Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 10:03 PM EDT

PDB ID	:	1CF2
Title	:	THREE-DIMENSIONAL STRUCTURE OF D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE FROM THE HYPERTHERMOPHILIC ARCHAEON METHANOTHERMUS FERVIDUS
Authors	:	Charron, C.; Talfournier, F.; Isuppov, 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 (i) 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 (i)) were used in the production of this report:

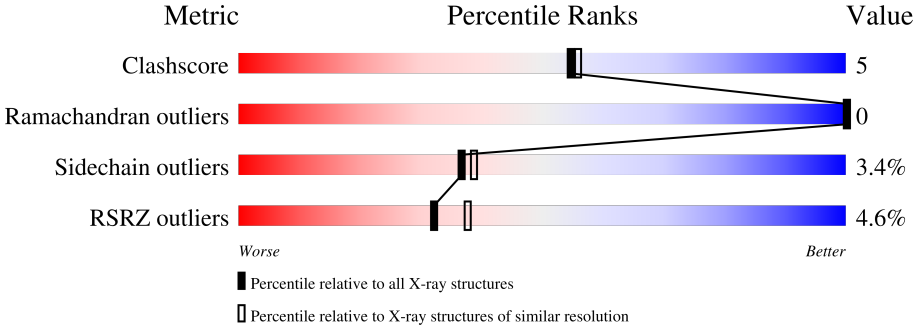
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	4% 84% 14% •
1	P	337	4% 83% 15% •
1	Q	337	5% 80% 19% •
1	R	337	5% 82% 17%

2 Entry composition (i)

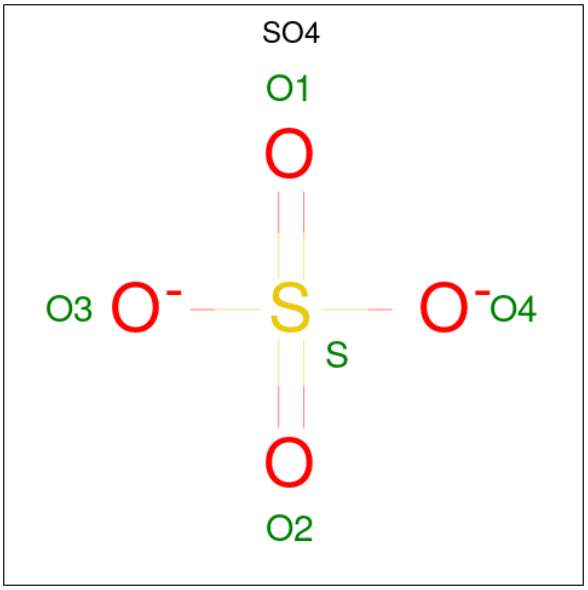
There are 4 unique types of molecules in this entry. The entry contains 11620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	P	336	2612	1645	441	511	15	0	0	0
1	R	336	2612	1645	441	511	15	0	0	0
1	O	336	2612	1645	441	511	15	0	0	0
1	Q	336	2612	1645	441	511	15	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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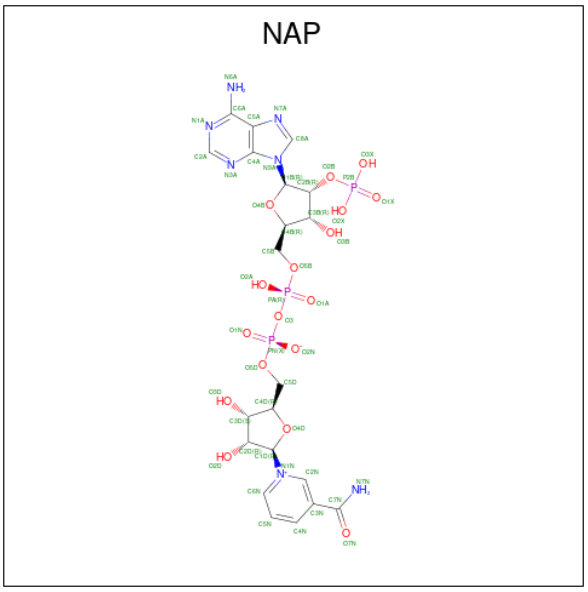
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	O	1	5	4	1		0	0
			Total	O	S			
2	Q	1	5	4	1		0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	P	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	R	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	O	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	Q	1	48	21	7	17	3	0	0

- Molecule 4 is water.

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

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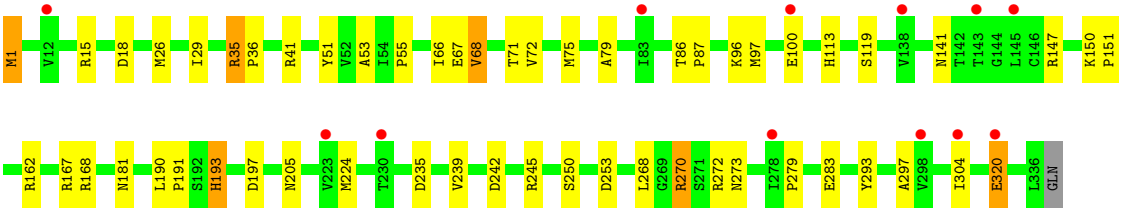
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	Q	250	250	250	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

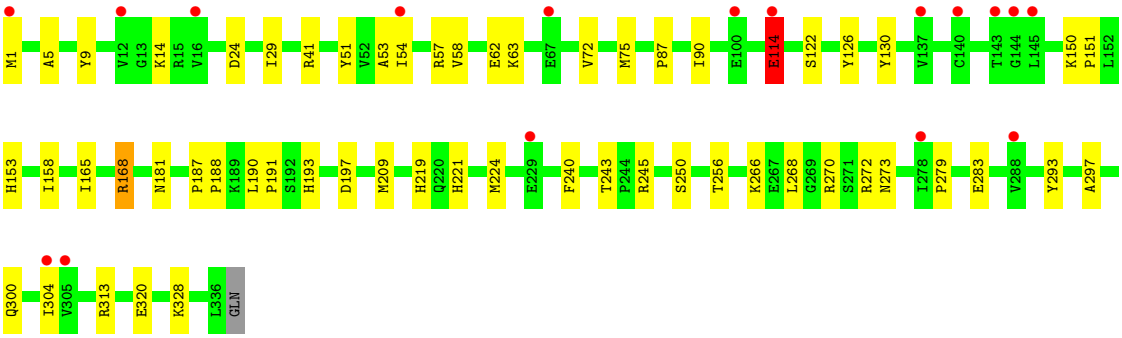
• Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

Chain P:



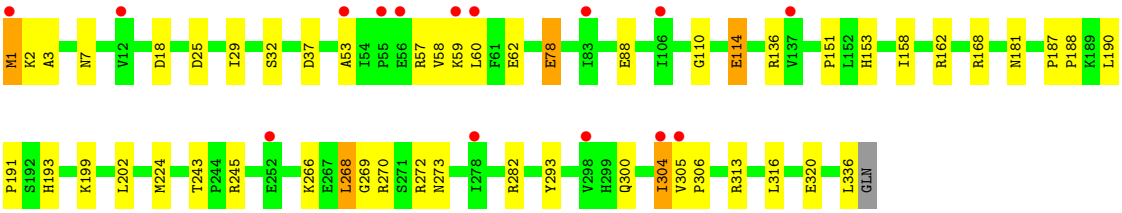
• Molecule 1: PROTEIN (GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

Chain R:



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

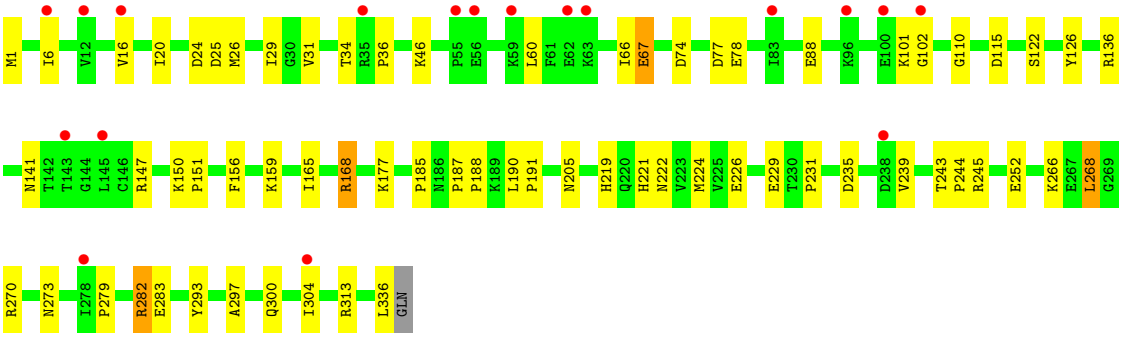
Chain O:



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

Chain Q:

5%
80%
19%


M1 I6 V12 V16 I20 D24 D25 M26 I29 G30 V31 T34 R35 P36 K46 P55 E56 K59 L60 F61 E62 K63 I66 E67 D74 D77 E78 I83 E88 K96 E100 K101 G102 G110 D115 S122 Y126 R136
N141 T142 T143 G144 L145 C146 R147 K150 P151 F156 K159 I165 R168 K177 P185 M186 P187 P188 K189 L190 P191 N205 H219 Q220 H221 N222 V223 M224 V225 E226 E229 T230 P231 D235 D238 V239 T243 P244 R245 E252 K266 E267 L268 G269
R270 N273 I278 P279 R282 E283 Y293 A297 Q300 I304 R313 L336 GLN

4 Data and refinement statistics (i)

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 33.10 – 2.01	Depositor EDS
% Data completeness (in resolution range)	91.7 (10.00-2.10) 85.6 (33.10-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	5.60	Depositor
$< I/\sigma(I) >$ [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)	0.34 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAP

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	0.47	0/2654	1.19	12/3593 (0.3%)
1	P	0.51	0/2654	1.21	11/3593 (0.3%)
1	Q	0.48	0/2654	1.20	14/3593 (0.4%)
1	R	0.51	0/2654	1.18	6/3593 (0.2%)
All	All	0.49	0/10616	1.20	43/14372 (0.3%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	245	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	O	272	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	P	15	ARG	NE-CZ-NH1	-9.03	115.78	120.30
1	Q	245	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	R	245	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	Q	115	ASP	CB-CG-OD2	-8.17	110.95	118.30
1	O	18	ASP	CB-CG-OD1	7.99	125.49	118.30
1	R	41	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	P	242	ASP	CB-CG-OD1	7.20	124.78	118.30
1	Q	147	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	P	147	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	O	282	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	P	245	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	Q	147	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	Q	168	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	Q	25	ASP	CB-CG-OD1	6.33	124.00	118.30
1	Q	24	ASP	CB-CG-OD1	6.22	123.90	118.30
1	R	313	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	R	272	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	O	1	MET	N-CA-CB	6.11	121.59	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	18	ASP	CB-CG-OD1	5.97	123.68	118.30
1	R	114	GLU	CA-CB-CG	5.96	126.51	113.40
1	P	270	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	O	313	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	P	253	ASP	CB-CG-OD1	5.79	123.51	118.30
1	Q	26	MET	CA-CB-CG	5.77	123.11	113.30
1	P	162	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	P	41	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	P	68	VAL	CA-CB-CG1	5.46	119.09	110.90
1	P	167	ARG	CD-NE-CZ	5.46	131.24	123.60
1	O	245	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	Q	168	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	Q	136	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	Q	282	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	O	78	GLU	CB-CA-C	-5.16	100.08	110.40
1	Q	34	THR	N-CA-CB	5.15	120.08	110.30
1	O	136	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	Q	313	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	O	162	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	O	282	ARG	CD-NE-CZ	5.07	130.70	123.60
1	O	25	ASP	CB-CG-OD1	5.06	122.86	118.30
1	O	37	ASP	CB-CG-OD1	5.04	122.83	118.30
1	Q	74	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2612	0	2637	28	0
1	P	2612	0	2637	25	0
1	Q	2612	0	2637	31	1
1	R	2612	0	2637	29	1
2	O	5	0	0	0	0
2	P	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	110	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 (110) 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: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: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: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:114:GLU:H	1:O:114:GLU:CD	2.03	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:P:67:GLU:H	1:P:67:GLU:CD	2.19	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:O:181:ASN:HB2	4:O:1216:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:R:209:MET:HE2	1:Q:222:ASN:HB3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:77:ASP:OD1	1:Q:101:LYS:NZ	2.41	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 (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	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
All	All	1336/1348 (99%)	1297 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	290/291 (100%)	281 (97%)	9 (3%)	40	43
1	P	290/291 (100%)	278 (96%)	12 (4%)	30	31
1	Q	290/291 (100%)	280 (97%)	10 (3%)	37	39
1	R	290/291 (100%)	282 (97%)	8 (3%)	43	47
All	All	1160/1164 (100%)	1121 (97%)	39 (3%)	37	39

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	1	MET
1	P	35	ARG
1	P	68	VAL
1	P	97	MET
1	P	168	ARG
1	P	193	HIS
1	P	197	ASP
1	P	205	ASN
1	P	268	LEU
1	P	270	ARG
1	P	304	ILE
1	P	320	GLU
1	R	1	MET
1	R	114	GLU
1	R	168	ARG
1	R	193	HIS
1	R	197	ASP
1	R	268	LEU
1	R	270	ARG
1	R	304	ILE
1	O	1	MET
1	O	60	LEU
1	O	78	GLU
1	O	114	GLU
1	O	168	ARG
1	O	193	HIS
1	O	268	LEU
1	O	270	ARG
1	O	304	ILE
1	Q	1	MET

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Mol	Chain	Res	Type
1	Q	60	LEU
1	Q	67	GLU
1	Q	168	ARG
1	Q	205	ASN
1	Q	229	GLU
1	Q	268	LEU
1	Q	270	ARG
1	Q	282	ARG
1	Q	304	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	113	HIS
1	P	205	ASN
1	P	273	ASN
1	P	334	ASN
1	R	273	ASN
1	O	153	HIS
1	O	273	ASN
1	Q	22	GLN
1	Q	205	ASN
1	Q	273	ASN
1	Q	334	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 monosaccharides 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	$\#\|Z\| > 2$
2	SO4	R	1002	-	4,4,4	0.68	0	6,6,6	0.15	0
3	NAP	Q	340	-	46,52,52	1.21	3 (6%)	61,80,80	2.08	11 (18%)
3	NAP	P	340	-	46,52,52	1.21	3 (6%)	61,80,80	1.95	10 (16%)
2	SO4	P	1001	-	4,4,4	0.70	0	6,6,6	0.27	0
2	SO4	Q	1004	-	4,4,4	0.72	0	6,6,6	0.29	0
3	NAP	O	340	-	46,52,52	1.34	5 (10%)	61,80,80	1.88	12 (19%)
3	NAP	R	340	-	46,52,52	1.12	3 (6%)	61,80,80	1.88	9 (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	Q	340	-	-	6/31/67/67	0/5/5/5
3	NAP	P	340	-	-	7/31/67/67	0/5/5/5
3	NAP	O	340	-	-	6/31/67/67	0/5/5/5
3	NAP	R	340	-	-	6/31/67/67	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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 (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	P	340	NAP	C1B-N9A-C4A	-3.57	120.38	126.64
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	C1B-N9A-C4A	-3.31	120.82	126.64
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
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-C5A-N7A	2.76	112.26	109.34
3	O	340	NAP	O4B-C1B-N9A	-2.69	105.18	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	340	NAP	C1B-N9A-C4A	-2.62	122.03	126.64
3	O	340	NAP	C1B-N9A-C4A	-2.59	122.08	126.64
3	Q	340	NAP	O4B-C1B-N9A	-2.58	105.33	108.75
3	Q	340	NAP	C4N-C3N-C7N	-2.54	114.13	121.06
3	O	340	NAP	C5A-C6A-N6A	2.41	123.98	120.31
3	O	340	NAP	P2B-O2B-C2B	-2.40	117.03	123.43
3	R	340	NAP	O4B-C1B-N9A	-2.37	105.60	108.75
3	O	340	NAP	C4A-C5A-N7A	2.24	111.70	109.34
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 (25) 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	PN-O3-PA-O1A
3	O	340	NAP	PN-O3-PA-O1A
3	O	340	NAP	PN-O3-PA-O2A
3	R	340	NAP	PN-O3-PA-O2A
3	Q	340	NAP	PN-O3-PA-O2A
3	P	340	NAP	O4B-C4B-C5B-O5B

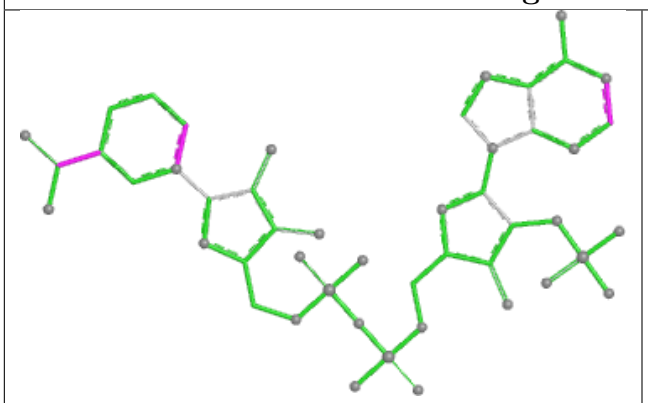
There are no ring outliers.

6 monomers are involved in 8 short contacts:

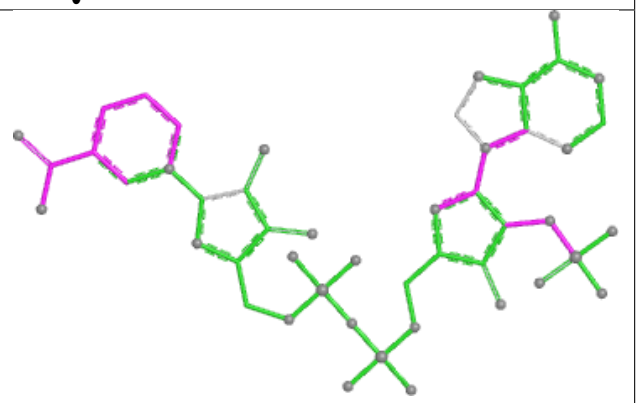
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	340	NAP	1	0
3	P	340	NAP	3	0
2	P	1001	SO4	1	0
2	Q	1004	SO4	1	0
3	O	340	NAP	1	0
3	R	340	NAP	1	0

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 then 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.

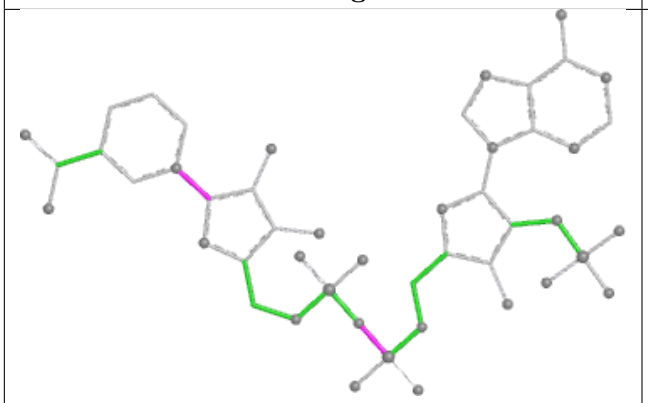
Ligand NAP Q 340



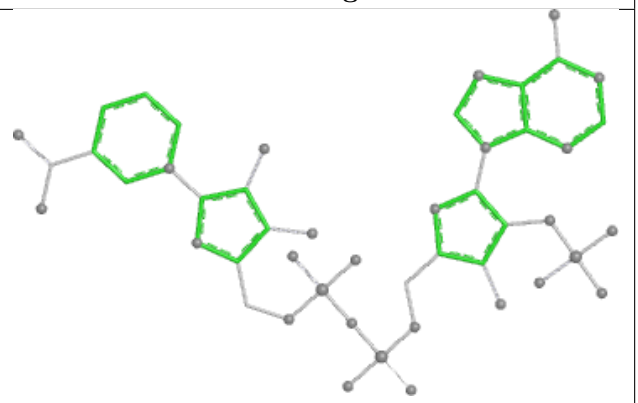
Bond lengths



Bond angles

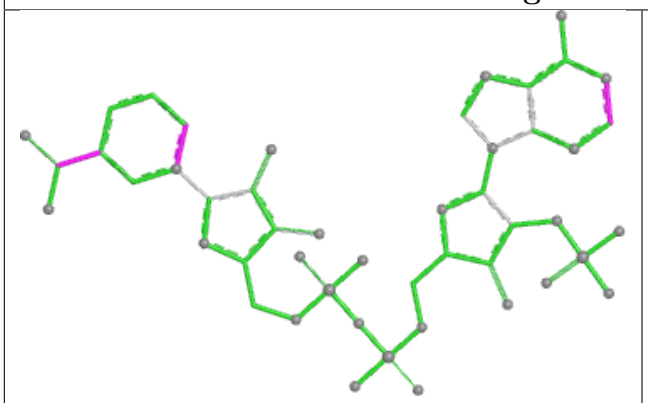


Torsions

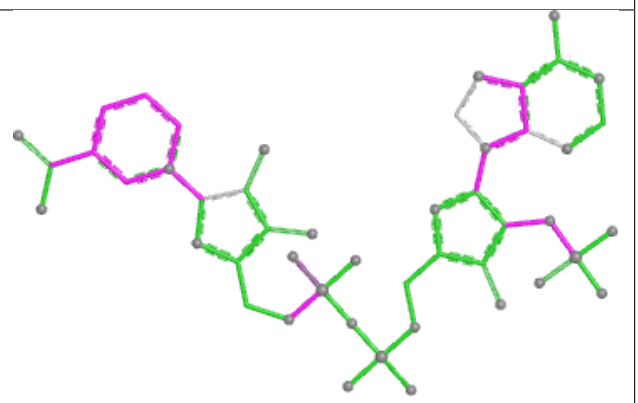


Rings

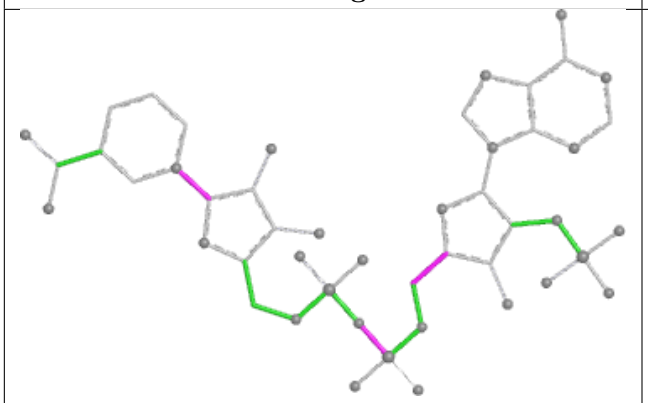
Ligand NAP P 340



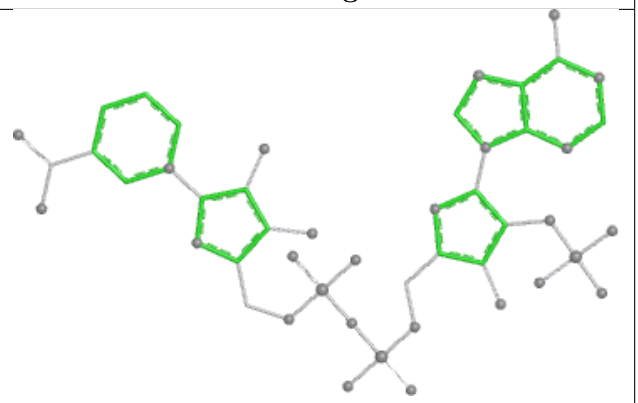
Bond lengths



Bond angles

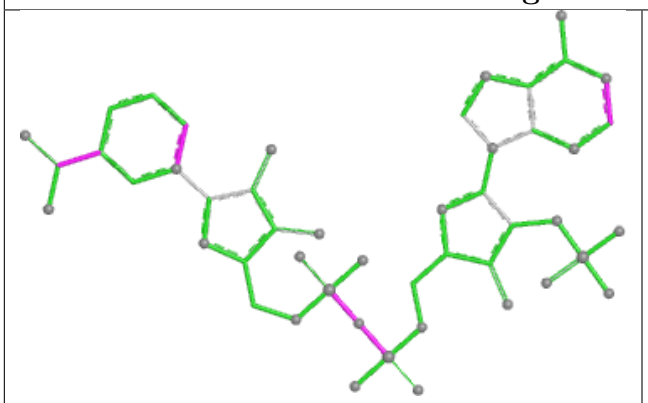


Torsions

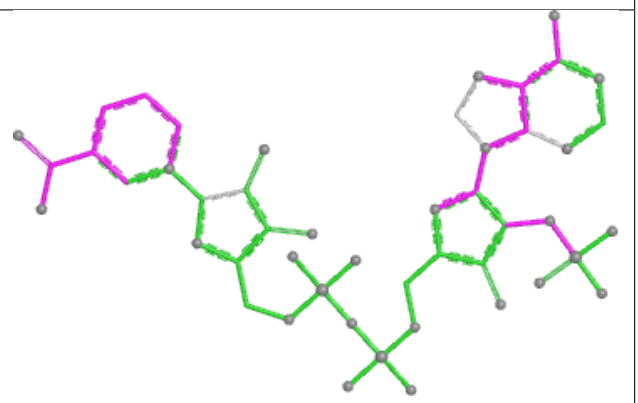


Rings

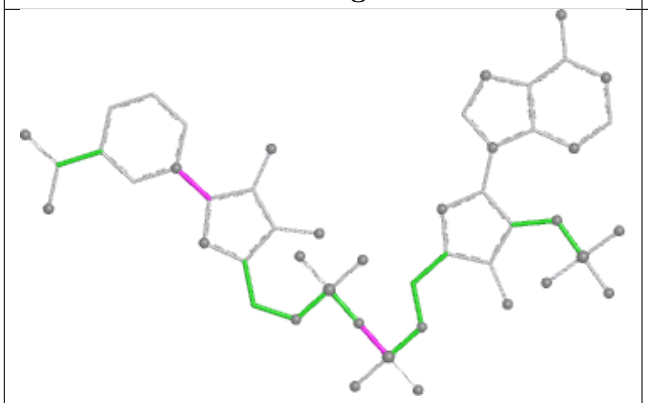
Ligand NAP O 340



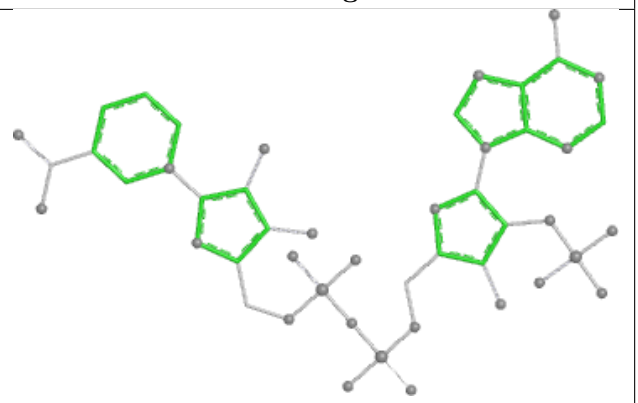
Bond lengths



Bond angles

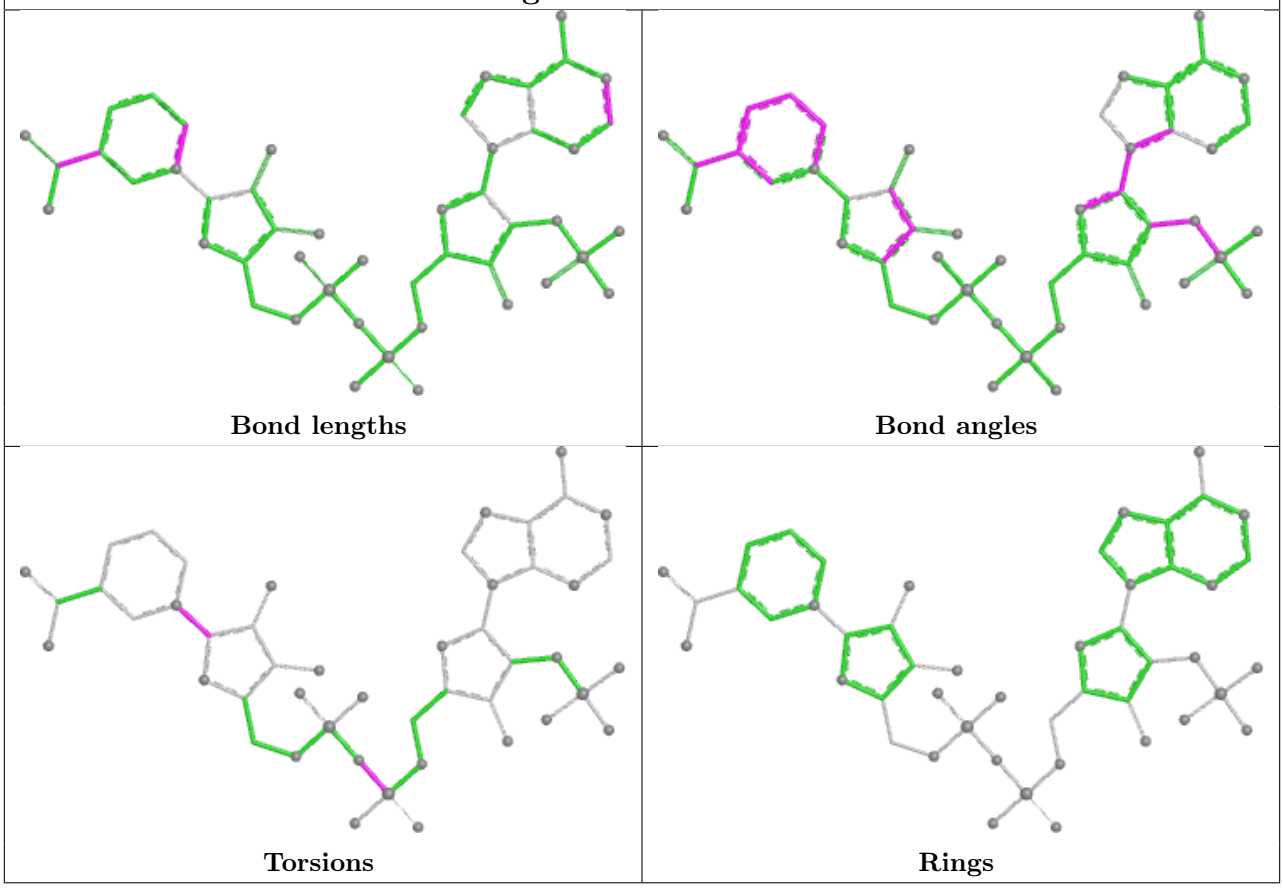


Torsions



Rings

Ligand NAP R 340



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%)	0.24	15 (4%)	33	38	22, 37, 60, 86	0
1	P	336/337 (99%)	0.21	12 (3%)	42	49	22, 33, 53, 70	0
1	Q	336/337 (99%)	0.23	18 (5%)	25	31	21, 36, 54, 81	0
1	R	336/337 (99%)	0.23	17 (5%)	28	33	20, 36, 54, 75	0
All	All	1344/1348 (99%)	0.23	62 (4%)	32	38	20, 35, 55, 86	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	304	ILE	3.9
1	P	145	LEU	3.5
1	Q	12	VAL	3.4
1	Q	83	ILE	3.3
1	Q	56	GLU	3.3
1	O	1	MET	3.3
1	R	145	LEU	3.2
1	Q	63	LYS	3.2
1	R	100	GLU	3.1
1	O	83	ILE	3.1
1	R	304	ILE	3.1
1	P	143	THR	3.0
1	Q	55	PRO	3.0
1	O	56	GLU	3.0
1	O	60	LEU	2.9
1	O	59	LYS	2.9
1	R	143	THR	2.7
1	R	54	ILE	2.7
1	Q	304	ILE	2.7
1	Q	145	LEU	2.7
1	R	278	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	Q	6	ILE	2.7
1	P	83	ILE	2.6
1	O	12	VAL	2.6
1	R	137	VAL	2.6
1	Q	16	VAL	2.6
1	O	55	PRO	2.5
1	Q	278	ILE	2.5
1	P	298	VAL	2.5
1	O	305	VAL	2.5
1	O	53	ALA	2.5
1	P	12	VAL	2.4
1	Q	238	ASP	2.4
1	R	114	GLU	2.4
1	O	106	ILE	2.4
1	R	288	VAL	2.4
1	R	67	GLU	2.4
1	O	304	ILE	2.4
1	R	144	GLY	2.4
1	O	252	GLU	2.3
1	R	140	CYS	2.3
1	O	278	ILE	2.3
1	R	16	VAL	2.3
1	Q	59	LYS	2.3
1	P	138	VAL	2.2
1	Q	100	GLU	2.2
1	R	12	VAL	2.2
1	P	278	ILE	2.2
1	O	137	VAL	2.2
1	Q	35	ARG	2.2
1	Q	96	LYS	2.2
1	P	230	THR	2.1
1	P	223	VAL	2.1
1	Q	62	GLU	2.1
1	P	100	GLU	2.1
1	P	320	GLU	2.1
1	R	1	MET	2.1
1	R	229	GLU	2.0
1	R	305	VAL	2.0
1	O	298	VAL	2.0
1	Q	143	THR	2.0
1	Q	102	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

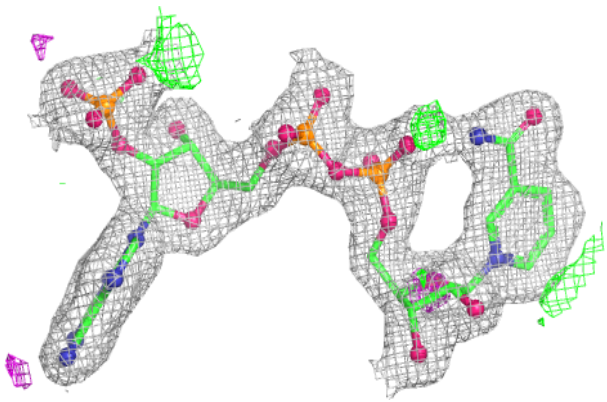
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

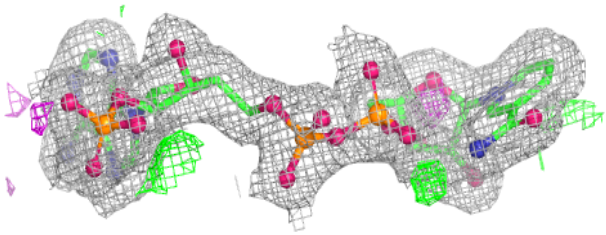
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAP	P	340	48/48	0.94	0.11	23,33,40,41	0
3	NAP	O	340	48/48	0.94	0.11	24,37,45,47	0
3	NAP	R	340	48/48	0.95	0.10	22,39,48,55	0
2	SO4	P	1001	5/5	0.95	0.11	69,69,71,74	0
3	NAP	Q	340	48/48	0.95	0.10	22,34,43,48	0
2	SO4	Q	1004	5/5	0.96	0.13	61,62,64,65	0
2	SO4	O	1003	5/5	0.97	0.11	46,49,51,52	0
2	SO4	R	1002	5/5	0.97	0.12	55,56,58,59	0

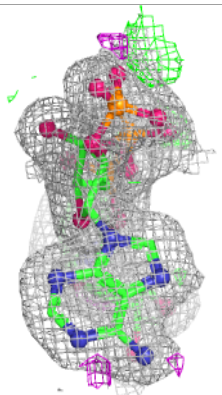
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAP 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)

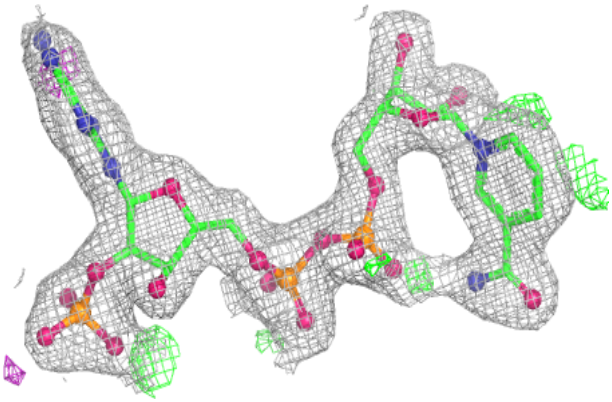


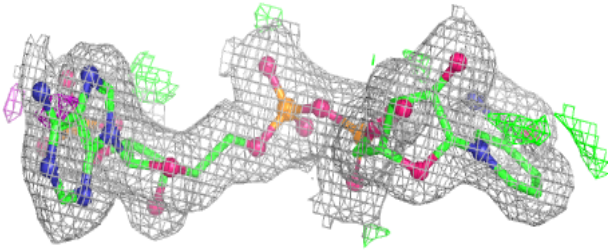


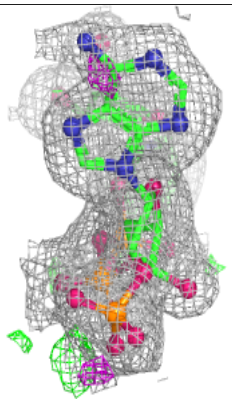


Electron density around NAP O 340:

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

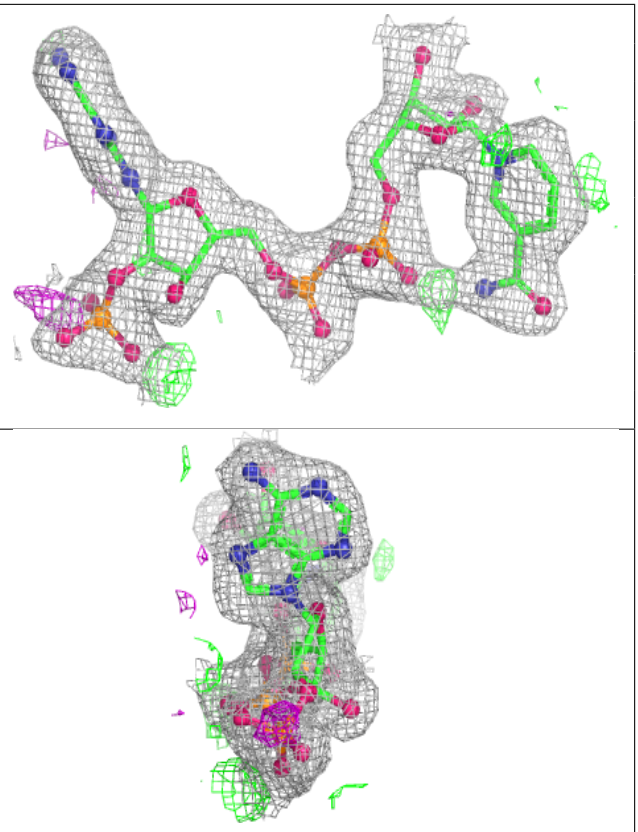






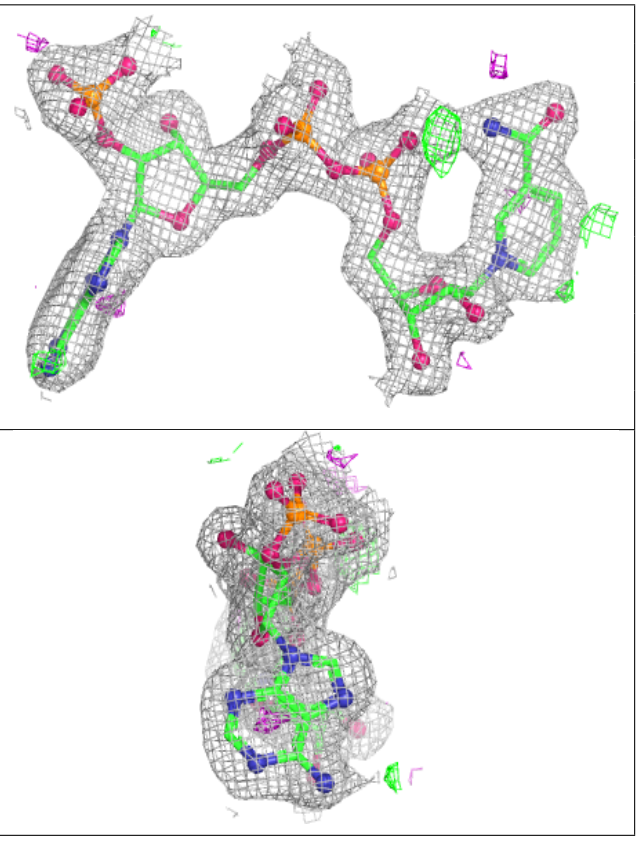
Electron density around NAP R 340:

$2mF_o$-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 Q 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.