



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:53 am BST

PDB ID : 3BUR
Title : Crystal structure of Delta(4)-3-ketosteroid 5-beta-reductase in complex with NADP and TESTOSTERONE. RESOLUTION: 1.62 Å.
Authors : Di Costanzo, L.; Christianson, D.W.
Deposited on : 2008-01-03
Resolution : 1.62 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

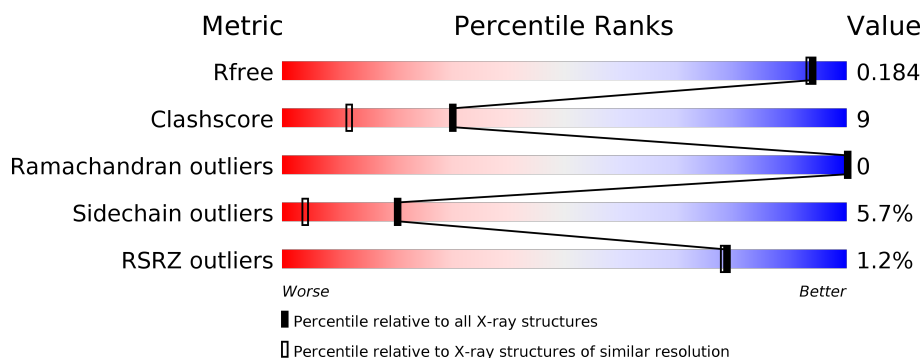
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	<div> <div>2%</div> <div>74%</div> <div>20%</div> <div>6%</div> </div>
1	B	326	<div> <div>85%</div> <div>13%</div> <div>.</div> </div>

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:

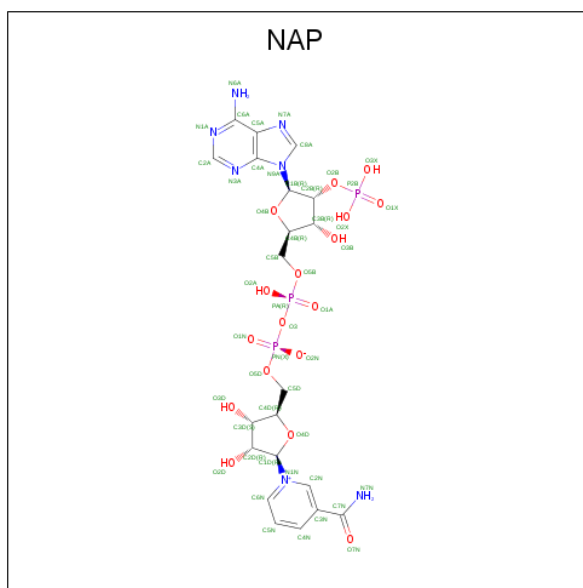
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	338	-	-	-	X

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 3-oxo-5-beta-steroid 4-dehydrogenase.

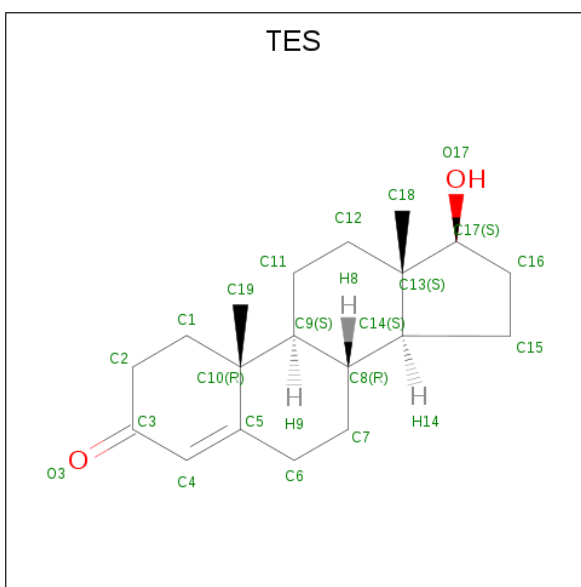
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2627	1680	455	481	11			
1	B	325	Total	C	N	O	S	0	0	0
			2627	1680	455	481	11			

- Molecule 2 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
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is TESTOSTERONE (three-letter code: TES) (formula: $C_{19}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	19	2		
3	B	1	Total	C	O	0	0
			21	19	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

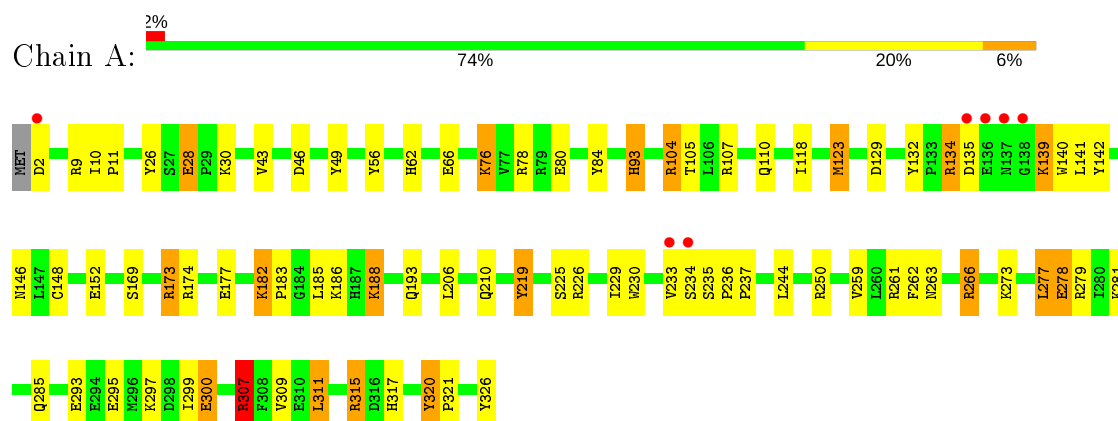
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	242	Total	O	0	0
			242	242		
5	B	256	Total	O	0	0
			256	256		

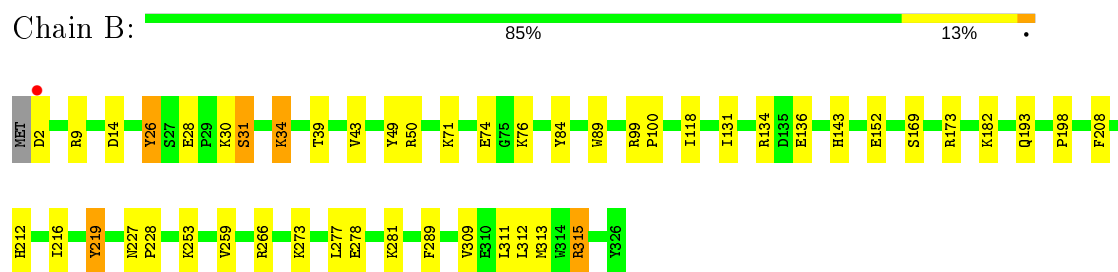
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: 3-oxo-5-beta-steroid 4-dehydrogenase



- Molecule 1: 3-oxo-5-beta-steroid 4-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.82Å 109.98Å 128.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.62 46.47 – 1.62	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.62) 95.0 (46.47-1.62)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 1.63Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.228 , 0.248 0.182 , 0.184	Depositor DCC
R_{free} test set	4317 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.9	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	0.96	EDS
Total number of atoms	5950	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: GOL, NAP, TES

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	0.44	1/2692 (0.0%)	1.20	17/3649 (0.5%)
1	B	0.39	0/2692	1.07	12/3649 (0.3%)
All	All	0.42	1/5384 (0.0%)	1.14	29/7298 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	326	TYR	C-OXT	9.95	1.42	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ARG	CD-NE-CZ	23.65	156.71	123.60
1	A	266	ARG	NE-CZ-NH1	12.71	126.65	120.30
1	A	104	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	A	266	ARG	CD-NE-CZ	10.79	138.71	123.60
1	A	104	ARG	NE-CZ-NH2	-10.77	114.92	120.30
1	A	174	ARG	NE-CZ-NH1	10.69	125.65	120.30
1	B	219	TYR	CB-CG-CD1	9.84	126.90	121.00
1	B	26	TYR	CB-CG-CD2	9.46	126.68	121.00
1	A	307	ARG	NE-CZ-NH1	-8.86	115.87	120.30
1	B	26	TYR	CB-CG-CD1	-8.67	115.80	121.00
1	A	174	ARG	CD-NE-CZ	8.40	135.36	123.60
1	A	219	TYR	CA-CB-CG	7.94	128.48	113.40
1	B	134	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	A	266	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	B	219	TYR	CA-CB-CG	7.62	127.88	113.40
1	A	9	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	A	250	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	B	9	ARG	NE-CZ-NH2	-6.51	117.05	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	TYR	CB-CG-CD1	-6.29	117.23	121.00
1	B	14	ASP	CB-CG-OD1	6.16	123.84	118.30
1	B	49	TYR	CA-CB-CG	5.90	124.61	113.40
1	B	50	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	173	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	219	TYR	CB-CG-CD1	5.50	124.30	121.00
1	B	266	ARG	CD-NE-CZ	5.47	131.26	123.60
1	A	320	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	A	49	TYR	CA-CB-CG	5.19	123.26	113.40
1	B	84	TYR	CB-CG-CD2	5.18	124.11	121.00
1	A	261	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2627	0	2622	67	0
1	B	2627	0	2622	25	0
2	A	48	0	25	4	0
2	B	48	0	25	5	0
3	A	21	0	28	3	0
3	B	21	0	28	4	0
4	A	36	0	48	11	0
4	B	24	0	32	3	0
5	A	242	0	0	9	0
5	B	256	0	0	2	0
All	All	5950	0	5430	101	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 9.

All (101) 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)
2:B:327:NAP:H5N	3:B:340:TES:H62	1.54	0.87
1:A:152:GLU:OE1	1:A:182:LYS:HE3	1.84	0.77
1:A:229:ILE:HG21	4:A:331:GOL:H32	1.66	0.77
1:A:188:LYS:HG3	5:A:1226:HOH:O	1.84	0.77
1:A:206:LEU:O	1:A:210:GLN:HG3	1.83	0.76
1:A:123:MET:HE2	1:A:321:PRO:HD3	1.71	0.70
1:B:152:GLU:HG3	1:B:182:LYS:HE3	1.72	0.70
1:A:277:LEU:HD23	1:A:278:GLU:OE2	1.92	0.69
1:B:277:LEU:HD23	1:B:278:GLU:OE2	1.94	0.67
1:A:110:GLN:HA	4:A:335:GOL:H12	1.78	0.66
1:A:182:LYS:HE2	1:A:183:PRO:O	1.96	0.66
1:A:263:ASN:O	1:A:266:ARG:HG2	1.97	0.65
1:A:104:ARG:HD2	5:A:1043:HOH:O	1.96	0.64
1:B:193:GLN:OE1	2:B:327:NAP:H2N	1.98	0.64
1:A:62:HIS:O	1:A:66:GLU:HG3	1.98	0.63
1:A:235:SER:HB2	5:A:1347:HOH:O	2.02	0.60
1:A:93:HIS:HD2	5:A:1126:HOH:O	1.84	0.60
1:B:28:GLU:HG2	1:B:31:SER:HB3	1.85	0.59
4:A:334:GOL:H11	4:A:338:GOL:H11	1.85	0.59
1:A:135:ASP:OD1	1:A:139:LYS:HB3	2.03	0.58
1:A:56:TYR:CE1	1:A:104:ARG:HD3	2.37	0.58
1:A:315:ARG:HG3	1:A:315:ARG:HH11	1.68	0.58
1:B:89:TRP:NE1	1:B:131:ILE:HG23	2.19	0.58
1:B:277:LEU:O	1:B:281:LYS:HE3	2.04	0.58
1:B:312:LEU:HD22	1:B:315:ARG:HH21	1.67	0.58
1:A:293:GLU:O	1:A:297:LYS:HG3	2.05	0.57
4:A:334:GOL:H11	4:A:338:GOL:C1	2.35	0.57
1:B:31:SER:HA	5:B:1300:HOH:O	2.04	0.56
1:A:132:TYR:HB3	1:A:140:TRP:CZ3	2.41	0.55
1:A:230:TRP:CZ2	4:A:331:GOL:H31	2.41	0.55
1:A:262:PHE:HZ	1:A:300:GLU:HG2	1.71	0.55
1:A:134:ARG:HB3	1:A:139:LYS:O	2.05	0.55
2:B:327:NAP:O2X	4:B:336:GOL:H12	2.06	0.55
1:A:148:CYS:O	1:A:152:GLU:HG3	2.07	0.55
1:A:236:PRO:HD2	5:A:1199:HOH:O	2.07	0.54
1:A:230:TRP:CD1	3:A:339:TES:H12	2.42	0.54
1:A:273:LYS:O	2:A:328:NAP:H8A	2.08	0.54
4:A:333:GOL:H11	1:B:100:PRO:HB2	1.88	0.54
1:B:26:TYR:CE2	3:B:340:TES:H11	2.42	0.53
1:A:277:LEU:HD21	1:A:281:LYS:NZ	2.24	0.53
1:A:107:ARG:HA	4:A:335:GOL:H32	1.89	0.53
1:A:263:ASN:HA	1:A:266:ARG:HD3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LYS:HD3	1:B:34:LYS:N	2.20	0.53
1:A:226:ARG:HD3	4:A:332:GOL:H31	1.91	0.53
1:A:46:ASP:HA	1:A:76:LYS:HE3	1.90	0.53
1:A:123:MET:CE	1:A:321:PRO:HD3	2.39	0.52
1:A:193:GLN:OE1	2:A:328:NAP:H2N	2.09	0.51
1:A:309:VAL:HG12	1:A:311:LEU:HD13	1.92	0.51
4:B:329:GOL:O3	4:B:337:GOL:H32	2.11	0.51
1:B:71:LYS:HA	1:B:74:GLU:HG2	1.92	0.51
1:A:225:SER:C	4:A:332:GOL:H32	2.32	0.50
1:A:118:ILE:HD12	1:A:169:SER:HB2	1.94	0.50
1:A:134:ARG:HA	1:A:141:LEU:HG	1.93	0.50
1:A:233:VAL:O	1:A:233:VAL:HG23	2.11	0.50
1:A:140:TRP:HB3	1:A:142:TYR:CE2	2.46	0.50
4:A:335:GOL:H31	5:A:1032:HOH:O	2.12	0.49
1:A:28:GLU:HG2	5:A:1238:HOH:O	2.12	0.49
2:A:328:NAP:H5N	3:A:339:TES:H62	1.94	0.49
4:A:332:GOL:H2	5:A:1486:HOH:O	2.13	0.49
1:B:26:TYR:CD2	3:B:340:TES:H193	2.48	0.48
1:A:26:TYR:CD2	3:A:339:TES:H193	2.48	0.48
1:A:277:LEU:HD11	1:A:281:LYS:HZ1	1.79	0.47
1:A:277:LEU:HD21	1:A:281:LYS:HZ2	1.79	0.47
1:A:244:LEU:HD13	1:A:259:VAL:CG2	2.44	0.47
1:A:78:ARG:NH1	1:A:80:GLU:OE1	2.48	0.47
1:A:185:LEU:HD21	1:A:188:LYS:HG2	1.96	0.46
1:A:186:LYS:HB3	1:A:186:LYS:HE2	1.46	0.46
1:B:273:LYS:O	2:B:327:NAP:H8A	2.16	0.46
1:A:315:ARG:HA	1:A:320:TYR:CD2	2.50	0.46
1:A:277:LEU:O	1:A:281:LYS:HG3	2.16	0.46
1:B:30:LYS:HD2	1:B:30:LYS:HA	1.47	0.46
1:B:198:PRO:HG2	1:B:259:VAL:HG22	1.98	0.46
1:B:89:TRP:CD1	1:B:131:ILE:HG23	2.51	0.46
1:A:10:ILE:HB	1:A:11:PRO:HD2	1.97	0.45
1:A:281:LYS:O	1:A:285:GLN:HG2	2.16	0.45
1:A:315:ARG:HG3	1:A:315:ARG:NH1	2.29	0.45
1:A:173:ARG:NH1	1:A:177:GLU:OE1	2.50	0.44
1:A:43:VAL:HG11	1:A:277:LEU:HD12	1.98	0.44
1:A:188:LYS:HE2	1:A:188:LYS:HB3	1.36	0.43
1:A:123:MET:HG2	1:A:317:HIS:CG	2.53	0.43
1:B:253:LYS:HE3	1:B:289:PHE:CD1	2.52	0.43
1:B:309:VAL:CG2	3:B:340:TES:H61	2.49	0.43
1:B:99:ARG:HB3	1:B:100:PRO:HD3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ARG:HA	1:A:320:TYR:CG	2.53	0.43
1:A:78:ARG:HD2	1:A:80:GLU:OE1	2.18	0.43
1:A:236:PRO:HA	1:A:237:PRO:HD3	1.73	0.42
1:A:186:LYS:HG3	5:A:1379:HOH:O	2.19	0.42
1:A:277:LEU:HD23	1:A:278:GLU:CD	2.39	0.42
1:A:295:GLU:O	1:A:299:ILE:HG13	2.20	0.42
1:B:28:GLU:HG3	5:B:1483:HOH:O	2.19	0.42
1:A:132:TYR:HB3	1:A:140:TRP:CH2	2.54	0.42
1:A:279:ARG:HD2	2:A:328:NAP:C5A	2.49	0.42
1:B:208:PHE:O	1:B:212:HIS:HD2	2.03	0.41
1:A:80:GLU:CD	1:A:80:GLU:H	2.23	0.41
1:B:118:ILE:HD12	1:B:169:SER:HB2	2.02	0.41
2:B:327:NAP:N3A	4:B:330:GOL:O1	2.50	0.41
1:A:307:ARG:HD3	1:A:307:ARG:HH11	1.58	0.41
1:B:39:THR:O	1:B:43:VAL:HG23	2.20	0.41
1:A:134:ARG:CA	1:A:141:LEU:HG	2.51	0.41
1:B:227:ASN:HA	1:B:228:PRO:HD3	1.68	0.41
1:A:132:TYR:HB3	1:A:140:TRP:HZ3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/326 (99%)	311 (96%)	12 (4%)	0	100	100
1	B	323/326 (99%)	315 (98%)	8 (2%)	0	100	100
All	All	646/652 (99%)	626 (97%)	20 (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	A	289/290 (100%)	267 (92%)	22 (8%)	13	2
1	B	289/290 (100%)	278 (96%)	11 (4%)	33	9
All	All	578/580 (100%)	545 (94%)	33 (6%)	20	4

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	28	GLU
1	A	30	LYS
1	A	76	LYS
1	A	93	HIS
1	A	105	THR
1	A	123	MET
1	A	129	ASP
1	A	134	ARG
1	A	139	LYS
1	A	146	ASN
1	A	173	ARG
1	A	182	LYS
1	A	188	LYS
1	A	219	TYR
1	A	234	SER
1	A	277	LEU
1	A	278	GLU
1	A	300	GLU
1	A	307	ARG
1	A	311	LEU
1	A	315	ARG
1	B	2	ASP
1	B	31	SER
1	B	34	LYS
1	B	76	LYS
1	B	136	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	143	HIS
1	B	216	ILE
1	B	219	TYR
1	B	311	LEU
1	B	313	MET
1	B	315	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	93	HIS
1	A	110	GLN
1	A	146	ASN
1	B	212	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 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	GOL	A	334	-	5,5,5	0.62	0	5,5,5	0.76	0
3	TES	A	339	-	24,24,24	0.74	0	39,39,39	0.90	0
2	NAP	B	327	-	45,52,52	2.27	17 (37%)	56,80,80	2.14	17 (30%)
4	GOL	B	329	-	5,5,5	0.51	0	5,5,5	0.71	0
4	GOL	B	330	-	5,5,5	0.45	0	5,5,5	1.10	0
4	GOL	B	337	-	5,5,5	0.50	0	5,5,5	0.61	0
4	GOL	A	338	-	5,5,5	0.68	0	5,5,5	0.82	0
4	GOL	A	335	-	5,5,5	0.43	0	5,5,5	0.67	0
3	TES	B	340	-	24,24,24	0.79	0	39,39,39	1.44	5 (12%)
4	GOL	A	331	-	5,5,5	0.53	0	5,5,5	0.78	0
4	GOL	A	332	-	5,5,5	0.56	0	5,5,5	0.48	0
4	GOL	B	336	-	5,5,5	0.59	0	5,5,5	0.75	0
4	GOL	A	333	-	5,5,5	0.60	0	5,5,5	0.88	0
2	NAP	A	328	-	45,52,52	2.14	13 (28%)	56,80,80	1.94	12 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	334	-	-	2/4/4/4	-
3	TES	A	339	-	-	-	0/4/4/4
2	NAP	B	327	-	-	6/31/67/67	0/5/5/5
4	GOL	B	329	-	-	1/4/4/4	-
4	GOL	B	330	-	-	4/4/4/4	-
4	GOL	B	337	-	-	3/4/4/4	-
3	TES	B	340	-	-	-	0/4/4/4
4	GOL	A	335	-	-	2/4/4/4	-
4	GOL	A	338	-	-	4/4/4/4	-
4	GOL	A	331	-	-	2/4/4/4	-
4	GOL	A	332	-	-	2/4/4/4	-
4	GOL	B	336	-	-	2/4/4/4	-
4	GOL	A	333	-	-	1/4/4/4	-
2	NAP	A	328	-	-	7/31/67/67	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	327	NAP	C4A-N3A	6.42	1.44	1.35
2	A	328	NAP	C4A-N3A	5.72	1.43	1.35
2	B	327	NAP	C6N-N1N	5.32	1.48	1.35
2	A	328	NAP	C6N-N1N	5.08	1.47	1.35
2	B	327	NAP	C2N-N1N	4.67	1.40	1.35
2	B	327	NAP	O5B-C5B	-4.61	1.27	1.44
2	A	328	NAP	O5B-C5B	-4.56	1.27	1.44
2	A	328	NAP	C2N-N1N	4.47	1.40	1.35
2	B	327	NAP	PN-O5D	-3.45	1.45	1.59
2	A	328	NAP	O4B-C4B	-3.27	1.37	1.45
2	A	328	NAP	PN-O5D	-3.20	1.46	1.59
2	A	328	NAP	PN-O1N	-3.14	1.39	1.50
2	B	327	NAP	PN-O1N	-3.09	1.40	1.50
2	A	328	NAP	C4N-C3N	2.99	1.44	1.39
2	A	328	NAP	PA-O1A	-2.99	1.40	1.50
2	B	327	NAP	C5N-C4N	2.90	1.45	1.38
2	B	327	NAP	O4D-C1D	2.84	1.45	1.41
2	B	327	NAP	C2N-C3N	2.71	1.43	1.39
2	B	327	NAP	PA-O1A	-2.66	1.41	1.50
2	B	327	NAP	C4N-C3N	2.52	1.43	1.39
2	B	327	NAP	O4B-C4B	-2.51	1.39	1.45
2	B	327	NAP	O4B-C1B	2.49	1.44	1.41
2	B	327	NAP	C3D-C4D	2.27	1.58	1.53
2	B	327	NAP	P2B-O2B	2.22	1.63	1.59
2	A	328	NAP	C5N-C4N	2.21	1.43	1.38
2	B	327	NAP	C8A-N7A	2.20	1.38	1.34
2	A	328	NAP	P2B-O2B	2.20	1.63	1.59
2	A	328	NAP	O4D-C1D	2.20	1.44	1.41
2	A	328	NAP	O3D-C3D	2.18	1.48	1.43
2	B	327	NAP	C2A-N1A	2.13	1.37	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	328	NAP	C5A-C6A-N6A	6.83	130.73	120.35
2	B	327	NAP	PN-O3-PA	6.45	154.97	132.83
2	A	328	NAP	PN-O3-PA	6.45	154.94	132.83
3	B	340	TES	C16-C17-C13	-5.59	100.09	104.53
2	B	327	NAP	C5A-C6A-N6A	5.30	128.41	120.35
2	B	327	NAP	N3A-C2A-N1A	-5.18	120.59	128.68
2	B	327	NAP	C3N-C7N-N7N	-5.03	111.72	117.75
2	A	328	NAP	O5D-C5D-C4D	3.72	121.78	108.99
2	A	328	NAP	O7N-C7N-N7N	3.69	127.81	122.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	327	NAP	O7N-C7N-N7N	3.48	127.52	122.58
2	B	327	NAP	C6N-N1N-C2N	-3.22	119.04	121.97
2	A	328	NAP	N3A-C2A-N1A	-3.15	123.76	128.68
2	B	327	NAP	O4D-C4D-C3D	-3.02	99.14	105.11
2	B	327	NAP	C2N-C3N-C4N	2.97	121.63	118.26
2	A	328	NAP	C2N-C3N-C4N	2.95	121.61	118.26
2	B	327	NAP	PN-O5D-C5D	2.71	137.58	121.68
2	B	327	NAP	O3D-C3D-C2D	2.69	120.53	111.82
2	B	327	NAP	O5D-C5D-C4D	2.69	118.25	108.99
2	B	327	NAP	C2A-N1A-C6A	2.49	123.01	118.75
2	A	328	NAP	PN-O5D-C5D	2.45	136.07	121.68
2	A	328	NAP	C3N-C7N-N7N	-2.42	114.85	117.75
2	A	328	NAP	C5A-C6A-N1A	-2.35	115.03	120.35
2	B	327	NAP	C5A-C6A-N1A	-2.32	115.10	120.35
3	B	340	TES	C19-C10-C9	2.27	114.39	111.68
3	B	340	TES	C10-C9-C8	2.27	116.14	112.73
2	B	327	NAP	O4B-C4B-C5B	-2.25	101.98	109.37
2	A	328	NAP	O4B-C4B-C5B	-2.25	101.98	109.37
3	B	340	TES	C18-C13-C12	2.23	114.11	110.59
2	B	327	NAP	C6N-C5N-C4N	-2.21	116.22	119.44
2	B	327	NAP	O5B-C5B-C4B	2.15	116.38	108.99
2	B	327	NAP	C5N-C6N-N1N	2.11	123.43	120.40
2	A	328	NAP	N6A-C6A-N1A	-2.09	114.24	118.57
3	B	340	TES	C12-C13-C14	2.06	110.46	107.27
2	A	328	NAP	C3N-C2N-N1N	-2.01	118.46	120.43

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	334	GOL	O1-C1-C2-C3
2	B	327	NAP	C5D-O5D-PN-O2N
2	B	327	NAP	O4D-C1D-N1N-C6N
4	B	330	GOL	O1-C1-C2-C3
4	B	337	GOL	O1-C1-C2-C3
4	A	338	GOL	O1-C1-C2-C3
4	A	338	GOL	C1-C2-C3-O3
4	A	331	GOL	O1-C1-C2-O2
4	A	331	GOL	O1-C1-C2-C3
4	A	332	GOL	C1-C2-C3-O3
4	B	336	GOL	C1-C2-C3-O3
2	A	328	NAP	C5D-O5D-PN-O2N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	328	NAP	O4D-C1D-N1N-C6N
4	B	330	GOL	O1-C1-C2-O2
4	B	337	GOL	O1-C1-C2-O2
4	B	330	GOL	C1-C2-C3-O3
4	A	335	GOL	O1-C1-C2-C3
4	A	334	GOL	O1-C1-C2-O2
4	A	338	GOL	O1-C1-C2-O2
4	B	336	GOL	O2-C2-C3-O3
2	A	328	NAP	C4D-C5D-O5D-PN
4	A	332	GOL	O2-C2-C3-O3
2	B	327	NAP	C4D-C5D-O5D-PN
2	B	327	NAP	PA-O3-PN-O5D
2	A	328	NAP	PA-O3-PN-O5D
4	B	330	GOL	O2-C2-C3-O3
4	A	338	GOL	O2-C2-C3-O3
4	A	333	GOL	O1-C1-C2-O2
2	A	328	NAP	C5D-O5D-PN-O3
2	A	328	NAP	C5D-O5D-PN-O1N
2	B	327	NAP	PN-O3-PA-O2A
2	A	328	NAP	PN-O3-PA-O2A
2	B	327	NAP	C5D-O5D-PN-O3
4	A	335	GOL	O1-C1-C2-O2
4	B	329	GOL	C1-C2-C3-O3
4	B	337	GOL	C1-C2-C3-O3

There are no ring outliers.

14 monomers are involved in 26 short contacts:

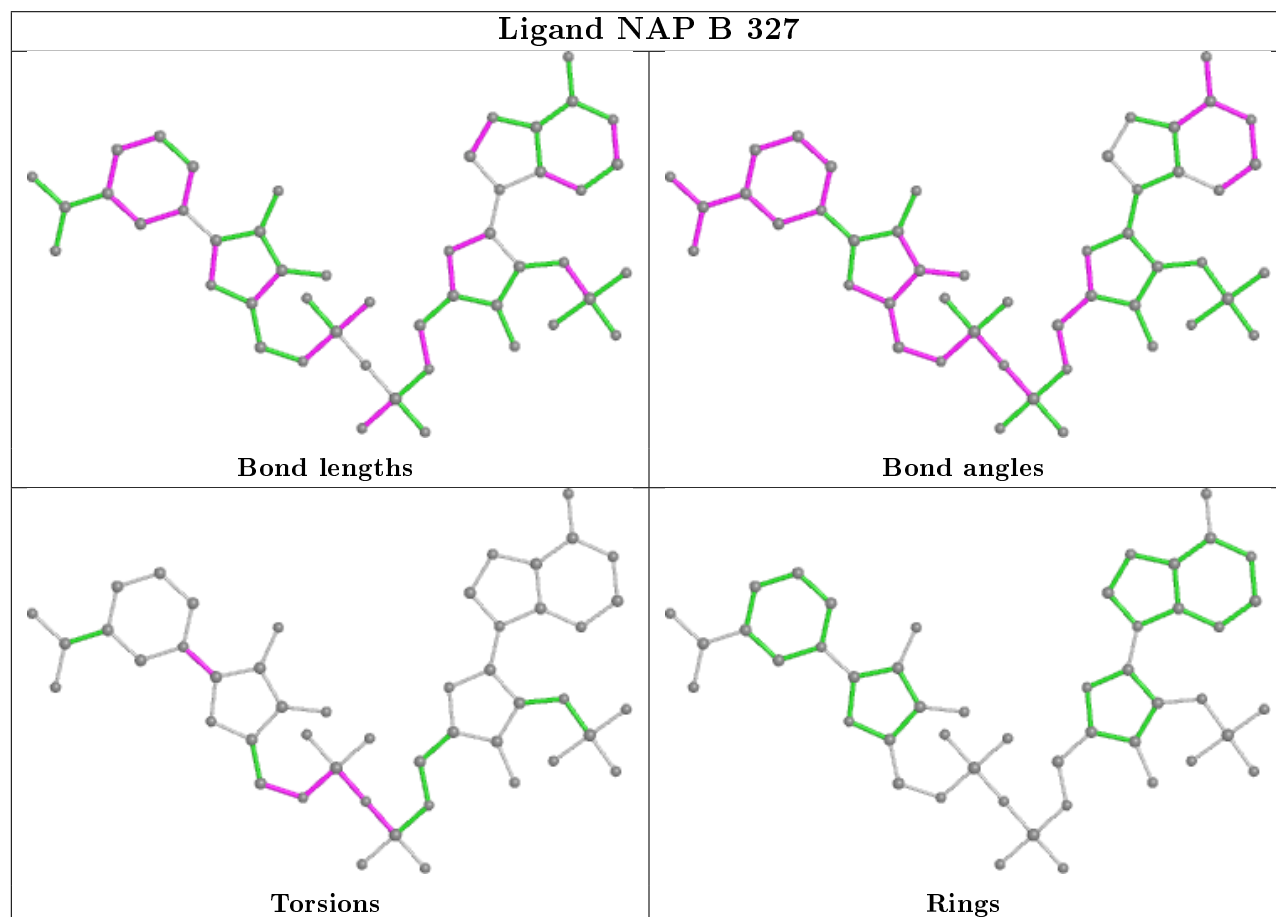
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	334	GOL	2	0
3	A	339	TES	3	0
2	B	327	NAP	5	0
4	B	329	GOL	1	0
4	B	330	GOL	1	0
4	B	337	GOL	1	0
4	A	338	GOL	2	0
4	A	335	GOL	3	0
3	B	340	TES	4	0
4	A	331	GOL	2	0
4	A	332	GOL	3	0
4	B	336	GOL	1	0
4	A	333	GOL	1	0

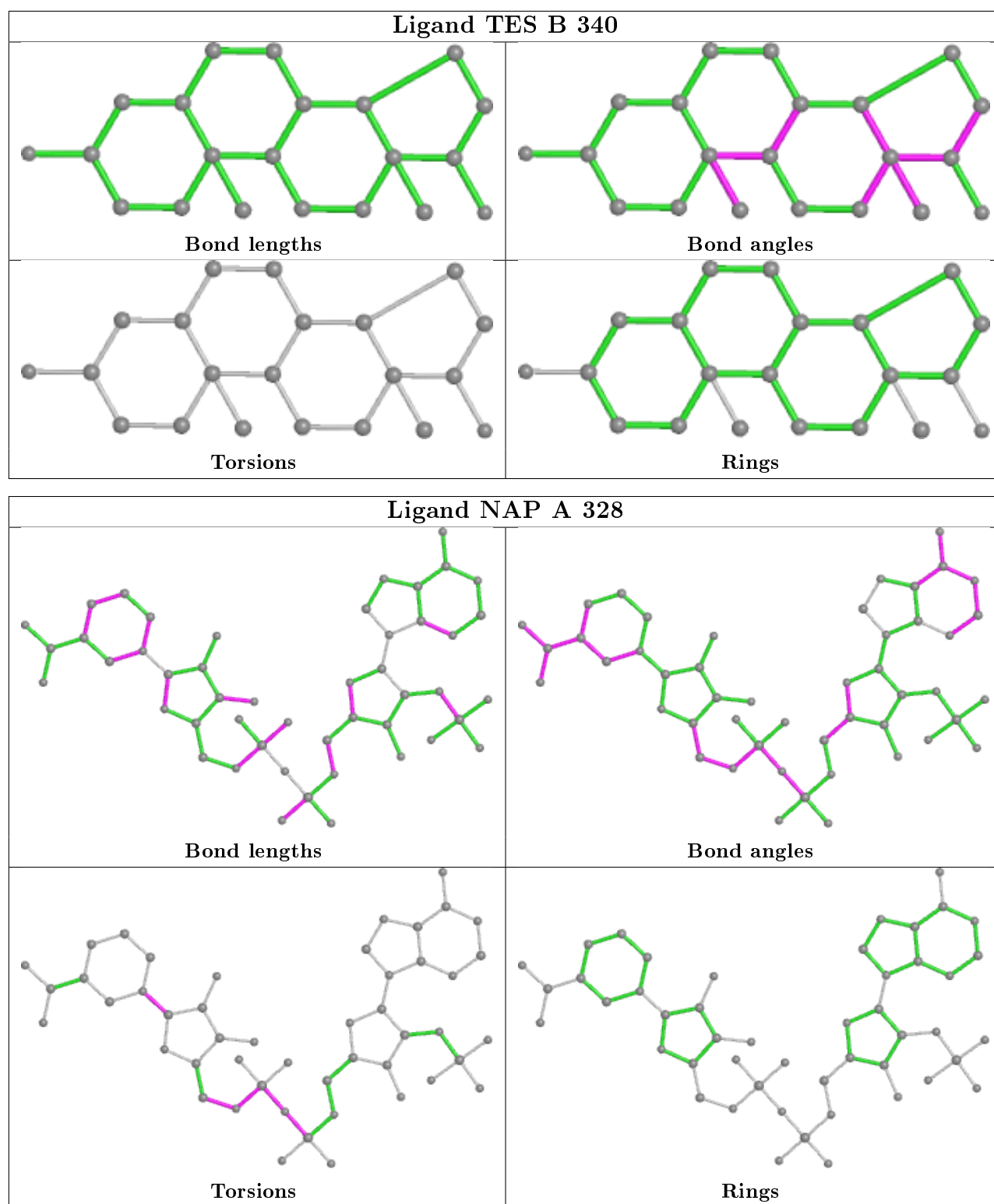
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	328	NAP	4	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	325/326 (99%)	-0.09	7 (2%) 62 60	9, 18, 45, 87	0
1	B	325/326 (99%)	-0.38	1 (0%) 94 93	10, 16, 33, 71	0
All	All	650/652 (99%)	-0.24	8 (1%) 79 78	9, 17, 39, 87	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	SER	4.3
1	B	2	ASP	3.2
1	A	137	ASN	3.1
1	A	135	ASP	2.6
1	A	2	ASP	2.6
1	A	138	GLY	2.5
1	A	136	GLU	2.3
1	A	233	VAL	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

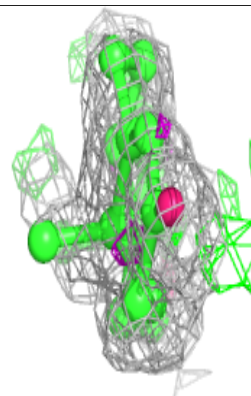
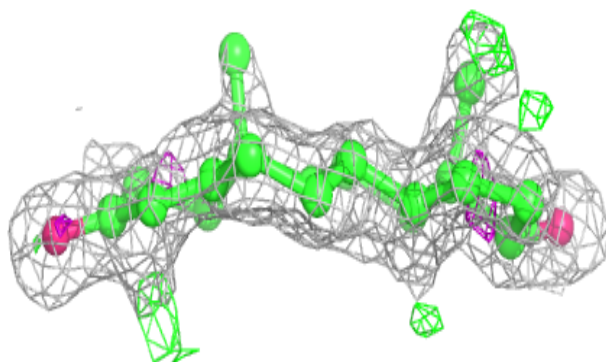
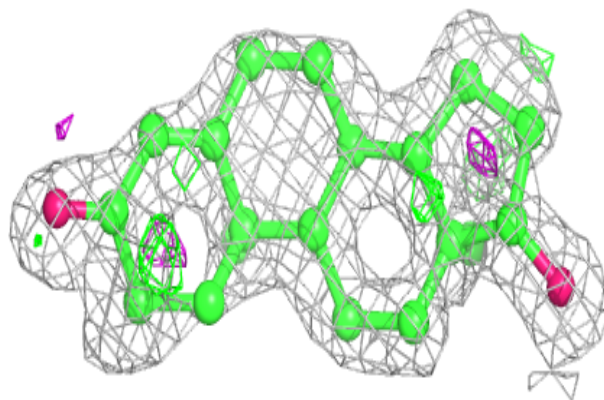
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	334	6/6	0.38	0.33	35,39,44,46	6
4	GOL	A	331	6/6	0.65	0.34	21,26,32,38	6
4	GOL	A	338	6/6	0.67	0.42	19,24,26,28	6
4	GOL	A	332	6/6	0.76	0.26	39,54,62,76	0
4	GOL	B	336	6/6	0.76	0.21	30,40,51,60	6
3	TES	B	340	21/21	0.80	0.20	27,35,49,51	0
4	GOL	A	335	6/6	0.80	0.31	34,38,39,50	0
4	GOL	B	329	6/6	0.81	0.16	26,36,41,57	0
4	GOL	B	330	6/6	0.84	0.15	20,38,47,62	0
3	TES	A	339	21/21	0.88	0.13	21,29,34,40	0
4	GOL	A	333	6/6	0.88	0.18	37,51,53,53	0
4	GOL	B	337	6/6	0.90	0.13	27,44,48,50	0
2	NAP	B	327	48/48	0.97	0.08	9,12,16,19	0
2	NAP	A	328	48/48	0.97	0.08	9,14,18,22	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.

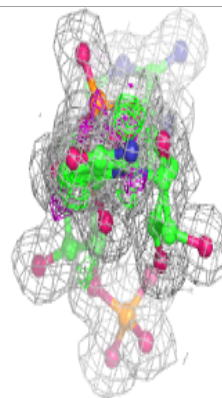
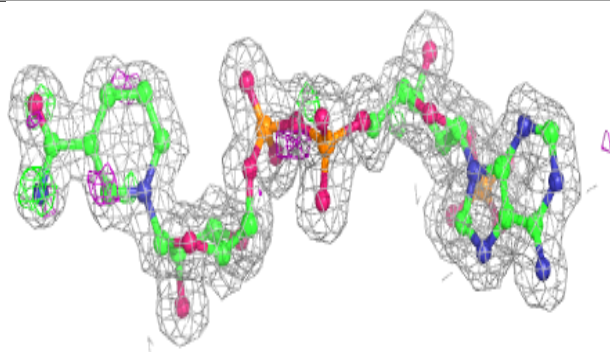
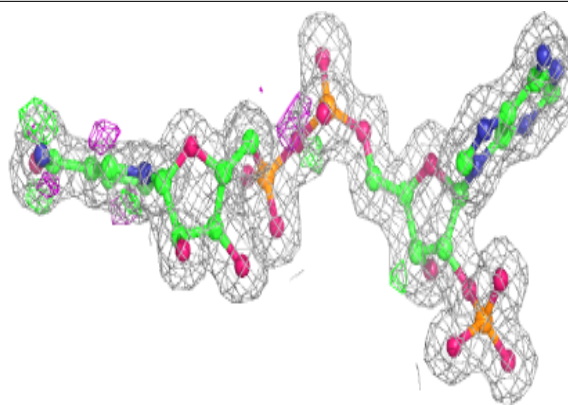
Electron density around TES B 340:

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

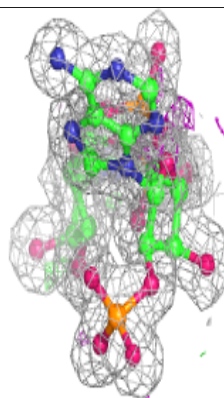
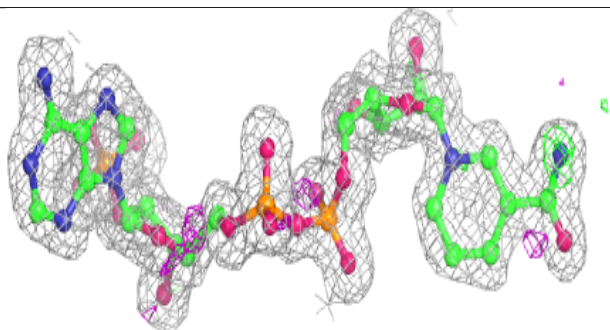
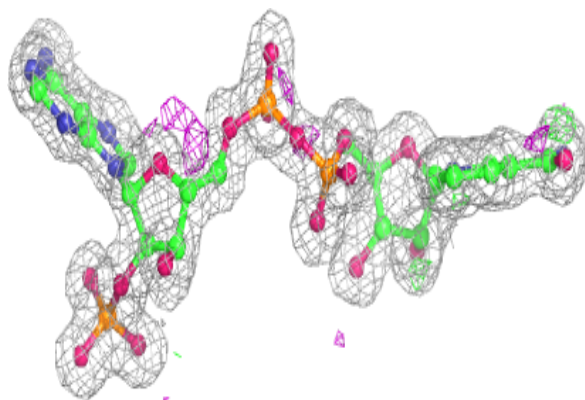


Electron density around NAP B 327:

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

**Electron density around NAP A 328:**

$2mF_o-DF_c$ (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.