B:521:THR:OG1	1:B:552:VAL:O	2.27	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: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
1:A:29:THR:HA	1:A:53:THR:CG2	2.47	0.44
1:A:179:ILE:HG12	1:A:299:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:A:104:ARG:HH21	1.83	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:A:71:THR:C	1:A:73:ALA:H	2.25	0.43
1:B:29:THR:HB	1:B:112:ALA:HB2	2.00	0.43
1:B:223:PRO:CD	1:B:302:MET:HE1	2.40	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:B:85:GLY:HA3	1:B:155:VAL:HA	1.99	0.43
1:A:104:ARG:HG2	1:A:104:ARG:NH2	2.32	0.43
1:A:274:GLU:CD	1:A:274:GLU:H	2.25	0.43
1:B:113:GLY:O	2:B:1301:NAP:H8A	2.18	0.43
1:B:319:ARG:HD3	1:B:319:ARG:N	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:HD12	1:B:21:LEU:HA	1.86	0.42
1:B:223:PRO:CD	1:B:302:MET:CE	2.96	0.42
1:A:193:VAL:HG11	1:A:444:MET:HE2	2.00	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

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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:99:VAL:O	1:B:103:GLY:N	2.52	0.42
1:B:347:LEU:HG	1:B:353:VAL:HG21	2.02	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: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:A:178:THR:HG21	1:A:191:TYR:CE2	2.56	0.41
1:B:485:ARG:HA	1:B:516:GLN:HE22	1.85	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%)	21	53
1	B	544/575 (95%)	504 (93%)	38 (7%)	2 (0%)	30	60
All	All	1087/1150 (94%)	1002 (92%)	80 (7%)	5 (0%)	24	57

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%)	365 (89%)	45 (11%)	6	24
1	B	411/431 (95%)	381 (93%)	30 (7%)	13	40
All	All	821/862 (95%)	746 (91%)	75 (9%)	9	31

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	53	THR
1	A	83	LEU
1	A	90	SER
1	A	95	ILE
1	A	99	VAL
1	A	100	GLN
1	A	122	GLU
1	A	123	ASN
1	A	129	GLU
1	A	137	THR

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Mol	Chain	Res	Type
1	A	144	THR
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	279	THR
1	A	304	VAL
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	381	ILE
1	A	387	LYS
1	A	400	THR
1	A	432	VAL
1	A	435	LEU
1	A	451	SER
1	A	461	LEU
1	A	471	HIS
1	A	521	THR
1	A	522	ASN
1	A	545	LEU
1	B	21	LEU
1	B	53	THR
1	B	59	ARG
1	B	60	THR
1	B	83	LEU
1	B	129	GLU
1	B	137	THR
1	B	144	THR

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Mol	Chain	Res	Type
1	B	150	ARG
1	B	182	ARG
1	B	183	THR
1	B	203	ARG
1	B	232	VAL
1	B	240	ARG
1	B	242	ASP
1	B	269	THR
1	B	285	SER
1	B	304	VAL
1	B	306	LYS
1	B	307	GLU
1	B	318	MET
1	B	369	ARG
1	B	370	CYS
1	B	376	THR
1	B	421	SER
1	B	429	ASP
1	B	435	LEU
1	B	448	ARG
1	B	485	ARG
1	B	527	ASN

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

Mol	Chain	Res	Type
1	A	42	HIS
1	A	110	ASN
1	A	111	ASN
1	A	166	HIS
1	A	175	ASN
1	A	217	ASN
1	A	264	ASN
1	A	294	HIS
1	A	352	GLN
1	A	457	HIS
1	A	515	ASN
1	A	516	GLN
1	B	34	ASN
1	B	166	HIS
1	B	294	HIS
1	B	344	GLN

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Mol	Chain	Res	Type
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	NAP	A	1301	-	50,52,52	1.33	5 (10%)	71,80,80	1.90	19 (26%)
3	SO4	B	1302	-	4,4,4	0.36	0	6,6,6	0.11	0
2	NAP	B	1301	-	50,52,52	1.21	6 (12%)	71,80,80	1.62	13 (18%)

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	A	1301	-	-	7/35/67/67	0/5/5/5
2	NAP	B	1301	-	-	12/35/67/67	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	NAP	C5A-C4A	5.01	1.48	1.39
2	A	1301	NAP	C5A-C4A	4.40	1.46	1.39
2	A	1301	NAP	O4D-C1D	3.31	1.45	1.40
2	A	1301	NAP	C5A-N7A	-3.15	1.33	1.39
2	A	1301	NAP	C4A-N9A	-2.72	1.32	1.37
2	B	1301	NAP	C5A-C6A	2.34	1.47	1.41
2	B	1301	NAP	O4D-C1D	2.28	1.43	1.40
2	B	1301	NAP	C8A-N7A	2.27	1.36	1.31
2	A	1301	NAP	C8A-N7A	2.17	1.35	1.31
2	B	1301	NAP	C5A-N7A	-2.13	1.35	1.39
2	B	1301	NAP	C4A-N9A	-2.08	1.33	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	NAP	C6N-N1N-C2N	-5.27	117.39	121.88
2	B	1301	NAP	C5A-C4A-N3A	-4.72	120.22	126.72
2	A	1301	NAP	C2B-C1B-N9A	-4.65	106.09	113.75
2	B	1301	NAP	N3A-C4A-N9A	4.64	135.06	127.17
2	A	1301	NAP	N3A-C2A-N1A	-4.19	122.24	128.58
2	B	1301	NAP	N3A-C2A-N1A	-3.94	122.62	128.58
2	A	1301	NAP	C2N-N1N-C1D	3.91	127.77	119.13
2	B	1301	NAP	C4A-N9A-C8A	3.82	109.75	105.74
2	A	1301	NAP	N3A-C4A-N9A	3.76	133.56	127.17
2	A	1301	NAP	C5A-C4A-N3A	-3.74	121.56	126.72
2	A	1301	NAP	C4A-N9A-C8A	3.57	109.49	105.74
2	B	1301	NAP	C2A-N3A-C4A	3.41	120.16	111.83
2	A	1301	NAP	C2A-N3A-C4A	3.07	119.33	111.83
2	B	1301	NAP	C2B-C1B-N9A	-2.54	109.57	113.75
2	A	1301	NAP	C2A-N1A-C6A	2.54	122.90	118.73
2	A	1301	NAP	C6N-N1N-C1D	-2.49	114.84	119.73
2	B	1301	NAP	C6N-N1N-C2N	-2.42	119.82	121.88
2	A	1301	NAP	C5N-C6N-N1N	2.34	123.57	120.38
2	A	1301	NAP	O4B-C1B-N9A	2.33	112.57	108.09
2	A	1301	NAP	O2N-PN-O1N	2.31	123.18	112.44
2	B	1301	NAP	N6A-C6A-N1A	2.30	123.50	118.38
2	B	1301	NAP	C4A-C5A-N7A	-2.28	107.97	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	NAP	N9A-C8A-N7A	-2.24	110.76	113.94
2	B	1301	NAP	C2A-N1A-C6A	2.22	122.37	118.73
2	A	1301	NAP	O4D-C4D-C5D	-2.22	102.24	109.33
2	A	1301	NAP	O5D-C5D-C4D	2.19	116.44	108.99
2	A	1301	NAP	C4A-N9A-C1B	-2.19	121.52	126.63
2	A	1301	NAP	N6A-C6A-N1A	2.18	123.23	118.38
2	B	1301	NAP	C5A-C6A-N6A	-2.15	117.97	123.29
2	B	1301	NAP	O2A-PA-O1A	2.12	122.29	112.44
2	B	1301	NAP	C2B-C3B-C4B	2.11	106.53	101.99
2	A	1301	NAP	C4N-C3N-C7N	-2.10	115.33	121.06

There are no chirality outliers.

All (19) torsion outliers are listed below:

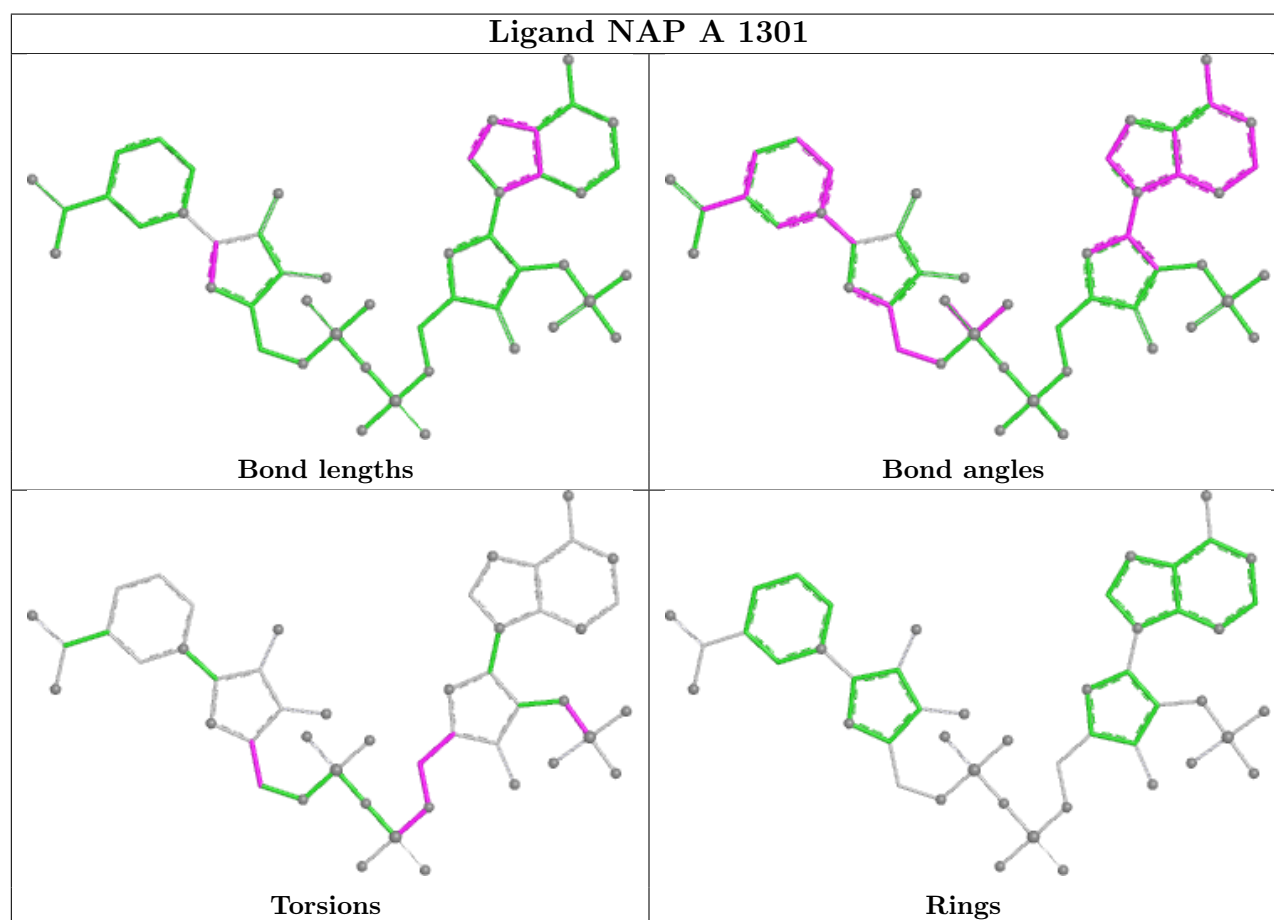
Mol	Chain	Res	Type	Atoms
2	A	1301	NAP	C4B-C5B-O5B-PA
2	B	1301	NAP	C5B-O5B-PA-O1A
2	B	1301	NAP	C5B-O5B-PA-O3
2	B	1301	NAP	C4B-C5B-O5B-PA
2	B	1301	NAP	C5D-O5D-PN-O1N
2	B	1301	NAP	C5D-O5D-PN-O2N
2	A	1301	NAP	C3B-C4B-C5B-O5B
2	A	1301	NAP	O4B-C4B-C5B-O5B
2	A	1301	NAP	C3D-C4D-C5D-O5D
2	A	1301	NAP	O4D-C4D-C5D-O5D
2	B	1301	NAP	C3D-C4D-C5D-O5D
2	A	1301	NAP	C2B-O2B-P2B-O1X
2	B	1301	NAP	O4D-C4D-C5D-O5D
2	A	1301	NAP	C5B-O5B-PA-O1A
2	B	1301	NAP	C5D-O5D-PN-O3
2	B	1301	NAP	C2B-O2B-P2B-O2X
2	B	1301	NAP	C3B-C4B-C5B-O5B
2	B	1301	NAP	C4N-C3N-C7N-N7N
2	B	1301	NAP	C4N-C3N-C7N-O7N

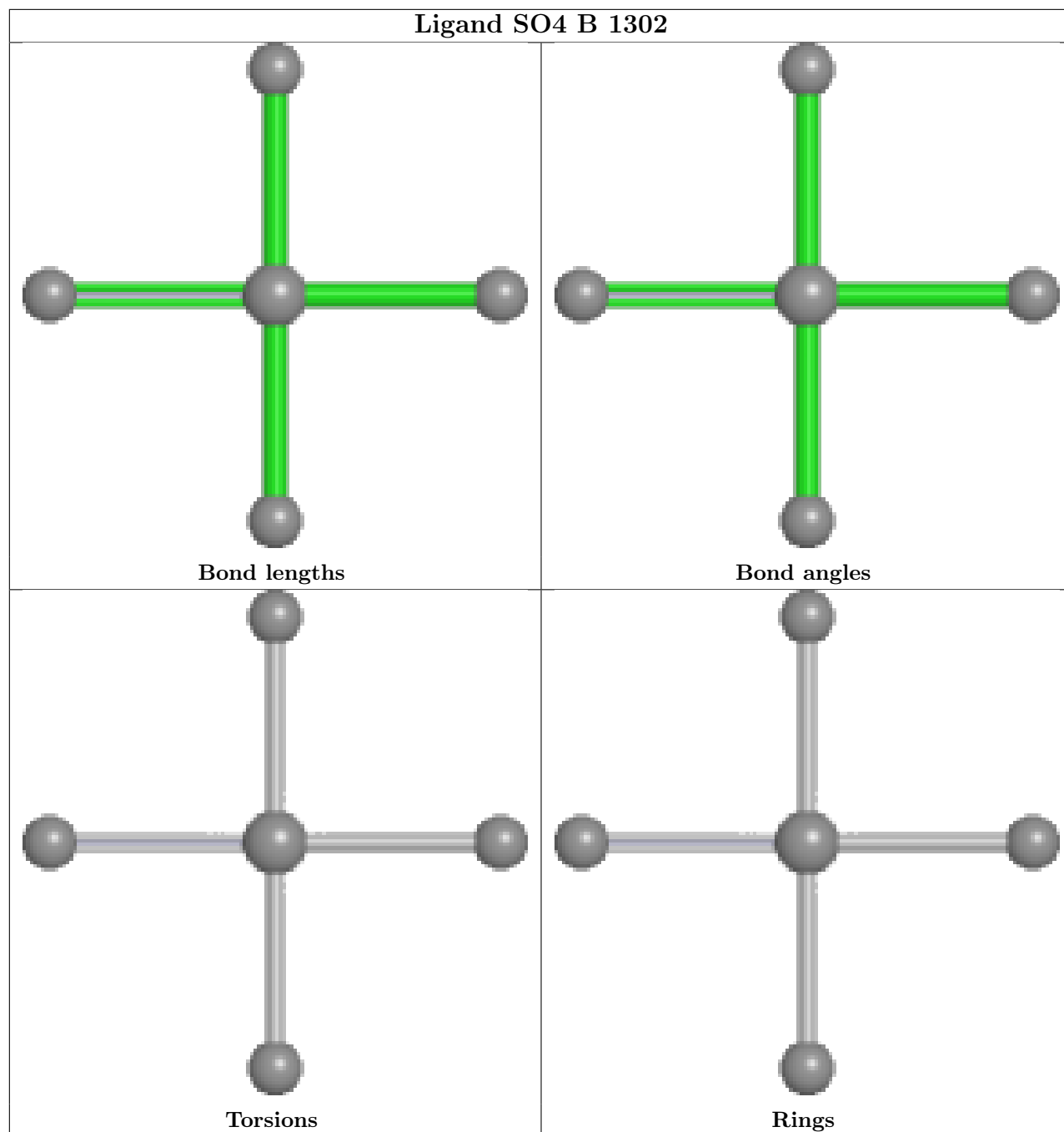
There are no ring outliers.

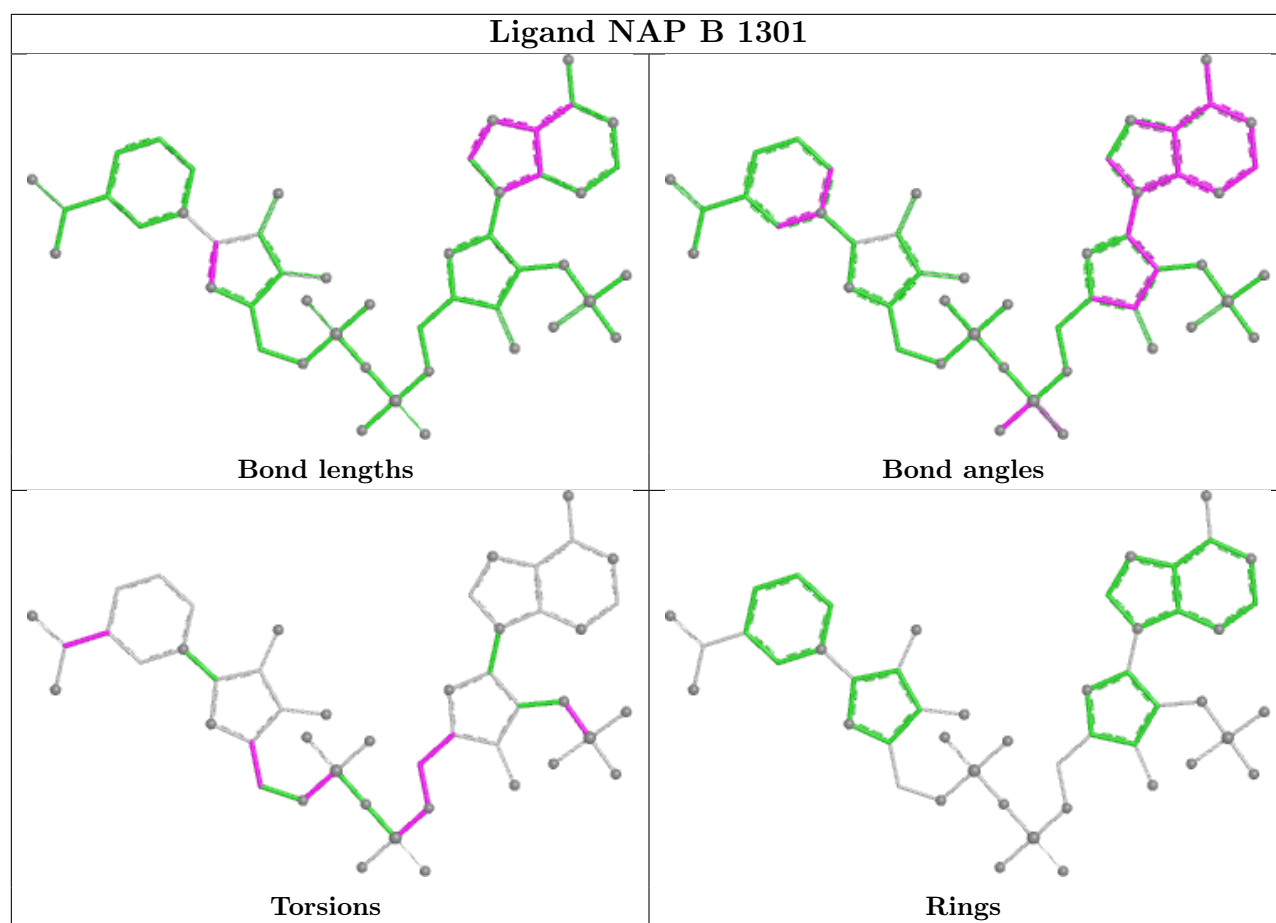
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	NAP	6	0
2	B	1301	NAP	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.11	3 (0%) 85 72	21, 43, 80, 131	0
1	B	545/575 (94%)	-0.15	1 (0%) 91 85	19, 41, 76, 119	1 (0%)
All	All	1090/1150 (94%)	-0.13	4 (0%) 88 78	19, 42, 79, 131	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458	ASP	5.3
1	A	229	ILE	3.4
1	A	400	THR	2.5
1	B	397	GLU	2.4

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(Å ²)	Q<0.9
3	SO4	B	1302	5/5	0.89	0.09	82,82,83,85	0

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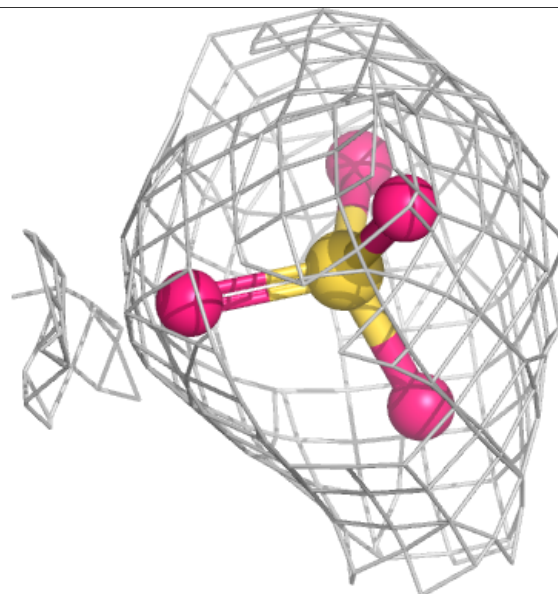
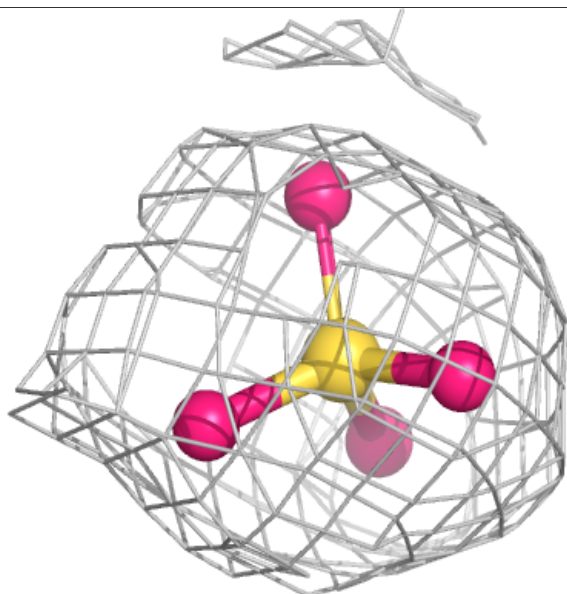
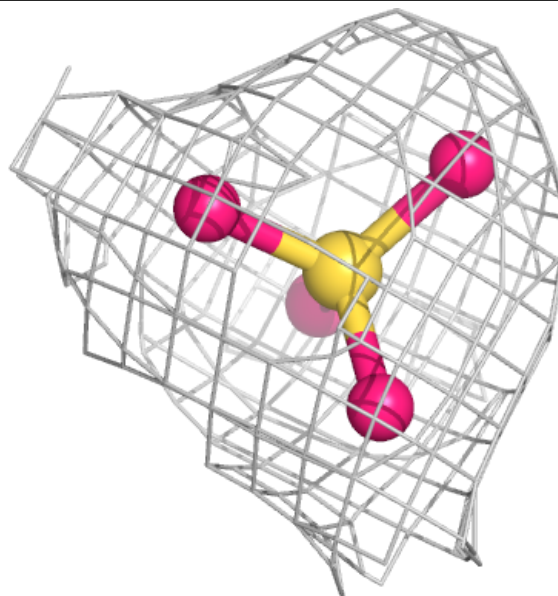
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	B	1301	48/48	0.92	0.10	58,70,77,78	0
2	NAP	A	1301	48/48	0.94	0.09	34,45,59,67	0

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.

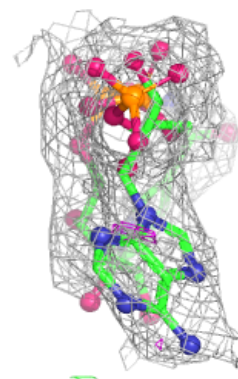
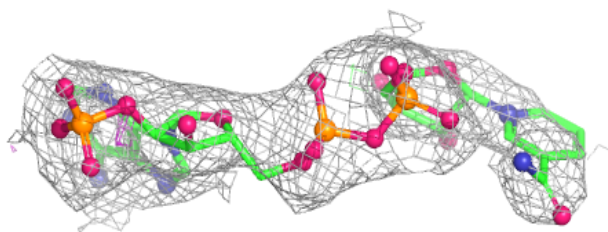
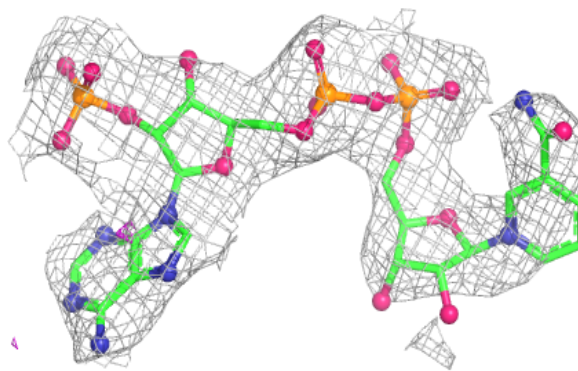
Electron density around SO4 B 1302:

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

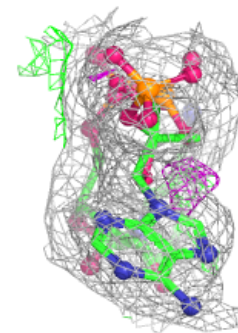
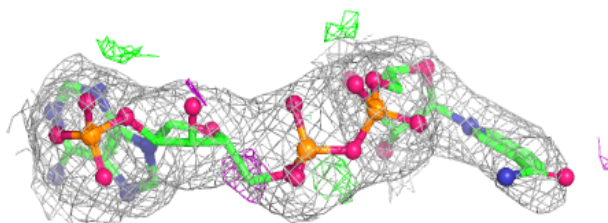
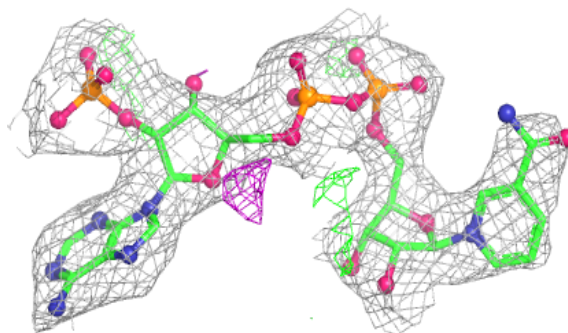


Electron density around NAP B 1301:

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

**Electron density around NAP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.