



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:21 PM UTC

PDB ID : 1CF2 / pdb_00001cf2
Title : THREE-DIMENSIONAL STRUCTURE OF D-GLYCERALDEHYDE-3-P
HOSPHATE DEHYDROGENASE FROM THE HYPERTHERMOPHILIC
ARCHAEON METHANOTHERMUS FERVIDUS
Authors : Charron, C.; Talfournier, F.; Isupov, M.N.; Branlant, G.; Littlechild, J.A.;
Vitoux, B.; Aubry, A.
Deposited on : 1999-03-24
Resolution : 2.10 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

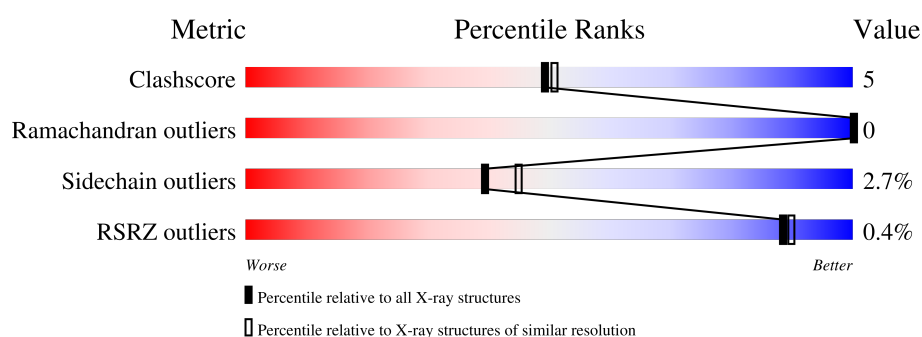
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	O	337	% 84% 14% .
1	P	337	82% 16% .
1	Q	337	81% 16% .
1	R	337	% 80% 19% .

2 Entry composition [i](#)

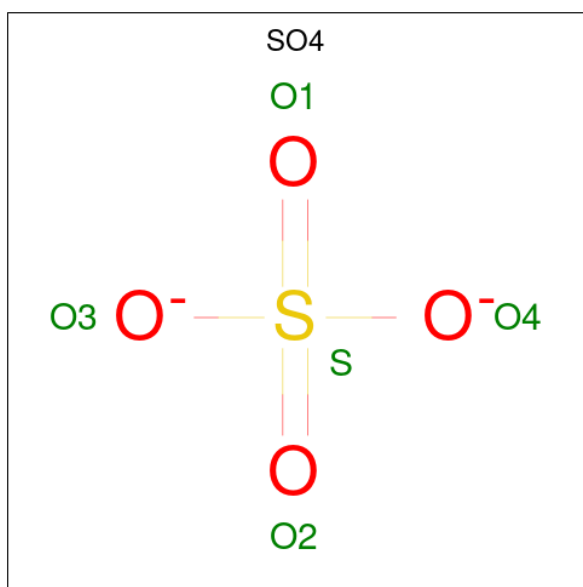
There are 4 unique types of molecules in this entry. The entry contains 11620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	336	Total	C	N	O	S	0	0	0
			2612	1645	441	511	15			
1	R	336	Total	C	N	O	S	0	0	0
			2612	1645	441	511	15			
1	O	336	Total	C	N	O	S	0	0	0
			2612	1645	441	511	15			
1	Q	336	Total	C	N	O	S	0	0	0
			2612	1645	441	511	15			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	P	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total 5	O 4	S 1	0	0
2	Q	1	Total 5	O 4	S 1	0	0

- # NAP

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	259	Total O 259 259	0	0
4	R	234	Total O 234 234	0	0
4	O	217	Total O 217 217	0	0

WORLDWIDE
PDB
PROTEIN DATA BANK

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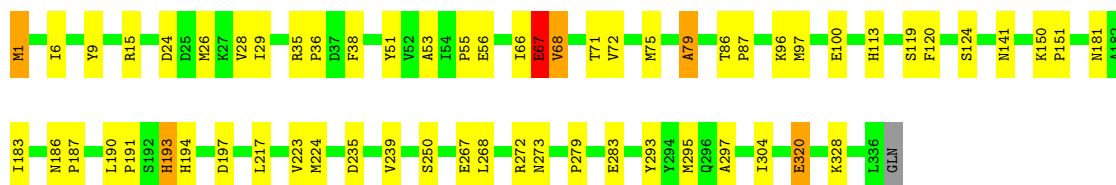
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	250	Total 250	O 250	0	0

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: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

Chain P: 



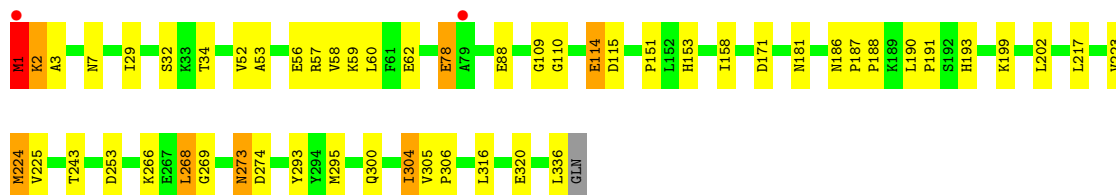
- Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

Chain R: 



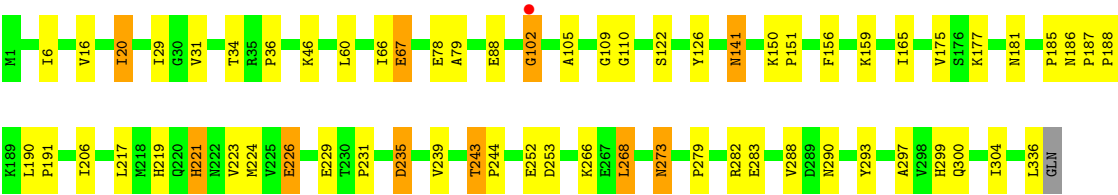
- Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

Chain O: 



- Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

Chain Q: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	136.66Å 153.28Å 74.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 10.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.7 (10.00-2.10) 90.8 (10.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	5.60	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.257 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11620	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.57% 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	O	0.62	0/2654	1.55	19/3593 (0.5%)
1	P	0.68	1/2654 (0.0%)	1.54	22/3593 (0.6%)
1	Q	0.62	0/2654	1.52	24/3593 (0.7%)
1	R	0.65	2/2654 (0.1%)	1.54	21/3593 (0.6%)
All	All	0.64	3/10616 (0.0%)	1.54	86/14372 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	327	ASN	CG-OD1	5.28	1.33	1.23
1	R	22	GLN	CD-OE1	5.05	1.33	1.23
1	P	186	ASN	CG-OD1	5.04	1.33	1.23

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	253	ASP	CA-CB-CG	9.74	122.34	112.60
1	O	253	ASP	CA-CB-CG	8.55	121.15	112.60
1	R	321	ASP	CA-CB-CG	8.13	120.73	112.60
1	R	217	LEU	N-CA-C	7.77	119.66	111.03
1	Q	181	ASN	OD1-CG-ND2	-7.59	115.01	122.60
1	Q	273	ASN	CA-CB-CG	7.55	120.15	112.60
1	P	217	LEU	N-CA-C	7.33	119.17	111.03
1	P	194	HIS	CA-CB-CG	-7.30	106.50	113.80
1	R	186	ASN	CA-CB-CG	7.25	119.85	112.60
1	Q	290	ASN	CA-CB-CG	7.21	119.81	112.60
1	Q	243	THR	CB-CA-C	7.16	118.97	108.87
1	R	253	ASP	CA-CB-CG	6.84	119.44	112.60
1	O	273	ASN	CA-CB-CG	6.79	119.39	112.60
1	Q	34	THR	N-CA-CB	6.77	120.08	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	194	HIS	CA-CB-CG	-6.75	107.05	113.80
1	R	273	ASN	CA-CB-CG	6.56	119.16	112.60
1	O	1	MET	N-CA-CB	6.52	121.59	110.50
1	R	120	PHE	CA-CB-CG	6.49	120.28	113.80
1	O	171	ASP	CA-CB-CG	-6.47	106.13	112.60
1	R	124	SER	N-CA-C	6.38	118.03	111.14
1	O	274	ASP	CA-CB-CG	6.37	118.97	112.60
1	Q	288	VAL	CA-C-O	-6.35	114.09	120.31
1	P	186	ASN	N-CA-CB	-6.29	103.29	111.09
1	R	114	GLU	CA-CB-CG	6.21	126.51	114.10
1	O	115	ASP	N-CA-C	-6.14	104.85	112.90
1	P	124	SER	CA-C-O	-6.14	112.41	119.60
1	O	186	ASN	CA-CB-CG	6.07	118.67	112.60
1	Q	223	VAL	N-CA-C	6.07	116.67	108.17
1	P	187	PRO	CA-C-N	6.07	125.62	119.19
1	P	187	PRO	C-N-CA	6.07	125.62	119.19
1	P	79	ALA	N-CA-C	6.06	119.42	109.85
1	Q	226	GLU	CB-CG-CD	6.05	122.89	112.60
1	P	28	VAL	CA-C-N	-6.01	113.14	122.09
1	P	28	VAL	C-N-CA	-6.01	113.14	122.09
1	O	78	GLU	CB-CA-C	-5.99	100.08	110.09
1	Q	20	ILE	CB-CA-C	-5.96	104.34	111.97
1	R	280	VAL	CA-C-O	-5.92	114.17	120.39
1	O	186	ASN	N-CA-CB	-5.90	103.77	111.09
1	Q	79	ALA	N-CA-C	5.89	119.32	109.95
1	O	34	THR	N-CA-CB	5.87	118.83	110.67
1	P	67	GLU	CA-C-N	5.78	131.94	122.64
1	P	67	GLU	C-N-CA	5.78	131.94	122.64
1	P	120	PHE	CA-C-N	5.77	130.93	122.39
1	P	120	PHE	C-N-CA	5.77	130.93	122.39
1	P	183	ILE	N-CA-CB	5.75	119.12	111.64
1	Q	235	ASP	CA-CB-CG	5.75	118.35	112.60
1	P	15	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	R	34	THR	N-CA-CB	5.69	118.66	110.40
1	R	304	ILE	CA-C-N	5.67	124.87	120.33
1	R	304	ILE	C-N-CA	5.67	124.87	120.33
1	P	38	PHE	CA-C-O	-5.60	113.77	120.10
1	R	322	LYS	CA-C-O	-5.60	114.62	120.55
1	R	222	ASN	CA-CB-CG	-5.53	107.07	112.60
1	Q	102	GLY	CA-C-O	-5.53	113.18	119.04
1	Q	34	THR	N-CA-C	-5.52	106.90	113.97
1	O	52	VAL	N-CA-C	5.48	115.84	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	114	GLU	N-CA-CB	5.47	118.17	110.12
1	Q	299	HIS	CA-CB-CG	-5.47	108.33	113.80
1	Q	141	ASN	CA-CB-CG	-5.45	107.15	112.60
1	O	223	VAL	N-CA-C	5.44	115.79	108.17
1	Q	105	ALA	N-CA-C	5.44	117.53	108.99
1	O	224	MET	CA-C-O	-5.42	114.50	120.24
1	O	186	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	Q	181	ASN	CB-CG-ND2	5.40	124.50	116.40
1	P	6	ILE	CA-C-N	-5.38	115.85	122.84
1	P	6	ILE	C-N-CA	-5.38	115.85	122.84
1	Q	221	HIS	CA-CB-CG	5.36	119.16	113.80
1	O	2	LYS	N-CA-C	-5.35	102.36	110.28
1	R	139	SER	N-CA-C	5.34	117.22	110.33
1	Q	175	VAL	N-CA-C	5.33	120.31	113.07
1	Q	186	ASN	N-CA-CB	-5.30	104.45	111.40
1	P	223	VAL	N-CA-C	5.29	115.51	108.11
1	Q	109	GLY	N-CA-C	5.29	120.75	113.99
1	O	217	LEU	N-CA-C	5.28	117.84	111.40
1	Q	206	ILE	CA-C-O	5.23	126.13	120.43
1	Q	217	LEU	N-CA-C	5.23	116.83	111.03
1	R	246	VAL	CA-C-O	-5.18	114.87	120.36
1	O	225	VAL	CB-CA-C	-5.14	103.47	110.77
1	R	150	LYS	CA-C-N	5.12	124.73	119.05
1	R	150	LYS	C-N-CA	5.12	124.73	119.05
1	P	68	VAL	CA-CB-CG1	5.11	119.09	110.40
1	P	9	TYR	N-CA-CB	-5.08	104.33	110.53
1	R	181	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	P	267	GLU	CA-C-O	5.05	125.59	119.38
1	O	225	VAL	N-CA-C	5.03	115.09	107.75
1	O	109	GLY	N-CA-C	5.01	119.94	113.27

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	O	2612	0	2637	32	0
1	P	2612	0	2637	29	0
1	Q	2612	0	2637	31	1
1	R	2612	0	2637	30	1
2	O	5	0	0	0	0
2	P	5	0	0	1	0
2	Q	5	0	0	1	0
2	R	5	0	0	0	0
3	O	48	0	25	1	0
3	P	48	0	25	3	0
3	Q	48	0	25	1	0
3	R	48	0	25	1	0
4	O	217	0	0	7	0
4	P	259	0	0	2	0
4	Q	250	0	0	1	0
4	R	234	0	0	1	0
All	All	11620	0	10648	116	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (116) 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:O:153:HIS:HD2	1:O:158:ILE:H	1.08	1.00
1:Q:159:LYS:HD3	1:Q:226:GLU:HB3	1.62	0.80
1:O:273:ASN:ND2	1:Q:273:ASN:ND2	2.34	0.76
1:O:153:HIS:CD2	1:O:158:ILE:H	2.00	0.75
1:R:224:MET:HE1	1:Q:224:MET:HE1	1.70	0.74
1:R:250:SER:HB2	1:R:283:GLU:OE2	1.90	0.71
1:O:88:GLU:HG2	1:O:110:GLY:HA3	1.70	0.71
1:P:224:MET:HE1	1:O:224:MET:HE1	1.74	0.69
1:Q:266:LYS:HG2	1:Q:273:ASN:ND2	2.09	0.68
1:O:57:ARG:HD3	4:O:1191:HOH:O	1.95	0.67
1:P:320:GLU:HG3	4:P:1157:HOH:O	1.96	0.65
1:O:114:GLU:H	1:O:114:GLU:CD	2.03	0.65
1:R:114:GLU:HG3	4:R:1117:HOH:O	1.98	0.63
1:R:150:LYS:HB3	1:R:151:PRO:HD3	1.80	0.63
1:R:266:LYS:HG2	1:R:273:ASN:ND2	2.15	0.62
1:R:266:LYS:HG2	1:R:273:ASN:HD22	1.64	0.60
1:O:190:LEU:HB3	1:O:191:PRO:HA	1.82	0.60
1:O:58:VAL:O	1:O:62:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:268:LEU:HD21	1:O:336:LEU:HD11	1.85	0.57
1:R:190:LEU:HB3	1:R:191:PRO:HA	1.86	0.57
1:O:3:ALA:HB1	1:O:29:ILE:HG12	1.86	0.57
1:O:266:LYS:HG2	1:O:273:ASN:ND2	2.20	0.57
1:O:53:ALA:HB3	4:O:1191:HOH:O	2.06	0.56
1:Q:159:LYS:HD3	1:Q:226:GLU:CB	2.33	0.56
1:O:59:LYS:HA	1:O:62:GLU:OE1	2.05	0.56
1:P:273:ASN:ND2	1:R:273:ASN:ND2	2.54	0.55
1:R:279:PRO:HD2	1:R:297:ALA:O	2.07	0.55
1:O:187:PRO:HB2	1:O:188:PRO:HD2	1.89	0.55
1:Q:224:MET:HG2	1:Q:293:TYR:CD1	2.43	0.54
1:R:224:MET:HG2	1:R:293:TYR:CD1	2.44	0.53
1:P:35:ARG:HG2	3:P:340:NAP:O2X	2.09	0.53
1:P:96:LYS:O	1:P:100:GLU:HG3	2.08	0.53
1:P:113:HIS:HD2	1:P:119:SER:OG	1.91	0.52
1:P:193:HIS:HB3	4:P:1040:HOH:O	2.09	0.52
1:P:235:ASP:O	1:P:239:VAL:HG23	2.10	0.52
1:P:55:PRO:HB3	1:P:71:THR:HG21	1.91	0.52
1:P:190:LEU:HB3	1:P:191:PRO:HA	1.92	0.52
1:Q:190:LEU:HB3	1:Q:191:PRO:HA	1.90	0.51
1:Q:16:VAL:O	1:Q:20:ILE:HG12	2.12	0.50
1:P:67:GLU:H	1:P:67:GLU:CD	2.19	0.50
1:R:58:VAL:O	1:R:62:GLU:HG3	2.12	0.50
4:O:1150:HOH:O	1:Q:46:LYS:HE3	2.12	0.50
1:Q:268:LEU:HD21	1:Q:336:LEU:HD11	1.94	0.50
1:Q:141:ASN:HB2	2:Q:1004:SO4:O2	2.12	0.50
1:R:24:ASP:OD1	1:R:328:LYS:NZ	2.45	0.49
1:O:320:GLU:HG3	4:O:1025:HOH:O	2.13	0.49
1:R:54:ILE:HG13	1:R:57:ARG:HG3	1.95	0.49
1:R:122:SER:O	1:R:126:TYR:HB2	2.13	0.49
1:Q:235:ASP:O	1:Q:239:VAL:HG23	2.13	0.48
1:Q:279:PRO:HD2	1:Q:297:ALA:O	2.13	0.48
1:O:300:GLN:O	3:O:340:NAP:H4N	2.14	0.48
1:O:2:LYS:HD2	1:O:316:LEU:HD13	1.95	0.48
1:Q:29:ILE:HD13	1:Q:78:GLU:HB2	1.95	0.48
1:Q:88:GLU:HG2	1:Q:110:GLY:HA3	1.95	0.48
1:Q:300:GLN:O	3:Q:340:NAP:H4N	2.14	0.47
1:R:256:THR:O	1:Q:185:PRO:HD2	2.15	0.47
3:P:340:NAP:O1N	3:P:340:NAP:N7N	2.48	0.46
1:P:141:ASN:HB2	2:P:1001:SO4:O2	2.16	0.46
1:R:130:TYR:CZ	1:R:320:GLU:HG2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:272:ARG:O	1:P:273:ASN:HB2	2.16	0.46
1:O:153:HIS:HE1	4:O:1187:HOH:O	1.99	0.46
1:Q:187:PRO:HB2	1:Q:188:PRO:HD2	1.98	0.45
1:Q:252:GLU:HG3	1:Q:283:GLU:OE2	2.16	0.45
1:R:51:TYR:CG	1:R:75:MET:HB2	2.51	0.45
1:O:304:ILE:H	1:O:304:ILE:HD13	1.82	0.45
1:P:190:LEU:HD21	1:O:295:MET:HE3	1.99	0.45
1:O:181:ASN:HB2	4:O:1216:HOH:O	2.16	0.45
1:P:36:PRO:HB2	1:P:66:ILE:HD12	1.98	0.44
1:P:150:LYS:N	1:P:151:PRO:HD2	2.33	0.44
1:P:295:MET:HE3	1:O:190:LEU:HD21	1.99	0.44
1:R:53:ALA:HA	1:R:72:VAL:HG23	1.99	0.44
1:O:305:VAL:HB	1:O:306:PRO:HD3	2.00	0.44
1:O:153:HIS:HD2	1:O:158:ILE:N	1.93	0.44
1:Q:67:GLU:HG2	4:Q:1010:HOH:O	2.18	0.44
1:Q:266:LYS:HA	1:Q:273:ASN:HB3	2.00	0.44
1:P:279:PRO:HD2	1:P:297:ALA:O	2.18	0.43
1:Q:156:PHE:CE1	1:Q:231:PRO:HB3	2.53	0.43
1:Q:122:SER:O	1:Q:126:TYR:HB2	2.19	0.43
1:P:86:THR:HB	1:P:87:PRO:HD2	2.01	0.43
1:R:300:GLN:O	3:R:340:NAP:H4N	2.19	0.43
1:O:199:LYS:HA	1:O:202:LEU:O	2.19	0.43
1:O:269:GLY:HA2	4:O:1134:HOH:O	2.19	0.42
1:Q:6:ILE:HB	1:Q:31:VAL:HG12	2.01	0.42
1:Q:243:THR:HA	1:Q:244:PRO:HD3	1.96	0.42
1:P:86:THR:HB	1:P:87:PRO:CD	2.49	0.42
1:P:53:ALA:HA	1:P:72:VAL:HG23	2.00	0.42
1:R:165:ILE:HD12	1:R:221:HIS:CD2	2.54	0.42
1:O:224:MET:HG2	1:O:293:TYR:CD1	2.55	0.42
1:R:29:ILE:C	1:R:29:ILE:HD12	2.45	0.42
1:R:266:LYS:HA	1:R:273:ASN:HB3	2.01	0.42
1:O:304:ILE:H	1:O:304:ILE:CD1	2.33	0.42
1:R:168:ARG:HG3	1:R:219:HIS:CE1	2.54	0.41
1:Q:266:LYS:HG2	1:Q:273:ASN:CG	2.44	0.41
1:P:29:ILE:HD11	1:P:79:ALA:HB2	2.02	0.41
1:P:250:SER:HB2	1:P:283:GLU:OE2	2.19	0.41
1:O:7:ASN:HA	1:O:32:SER:OG	2.20	0.41
1:Q:177:LYS:HE2	1:Q:177:LYS:HB3	1.83	0.41
1:P:1:MET:HG2	1:P:26:MET:N	2.35	0.41
1:Q:165:ILE:HD12	1:Q:221:HIS:CD2	2.55	0.41
1:P:224:MET:HG2	1:P:293:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:9:TYR:CE1	1:R:14:LYS:HA	2.55	0.41
1:Q:150:LYS:N	1:Q:151:PRO:HD2	2.35	0.41
3:P:340:NAP:H2D	3:P:340:NAP:H2N	1.77	0.41
1:R:153:HIS:HA	1:R:158:ILE:HG13	2.03	0.41
1:P:51:TYR:CE1	1:P:75:MET:HG3	2.56	0.41
1:R:87:PRO:O	1:R:90:ILE:HB	2.21	0.41
1:P:24:ASP:OD1	1:P:328:LYS:NZ	2.50	0.41
1:P:53:ALA:HA	1:P:72:VAL:CG2	2.50	0.41
1:Q:219:HIS:CD2	1:Q:300:GLN:HB3	2.56	0.41
1:R:240:PHE:HA	1:R:243:THR:HG22	2.02	0.40
1:P:181:ASN:ND2	1:R:181:ASN:HD22	2.18	0.40
1:O:1:MET:N	1:O:1:MET:SD	2.84	0.40
1:O:151:PRO:HG3	1:O:243:THR:OG1	2.21	0.40
1:R:5:ALA:HB2	1:R:29:ILE:HD11	2.03	0.40
1:Q:36:PRO:HB2	1:Q:66:ILE:HD12	2.03	0.40
1:R:187:PRO:HB2	1:R:188:PRO:HD2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:63:LYS:NZ	1:Q:102:GLY:O[4_555]	2.18	0.02

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	O	334/337 (99%)	324 (97%)	10 (3%)	0	100	100
1	P	334/337 (99%)	324 (97%)	10 (3%)	0	100	100
1	Q	334/337 (99%)	326 (98%)	8 (2%)	0	100	100
1	R	334/337 (99%)	323 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1336/1348 (99%)	1297 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	290/291 (100%)	282 (97%)	8 (3%)	38	43
1	P	290/291 (100%)	280 (97%)	10 (3%)	32	35
1	Q	290/291 (100%)	284 (98%)	6 (2%)	47	54
1	R	290/291 (100%)	283 (98%)	7 (2%)	43	49
All	All	1160/1164 (100%)	1129 (97%)	31 (3%)	39	45

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	1	MET
1	P	56	GLU
1	P	67	GLU
1	P	68	VAL
1	P	97	MET
1	P	193	HIS
1	P	197	ASP
1	P	268	LEU
1	P	304	ILE
1	P	320	GLU
1	R	1	MET
1	R	68	VAL
1	R	114	GLU
1	R	193	HIS
1	R	197	ASP
1	R	268	LEU
1	R	304	ILE

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Mol	Chain	Res	Type
1	O	1	MET
1	O	56	GLU
1	O	60	LEU
1	O	78	GLU
1	O	114	GLU
1	O	193	HIS
1	O	268	LEU
1	O	304	ILE
1	Q	60	LEU
1	Q	67	GLU
1	Q	229	GLU
1	Q	268	LEU
1	Q	282	ARG
1	Q	304	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	108	GLN
1	P	113	HIS
1	P	205	ASN
1	P	273	ASN
1	P	290	ASN
1	P	308	ASN
1	P	334	ASN
1	R	181	ASN
1	R	273	ASN
1	O	108	GLN
1	O	153	HIS
1	O	273	ASN
1	O	308	ASN
1	Q	22	GLN
1	Q	205	ASN
1	Q	273	ASN
1	Q	334	ASN

5.3.3 RNA ⓘ

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](#)

8 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	NAP	R	340	-	50,52,52	1.12	3 (6%)	71,80,80	1.74	7 (9%)
2	SO4	R	1002	-	4,4,4	0.68	0	6,6,6	0.15	0
3	NAP	Q	340	-	50,52,52	1.15	3 (6%)	71,80,80	1.91	11 (15%)
2	SO4	P	1001	-	4,4,4	0.70	0	6,6,6	0.27	0
3	NAP	O	340	-	50,52,52	1.30	5 (10%)	71,80,80	1.69	8 (11%)
2	SO4	Q	1004	-	4,4,4	0.72	0	6,6,6	0.29	0
3	NAP	P	340	-	50,52,52	1.23	3 (6%)	71,80,80	1.82	10 (14%)
2	SO4	O	1003	-	4,4,4	0.70	0	6,6,6	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	O	340	-	-	7/35/67/67	0/5/5/5
3	NAP	R	340	-	-	7/35/67/67	0/5/5/5
3	NAP	P	340	-	-	8/35/67/67	0/5/5/5
3	NAP	Q	340	-	-	7/35/67/67	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	340	NAP	C3N-C7N	4.45	1.57	1.50
3	R	340	NAP	C3N-C7N	4.13	1.56	1.50
3	Q	340	NAP	C3N-C7N	4.06	1.56	1.50
3	P	340	NAP	C3N-C7N	4.02	1.56	1.50
3	Q	340	NAP	C6N-N1N	3.51	1.43	1.35
3	R	340	NAP	C6N-N1N	3.45	1.43	1.35
3	O	340	NAP	PA-O3	3.42	1.63	1.59
3	O	340	NAP	C6N-N1N	3.38	1.43	1.35
3	P	340	NAP	C6N-N1N	3.27	1.42	1.35
3	P	340	NAP	C2A-N1A	2.51	1.38	1.33
3	O	340	NAP	C2A-N1A	2.45	1.38	1.33
3	R	340	NAP	C2A-N1A	2.09	1.37	1.33
3	Q	340	NAP	C2A-N1A	2.05	1.37	1.33
3	O	340	NAP	PN-O3	2.05	1.61	1.59

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	340	NAP	C5N-C4N-C3N	-7.71	112.79	120.36
3	P	340	NAP	C5N-C4N-C3N	-7.60	112.89	120.36
3	Q	340	NAP	C5N-C4N-C3N	-7.30	113.19	120.36
3	R	340	NAP	C5N-C4N-C3N	-7.20	113.29	120.36
3	Q	340	NAP	O7N-C7N-C3N	6.56	127.63	119.60
3	P	340	NAP	C6N-C5N-C4N	6.14	128.30	119.45
3	R	340	NAP	C6N-C5N-C4N	6.03	128.14	119.45
3	Q	340	NAP	C6N-C5N-C4N	6.02	128.12	119.45
3	R	340	NAP	C5N-C6N-N1N	-5.40	113.02	120.38
3	P	340	NAP	C5N-C6N-N1N	-5.27	113.20	120.38
3	O	340	NAP	C2N-C3N-C4N	5.25	124.37	118.26
3	Q	340	NAP	C5N-C6N-N1N	-5.13	113.39	120.38
3	O	340	NAP	C6N-C5N-C4N	4.82	126.39	119.45
3	R	340	NAP	C2N-C3N-C4N	4.08	123.00	118.26
3	P	340	NAP	C2N-C3N-C4N	3.87	122.76	118.26
3	O	340	NAP	O7N-C7N-C3N	3.59	123.98	119.60
3	O	340	NAP	C5N-C6N-N1N	-3.42	115.72	120.38
3	Q	340	NAP	C2N-C3N-C4N	3.41	122.22	118.26
3	Q	340	NAP	P2B-O2B-C2B	-3.10	115.16	123.43
3	Q	340	NAP	C3N-C7N-N7N	-3.09	113.92	117.74
3	R	340	NAP	C4N-C3N-C7N	-2.97	112.97	121.06
3	P	340	NAP	P2B-O2B-C2B	-2.92	115.64	123.43
3	O	340	NAP	C4N-C3N-C7N	-2.89	113.19	121.06
3	Q	340	NAP	O7N-C7N-N7N	-2.89	118.44	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	340	NAP	C4N-C3N-C7N	-2.82	113.38	121.06
3	R	340	NAP	P2B-O2B-C2B	-2.79	115.99	123.43
3	P	340	NAP	C4A-N9A-C1B	-2.68	120.38	126.63
3	Q	340	NAP	C4N-C3N-C7N	-2.54	114.13	121.06
3	Q	340	NAP	C1B-N9A-C8A	2.51	132.67	127.09
3	Q	340	NAP	C4A-N9A-C1B	-2.48	120.82	126.63
3	O	340	NAP	P2B-O2B-C2B	-2.40	117.03	123.43
3	P	340	NAP	C4A-N9A-C8A	2.23	108.08	105.74
3	P	340	NAP	O2N-PN-O5D	2.21	117.60	107.57
3	R	340	NAP	C2D-C3D-C4D	-2.18	98.40	102.61
3	O	340	NAP	C3N-C7N-N7N	-2.09	115.17	117.74
3	P	340	NAP	C2N-N1N-C1D	-2.06	114.59	119.13

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	340	NAP	O4D-C1D-N1N-C2N
3	P	340	NAP	O4D-C1D-N1N-C6N
3	P	340	NAP	C2D-C1D-N1N-C2N
3	P	340	NAP	C2D-C1D-N1N-C6N
3	R	340	NAP	O4D-C1D-N1N-C2N
3	R	340	NAP	O4D-C1D-N1N-C6N
3	R	340	NAP	C2D-C1D-N1N-C2N
3	R	340	NAP	C2D-C1D-N1N-C6N
3	O	340	NAP	O4D-C1D-N1N-C2N
3	O	340	NAP	O4D-C1D-N1N-C6N
3	O	340	NAP	C2D-C1D-N1N-C2N
3	O	340	NAP	C2D-C1D-N1N-C6N
3	Q	340	NAP	O4D-C1D-N1N-C2N
3	Q	340	NAP	O4D-C1D-N1N-C6N
3	Q	340	NAP	C2D-C1D-N1N-C2N
3	Q	340	NAP	C2D-C1D-N1N-C6N
3	P	340	NAP	PN-O3-PA-O1A
3	Q	340	NAP	PN-O3-PA-O1A
3	P	340	NAP	PN-O3-PA-O2A
3	R	340	NAP	C2B-C1B-N9A-C8A
3	R	340	NAP	PN-O3-PA-O1A
3	O	340	NAP	PN-O3-PA-O1A
3	O	340	NAP	PN-O3-PA-O2A
3	P	340	NAP	C2B-C1B-N9A-C8A
3	O	340	NAP	C2B-C1B-N9A-C8A

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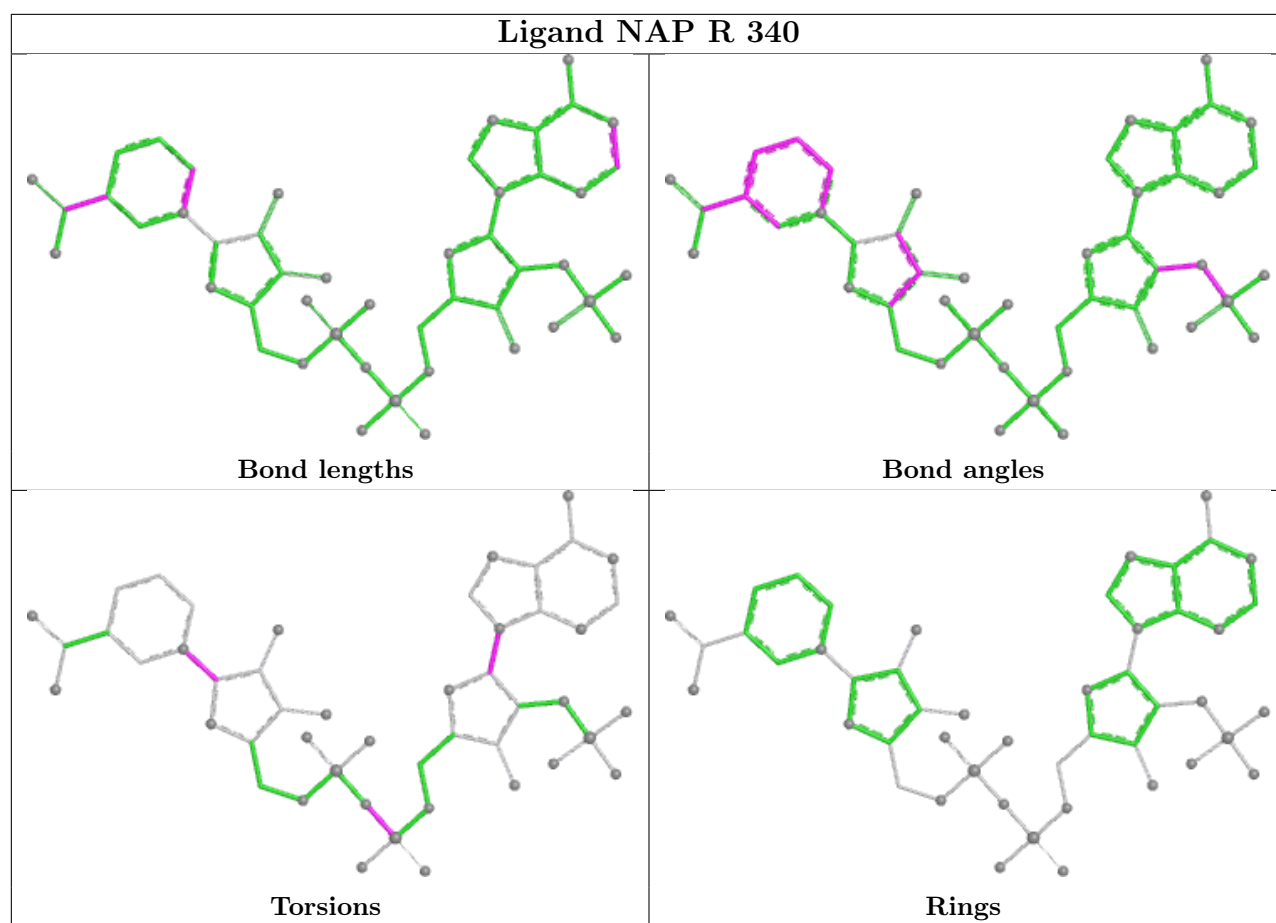
Mol	Chain	Res	Type	Atoms
3	Q	340	NAP	C2B-C1B-N9A-C8A
3	R	340	NAP	PN-O3-PA-O2A
3	Q	340	NAP	PN-O3-PA-O2A
3	P	340	NAP	O4B-C4B-C5B-O5B

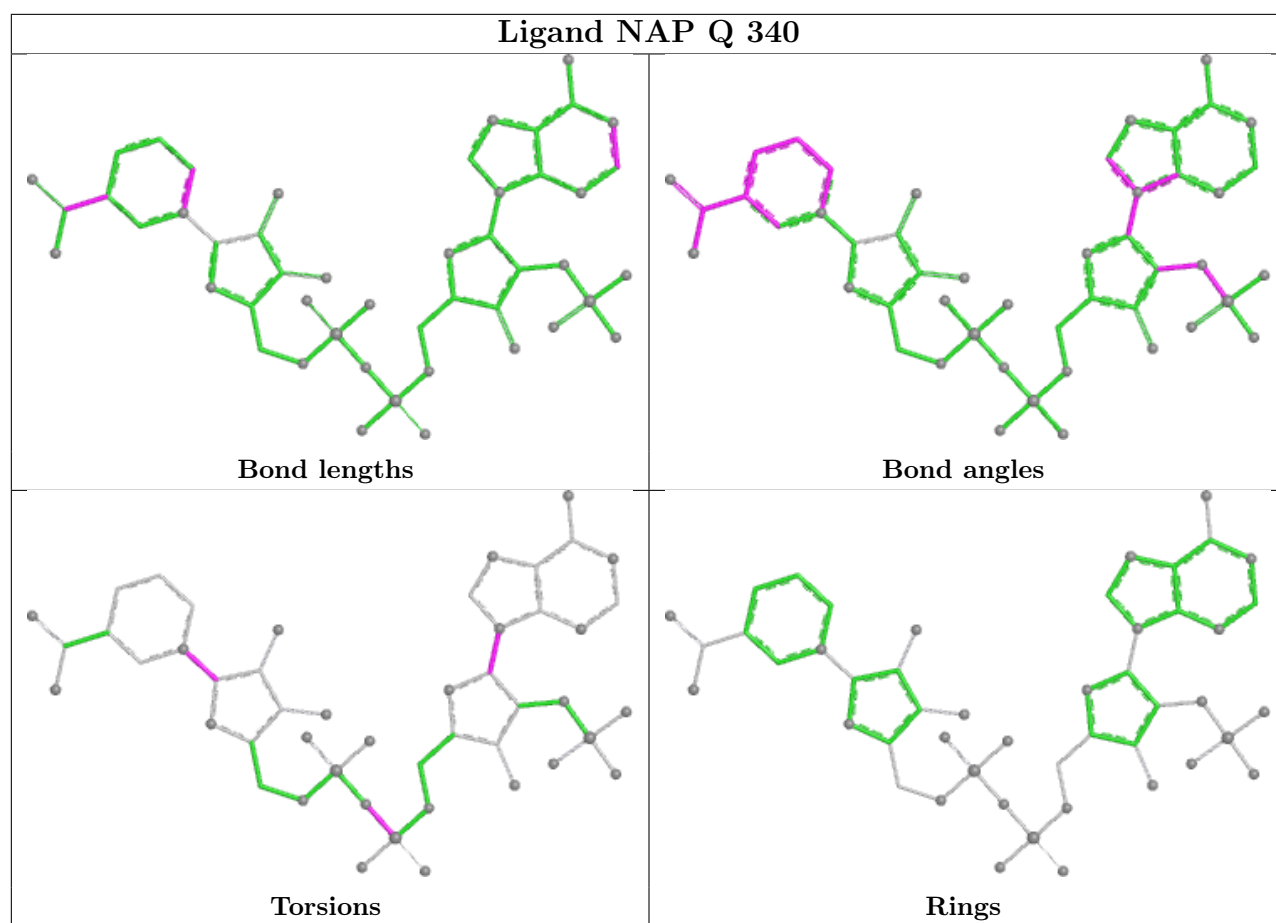
There are no ring outliers.

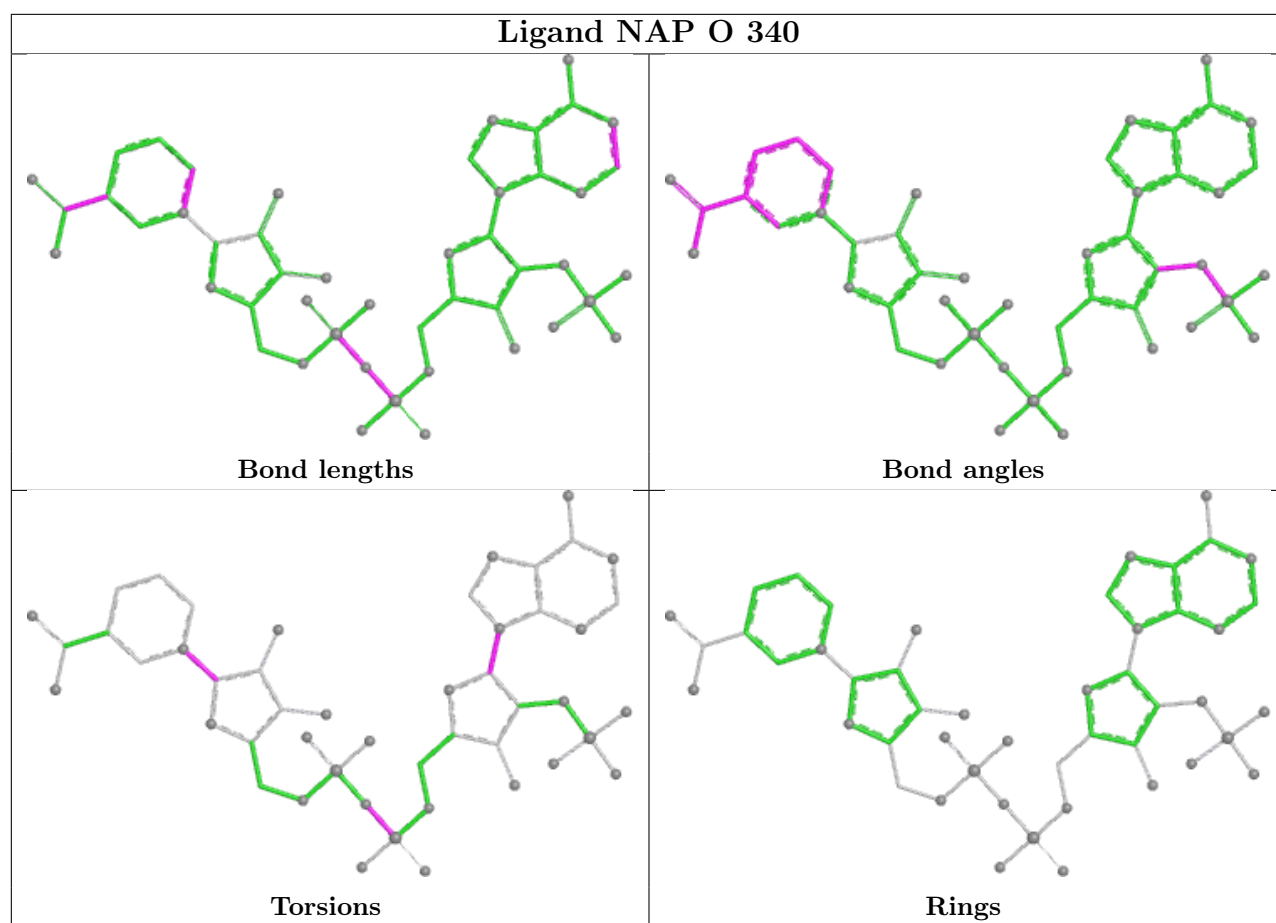
6 monomers are involved in 8 short contacts:

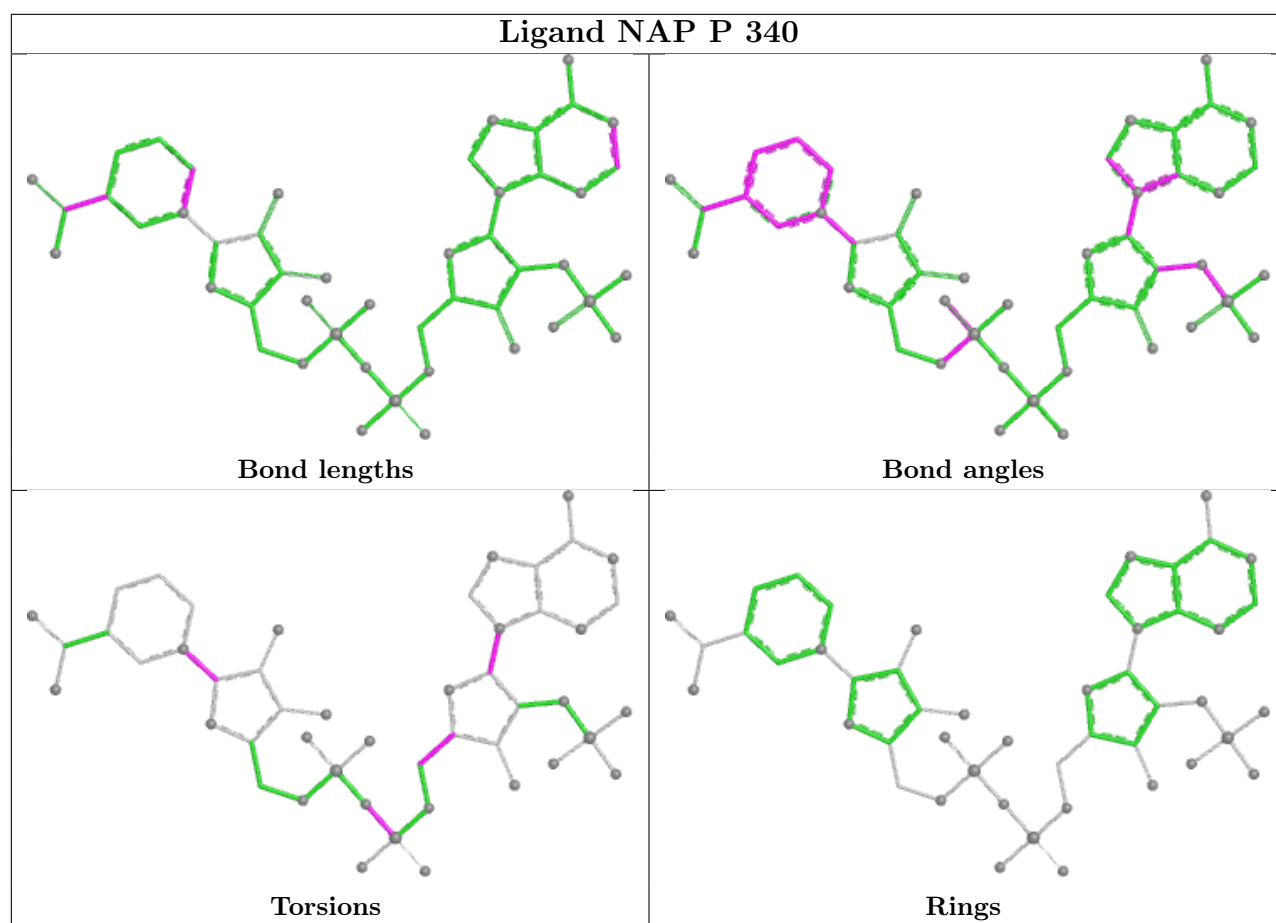
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	340	NAP	1	0
3	Q	340	NAP	1	0
2	P	1001	SO4	1	0
3	O	340	NAP	1	0
2	Q	1004	SO4	1	0
3	P	340	NAP	3	0

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	O	336/337 (99%)	-0.26	2 (0%) 85 87	22, 37, 60, 86	0
1	P	336/337 (99%)	-0.44	0 100 100	22, 33, 53, 70	0
1	Q	336/337 (99%)	-0.34	1 (0%) 90 91	21, 36, 54, 81	0
1	R	336/337 (99%)	-0.38	2 (0%) 85 87	20, 36, 54, 75	0
All	All	1344/1348 (99%)	-0.36	5 (0%) 88 90	20, 35, 55, 86	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	102	GLY	4.1
1	O	1	MET	3.6
1	O	79	ALA	2.3
1	R	191	PRO	2.1
1	R	63	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

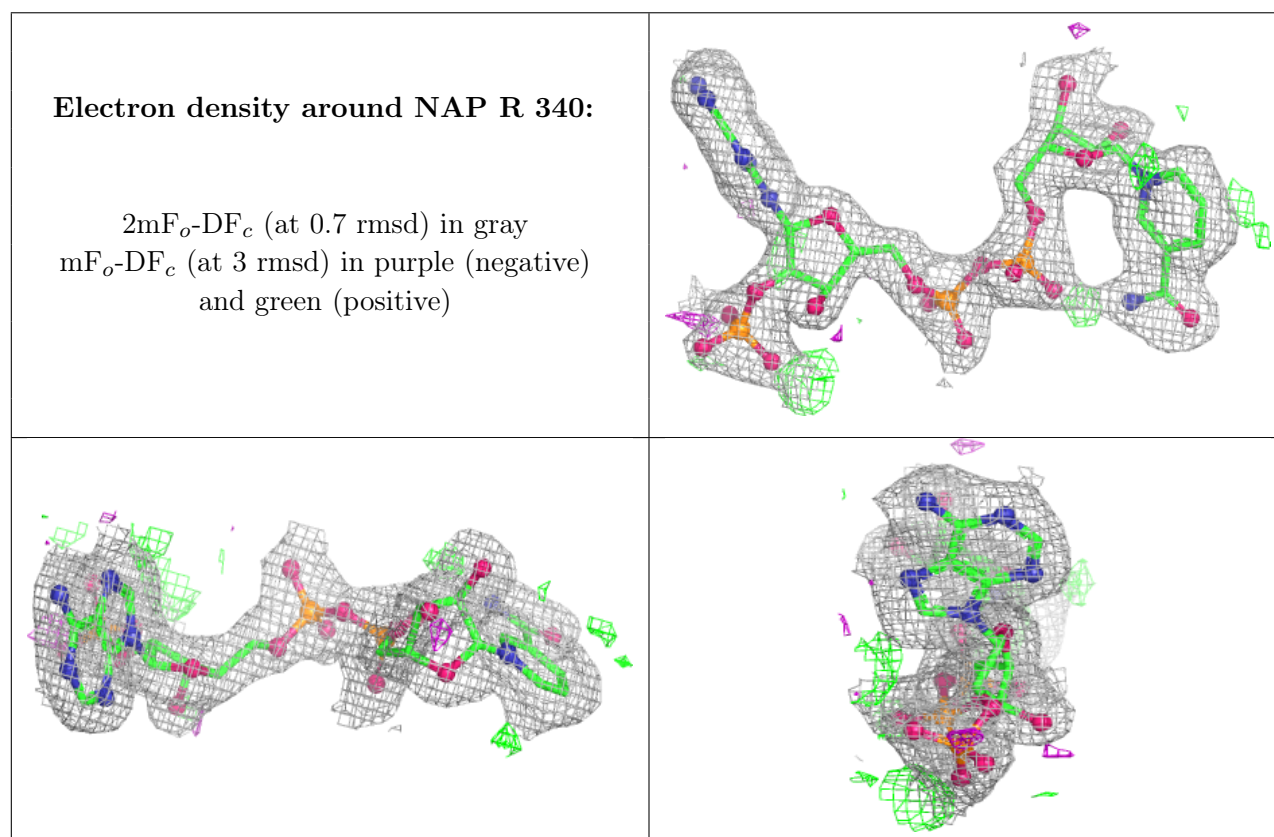
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

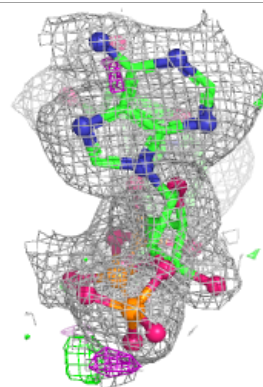
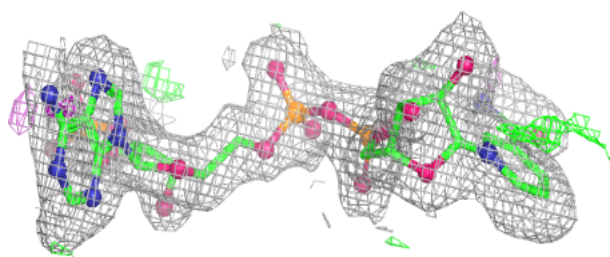
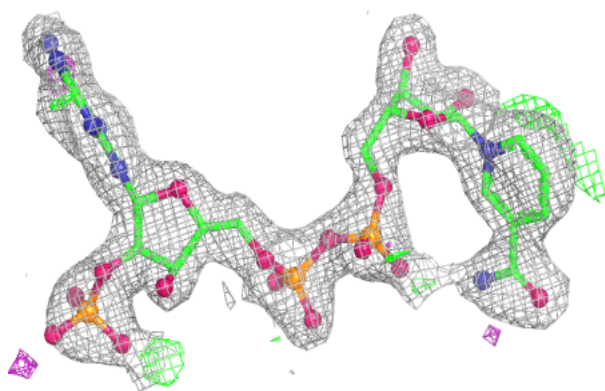
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	P	1001	5/5	0.91	0.11	69,69,71,74	0
2	SO4	R	1002	5/5	0.95	0.13	55,56,58,59	0
2	SO4	Q	1004	5/5	0.95	0.12	61,62,64,65	0
3	NAP	R	340	48/48	0.95	0.06	22,39,48,55	0
3	NAP	O	340	48/48	0.95	0.07	24,37,45,47	0
3	NAP	P	340	48/48	0.96	0.06	23,33,40,41	0
3	NAP	Q	340	48/48	0.96	0.06	22,34,43,48	0
2	SO4	O	1003	5/5	0.97	0.13	46,49,51,52	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.

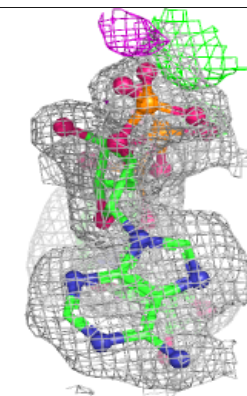
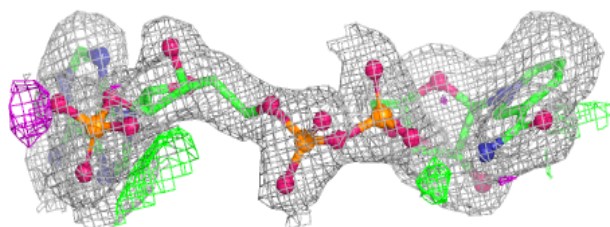
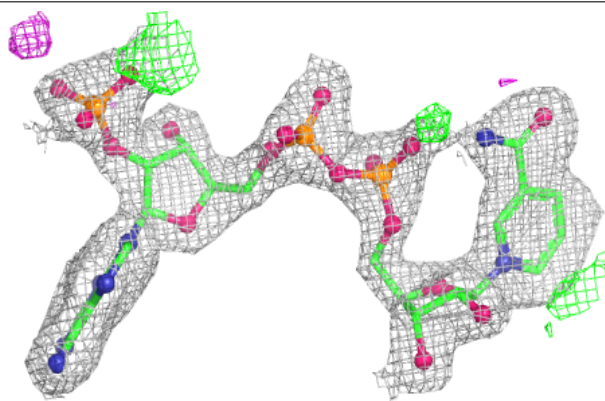


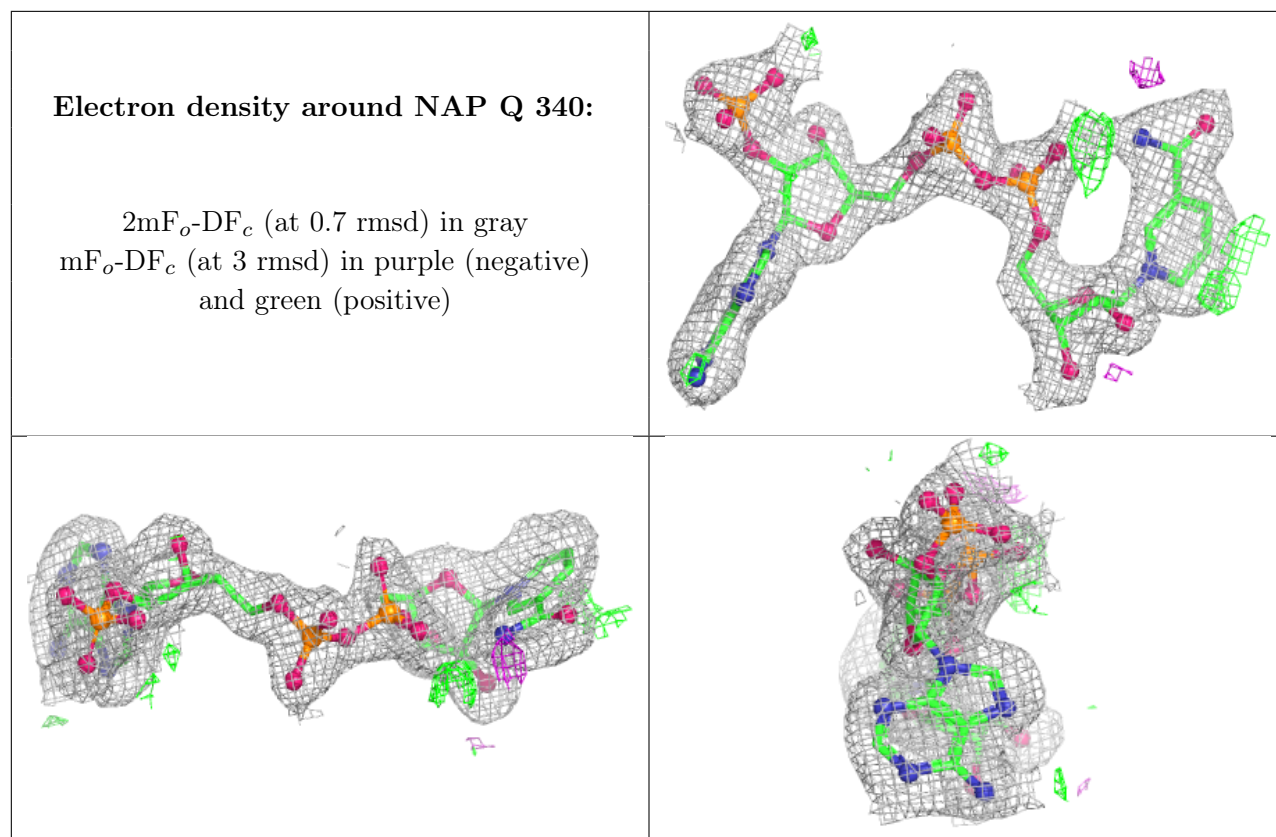
Electron density around NAP O 340:

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

**Electron density around NAP P 340:**

$2mF_o-DF_c$ (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.