



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:07 PM UTC

PDB ID : 1N9G / pdb_00001n9g
Title : Mitochondrial 2-enoyl thioester reductase Etr1p/Etr2p heterodimer from *Candida tropicalis*
Authors : Torkko, J.M.; Koivuranta, K.T.; Kastaniotis, A.J.; Airenne, T.T.; Glumoff, T.; Ilves, M.; Hartig, A.; Gurvitz, A.; Hiltunen, J.K.
Deposited on : 2002-11-25
Resolution : 1.98 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

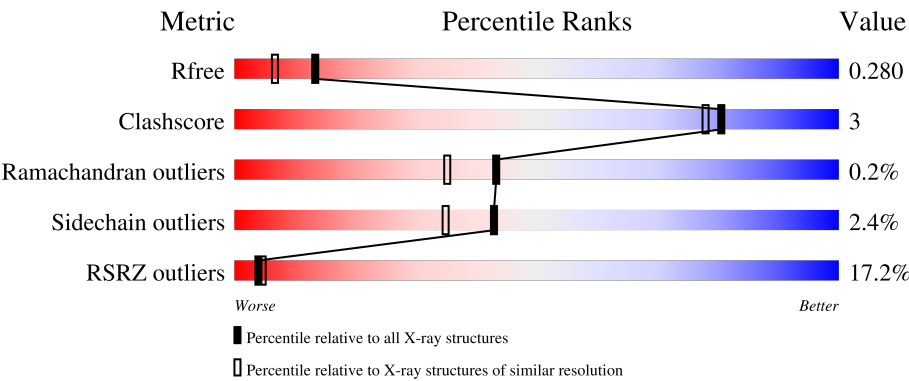
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	386	
1	C	386	
1	F	386	
2	B	386	

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Mol	Chain	Length	Quality of chain
2	D	386	 9% 89% 5% 6%
2	E	386	 17% 86% 8% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1532	-	-	X	-
3	SO4	B	1535	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18417 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.

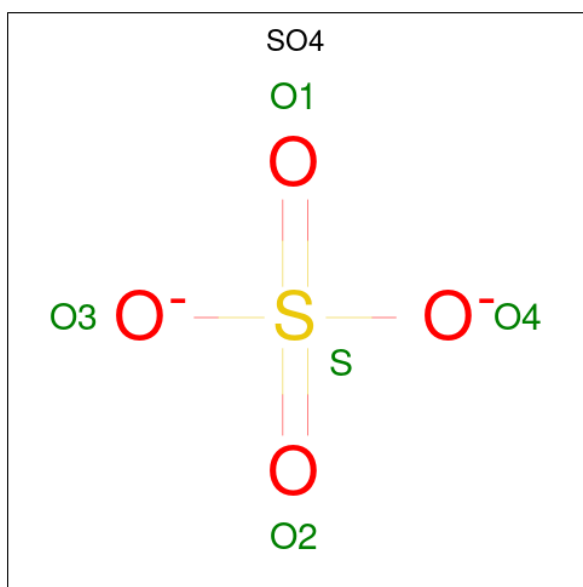
- Molecule 1 is a protein called 2,4-dienoyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	4	0	0
			2785	1768	464	547	6			
1	C	364	Total	C	N	O	S	0	0	0
			2785	1768	464	547	6			
1	F	364	Total	C	N	O	S	0	0	0
			2785	1768	464	547	6			

- Molecule 2 is a protein called 2,4-dienoyl-CoA reductase.

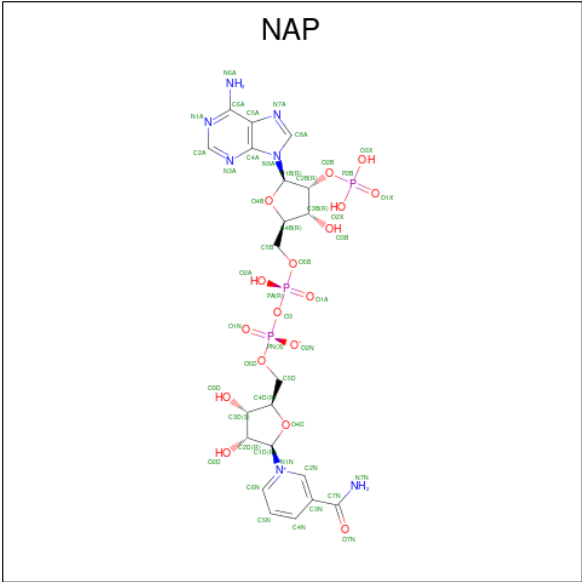
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	4	0	0
			2788	1768	466	548	6			
2	D	364	Total	C	N	O	S	0	0	0
			2787	1767	466	548	6			
2	E	364	Total	C	N	O	S	0	0	0
			2788	1768	466	548	6			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	2	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	1	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	296	Total	O	0	0
			296	296		
5	B	234	Total	O	0	0
			234	234		
5	C	183	Total	O	0	0
			183	183		
5	D	318	Total	O	2	0
			318	318		
5	E	206	Total	O	0	0
			206	206		
5	F	283	Total	O	2	0
			283	283		

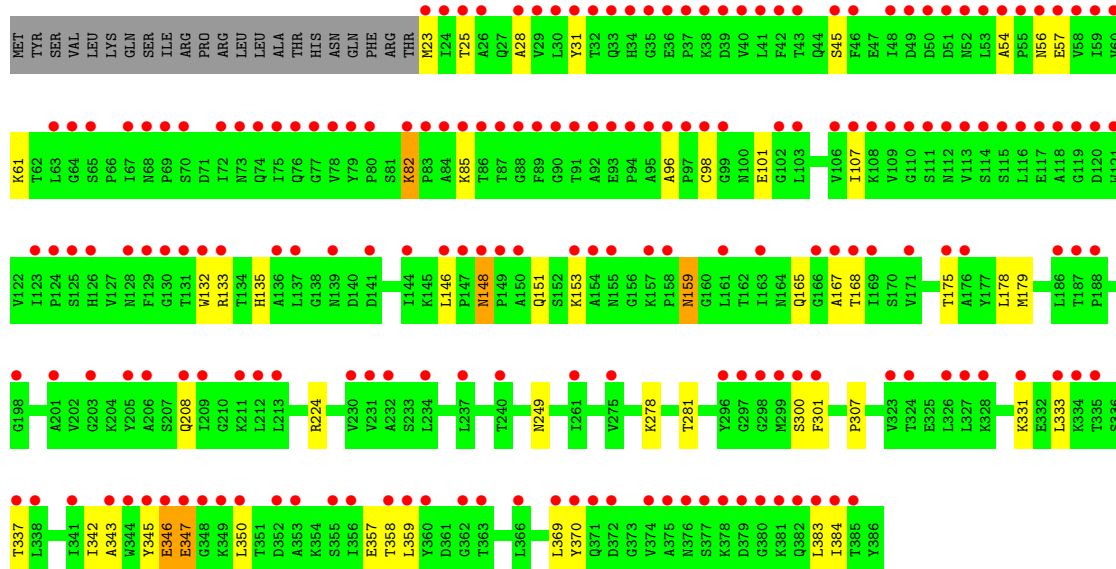
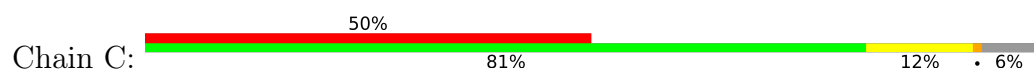
3 Residue-property plots

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.

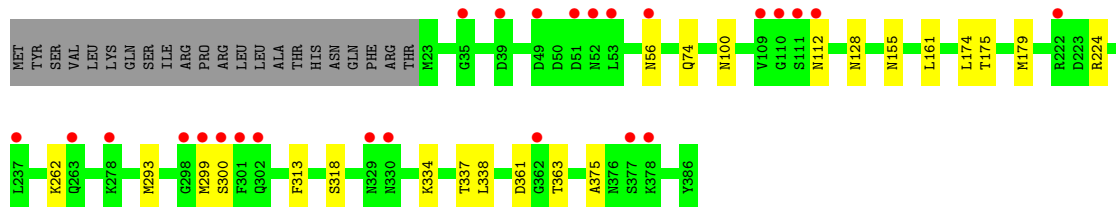
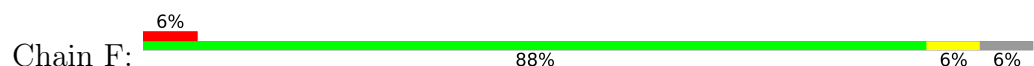
- Molecule 1: 2,4-dienoyl-CoA reductase



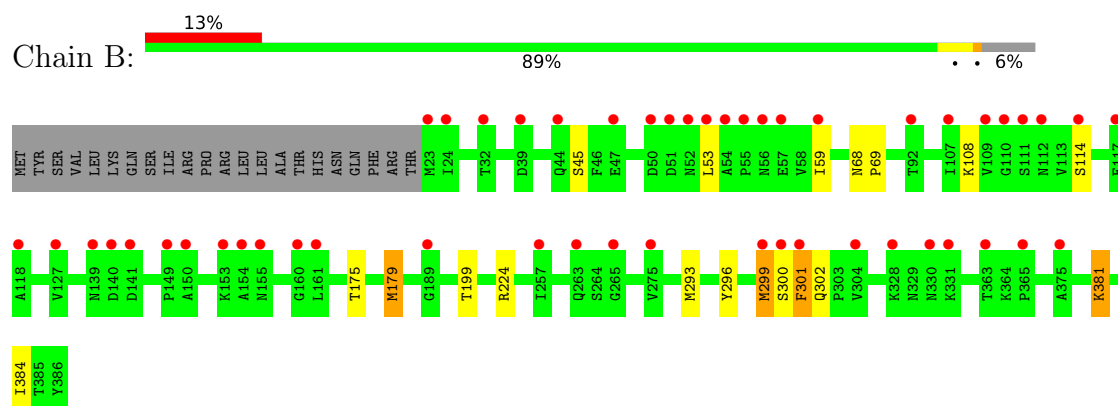
- Molecule 1: 2,4-dienoyl-CoA reductase



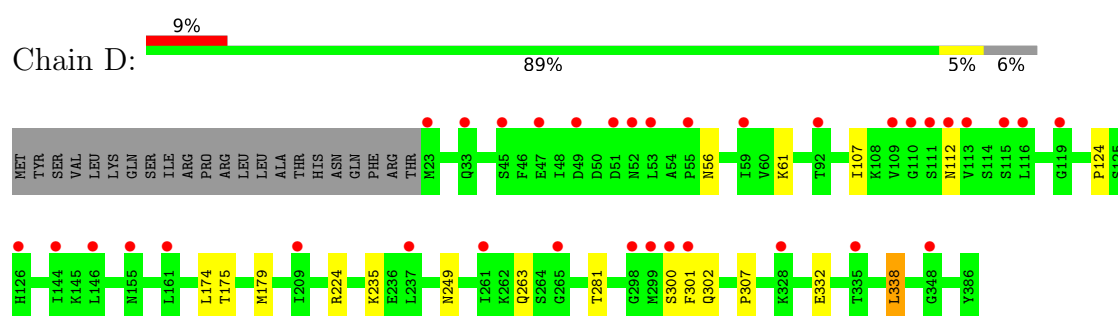
- Molecule 1: 2,4-dienoyl-CoA reductase



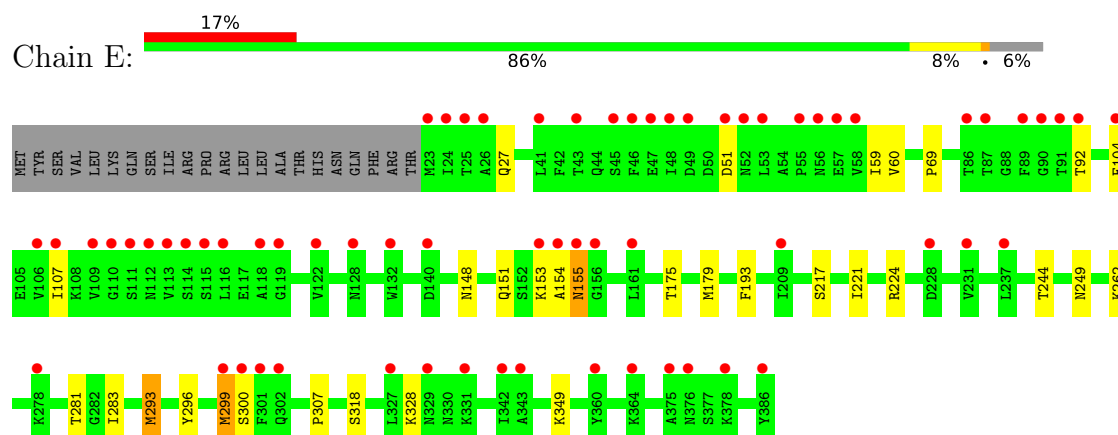
- Molecule 2: 2,4-dienoyl-CoA reductase



- Molecule 2: 2,4-dienoyl-CoA reductase



- Molecule 2: 2,4-dienoyl-CoA reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.45Å 95.50Å 164.23Å 90.00° 124.71° 90.00°	Depositor
Resolution (Å)	19.43 – 1.98 19.43 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.43-1.98) 99.7 (19.43-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.97Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.235 0.257 , 0.280	Depositor DCC
R_{free} test set	10101 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18417	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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	0.78	3/2844 (0.1%)	0.86	0/3865
1	C	0.75	0/2844	0.91	1/3865 (0.0%)
1	F	0.76	2/2844 (0.1%)	0.86	0/3865
2	B	0.83	3/2847 (0.1%)	0.86	2/3870 (0.1%)
2	D	0.74	0/2846	0.88	0/3869
2	E	0.75	1/2847 (0.0%)	0.87	1/3870 (0.0%)
All	All	0.77	9/17072 (0.1%)	0.88	4/23204 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	B	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	199	THR	CB-OG1	-17.91	1.15	1.43
2	E	293	MET	SD-CE	-15.94	1.39	1.79
1	A	296	TYR	C-O	-12.31	1.07	1.24
2	B	293	MET	SD-CE	-12.20	1.49	1.79
1	F	293	MET	SD-CE	-8.92	1.57	1.79
1	A	269	LYS	C-O	-8.71	1.13	1.23
2	B	179	MET	SD-CE	-6.49	1.63	1.79
1	F	313	PHE	N-CA	5.37	1.53	1.46
1	A	293	MET	SD-CE	-5.31	1.66	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	199	THR	CA-CB-OG1	7.71	121.17	109.60
1	C	347	GLU	N-CA-C	-7.35	104.28	113.18
2	E	155	ASN	N-CA-C	-6.64	101.95	110.19
2	B	199	THR	OG1-CB-CG2	5.24	119.77	109.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	299	MET	Peptide
1	C	346	GLU	Peptide

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	2785	0	2767	6	0
1	C	2785	0	2767	32	0
1	F	2785	0	2767	12	0
2	B	2788	0	2767	8	0
2	D	2787	0	2764	9	0
2	E	2788	0	2767	19	0
3	A	5	0	0	2	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
4	A	48	0	25	1	0
4	B	48	0	25	4	0
4	E	48	0	25	6	0
5	A	296	0	0	3	0
5	B	234	0	0	1	0
5	C	183	0	0	9	0
5	D	318	0	0	4	0
5	E	206	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	283	0	0	3	0
All	All	18417	0	16674	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (87) 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:C:159:ASN:HB2	1:C:346:GLU:HB3	1.59	0.85
2:B:300:SER:HB3	5:B:3487:HOH:O	1.80	0.82
2:B:296:TYR:O	4:B:3387:NAP:H2N	1.85	0.76
2:B:69:PRO:HG2	4:B:3387:NAP:H52N	1.68	0.74
2:D:56:ASN:HD21	2:D:112:ASN:HD22	1.36	0.73
1:C:82:LYS:NZ	5:C:1591:HOH:O	2.25	0.69
1:A:221:ILE:HA	3:A:1532:SO4:O3	1.93	0.69
1:C:175:THR:OG1	5:C:1624:HOH:O	2.12	0.68
1:F:334:LYS:CD	5:F:1784:HOH:O	2.44	0.66
1:F:334:LYS:HD3	5:F:1784:HOH:O	1.96	0.66
1:A:236:GLU:OE1	5:A:2472:HOH:O	2.14	0.64
1:C:208:GLN:NE2	5:C:1668:HOH:O	2.31	0.64
3:B:1535:SO4:O2	4:B:3387:NAP:O3B	2.14	0.62
1:C:178:LEU:HD21	1:C:337:THR:HG21	1.83	0.59
1:F:100:ASN:HD22	1:F:128:ASN:H	1.50	0.59
1:F:56:ASN:HD21	1:F:112:ASN:HD22	1.51	0.58
1:C:56:ASN:N	5:C:1556:HOH:O	2.20	0.58
2:D:302:GLN:NE2	5:D:1623:HOH:O	2.29	0.57
2:E:69:PRO:HG2	4:E:4387:NAP:H52N	1.87	0.57
2:E:221:ILE:O	2:E:244:THR:HA	2.05	0.57
1:F:174:LEU:HD22	1:F:337:THR:HG22	1.85	0.57
1:C:61:LYS:HG2	1:C:135:HIS:CD2	2.40	0.56
1:C:333:LEU:O	1:C:337:THR:HG23	2.05	0.56
2:E:299:MET:HE2	4:E:4387:NAP:O4B	2.06	0.56
2:E:249:ASN:ND2	5:E:4531:HOH:O	2.30	0.55
1:A:334:LYS:NZ	5:A:2674:HOH:O	2.38	0.55
1:C:98:CYS:HB3	1:C:132:TRP:CE3	2.43	0.54
1:A:53:LEU:HD11	1:A:59:ILE:HG23	1.89	0.54
1:F:74:GLN:HE22	1:F:100:ASN:HD21	1.56	0.53
1:C:249:ASN:ND2	5:C:1604:HOH:O	2.29	0.53
2:E:283:ILE:HG13	2:E:293:MET:CE	2.39	0.53
1:A:101:GLU:HG2	1:A:167:ALA:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:LEU:HD13	5:C:1639:HOH:O	2.10	0.52
2:E:283:ILE:HG13	2:E:293:MET:HE2	1.91	0.52
2:D:249:ASN:ND2	5:D:1704:HOH:O	2.28	0.51
2:E:59:ILE:HG22	2:E:107:ILE:HD11	1.93	0.51
2:E:296:TYR:O	4:E:4387:NAP:H2N	2.11	0.50
2:B:68:ASN:HD22	2:B:381:LYS:NZ	2.11	0.49
2:E:281:THR:HG23	2:E:307:PRO:HD3	1.94	0.49
2:D:174:LEU:HD21	2:D:338:LEU:HD13	1.94	0.49
1:F:175:THR:HG22	1:F:179:MET:HE2	1.95	0.49
1:F:375:ALA:O	5:F:1798:HOH:O	2.20	0.49
1:C:148:ASN:HD22	1:C:148:ASN:C	2.22	0.48
1:C:281:THR:HG23	1:C:307:PRO:HD3	1.94	0.48
2:B:296:TYR:O	4:B:3387:NAP:C2N	2.59	0.47
2:E:299:MET:HG2	4:E:4387:NAP:C5A	2.44	0.47
1:C:345:TYR:CE2	1:C:350:LEU:HD12	2.49	0.46
2:D:281:THR:HG23	2:D:307:PRO:HD3	1.98	0.46
1:C:159:ASN:C	1:C:346:GLU:HB3	2.42	0.45
2:D:124:PRO:HD2	5:D:1721:HOH:O	2.16	0.45
1:F:100:ASN:ND2	1:F:128:ASN:H	2.12	0.45
2:B:175:THR:HG22	2:B:179:MET:HE2	1.98	0.45
2:D:175:THR:HG22	2:D:179:MET:HE2	1.99	0.45
2:E:349:LYS:NZ	5:E:4464:HOH:O	2.49	0.45
2:E:148:ASN:H	2:E:151:GLN:NE2	2.15	0.45
1:C:175:THR:HG22	1:C:179:MET:HE2	2.00	0.44
2:E:60:VAL:HB	2:E:104:PHE:HB3	1.98	0.44
1:C:28:ALA:HA	1:C:133:ARG:HB3	2.00	0.44
1:C:31:TYR:CZ	1:C:96:ALA:HB3	2.52	0.44
1:C:101:GLU:HG2	1:C:167:ALA:O	2.17	0.44
1:C:357:GLU:HA	1:C:383:LEU:O	2.17	0.44
2:D:235:LYS:CE	5:D:1554:HOH:O	2.66	0.43
2:E:175:THR:HG22	2:E:179:MET:HE2	2.00	0.43
2:E:318:SER:HB3	1:F:318:SER:HB3	2.01	0.43
2:B:300:SER:C	2:B:302:GLN:H	2.26	0.43
1:C:383:LEU:HD21	5:C:1587:HOH:O	2.19	0.43
1:C:165:GLN:HG2	1:C:345:TYR:CE2	2.54	0.43
1:C:343:ALA:O	1:C:347:GLU:HB2	2.19	0.43
3:A:1532:SO4:O1	4:A:2387:NAP:O2B	2.36	0.42
1:C:148:ASN:ND2	1:C:151:GLN:H	2.17	0.42
1:C:148:ASN:HD22	1:C:151:GLN:H	1.66	0.42
2:E:193:PHE:CE2	2:E:217:SER:HB3	2.54	0.42
2:E:299:MET:CE	4:E:4387:NAP:O4B	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:THR:HG23	5:C:1628:HOH:O	2.19	0.42
2:E:154:ALA:C	2:E:155:ASN:O	2.59	0.42
2:E:148:ASN:H	2:E:151:GLN:HE21	1.68	0.42
1:C:54:ALA:HB3	1:C:57:GLU:CD	2.45	0.41
1:F:361:ASP:HB3	1:F:363:THR:HG23	2.02	0.41
2:B:53:LEU:HD21	2:B:59:ILE:CD1	2.51	0.41
1:F:56:ASN:ND2	1:F:112:ASN:HD22	2.17	0.41
1:C:146:LEU:CD2	1:C:342:ILE:HD11	2.51	0.41
1:A:235:LYS:NZ	5:A:2591:HOH:O	2.54	0.41
1:C:45:SER:HB3	5:C:1628:HOH:O	2.21	0.40
1:C:369:LEU:HB3	1:C:384:ILE:HD12	2.02	0.40
1:C:278:LYS:NZ	2:D:263:GLN:O	2.54	0.40
1:C:370:TYR:CE2	1:C:384:ILE:HG13	2.57	0.40
3:E:1536:SO4:S	4:E:4387:NAP:O2B	2.78	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	362/386 (94%)	354 (98%)	8 (2%)	0	100	100
1	C	362/386 (94%)	350 (97%)	11 (3%)	1 (0%)	36	27
1	F	362/386 (94%)	351 (97%)	10 (3%)	1 (0%)	36	27
2	B	362/386 (94%)	353 (98%)	8 (2%)	1 (0%)	36	27
2	D	362/386 (94%)	351 (97%)	10 (3%)	1 (0%)	36	27
2	E	362/386 (94%)	350 (97%)	11 (3%)	1 (0%)	36	27
All	All	2172/2316 (94%)	2109 (97%)	58 (3%)	5 (0%)	43	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	300	SER
2	E	300	SER
1	F	300	SER
2	B	301	PHE
1	C	300	SER

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	306/327 (94%)	302 (99%)	4 (1%)	61	57
1	C	306/327 (94%)	293 (96%)	13 (4%)	26	15
1	F	306/327 (94%)	300 (98%)	6 (2%)	48	42
2	B	307/328 (94%)	299 (97%)	8 (3%)	40	32
2	D	306/328 (93%)	300 (98%)	6 (2%)	48	42
2	E	307/328 (94%)	299 (97%)	8 (3%)	40	32
All	All	1838/1965 (94%)	1793 (98%)	45 (2%)	43	35

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	300	SER
1	A	328	LYS
1	A	378	LYS
2	B	45	SER
2	B	108	LYS
2	B	114	SER
2	B	224	ARG
2	B	299	MET
2	B	301	PHE
2	B	381	LYS
2	B	384	ILE
1	C	23	MET
1	C	82	LYS

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Mol	Chain	Res	Type
1	C	85	LYS
1	C	107	ILE
1	C	148	ASN
1	C	153	LYS
1	C	159	ASN
1	C	168	THR
1	C	224	ARG
1	C	301	PHE
1	C	331	LYS
1	C	358	THR
1	C	359	LEU
2	D	61	LYS
2	D	107	ILE
2	D	224	ARG
2	D	301	PHE
2	D	332	GLU
2	D	338	LEU
2	E	27	GLN
2	E	51	ASP
2	E	92	THR
2	E	153	LYS
2	E	224	ARG
2	E	262	LYS
2	E	299	MET
2	E	328	LYS
1	F	155	ASN
1	F	161	LEU
1	F	224	ARG
1	F	262	LYS
1	F	299	MET
1	F	338	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	56	ASN
1	A	112	ASN
1	A	155	ASN
2	B	68	ASN
2	B	135	HIS
2	B	376	ASN

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Mol	Chain	Res	Type
1	C	126	HIS
1	C	148	ASN
1	C	249	ASN
1	C	289	ASN
2	D	56	ASN
2	D	73	ASN
2	D	74	GLN
2	D	128	ASN
2	D	139	ASN
2	E	56	ASN
2	E	73	ASN
2	E	112	ASN
2	E	139	ASN
2	E	151	GLN
2	E	155	ASN
2	E	182	HIS
1	F	74	GLN
1	F	112	ASN
1	F	249	ASN
1	F	302	GLN
1	F	330	ASN
1	F	376	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](#)

10 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
4	NAP	E	4387	3	50,52,52	1.67	6 (12%)	71,80,80	1.81	18 (25%)
3	SO4	F	1537	-	4,4,4	0.25	0	6,6,6	0.21	0
3	SO4	D	1533	-	4,4,4	0.32	0	6,6,6	0.54	0
3	SO4	A	1532	-	4,4,4	0.33	0	6,6,6	0.32	0
3	SO4	D	1531	-	4,4,4	0.28	0	6,6,6	0.26	0
4	NAP	B	3387	3	50,52,52	1.89	7 (14%)	71,80,80	1.85	17 (23%)
3	SO4	B	1535	4	4,4,4	4.34	4 (100%)	6,6,6	3.81	5 (83%)
3	SO4	E	1536	4	4,4,4	1.45	1 (25%)	6,6,6	1.98	2 (33%)
3	SO4	C	1534	-	4,4,4	0.28	0	6,6,6	0.41	0
4	NAP	A	2387	-	50,52,52	1.61	4 (8%)	71,80,80	1.56	11 (15%)

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
4	NAP	B	3387	3	-	7/35/67/67	0/5/5/5
4	NAP	A	2387	-	-	10/35/67/67	0/5/5/5
4	NAP	E	4387	3	-	7/35/67/67	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3387	NAP	O7N-C7N	9.72	1.42	1.24
4	A	2387	NAP	O7N-C7N	8.74	1.40	1.24
4	E	4387	NAP	O7N-C7N	8.70	1.40	1.24
3	B	1535	SO4	O4-S	-6.43	0.95	1.48
4	B	3387	NAP	PA-O3	4.03	1.63	1.59
3	B	1535	SO4	O2-S	-3.96	1.21	1.44
3	B	1535	SO4	O1-S	3.07	1.63	1.44
3	B	1535	SO4	O3-S	-3.00	1.23	1.48
4	B	3387	NAP	C2A-N1A	2.95	1.39	1.33
4	B	3387	NAP	C2A-N3A	2.91	1.39	1.33
3	E	1536	SO4	O4-S	-2.87	1.24	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2387	NAP	C2A-N3A	2.77	1.38	1.33
4	E	4387	NAP	C2A-N3A	2.77	1.38	1.33
4	A	2387	NAP	C2A-N1A	2.70	1.38	1.33
4	E	4387	NAP	P2B-O2B	2.63	1.64	1.59
4	E	4387	NAP	C2A-N1A	2.55	1.38	1.33
4	B	3387	NAP	O4D-C1D	2.47	1.44	1.40
4	B	3387	NAP	PN-O3	2.38	1.62	1.59
4	E	4387	NAP	C8A-N7A	2.28	1.36	1.31
4	A	2387	NAP	C8A-N7A	2.10	1.35	1.31
4	E	4387	NAP	O4D-C1D	2.10	1.43	1.40
4	B	3387	NAP	C7N-N7N	2.02	1.36	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2387	NAP	N3A-C2A-N1A	-5.77	119.85	128.58
4	E	4387	NAP	N3A-C2A-N1A	-5.66	120.01	128.58
4	B	3387	NAP	N3A-C2A-N1A	-5.63	120.05	128.58
3	B	1535	SO4	O4-S-O3	5.14	136.89	108.54
4	E	4387	NAP	C5A-C4A-N3A	-4.88	120.00	126.72
3	B	1535	SO4	O4-S-O2	-4.71	84.95	109.56
4	B	3387	NAP	O7N-C7N-C3N	-4.45	114.16	119.60
4	B	3387	NAP	N9A-C8A-N7A	-4.30	107.84	113.94
4	B	3387	NAP	C5A-C4A-N3A	-4.24	120.88	126.72
4	A	2387	NAP	C5A-C4A-N3A	-4.23	120.89	126.72
4	E	4387	NAP	N9A-C8A-N7A	-4.06	108.18	113.94
4	E	4387	NAP	C6N-N1N-C2N	-4.01	118.46	121.88
3	B	1535	SO4	O3-S-O2	4.01	130.52	109.56
4	A	2387	NAP	N9A-C8A-N7A	-3.93	108.37	113.94
3	B	1535	SO4	O4-S-O1	-3.80	89.70	109.56
3	E	1536	SO4	O4-S-O2	-3.78	89.81	109.56
4	E	4387	NAP	C5A-N7A-C8A	3.67	109.22	103.45
4	E	4387	NAP	C2A-N3A-C4A	3.61	120.65	111.83
4	B	3387	NAP	N3A-C4A-N9A	3.56	133.22	127.17
4	B	3387	NAP	C5A-N7A-C8A	3.54	109.01	103.45
4	A	2387	NAP	C5A-N7A-C8A	3.40	108.79	103.45
4	A	2387	NAP	C2A-N3A-C4A	3.34	119.99	111.83
4	E	4387	NAP	C5D-C4D-C3D	-3.20	103.68	115.21
4	E	4387	NAP	N3A-C4A-N9A	3.17	132.56	127.17
4	B	3387	NAP	C2A-N3A-C4A	3.05	119.29	111.83
4	B	3387	NAP	C4A-N9A-C8A	3.02	108.91	105.74
4	B	3387	NAP	O5B-C5B-C4B	2.99	119.18	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3387	NAP	C6N-N1N-C2N	-2.98	119.34	121.88
4	E	4387	NAP	C5N-C4N-C3N	-2.95	117.47	120.36
3	E	1536	SO4	O4-S-O3	2.91	124.57	108.54
4	A	2387	NAP	N3A-C4A-N9A	2.89	132.08	127.17
4	B	3387	NAP	C3N-C7N-N7N	2.84	121.24	117.74
3	B	1535	SO4	O2-S-O1	-2.84	89.08	109.06
4	B	3387	NAP	O5D-C5D-C4D	2.83	118.63	108.99
4	E	4387	NAP	C2B-C3B-C4B	2.60	107.57	101.99
4	E	4387	NAP	C4A-C5A-N7A	-2.59	107.62	110.58
4	B	3387	NAP	C5D-C4D-C3D	-2.43	106.47	115.21
4	E	4387	NAP	O3B-C3B-C4B	-2.42	104.13	111.08
4	E	4387	NAP	C3B-C2B-C1B	-2.37	98.26	102.81
4	B	3387	NAP	O5D-PN-O1N	-2.33	99.71	108.94
4	A	2387	NAP	C4A-C5A-N7A	-2.30	107.95	110.58
4	E	4387	NAP	O2N-PN-O1N	2.29	123.11	112.44
4	B	3387	NAP	C5N-C4N-C3N	-2.28	118.13	120.36
4	B	3387	NAP	O4B-C1B-C2B	-2.23	102.74	106.59
4	A	2387	NAP	O2N-PN-O1N	2.22	122.79	112.44
4	A	2387	NAP	C5D-C4D-C3D	-2.18	107.38	115.21
4	E	4387	NAP	O5D-PN-O1N	-2.17	100.35	108.94
4	E	4387	NAP	O7N-C7N-C3N	-2.13	116.99	119.60
4	E	4387	NAP	O7N-C7N-N7N	2.12	125.69	122.62
4	A	2387	NAP	O7N-C7N-C3N	-2.12	117.01	119.60
4	E	4387	NAP	C2B-C1B-N9A	2.03	117.10	113.75
4	A	2387	NAP	C4A-N9A-C8A	2.03	107.86	105.74
4	B	3387	NAP	C6A-C5A-C4A	2.01	119.92	117.18

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2387	NAP	C5D-O5D-PN-O1N
4	A	2387	NAP	C5D-O5D-PN-O2N
4	A	2387	NAP	O4D-C4D-C5D-O5D
4	B	3387	NAP	C5D-O5D-PN-O3
4	B	3387	NAP	C5D-O5D-PN-O1N
4	B	3387	NAP	C5D-O5D-PN-O2N
4	B	3387	NAP	O4D-C4D-C5D-O5D
4	B	3387	NAP	C3D-C4D-C5D-O5D
4	E	4387	NAP	C5D-O5D-PN-O1N
4	E	4387	NAP	C5D-O5D-PN-O2N
4	A	2387	NAP	C3D-C4D-C5D-O5D

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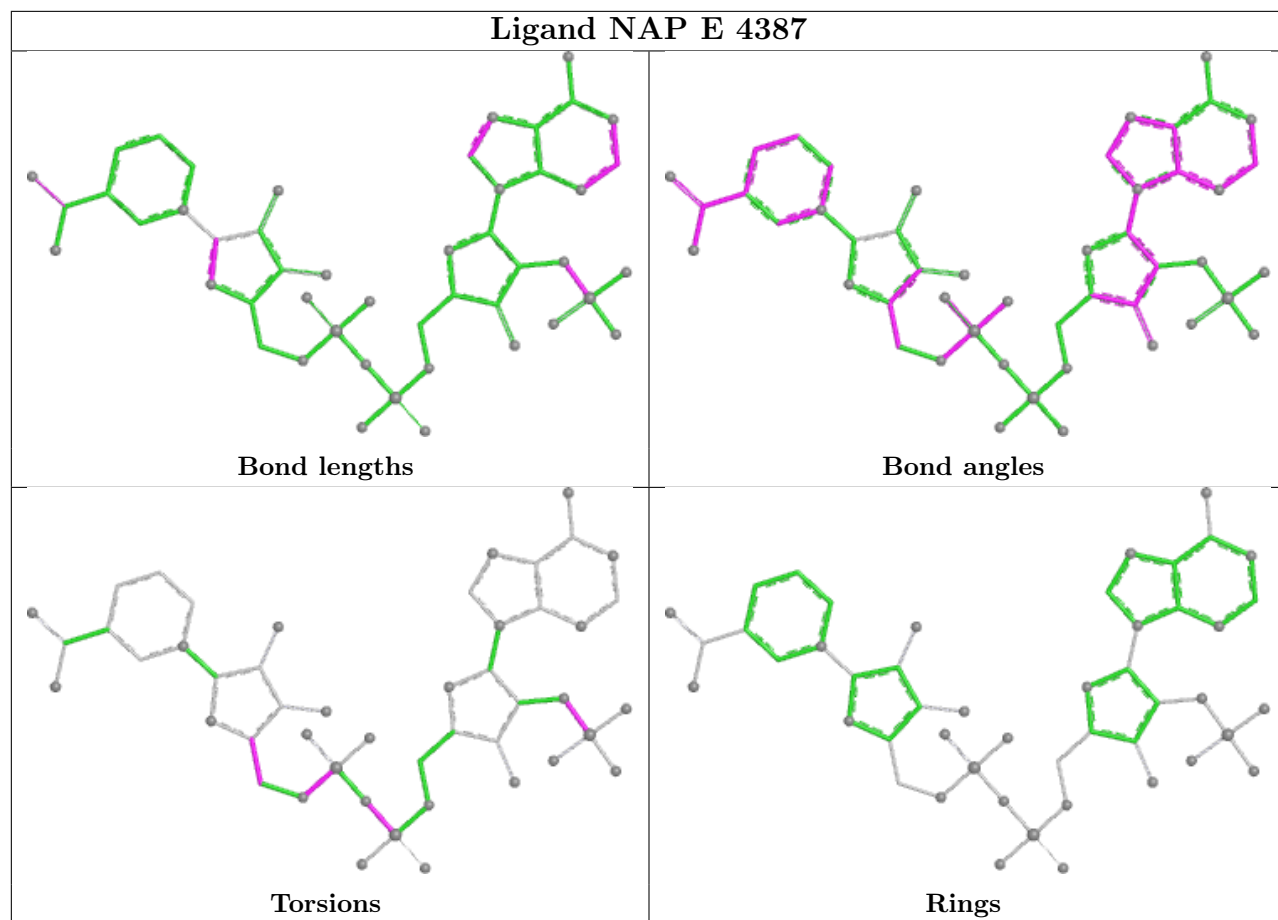
Mol	Chain	Res	Type	Atoms
4	E	4387	NAP	C3D-C4D-C5D-O5D
4	A	2387	NAP	C2B-O2B-P2B-O2X
4	E	4387	NAP	O4D-C4D-C5D-O5D
4	A	2387	NAP	C5D-O5D-PN-O3
4	E	4387	NAP	C5D-O5D-PN-O3
4	B	3387	NAP	C2B-O2B-P2B-O1X
4	E	4387	NAP	C2B-O2B-P2B-O1X
4	A	2387	NAP	O4B-C4B-C5B-O5B
4	A	2387	NAP	PN-O3-PA-O2A
4	B	3387	NAP	PN-O3-PA-O2A
4	E	4387	NAP	PN-O3-PA-O2A
4	A	2387	NAP	C2B-O2B-P2B-O3X
4	A	2387	NAP	C2B-O2B-P2B-O1X

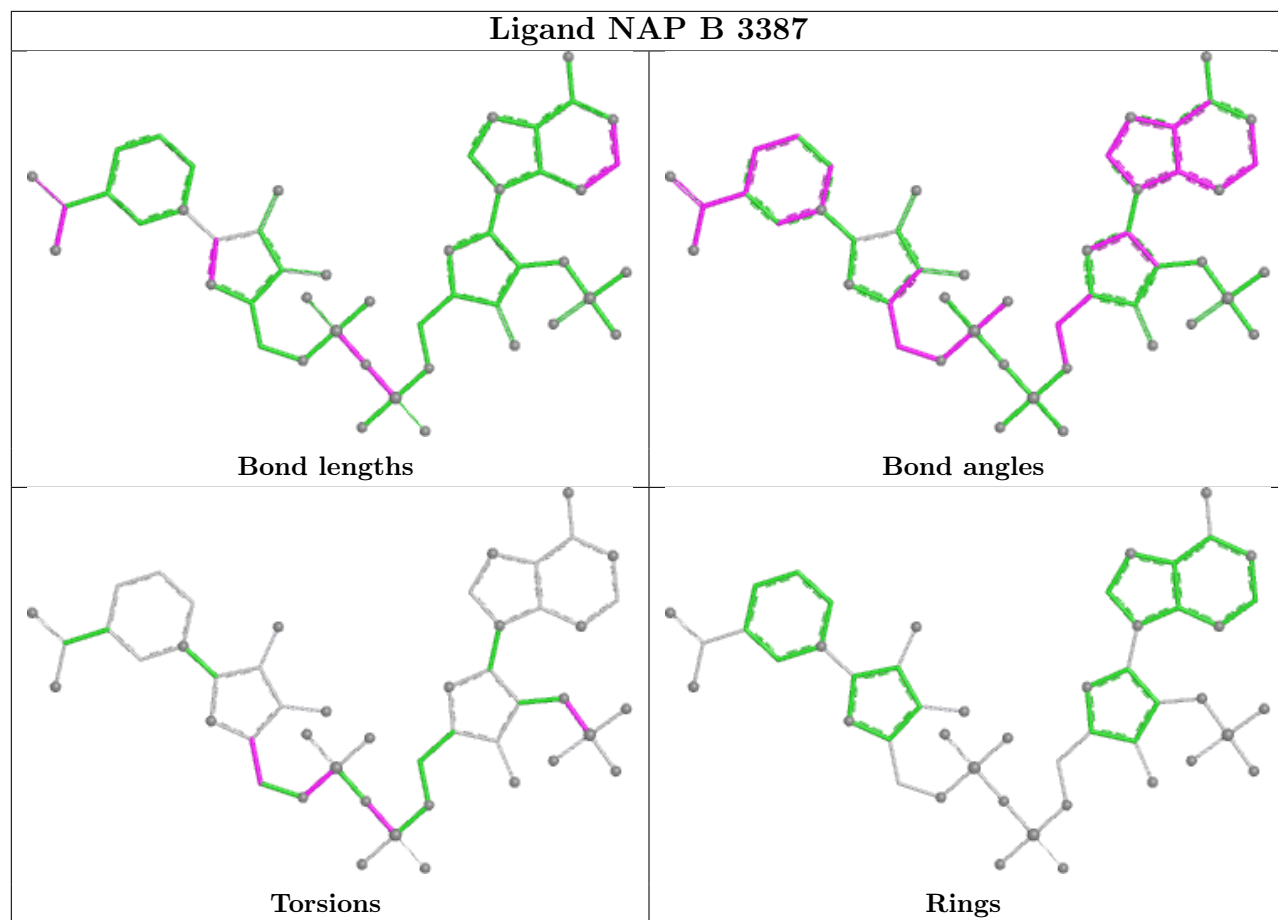
There are no ring outliers.

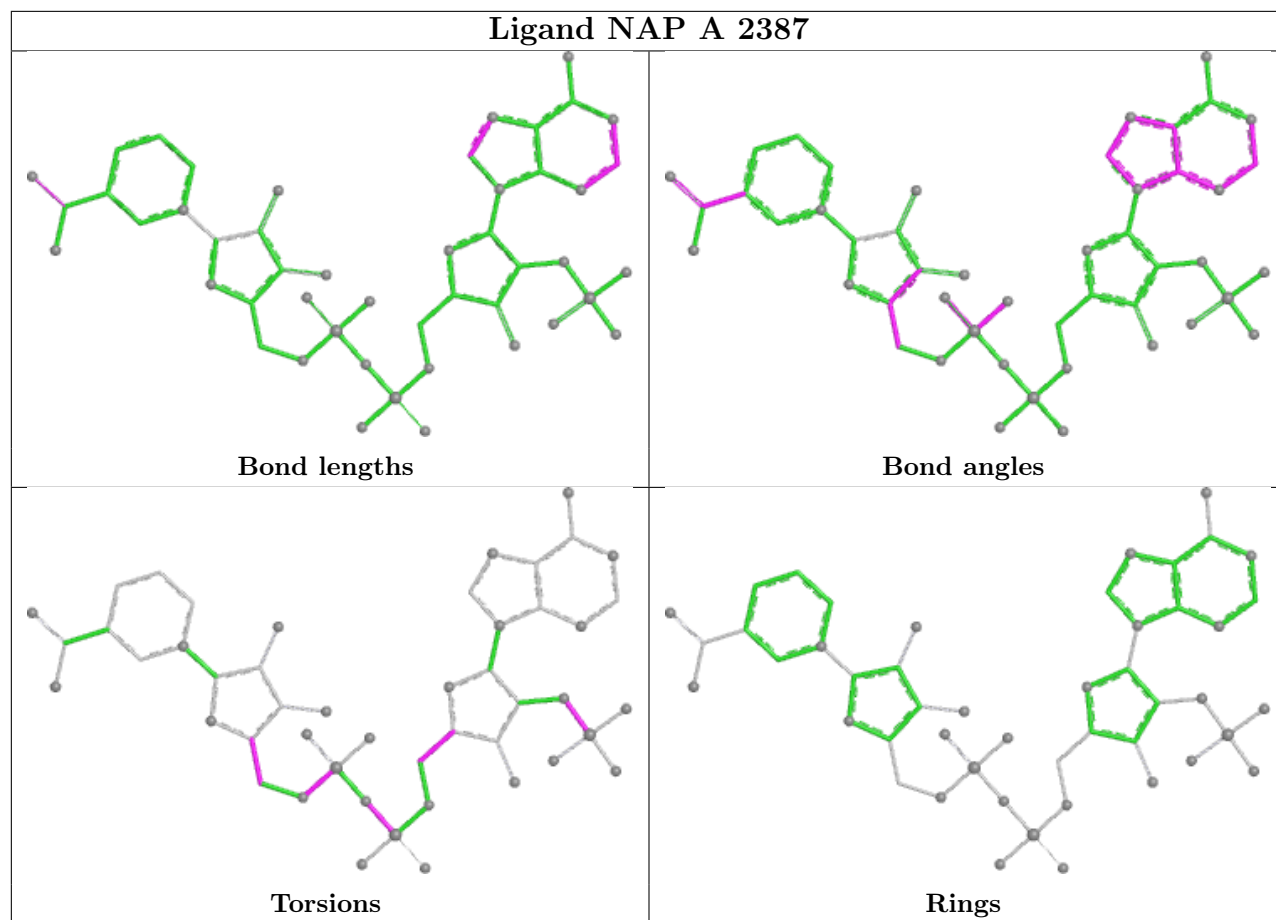
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	4387	NAP	6	0
3	A	1532	SO4	2	0
4	B	3387	NAP	4	0
3	B	1535	SO4	1	0
3	E	1536	SO4	1	0
4	A	2387	NAP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	364/386 (94%)	0.05	5 (1%) 73 81	11, 18, 27, 41	12 (3%)
1	C	364/386 (94%)	2.44	194 (53%) 0 0	11, 32, 58, 70	13 (3%)
1	F	364/386 (94%)	0.85	25 (6%) 23 30	13, 29, 43, 71	3 (0%)
2	B	364/386 (94%)	1.03	50 (13%) 6 9	12, 27, 50, 62	8 (2%)
2	D	364/386 (94%)	0.84	35 (9%) 13 19	12, 27, 40, 51	4 (1%)
2	E	364/386 (94%)	1.29	66 (18%) 3 4	11, 29, 49, 60	4 (1%)
All	All	2184/2316 (94%)	1.08	375 (17%) 4 5	11, 27, 49, 71	44 (2%)

All (375) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	301	PHE	11.8
1	C	41	LEU	8.5
1	F	301	PHE	8.0
1	C	55	PRO	7.7
1	A	301	PHE	7.4
1	C	32	THR	7.3
1	C	301	PHE	6.2
1	C	112	ASN	6.2
1	C	52	ASN	6.1
2	D	301	PHE	6.0
1	C	94	PRO	6.0
1	C	84	ALA	6.0
2	B	301	PHE	6.0
1	C	58	VAL	6.0
1	C	56	ASN	5.9
1	C	95	ALA	5.9
1	C	88	GLY	5.8
1	C	70	SER	5.8
1	C	378	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	35	GLY	5.7
1	C	131	THR	5.7
1	C	153	LYS	5.6
1	C	60	VAL	5.6
1	C	353	ALA	5.5
1	C	31	TYR	5.4
1	C	37	PRO	5.3
2	B	300	SER	5.2
1	C	111	SER	5.2
1	C	75	ILE	5.1
1	C	89	PHE	5.1
1	C	59	ILE	5.0
1	C	90	GLY	5.0
1	C	26	ALA	4.9
1	C	370	TYR	4.9
2	E	111	SER	4.9
1	C	25	THR	4.9
2	E	92	THR	4.8
1	C	79	TYR	4.8
1	C	154	ALA	4.8
2	E	116	LEU	4.8
2	E	23	MET	4.8
1	C	43	THR	4.7
1	C	69	PRO	4.7
2	E	112	ASN	4.7
1	C	42	PHE	4.7
2	E	154	ALA	4.7
1	C	78	VAL	4.7
1	C	92	ALA	4.6
1	C	163	ILE	4.6
1	C	130	GLY	4.6
2	E	90	GLY	4.6
2	D	92	THR	4.6
1	C	102	GLY	4.6
2	E	299	MET	4.5
1	C	348	GLY	4.5
1	F	299	MET	4.5
1	C	110	GLY	4.5
2	D	298	GLY	4.4
1	F	300	SER	4.4
2	E	51	ASP	4.4
1	C	118	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
2	E	113	VAL	4.3
1	C	39	ASP	4.3
1	C	53	LEU	4.3
2	D	55	PRO	4.3
2	E	52	ASN	4.3
1	C	120	ASP	4.3
1	C	24	ILE	4.2
1	C	34	HIS	4.1
1	C	103	LEU	4.1
2	E	25	THR	4.1
1	C	87	THR	4.1
1	C	380	GLY	4.1
1	C	96	ALA	4.0
1	C	86	THR	4.0
2	B	299	MET	4.0
1	C	28	ALA	4.0
1	C	54	ALA	4.0
1	C	157	LYS	4.0
1	C	117	GLU	4.0
1	C	64	GLY	4.0
1	C	48	ILE	4.0
1	C	384	ILE	4.0
2	D	52	ASN	4.0
2	D	112	ASN	4.0
1	C	97	PRO	4.0
1	C	136	ALA	3.9
1	C	72	ILE	3.9
1	C	46	PHE	3.9
1	C	128	ASN	3.9
1	C	369	LEU	3.9
1	C	298	GLY	3.9
1	C	299	MET	3.9
2	B	111	SER	3.8
1	C	109	VAL	3.8
1	C	40	VAL	3.8
2	E	53	LEU	3.7
1	C	68	ASN	3.7
1	C	125	SER	3.7
2	E	118	ALA	3.7
1	C	383	LEU	3.7
1	C	375	ALA	3.6
1	C	171	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	300	SER	3.6
1	C	50	ASP	3.6
1	C	124	PRO	3.6
1	C	374	VAL	3.6
2	E	114	SER	3.6
1	C	167	ALA	3.5
1	C	346	GLU	3.5
2	D	119	GLY	3.5
1	C	65	SER	3.5
1	C	212	LEU	3.5
1	C	108	LYS	3.5
2	D	300	SER	3.5
1	C	132	TRP	3.5
2	B	257	ILE	3.5
1	C	148	ASN	3.4
1	C	343	ALA	3.4
1	C	74	GLN	3.4
2	B	92	THR	3.4
1	C	23	MET	3.4
1	C	51	ASP	3.4
1	F	298	GLY	3.4
1	C	57	GLU	3.3
1	F	329	ASN	3.3
2	B	154	ALA	3.3
1	C	49	ASP	3.3
1	C	107	ILE	3.3
1	C	123	ILE	3.3
1	C	98	CYS	3.3
2	E	55	PRO	3.3
1	A	300	SER	3.3
1	C	381	LYS	3.2
1	C	113	VAL	3.2
1	C	83	PRO	3.2
2	D	53	LEU	3.2
2	E	302	GLN	3.2
2	B	55	PRO	3.2
2	E	56	ASN	3.2
2	E	153	LYS	3.2
1	C	323	VAL	3.2
2	D	109	VAL	3.2
1	C	327	LEU	3.2
2	E	110	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	121	TRP	3.1
1	C	91	THR	3.1
1	C	209	ILE	3.1
1	C	350	LEU	3.1
1	F	112	ASN	3.1
1	C	168	THR	3.1
1	C	169	ILE	3.1
1	C	30	LEU	3.1
1	C	333	LEU	3.1
1	C	85	LYS	3.1
1	F	111	SER	3.1
2	D	111	SER	3.1
2	E	26	ALA	3.1
1	C	77	GLY	3.1
2	D	328	LYS	3.1
1	F	52	ASN	3.1
1	C	337	THR	3.1
2	E	115	SER	3.1
1	C	119	GLY	3.1
1	C	176	ALA	3.1
1	C	345	TYR	3.0
1	A	329	ASN	3.0
1	C	161	LEU	3.0
2	B	53	LEU	3.0
1	C	93	GLU	3.0
1	C	114	SER	3.0
1	F	53	LEU	3.0
1	C	208	GLN	3.0
2	B	149	PRO	3.0
2	B	117	GLU	3.0
2	E	48	ILE	3.0
1	C	116	LEU	2.9
2	B	140	ASP	2.9
1	C	324	THR	2.9
2	B	23	MET	2.9
1	C	344	TRP	2.9
2	B	112	ASN	2.9
1	C	126	HIS	2.9
1	C	76	GLN	2.9
2	E	122	VAL	2.9
2	B	328	LYS	2.9
2	B	114	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	237	LEU	2.9
1	C	326	LEU	2.9
2	B	109	VAL	2.9
1	C	366	LEU	2.9
1	C	147	PRO	2.8
2	E	57	GLU	2.8
1	C	186	LEU	2.8
2	B	150	ALA	2.8
2	B	107	ILE	2.8
1	C	358	THR	2.8
2	B	56	ASN	2.8
1	C	297	GLY	2.8
1	C	359	LEU	2.8
2	D	144	ILE	2.8
1	F	49	ASP	2.8
2	D	23	MET	2.8
1	A	299	MET	2.7
1	C	36	GLU	2.7
1	C	331	LYS	2.7
1	C	360	TYR	2.7
2	B	363	THR	2.7
2	E	87	THR	2.7
2	E	228	ASP	2.7
1	C	234	LEU	2.7
2	E	329	ASN	2.7
1	C	347	GLU	2.7
1	C	377	SER	2.7
1	C	67	ILE	2.7
1	C	106	VAL	2.7
2	E	119	GLY	2.6
1	C	205	TYR	2.6
2	B	59	ILE	2.6
1	C	29	VAL	2.6
1	C	231	VAL	2.6
2	D	49	ASP	2.6
2	D	51	ASP	2.6
2	E	132	TRP	2.6
2	E	104	PHE	2.6
1	C	338	LEU	2.6
1	C	341	ILE	2.6
2	D	59	ILE	2.6
1	C	99	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	110	GLY	2.6
2	B	54	ALA	2.6
2	D	335	THR	2.6
2	E	24	ILE	2.6
1	C	201	ALA	2.6
2	D	113	VAL	2.6
2	E	375	ALA	2.6
1	C	115	SER	2.6
2	E	45	SER	2.6
2	E	327	LEU	2.5
1	C	82	LYS	2.5
1	C	144	ILE	2.5
1	C	362	GLY	2.5
2	B	265	GLY	2.5
1	C	73	ASN	2.5
2	E	231	VAL	2.5
1	C	363	THR	2.5
1	C	133	ARG	2.5
1	C	371	GLN	2.5
2	B	375	ALA	2.5
2	E	106	VAL	2.5
2	B	141	ASP	2.5
1	C	146	LEU	2.5
1	C	198	GLY	2.5
1	C	213	LEU	2.5
1	C	355	SER	2.5
1	C	356	ILE	2.5
1	C	175	THR	2.5
2	E	43	THR	2.5
2	B	50	ASP	2.5
2	B	51	ASP	2.5
2	E	41	LEU	2.4
2	D	33	GLN	2.4
2	E	300	SER	2.4
2	D	209	ILE	2.4
2	E	331	LYS	2.4
1	F	51	ASP	2.4
1	C	80	PRO	2.4
2	E	47	GLU	2.4
2	D	299	MET	2.4
2	B	153	LYS	2.4
2	E	49	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	240	THR	2.4
1	C	335	THR	2.4
1	C	149	PRO	2.4
2	B	189	GLY	2.4
1	C	349	LYS	2.4
2	B	44	GLN	2.4
2	D	155	ASN	2.4
1	F	110	GLY	2.4
1	F	362	GLY	2.4
2	E	58	VAL	2.4
2	D	45	SER	2.4
1	C	38	LYS	2.4
1	C	137	LEU	2.3
2	E	360	TYR	2.3
1	F	302	GLN	2.3
1	F	56	ASN	2.3
2	E	155	ASN	2.3
1	C	166	GLY	2.3
1	C	203	GLY	2.3
2	B	160	GLY	2.3
1	F	222	ARG	2.3
1	C	63	LEU	2.3
2	D	161	LEU	2.3
2	D	126	HIS	2.3
2	B	118	ALA	2.3
2	B	110	GLY	2.3
1	C	352	ASP	2.3
2	E	109	VAL	2.3
1	F	237	LEU	2.3
1	F	378	LYS	2.3
2	E	89	PHE	2.3
1	C	158	PRO	2.3
1	C	188	PRO	2.3
2	D	47	GLU	2.3
1	C	275	VAL	2.3
2	B	304	VAL	2.3
1	C	211	LYS	2.3
1	C	296	TYR	2.2
1	F	39	ASP	2.2
2	E	140	ASP	2.2
2	B	275	VAL	2.2
1	C	376	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	139	ASN	2.2
1	F	278	LYS	2.2
1	C	45	SER	2.2
1	C	382	GLN	2.2
2	E	46	PHE	2.2
1	C	155	ASN	2.2
1	C	334	LYS	2.2
2	B	127	VAL	2.2
1	C	33	GLN	2.2
2	B	161	LEU	2.2
2	B	263	GLN	2.2
2	E	161	LEU	2.2
2	B	47	GLU	2.2
1	C	372	ASP	2.2
2	D	237	LEU	2.2
2	B	365	PRO	2.2
1	C	150	ALA	2.2
2	D	261	ILE	2.1
1	F	109	VAL	2.1
2	E	86	THR	2.1
2	E	91	THR	2.1
2	E	156	GLY	2.1
1	C	139	ASN	2.1
1	F	330	ASN	2.1
2	E	128	ASN	2.1
2	E	343	ALA	2.1
1	F	263	GLN	2.1
2	E	209	ILE	2.1
1	C	385	THR	2.1
2	D	115	SER	2.1
1	C	328	LYS	2.1
2	B	331	LYS	2.1
2	B	155	ASN	2.1
2	B	330	ASN	2.1
2	D	116	LEU	2.1
2	E	237	LEU	2.1
1	A	313	PHE	2.1
1	C	141	ASP	2.1
2	B	24	ILE	2.1
2	E	342	ILE	2.1
2	E	386	TYR	2.1
2	E	364	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	378	LYS	2.1
2	D	265	GLY	2.1
1	C	230	VAL	2.1
2	E	376	ASN	2.1
1	C	232	ALA	2.1
1	C	379	ASP	2.1
2	B	39	ASP	2.1
1	C	129	PHE	2.0
1	C	261	ILE	2.0
2	E	107	ILE	2.0
2	D	348	GLY	2.0
2	B	52	ASN	2.0
2	D	146	LEU	2.0
1	C	206	ALA	2.0
2	B	57	GLU	2.0
2	E	278	LYS	2.0
1	F	377	SER	2.0
1	C	187	THR	2.0
1	F	35	GLY	2.0
2	B	32	THR	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAP	E	4387	48/48	0.83	0.23	21,43,46,47	41
4	NAP	B	3387	48/48	0.84	0.19	22,48,53,54	41
3	SO4	D	1531	5/5	0.85	0.16	60,62,63,63	0

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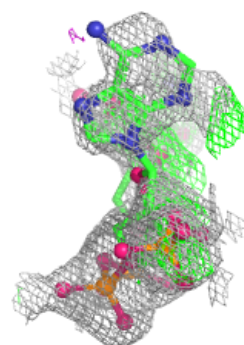
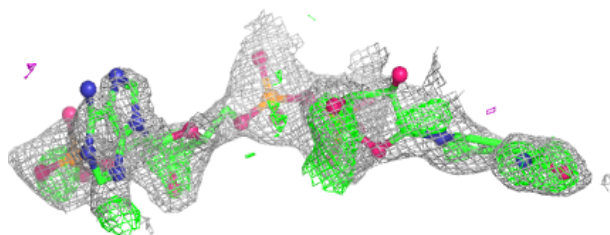
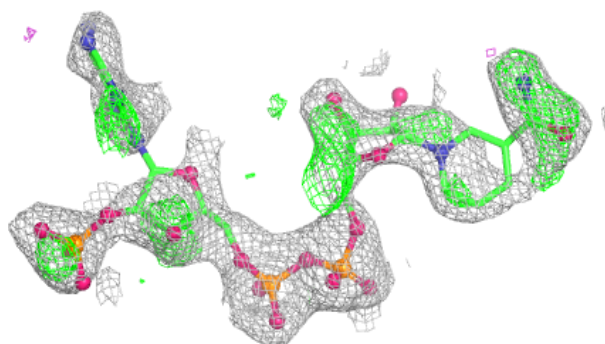
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	1534	5/5	0.88	0.17	60,61,62,63	0
4	NAP	A	2387	48/48	0.88	0.13	6,16,21,22	41
3	SO4	B	1535	5/5	0.90	0.24	30,30,40,66	2
3	SO4	A	1532	5/5	0.93	0.15	43,45,48,49	0
3	SO4	E	1536	5/5	0.95	0.09	30,57,60,61	1
3	SO4	F	1537	5/5	0.97	0.09	38,39,41,41	0
3	SO4	D	1533	5/5	0.97	0.07	38,39,39,40	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.

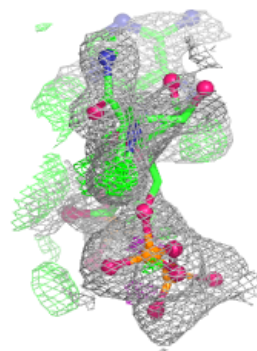
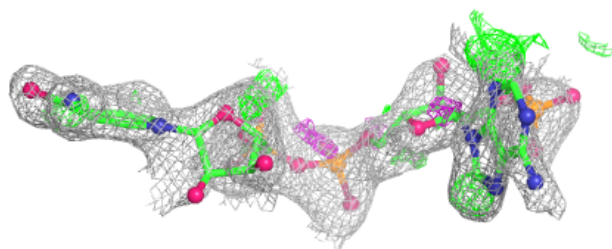
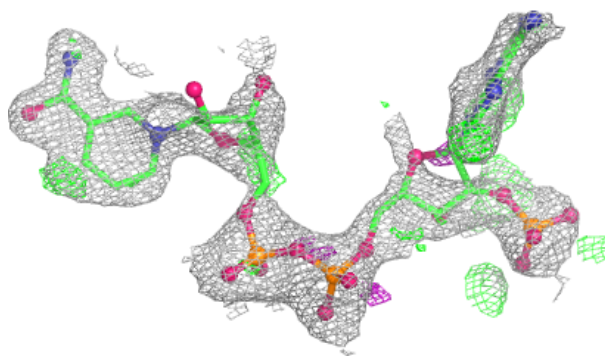
Electron density around NAP E 4387:

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

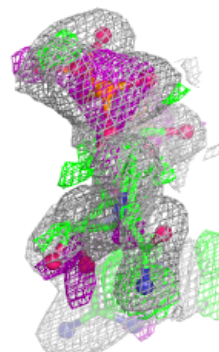
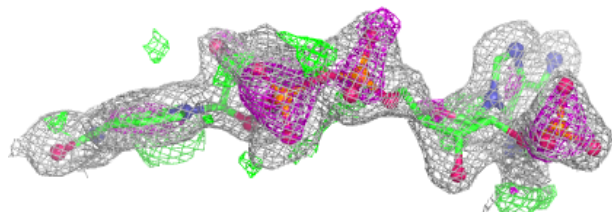
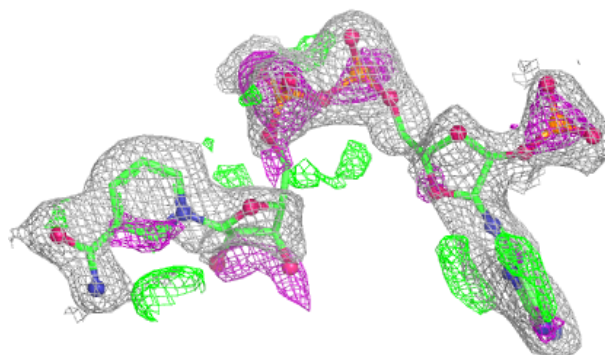


Electron density around NAP B 3387:

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

**Electron density around NAP A 2387:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.