



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:38 PM UTC

PDB ID : 2CDC / pdb\_00002cdc  
Title : Sulfolobus solfataricus Glucose Dehydrogenase 1 in complex with NADP and Xylose  
Authors : Milburn, C.C.; Lambie, H.J.; Theodossis, A.; Hough, D.W.; Danson, M.J.; Taylor, G.L.  
Deposited on : 2006-01-23  
Resolution : 1.50 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

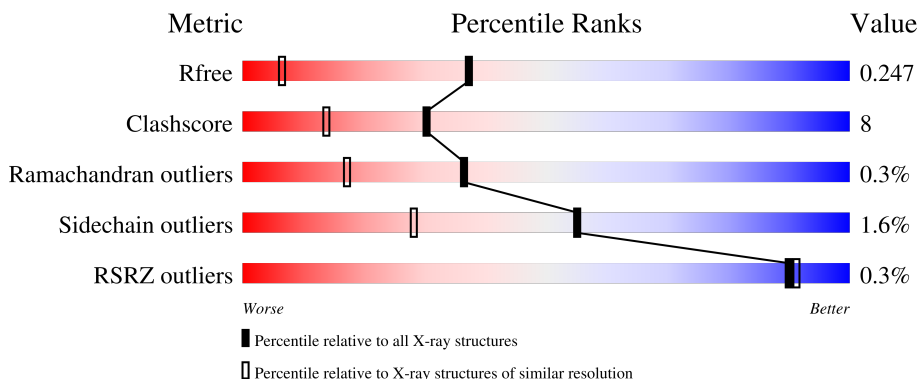
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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  $\geq 3$ , 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	366	 83% 15% ..
1	B	366	 85% 13% .
1	C	366	 86% 12% ..
1	D	366	 85% 11% ..

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13649 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 GLUCOSE DEHYDROGENASE GLUCOSE 1-DEHYDROGENASE, DHG-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	359	Total 2969	C 1902	N 501	O 552	S 14	0	34	0
1	B	359	Total 2937	C 1881	N 497	O 546	S 13	0	26	0
1	C	359	Total 2929	C 1875	N 497	O 543	S 14	0	22	0
1	D	359	Total 2922	C 1868	N 496	O 543	S 15	0	22	0

There are 4 discrepancies between the modelled and reference sequences:

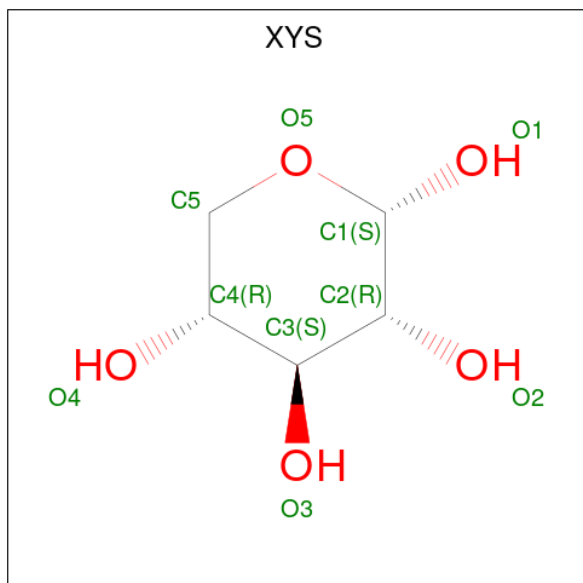
Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	THR	engineered mutation	UNP O93715
B	41	ALA	THR	engineered mutation	UNP O93715
C	41	ALA	THR	engineered mutation	UNP O93715
D	41	ALA	THR	engineered mutation	UNP O93715

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



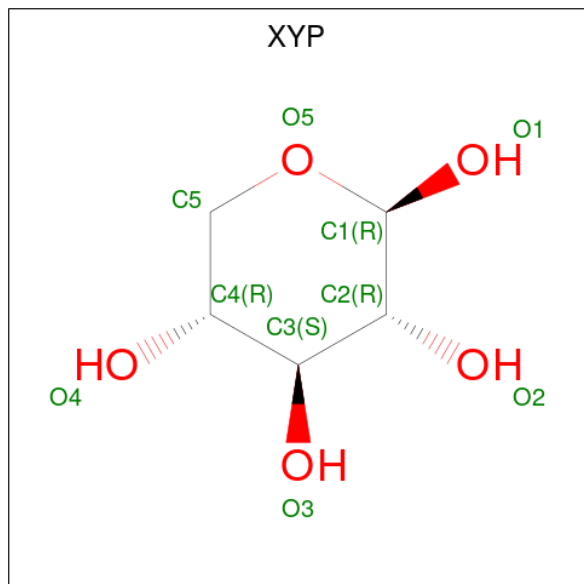
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			
2	A	1	Total	48	21	7	17	3	0	0
2	B	1	Total	48	21	7	17	3	0	0
2	C	1	Total	48	21	7	17	3	0	0
2	D	1	Total	48	21	7	17	3	0	0

- Molecule 3 is alpha-D-xylopyranose (CCD ID: YYS) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 5	0	1
3	A	1	Total C O 10 5 5	0	0
3	B	1	Total C O 10 5 5	0	0
3	C	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	1
3	D	1	Total C O 10 5 5	0	0

- Molecule 4 is beta-D-xylopyranose (CCD ID: XYP) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).

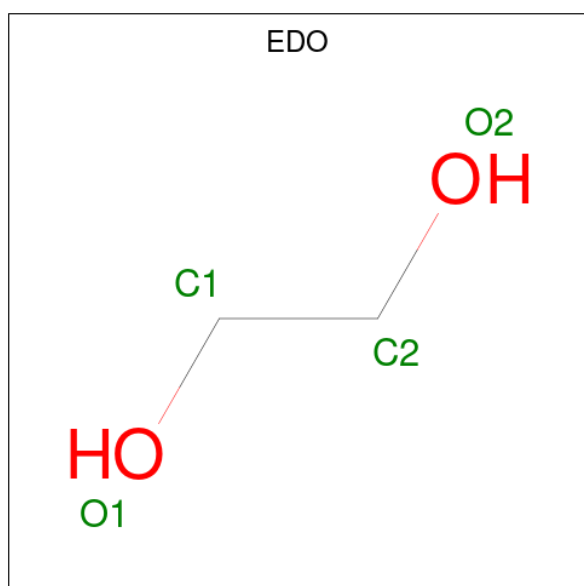


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 5 5	0	1
4	B	1	Total C O 10 5 5	0	0
4	C	1	Total C O 10 5 5	0	0
4	D	1	Total C O 10 5 5	0	1

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Zn 2 2	0	0
5	B	2	Total Zn 2 2	0	0
5	C	2	Total Zn 2 2	0	0
5	D	2	Total Zn 2 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	376	Total O 376 376	0	0
7	B	401	Total O 401 401	0	0
7	C	411	Total O 411 411	0	0

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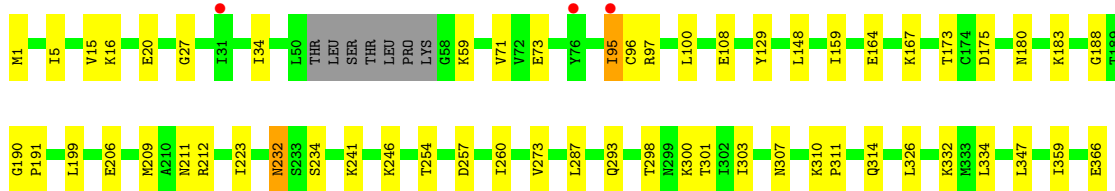
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	D	392	Total 392	O 392	0	0

### 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.

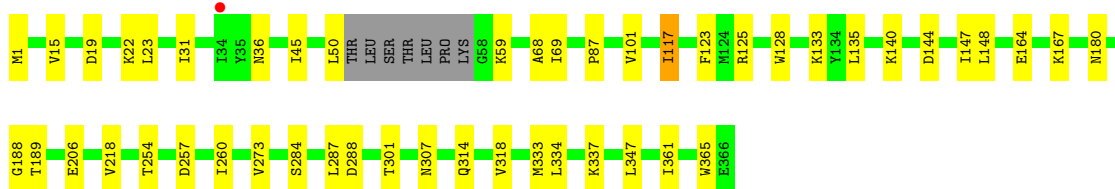
- Molecule 1: GLUCOSE DEHYDROGENASE GLUCOSE 1-DEHYDROGENASE, DHG-1

Chain A: 




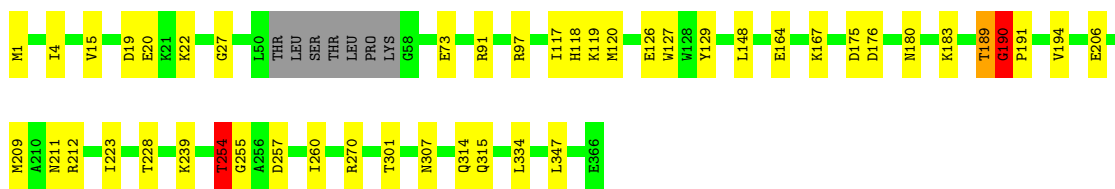
- Molecule 1: GLUCOSE DEHYDROGENASE GLUCOSE 1-DEHYDROGENASE, DHG-1

Chain B: 




- Molecule 1: GLUCOSE DEHYDROGENASE GLUCOSE 1-DEHYDROGENASE, DHG-1

Chain C: 



- Molecule 1: GLUCOSE DEHYDROGENASE GLUCOSE 1-DEHYDROGENASE, DHG-1

Chain D: 





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.64Å 91.03Å 138.72Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	138.68 – 1.50 138.68 – 1.50	Depositor EDS
% Data completeness (in resolution range)	93.0 (138.68-1.50) 92.9 (138.68-1.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.50Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.204 , 0.239 0.213 , 0.247	Depositor DCC
$R_{free}$ test set	12721 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.1	Xtrriage
Anisotropy	0.490	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.279 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13649	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4868e-03.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, XYS, XYP, EDO, ZN

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	0.85	2/3145 (0.1%)	0.93	4/4250 (0.1%)
1	B	0.59	0/3072	0.81	1/4147 (0.0%)
1	C	0.82	6/3047 (0.2%)	0.96	18/4118 (0.4%)
1	D	0.88	4/3038 (0.1%)	1.01	14/4104 (0.3%)
All	All	0.79	12/12302 (0.1%)	0.93	37/16619 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	1	0
All	All	1	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95[A]	ILE	CG1-CD1	23.65	2.44	1.51
1	A	95[B]	ILE	CG1-CD1	23.65	2.44	1.51
1	D	189[A]	THR	N-CA	-21.41	1.10	1.45
1	D	189[B]	THR	N-CA	-21.41	1.10	1.45
1	C	254[A]	THR	CA-C	15.25	1.73	1.52
1	C	254[B]	THR	CA-C	15.25	1.73	1.52
1	C	189[A]	THR	CA-C	-14.61	1.34	1.52
1	C	189[B]	THR	CA-C	-14.61	1.34	1.52
1	D	189[A]	THR	CA-CB	13.04	1.69	1.53
1	D	189[B]	THR	CA-CB	13.04	1.69	1.53
1	C	190[A]	GLY	C-N	-8.46	1.24	1.34
1	C	190[B]	GLY	C-N	-8.46	1.24	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95[A]	ILE	CB-CG1-CD1	-16.75	78.63	113.80
1	A	95[B]	ILE	CB-CG1-CD1	-16.75	78.63	113.80
1	D	189[A]	THR	CA-CB-OG1	14.81	131.82	109.60
1	D	189[B]	THR	CA-CB-OG1	14.81	131.82	109.60
1	A	95[A]	ILE	CG1-CB-CG2	-14.76	66.43	110.70
1	A	95[B]	ILE	CG1-CB-CG2	-14.76	66.43	110.70
1	D	189[A]	THR	N-CA-CB	11.12	122.64	108.96
1	D	189[B]	THR	N-CA-CB	11.12	122.64	108.96
1	D	189[A]	THR	CA-C-N	-10.10	106.01	121.87
1	D	189[A]	THR	C-N-CA	-10.10	106.01	121.87
1	D	189[B]	THR	CA-C-N	-10.10	106.01	121.87
1	D	189[B]	THR	C-N-CA	-10.10	106.01	121.87
1	D	188[A]	GLY	CA-C-N	-10.07	104.10	123.13
1	D	188[A]	GLY	C-N-CA	-10.07	104.10	123.13
1	D	188[B]	GLY	CA-C-N	-10.07	104.10	123.13
1	D	188[B]	GLY	C-N-CA	-10.07	104.10	123.13
1	C	189[A]	THR	CB-CA-C	-10.00	95.03	111.13
1	C	189[B]	THR	CB-CA-C	-10.00	95.03	111.13
1	C	254[A]	THR	CA-C-O	9.40	133.96	120.51
1	C	254[B]	THR	CA-C-O	9.40	133.96	120.51
1	C	190[A]	GLY	CA-C-N	8.68	130.69	119.84
1	C	190[A]	GLY	C-N-CA	8.68	130.69	119.84
1	C	190[B]	GLY	CA-C-N	8.68	130.69	119.84
1	C	190[B]	GLY	C-N-CA	8.68	130.69	119.84
1	C	254[A]	THR	N-CA-C	8.64	129.20	110.80
1	C	254[B]	THR	N-CA-C	8.64	129.20	110.80
1	D	189[A]	THR	CB-CA-C	8.11	124.54	114.40
1	D	189[B]	THR	CB-CA-C	8.11	124.54	114.40
1	C	189[A]	THR	N-CA-C	8.02	122.84	112.26
1	C	189[B]	THR	N-CA-C	8.02	122.84	112.26
1	C	190[A]	GLY	O-C-N	7.68	129.45	121.77
1	C	190[B]	GLY	O-C-N	7.68	129.45	121.77
1	C	254[A]	THR	CA-C-N	-6.16	111.68	122.09
1	C	254[A]	THR	C-N-CA	-6.16	111.68	122.09
1	C	254[B]	THR	CA-C-N	-6.16	111.68	122.09
1	C	254[B]	THR	C-N-CA	-6.16	111.68	122.09
1	B	144	ASP	N-CA-C	5.97	117.87	111.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	189[B]	THR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	190[B]	GLY	Mainchain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2969	0	3029	54	0
1	B	2937	0	3007	49	0
1	C	2929	0	2981	57	0
1	D	2922	0	2973	56	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	1	0
2	D	48	0	25	4	0
3	A	20	0	20	1	0
3	B	10	0	10	0	0
3	C	10	0	10	0	0
3	D	20	0	20	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	B	4	0	6	0	0
6	C	4	0	6	0	0
6	D	4	0	6	1	0
7	A	376	0	0	8	0
7	B	401	0	0	15	0
7	C	411	0	0	7	0
7	D	392	0	0	12	0
All	All	13649	0	12168	203	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 8.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34[B]:ILE:HD11	1:A:71[B]:VAL:CG2	1.26	1.58
1:C:254[B]:THR:CA	1:C:254[B]:THR:C	1.75	1.56
1:C:189[A]:THR:C	1:C:189[A]:THR:CA	1.83	1.52
1:C:255[A]:GLY:N	1:C:255[A]:GLY:CA	1.68	1.51
1:D:190[A]:GLY:N	1:D:190[A]:GLY:CA	1.88	1.36
1:D:189[A]:THR:CA	1:D:189[A]:THR:CB	2.05	1.34
1:A:34[B]:ILE:CD1	1:A:71[B]:VAL:CG2	2.16	1.22
1:D:189[A]:THR:CA	1:D:189[A]:THR:N	2.07	1.17
1:D:267:LEU:HD21	7:D:2256:HOH:O	1.45	1.13
1:A:34[B]:ILE:HD11	1:A:71[B]:VAL:HG21	1.28	1.08
1:A:34[B]:ILE:HD11	1:A:71[B]:VAL:HG23	1.29	1.07
1:A:34[B]:ILE:HD11	1:A:71[B]:VAL:HG22	1.37	1.02
1:C:254[B]:THR:C	1:C:254[B]:THR:CB	2.32	1.02
1:B:189[A]:THR:O	7:B:2232:HOH:O	1.78	1.01
1:C:254[B]:THR:C	1:C:254[B]:THR:N	2.18	1.00
1:C:254[B]:THR:O	7:C:2294:HOH:O	1.79	1.00
1:C:117:ILE:HD12	7:C:2152:HOH:O	1.63	0.98
1:D:189[A]:THR:CB	1:D:189[A]:THR:C	2.37	0.96
1:A:95[A]:ILE:CD1	1:A:95[A]:ILE:CG1	2.44	0.94
1:A:180:ASN:HD21	1:B:314:GLN:HE22	1.17	0.93
1:D:254[A]:THR:O	7:D:2279:HOH:O	1.86	0.92
1:A:148:LEU:HD11	1:A:334:LEU:HB3	1.51	0.92
1:C:254[B]:THR:C	1:C:254[B]:THR:OG1	2.12	0.92
1:A:211:ASN:HD22	1:A:212:ARG:H	1.18	0.91
1:C:190[B]:GLY:O	1:C:191[B]:PRO:C	2.05	0.91
1:A:34[B]:ILE:CD1	1:A:71[B]:VAL:HG23	1.91	0.90
1:C:211:ASN:HD22	1:C:212:ARG:H	1.17	0.89
1:A:314:GLN:HE22	1:B:180:ASN:HD21	1.15	0.87
1:A:183:LYS:HE3	7:A:2240:HOH:O	1.73	0.87
1:C:314:GLN:HE22	1:D:180:ASN:HD21	1.18	0.85
1:B:45:ILE:HD11	1:B:117:ILE:HG13	1.57	0.85
1:C:254[A]:THR:C	1:C:255[A]:GLY:CA	2.50	0.84
1:C:189[A]:THR:C	1:C:189[A]:THR:CB	2.51	0.84
1:C:148:LEU:HD11	1:C:334:LEU:HB3	1.59	0.83
1:D:240:LEU:HB3	7:D:2256:HOH:O	1.80	0.82
1:D:45[A]:ILE:HD11	1:D:117:ILE:HG13	1.61	0.81
1:C:180:ASN:HD21	1:D:314:GLN:HE22	1.30	0.80
1:C:254[B]:THR:C	1:C:254[B]:THR:HG1	1.87	0.79
1:A:34[B]:ILE:CD1	1:A:71[B]:VAL:HG22	2.02	0.79
1:A:254[A]:THR:O	7:A:2251:HOH:O	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254[B]:THR:CA	1:C:255[B]:GLY:N	2.45	0.79
1:D:211[A]:ASN:HD21	2:D:1368:NAP:H1B	1.47	0.79
1:A:95[A]:ILE:CD1	1:A:95[A]:ILE:CB	2.61	0.78
1:D:148:LEU:HD11	1:D:334:LEU:HB3	1.65	0.77
1:B:128:TRP:CH2	7:B:2107:HOH:O	2.38	0.77
1:B:254[A]:THR:O	7:B:2296:HOH:O	2.02	0.77
1:C:183:LYS:HE3	7:C:2286:HOH:O	1.86	0.76
1:C:176:ASP:HB3	1:D:133[B]:LYS:HD2	1.67	0.76
1:D:45[A]:ILE:HG12	1:D:50:LEU:HD12	1.68	0.75
1:D:189[A]:THR:C	1:D:190[A]:GLY:CA	2.59	0.75
1:A:97:ARG:NH1	1:C:175:ASP:OD1	2.22	0.73
1:A:175:ASP:OD1	1:C:97[B]:ARG:NH1	2.22	0.73
1:A:211:ASN:HD22	1:A:212:ARG:N	1.89	0.71
1:D:189[A]:THR:C	1:D:189[A]:THR:HB	2.15	0.71
1:C:1:MET:HE3	1:C:20:GLU:HG2	1.71	0.70
1:C:211:ASN:HD22	1:C:212:ARG:N	1.90	0.70
1:D:100[A]:LEU:HD23	7:D:2038:HOH:O	1.92	0.70
1:B:1:MET:CE	1:B:23:LEU:CD1	2.70	0.69
1:A:326[A]:LEU:HD13	7:B:2400:HOH:O	1.92	0.69
1:D:189[A]:THR:CB	1:D:189[A]:THR:N	2.55	0.69
1:D:189[A]:THR:HB	1:D:189[A]:THR:O	1.92	0.69
1:A:15:VAL:HG21	1:A:347:LEU:HD23	1.74	0.68
1:D:237:TYR:HB3	7:D:2256:HOH:O	1.94	0.66
1:D:189[A]:THR:HG1	2:D:1368:NAP:HO3A	1.44	0.66
1:A:96:CYS:O	1:A:100[B]:LEU:HD13	1.97	0.65
1:C:270[B]:ARG:NH1	7:C:2308:HOH:O	2.30	0.64
1:B:140:LYS:HG3	7:B:2193:HOH:O	1.98	0.64
1:C:4:ILE:HG12	1:C:15:VAL:HG22	1.80	0.64
1:C:164:GLU:HA	1:C:167:LYS:HE2	1.80	0.64
1:B:19:ASP:HB3	1:B:22:LYS:HE2	1.79	0.63
1:A:100[A]:LEU:HD23	7:A:2037:HOH:O	1.98	0.63
1:B:1:MET:HE1	1:B:23:LEU:CD1	2.27	0.63
1:C:148:LEU:CD1	1:C:334:LEU:HB3	2.29	0.63
1:B:1:MET:HE1	1:B:23:LEU:HD13	1.81	0.63
1:D:188[A]:GLY:C	1:D:189[A]:THR:CA	2.72	0.63
1:D:337:LYS:HG2	1:D:361:ILE:HD13	1.80	0.62
1:D:354:LYS:HB2	1:D:354:LYS:NZ	2.14	0.62
1:B:1:MET:HE2	1:B:23:LEU:CD1	2.31	0.61
1:A:232:ASN:C	1:A:232:ASN:HD22	2.09	0.61
1:A:188[A]:GLY:HA3	1:A:254[A]:THR:HG22	1.82	0.61
1:C:189[A]:THR:HG22	1:C:209[A]:MET:HE2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:CD1	1:A:334:LEU:HB3	2.28	0.60
1:A:173:THR:O	1:C:97[A]:ARG:NH1	2.26	0.59
1:D:36:ASN:ND2	1:D:365:TRP:HE1	2.00	0.59
1:A:209[A]:MET:CE	1:A:223:ILE:HG13	2.33	0.59
1:A:34[B]:ILE:CG1	1:A:71[B]:VAL:HG23	2.31	0.58
1:A:366:GLU:HB2	7:A:2320:HOH:O	2.04	0.58
1:B:68:ALA:HB3	7:B:2107:HOH:O	2.03	0.58
1:D:45[A]:ILE:CD1	1:D:117:ILE:HG13	2.34	0.58
1:C:189[A]:THR:CA	1:C:190[A]:GLY:N	2.60	0.58
1:C:118:HIS:NE2	1:C:119:LYS:HE2	2.19	0.58
1:A:1:MET:HE3	1:A:20[A]:GLU:HG2	1.84	0.58
1:D:189[B]:THR:CG2	1:D:209[B]:MET:HE2	2.34	0.57
1:B:68:ALA:CB	7:B:2107:HOH:O	2.52	0.57
1:A:303[B]:ILE:HG12	1:C:301[B]:THR:HG22	1.85	0.57
1:A:95[B]:ILE:CG1	1:A:95[B]:ILE:CG2	2.82	0.57
1:D:148:LEU:HD13	1:D:334:LEU:HD13	1.87	0.56
3:A:1368[A]:XYS:H52	7:A:2358:HOH:O	2.06	0.56
1:B:148[A]:LEU:HD11	1:B:334:LEU:HB3	1.88	0.56
1:B:1:MET:HE2	1:B:23:LEU:HD11	1.88	0.55
1:B:36:ASN:ND2	1:B:365:TRP:HE1	2.05	0.55
1:B:148[A]:LEU:HD13	1:B:334:LEU:HD13	1.89	0.54
1:C:254[B]:THR:C	1:C:254[B]:THR:H	2.09	0.54
1:B:87:PRO:HG3	7:B:2107:HOH:O	2.07	0.54
1:D:45[A]:ILE:CG1	1:D:50:LEU:HD12	2.38	0.54
1:B:123:PHE:HB3	7:B:2107:HOH:O	2.07	0.54
1:C:1:MET:HE2	1:C:127[B]:TRP:CE2	2.43	0.53
1:C:148:LEU:HD13	1:C:334:LEU:HD13	1.89	0.53
1:C:15:VAL:HG21	1:C:347:LEU:HD23	1.89	0.53
1:B:1:MET:HE3	1:B:125:ARG:HB2	1.90	0.53
1:D:36:ASN:HD22	1:D:365:TRP:HE1	1.54	0.53
2:D:1368:NAP:H2A	7:D:2253:HOH:O	2.09	0.53
1:A:164[A]:GLU:HA	1:A:167:LYS:HE2	1.90	0.53
1:A:298:THR:CB	1:A:300[B]:LYS:HZ3	2.22	0.53
1:D:189[B]:THR:HG22	1:D:209[B]:MET:HE2	1.90	0.53
1:A:206:GLU:HG2	7:A:2187:HOH:O	2.09	0.53
1:C:257:ASP:O	1:C:260[A]:ILE:HG22	2.08	0.52
1:A:95[B]:ILE:CG1	1:A:95[B]:ILE:CD1	2.88	0.52
1:A:273:VAL:HG22	1:A:301[B]:THR:CG2	2.39	0.52
1:C:189[B]:THR:O	2:C:1368:NAP:H4B	2.09	0.52
1:D:148:LEU:CD1	1:D:334:LEU:HB3	2.39	0.52
1:B:45:ILE:HG12	1:B:50:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189[A]:THR:OG1	2:D:1368:NAP:O3B	2.19	0.51
1:B:206:GLU:HG2	7:B:2235:HOH:O	2.10	0.51
1:C:1:MET:HG2	1:C:126:GLU:HB2	1.92	0.51
1:D:189[A]:THR:CA	1:D:189[A]:THR:CG2	2.87	0.51
1:D:273:VAL:HG22	1:D:301[B]:THR:CG2	2.41	0.50
1:A:232:ASN:HD22	1:A:234:SER:H	1.60	0.50
1:D:261:LEU:O	1:D:265:ILE:HG13	2.12	0.50
1:B:288:ASP:HA	1:D:284:SER:HA	1.93	0.49
1:A:159:ILE:HD12	1:A:199:LEU:HD23	1.93	0.49
1:A:257:ASP:O	1:A:260:ILE:HG22	2.12	0.49
1:B:337:LYS:HG2	1:B:361:ILE:HD12	1.95	0.49
1:A:108:GLU:C	1:C:270[B]:ARG:HE	2.20	0.49
1:A:190[A]:GLY:HA2	7:A:2204:HOH:O	2.12	0.49
1:C:1:MET:CG	1:C:126:GLU:HB2	2.43	0.49
1:B:284:SER:HA	1:D:288:ASP:HA	1.94	0.49
1:B:45:ILE:CD1	1:B:117:ILE:HG13	2.35	0.49
1:A:209[A]:MET:HE3	1:A:223:ILE:HG13	1.93	0.49
1:C:189[A]:THR:C	1:C:189[A]:THR:HB	2.37	0.49
1:C:118:HIS:CD2	1:C:119:LYS:HE2	2.48	0.48
1:C:211:ASN:ND2	1:C:212:ARG:H	1.99	0.48
1:D:315[A]:GLN:NE2	7:D:2321:HOH:O	2.45	0.48
1:B:337:LYS:HG2	1:B:361:ILE:CD1	2.44	0.48
1:A:95[A]:ILE:CD1	1:A:95[A]:ILE:HB	2.42	0.47
1:B:318:VAL:HG22	7:B:2400:HOH:O	2.13	0.47
1:D:354:LYS:HB2	1:D:354:LYS:HZ2	1.80	0.47
1:B:188[A]:GLY:HA3	1:B:254[A]:THR:HG22	1.97	0.47
1:C:206:GLU:HG2	7:C:2224:HOH:O	2.14	0.47
1:C:127[A]:TRP:HZ3	1:C:129:TYR:CE2	2.33	0.47
1:A:332:LYS:HG3	7:A:2307:HOH:O	2.13	0.47
1:B:218:VAL:HG22	1:B:333:MET:HE2	1.96	0.47
1:C:27:GLY:O	1:C:129:TYR:HB3	2.14	0.47
1:D:24:ASP:HB2	1:D:121:ASP:HB2	1.97	0.47
1:A:232:ASN:ND2	1:A:234:SER:H	2.13	0.47
1:B:36:ASN:HD22	1:B:365:TRP:HE1	1.62	0.47
1:B:15:VAL:HG21	1:B:347:LEU:HD23	1.97	0.46
1:A:191[A]:PRO:HD3	1:A:359:ILE:HA	1.96	0.46
1:B:257:ASP:O	1:B:260:ILE:HG22	2.16	0.46
1:C:257:ASP:O	1:C:260[B]:ILE:HG23	2.15	0.46
1:A:27:GLY:O	1:A:129:TYR:HB3	2.16	0.46
1:A:180:ASN:ND2	1:B:314:GLN:HE22	1.99	0.46
1:A:310:LYS:N	1:A:311:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:CE	1:B:125:ARG:HB2	2.46	0.45
1:C:190[B]:GLY:H	1:C:194:VAL:HG23	1.82	0.45
1:D:1:MET:HE2	1:D:127:TRP:CE2	2.51	0.45
1:D:189[B]:THR:O	1:D:190[B]:GLY:O	2.35	0.45
1:D:190[A]:GLY:N	1:D:190[A]:GLY:C	2.69	0.45
1:C:315[B]:GLN:HG3	7:C:2339:HOH:O	2.17	0.44
1:B:101:VAL:HA	1:C:97[A]:ARG:HE	1.81	0.44
1:B:59[B]:LYS:NZ	7:B:2098:HOH:O	2.50	0.44
1:D:206:GLU:HG2	7:D:2218:HOH:O	2.18	0.44
1:D:133[B]:LYS:HG2	7:D:2049:HOH:O	2.18	0.44
1:B:273:VAL:HG22	1:B:301[B]:THR:CG2	2.48	0.43
1:B:69[A]:ILE:HD11	1:B:147:ILE:N	2.34	0.43
1:B:117:ILE:HD13	7:B:2163:HOH:O	2.18	0.43
1:B:148[A]:LEU:CD1	1:B:334:LEU:HB3	2.48	0.43
1:B:128:TRP:CZ2	7:B:2107:HOH:O	2.69	0.42
1:D:354:LYS:HB2	1:D:354:LYS:HZ3	1.84	0.42
1:C:1:MET:HB2	1:C:20:GLU:HG3	2.01	0.42
1:A:100[B]:LEU:HD23	1:D:100[B]:LEU:HD11	2.01	0.42
1:D:189[A]:THR:O	1:D:190[A]:GLY:CA	2.68	0.42
1:A:5[A]:ILE:HD11	1:A:16:LYS:HD3	2.02	0.42
1:B:337:LYS:CG	1:B:361:ILE:HD12	2.50	0.42
1:D:354:LYS:NZ	1:D:354:LYS:CB	2.80	0.41
1:D:19:ASP:HB3	1:D:22:LYS:HE2	2.03	0.41
1:D:355:GLU:HG3	7:D:2368:HOH:O	2.19	0.41
1:B:45:ILE:CG1	1:B:50:LEU:HD12	2.50	0.41
1:D:140:LYS:HD2	6:D:1367:EDO:O1	2.20	0.41
1:B:164:GLU:HG3	7:B:2207:HOH:O	2.19	0.41
1:C:255[B]:GLY:HA2	7:C:2294:HOH:O	2.21	0.41
1:D:218:VAL:HG23	7:D:2231:HOH:O	2.20	0.41
1:D:315[A]:GLN:NE2	7:D:2322:HOH:O	2.53	0.41
1:B:164:GLU:HA	1:B:167:LYS:HE3	2.02	0.41
1:A:241:LYS:HE3	1:A:246:LYS:HE2	2.02	0.41
1:B:31:ILE:HD11	1:B:135:LEU:HD11	2.02	0.41
1:C:223:ILE:HG23	1:C:228:THR:O	2.20	0.41
1:C:1:MET:HE2	1:C:127[A]:TRP:CE2	2.56	0.41
1:C:19:ASP:HB3	1:C:22:LYS:NZ	2.36	0.41
1:C:91:ARG:HG3	1:C:120:MET:SD	2.62	0.40
1:D:15:VAL:HG21	1:D:347:LEU:HD23	2.04	0.40
1:A:232:ASN:C	1:A:232:ASN:ND2	2.79	0.40
1:B:1:MET:CE	1:B:23:LEU:HD13	2.46	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/366 (106%)	380 (98%)	8 (2%)	1 (0%)	36	17
1	B	381/366 (104%)	371 (97%)	9 (2%)	1 (0%)	36	17
1	C	377/366 (103%)	364 (97%)	12 (3%)	1 (0%)	36	17
1	D	377/366 (103%)	368 (98%)	8 (2%)	1 (0%)	36	17
All	All	1524/1464 (104%)	1483 (97%)	37 (2%)	4 (0%)	36	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	B	307	ASN
1	C	307	ASN
1	D	307	ASN

### 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	A	339/317 (107%)	333 (98%)	6 (2%)	51	24
1	B	331/317 (104%)	328 (99%)	3 (1%)	70	49
1	C	327/317 (103%)	323 (99%)	4 (1%)	63	38
1	D	327/317 (103%)	317 (97%)	10 (3%)	35	9
All	All	1324/1268 (104%)	1301 (98%)	23 (2%)	55	26

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	73	GLU
1	A	232	ASN
1	A	287	LEU
1	A	293[A]	GLN
1	A	293[B]	GLN
1	B	117	ILE
1	B	133	LYS
1	B	287	LEU
1	C	73	GLU
1	C	239	LYS
1	C	254[A]	THR
1	C	254[B]	THR
1	D	34	ILE
1	D	59	LYS
1	D	140	LYS
1	D	211[A]	ASN
1	D	211[B]	ASN
1	D	287	LEU
1	D	293	GLN
1	D	354	LYS
1	D	361	ILE
1	D	362	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	180	ASN
1	A	211	ASN
1	A	232	ASN
1	A	299	ASN
1	B	36	ASN
1	B	81	GLN
1	B	180	ASN
1	B	263	ASN
1	B	293	GLN
1	C	10	ASN
1	C	180	ASN
1	C	211	ASN
1	D	36	ASN

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Mol	Chain	Res	Type
1	D	77	HIS
1	D	81	GLN
1	D	180	ASN
1	D	263	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 for Mogul analysis.

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	XYP	D	1370[B]	-	10,10,10	1.12	1 (10%)	14,14,14	0.77	0
2	NAP	B	1368	-	50,52,52	1.51	6 (12%)	71,80,80	1.62	13 (18%)
3	XYS	A	1368[A]	-	10,10,10	1.06	1 (10%)	14,14,14	0.88	0
3	XYS	C	1370	-	10,10,10	1.04	1 (10%)	14,14,14	1.03	1 (7%)
6	EDO	C	1367	-	3,3,3	0.55	0	2,2,2	0.15	0
6	EDO	D	1367	-	3,3,3	0.58	0	2,2,2	0.06	0
2	NAP	C	1368	-	50,52,52	1.53	7 (14%)	71,80,80	1.56	9 (12%)
4	XYP	B	1369	-	10,10,10	1.05	1 (10%)	14,14,14	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	XYS	D	1369[A]	-	10,10,10	1.10	1 (10%)	14,14,14	0.79	0
4	XYP	C	1369	-	10,10,10	1.05	0	14,14,14	0.61	0
3	XYS	B	1370	-	10,10,10	1.15	1 (10%)	14,14,14	0.83	0
4	XYP	A	1369[B]	-	10,10,10	1.14	1 (10%)	14,14,14	0.89	0
3	XYS	D	1371	-	10,10,10	0.87	1 (10%)	14,14,14	0.89	0
6	EDO	B	1367	-	3,3,3	0.58	0	2,2,2	0.17	0
3	XYS	A	1370	-	10,10,10	0.77	0	14,14,14	1.08	1 (7%)
2	NAP	A	1367	-	50,52,52	1.72	9 (18%)	71,80,80	1.63	13 (18%)
2	NAP	D	1368	-	50,52,52	1.61	9 (18%)	71,80,80	1.64	12 (16%)

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	XYP	D	1370[B]	-	-	-	0/1/1/1
2	NAP	B	1368	-	-	8/35/67/67	0/5/5/5
3	XYS	A	1368[A]	-	-	-	0/1/1/1
3	XYS	C	1370	-	-	-	0/1/1/1
6	EDO	C	1367	-	-	0/1/1/1	-
6	EDO	D	1367	-	-	0/1/1/1	-
2	NAP	C	1368	-	-	6/35/67/67	0/5/5/5
4	XYP	B	1369	-	-	-	0/1/1/1
3	XYS	D	1369[A]	-	-	-	0/1/1/1
4	XYP	C	1369	-	-	-	0/1/1/1
3	XYS	B	1370	-	-	-	0/1/1/1
4	XYP	A	1369[B]	-	-	-	0/1/1/1
6	EDO	B	1367	-	-	0/1/1/1	-
3	XYS	D	1371	-	-	-	0/1/1/1
3	XYS	A	1370	-	-	-	0/1/1/1
2	NAP	A	1367	-	-	8/35/67/67	0/5/5/5
2	NAP	D	1368	-	-	9/35/67/67	0/5/5/5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1367	NAP	PN-O3	6.73	1.66	1.59
2	A	1367	NAP	C2N-N1N	5.12	1.40	1.35
2	D	1368	NAP	C2N-N1N	5.11	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1368	NAP	C2N-N1N	5.00	1.40	1.35
2	C	1368	NAP	C2N-N1N	4.77	1.40	1.35
2	D	1368	NAP	O4D-C1D	4.26	1.46	1.40
2	C	1368	NAP	P2B-O1X	4.25	1.63	1.50
2	B	1368	NAP	PN-O3	4.17	1.64	1.59
2	C	1368	NAP	PN-O3	4.03	1.63	1.59
2	B	1368	NAP	P2B-O1X	3.92	1.62	1.50
2	D	1368	NAP	PA-O3	3.76	1.63	1.59
2	C	1368	NAP	O4D-C1D	3.63	1.45	1.40
2	D	1368	NAP	PN-O3	3.42	1.63	1.59
2	D	1368	NAP	P2B-O1X	3.30	1.60	1.50
2	A	1367	NAP	P2B-O1X	3.10	1.60	1.50
2	B	1368	NAP	C5A-N7A	-2.95	1.33	1.39
2	B	1368	NAP	C6N-N1N	2.90	1.41	1.35
3	D	1369[A]	XYS	O5-C5	2.85	1.48	1.43
4	D	1370[B]	XYP	O5-C5	2.85	1.48	1.43
2	A	1367	NAP	PA-O3	2.80	1.62	1.59
2	C	1368	NAP	C5A-N7A	-2.75	1.34	1.39
2	A	1367	NAP	O4D-C1D	2.68	1.44	1.40
2	A	1367	NAP	C5A-N7A	-2.64	1.34	1.39
2	D	1368	NAP	C4A-N9A	-2.52	1.32	1.37
2	D	1368	NAP	C5A-N7A	-2.50	1.34	1.39
3	C	1370	XYS	O5-C1	2.44	1.47	1.43
2	D	1368	NAP	C6N-N1N	2.41	1.40	1.35
3	A	1368[A]	XYS	O5-C5	2.38	1.47	1.43
4	A	1369[B]	XYP	O5-C5	2.38	1.47	1.43
2	C	1368	NAP	P2B-O2X	2.35	1.63	1.54
2	C	1368	NAP	C6N-N1N	2.32	1.40	1.35
2	A	1367	NAP	C4A-N9A	-2.25	1.33	1.37
2	A	1367	NAP	C6N-N1N	2.20	1.40	1.35
3	D	1371	XYS	O5-C1	2.18	1.46	1.43
4	B	1369	XYP	O5-C5	2.17	1.47	1.43
2	A	1367	NAP	P2B-O2X	2.10	1.62	1.54
2	B	1368	NAP	PA-O3	2.06	1.61	1.59
2	D	1368	NAP	C3N-C7N	2.04	1.53	1.50
3	B	1370	XYS	O5-C1	2.04	1.46	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1367	NAP	N3A-C2A-N1A	-5.70	119.96	128.58
2	B	1368	NAP	N3A-C2A-N1A	-5.14	120.80	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1368	NAP	C5A-C4A-N3A	-4.95	119.90	126.72
2	B	1368	NAP	C5A-C4A-N3A	-4.75	120.17	126.72
2	D	1368	NAP	N3A-C2A-N1A	-4.70	121.47	128.58
2	C	1368	NAP	N3A-C2A-N1A	-4.63	121.57	128.58
2	D	1368	NAP	C5A-C4A-N3A	-4.44	120.61	126.72
2	A	1367	NAP	C5A-C4A-N3A	-4.35	120.73	126.72
2	D	1368	NAP	N9A-C8A-N7A	-3.84	108.50	113.94
2	A	1367	NAP	N9A-C8A-N7A	-3.64	108.78	113.94
2	A	1367	NAP	C2A-N3A-C4A	3.63	120.70	111.83
2	D	1368	NAP	C4A-N9A-C8A	3.63	109.55	105.74
2	B	1368	NAP	C2A-N3A-C4A	3.55	120.51	111.83
2	B	1368	NAP	N9A-C8A-N7A	-3.47	109.01	113.94
2	C	1368	NAP	C2A-N3A-C4A	3.43	120.22	111.83
2	C	1368	NAP	N9A-C8A-N7A	-3.35	109.19	113.94
2	D	1368	NAP	N3A-C4A-N9A	3.35	132.86	127.17
2	B	1368	NAP	N3A-C4A-N9A	3.34	132.85	127.17
2	D	1368	NAP	C2A-N3A-C4A	3.15	119.53	111.83
2	C	1368	NAP	C4A-C5A-N7A	-3.14	106.99	110.58
3	C	1370	XYS	C5-O5-C1	3.11	118.93	112.46
3	A	1370	XYS	C5-O5-C1	3.05	118.79	112.46
2	D	1368	NAP	C4D-O4D-C1D	-2.98	107.19	109.92
2	A	1367	NAP	N3A-C4A-N9A	2.95	132.19	127.17
2	C	1368	NAP	C5A-N7A-C8A	2.93	108.05	103.45
2	B	1368	NAP	C5A-N7A-C8A	2.91	108.02	103.45
2	C	1368	NAP	N3A-C4A-N9A	2.83	131.97	127.17
2	A	1367	NAP	C5A-N7A-C8A	2.81	107.86	103.45
2	C	1368	NAP	O3-PA-O1A	-2.80	102.27	110.70
2	A	1367	NAP	C4A-N9A-C8A	2.80	108.68	105.74
2	D	1368	NAP	C5A-N7A-C8A	2.70	107.69	103.45
2	B	1368	NAP	O2A-PA-O3	2.64	114.40	107.27
2	D	1368	NAP	C3N-C7N-N7N	-2.61	114.53	117.74
2	B	1368	NAP	C4A-C5A-N7A	-2.60	107.61	110.58
2	A	1367	NAP	C4A-C5A-N7A	-2.59	107.61	110.58
2	B	1368	NAP	C4A-N9A-C8A	2.52	108.38	105.74
2	D	1368	NAP	C4A-C5A-N7A	-2.49	107.73	110.58
2	A	1367	NAP	O3-PA-O1A	-2.47	103.28	110.70
2	A	1367	NAP	O3X-P2B-O2X	2.41	116.85	107.80
2	D	1368	NAP	O3-PA-O1A	-2.35	103.63	110.70
2	A	1367	NAP	C2A-N1A-C6A	2.30	122.51	118.73
2	B	1368	NAP	C3N-C7N-N7N	-2.28	114.92	117.74
2	B	1368	NAP	C2N-C3N-C4N	2.25	120.87	118.26
2	A	1367	NAP	C4D-O4D-C1D	-2.22	107.89	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1368	NAP	O3-PA-O1A	-2.21	104.04	110.70
2	C	1368	NAP	C5A-C4A-N9A	2.12	108.12	105.81
2	A	1367	NAP	O2N-PN-O1N	2.10	122.22	112.44
2	D	1368	NAP	C4A-N9A-C1B	-2.03	121.88	126.63
2	B	1368	NAP	O2N-PN-O1N	2.00	121.76	112.44

There are no chirality outliers.

All (31) torsion outliers are listed below:

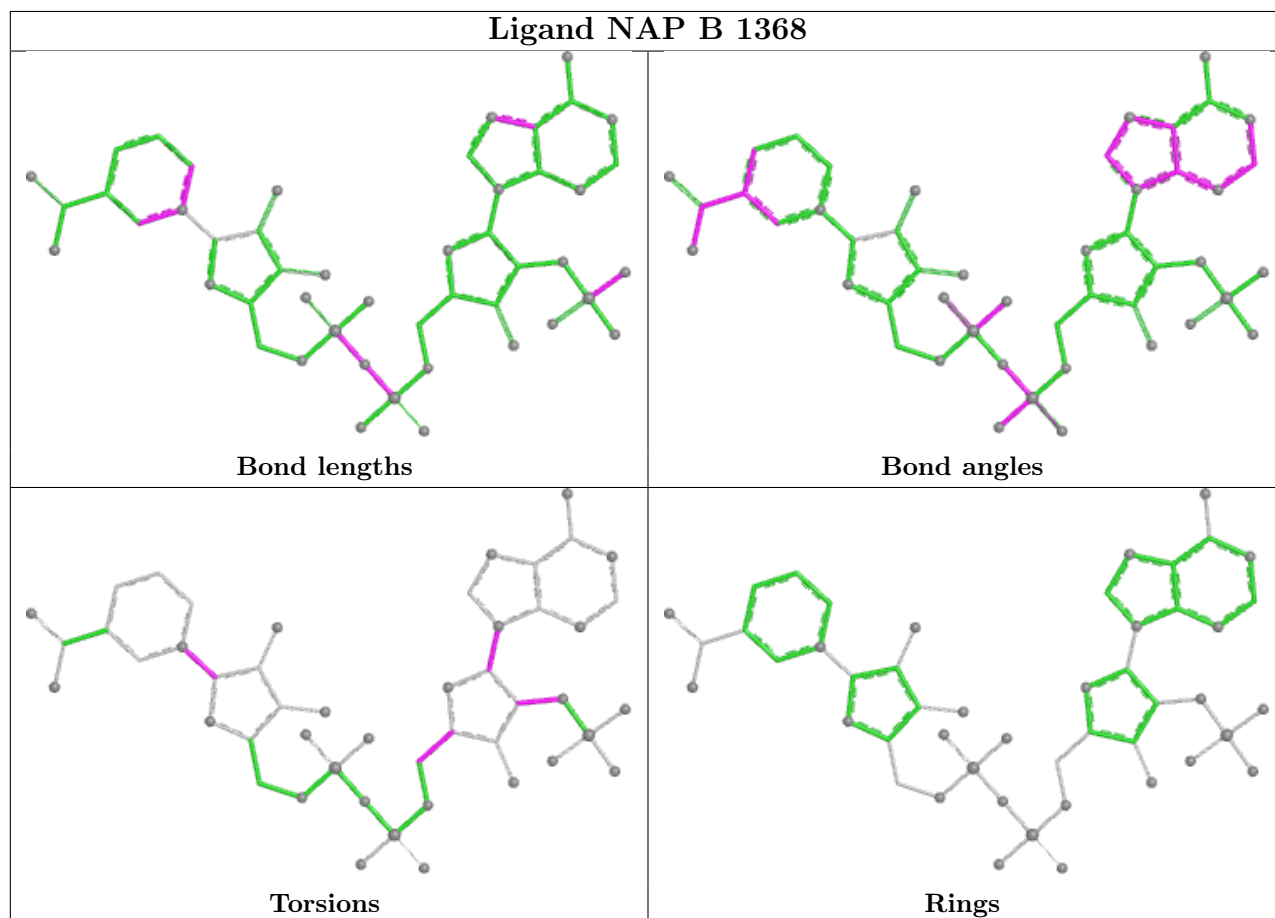
Mol	Chain	Res	Type	Atoms
2	A	1367	NAP	O4D-C1D-N1N-C2N
2	A	1367	NAP	O4D-C1D-N1N-C6N
2	A	1367	NAP	C2D-C1D-N1N-C2N
2	A	1367	NAP	C2D-C1D-N1N-C6N
2	B	1368	NAP	O4D-C1D-N1N-C2N
2	B	1368	NAP	O4D-C1D-N1N-C6N
2	B	1368	NAP	C2D-C1D-N1N-C2N
2	B	1368	NAP	C2D-C1D-N1N-C6N
2	C	1368	NAP	O4D-C1D-N1N-C2N
2	C	1368	NAP	O4D-C1D-N1N-C6N
2	C	1368	NAP	C2D-C1D-N1N-C2N
2	C	1368	NAP	C2D-C1D-N1N-C6N
2	D	1368	NAP	O4D-C1D-N1N-C2N
2	D	1368	NAP	O4D-C1D-N1N-C6N
2	D	1368	NAP	C2D-C1D-N1N-C2N
2	D	1368	NAP	C2D-C1D-N1N-C6N
2	A	1367	NAP	C3B-C2B-O2B-P2B
2	B	1368	NAP	C3B-C2B-O2B-P2B
2	C	1368	NAP	C3B-C2B-O2B-P2B
2	D	1368	NAP	C3B-C2B-O2B-P2B
2	A	1367	NAP	C1B-C2B-O2B-P2B
2	B	1368	NAP	C1B-C2B-O2B-P2B
2	C	1368	NAP	C1B-C2B-O2B-P2B
2	D	1368	NAP	C1B-C2B-O2B-P2B
2	D	1368	NAP	C2B-O2B-P2B-O1X
2	B	1368	NAP	O4B-C4B-C5B-O5B
2	B	1368	NAP	C2B-C1B-N9A-C8A
2	D	1368	NAP	C2B-O2B-P2B-O3X
2	A	1367	NAP	C2B-C1B-N9A-C8A
2	D	1368	NAP	C2B-C1B-N9A-C8A
2	A	1367	NAP	O4B-C4B-C5B-O5B

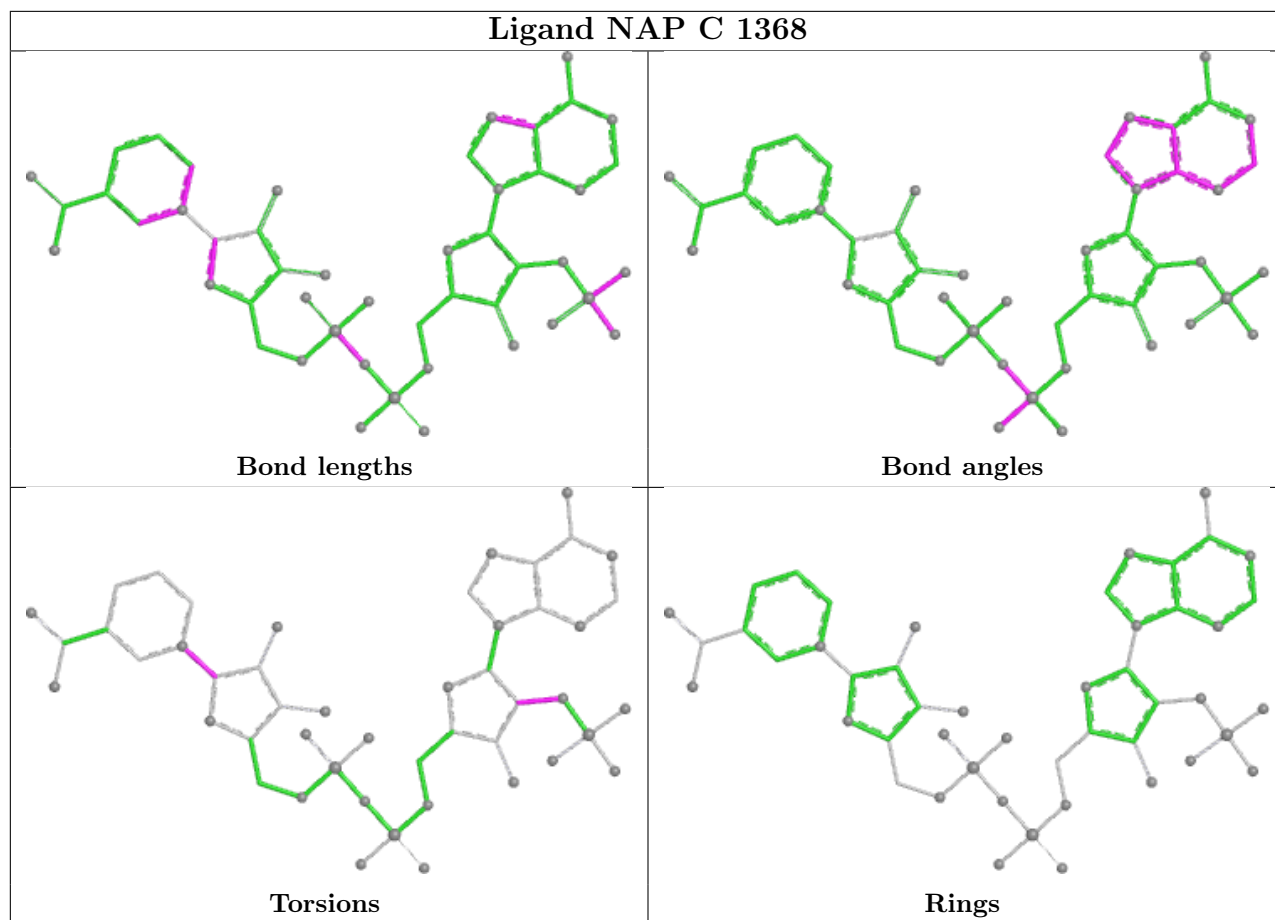
There are no ring outliers.

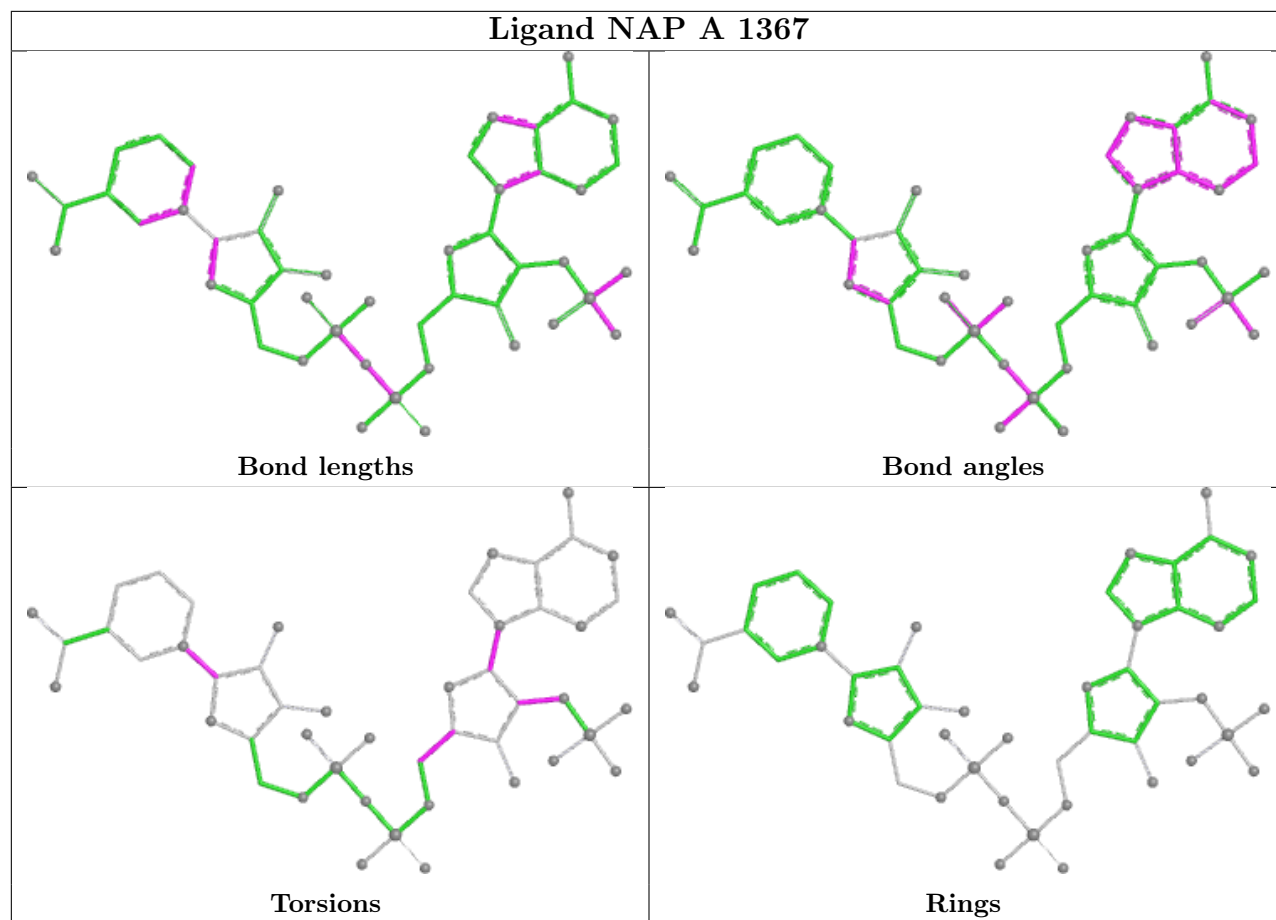
4 monomers are involved in 7 short contacts:

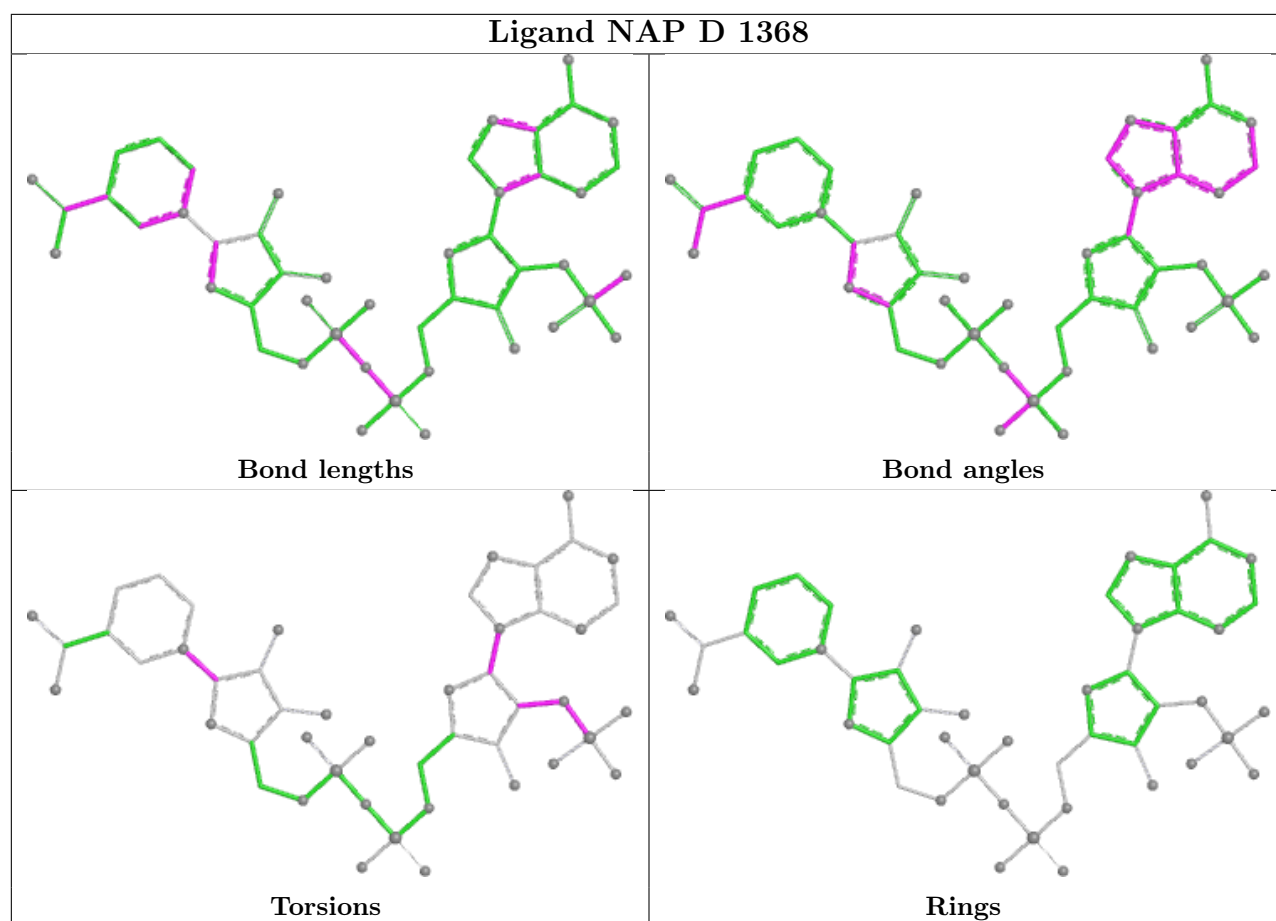
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1368[A]	XYS	1	0
6	D	1367	EDO	1	0
2	C	1368	NAP	1	0
2	D	1368	NAP	4	0

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 [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	190[A]:GLY	C	191[A]:PRO	N	1.67

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	359/366 (98%)	-0.88	3 (0%) 82   86	4, 13, 23, 31	36 (10%)
1	B	359/366 (98%)	-0.87	1 (0%) 90   91	4, 14, 25, 34	27 (7%)
1	C	359/366 (98%)	-0.96	0 100   100	4, 13, 25, 35	23 (6%)
1	D	359/366 (98%)	-0.91	1 (0%) 90   91	5, 13, 25, 33	22 (6%)
All	All	1436/1464 (98%)	-0.91	5 (0%) 90   91	4, 13, 25, 35	108 (7%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31[A]	ILE	2.5
1	A	76[A]	TYR	2.4
1	D	45[A]	ILE	2.1
1	A	95[A]	ILE	2.0
1	B	34[A]	ILE	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

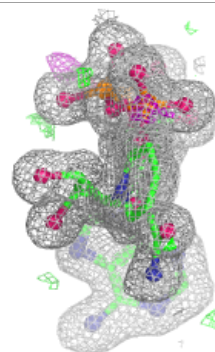
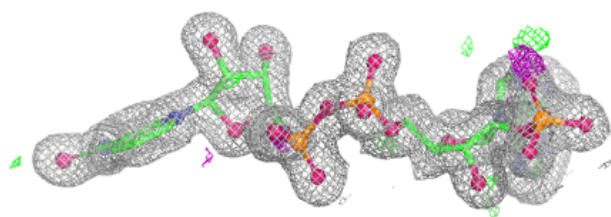
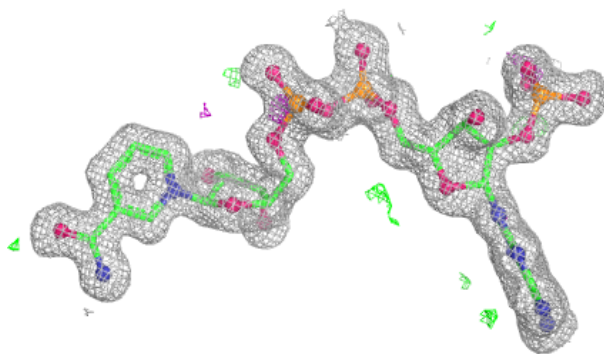
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	XYP	A	1369[B]	10/10	0.97	0.05	13,17,19,20	10
4	XYP	D	1370[B]	10/10	0.97	0.06	18,21,22,23	10
3	XYS	C	1370	10/10	0.98	0.04	16,19,20,23	0
3	XYS	D	1369[A]	10/10	0.98	0.05	18,21,22,23	10
3	XYS	D	1371	10/10	0.98	0.04	12,15,17,18	0
3	XYS	A	1370	10/10	0.98	0.04	15,17,19,20	0
4	XYP	B	1369	10/10	0.98	0.04	18,21,24,24	0
4	XYP	C	1369	10/10	0.98	0.05	16,19,20,22	0
3	XYS	B	1370	10/10	0.98	0.04	13,15,17,19	0
3	XYS	A	1368[A]	10/10	0.99	0.04	13,17,19,20	10
2	NAP	A	1367	48/48	0.99	0.03	10,13,16,17	0
2	NAP	B	1368	48/48	0.99	0.04	12,16,18,21	0
2	NAP	C	1368	48/48	0.99	0.03	9,13,17,17	0
2	NAP	D	1368	48/48	0.99	0.03	12,15,17,20	0
6	EDO	B	1367	4/4	0.99	0.03	16,17,18,18	0
6	EDO	C	1367	4/4	0.99	0.03	13,15,16,16	0
6	EDO	D	1367	4/4	0.99	0.03	17,18,19,20	0
5	ZN	B	1372	1/1	1.00	0.01	12,12,12,12	0
5	ZN	C	1371	1/1	1.00	0.01	10,10,10,10	1
5	ZN	C	1372	1/1	1.00	0.01	10,10,10,10	0
5	ZN	D	1372	1/1	1.00	0.01	11,11,11,11	1
5	ZN	D	1373	1/1	1.00	0.01	11,11,11,11	0
5	ZN	A	1371	1/1	1.00	0.01	10,10,10,10	1
5	ZN	A	1372	1/1	1.00	0.01	10,10,10,10	0
5	ZN	B	1371	1/1	1.00	0.02	10,10,10,10	1

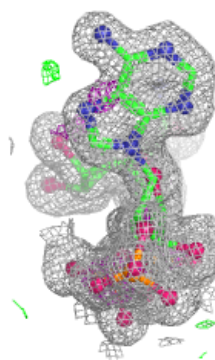
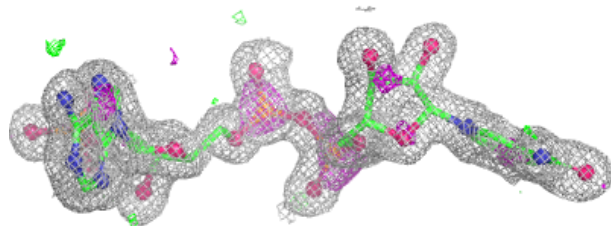
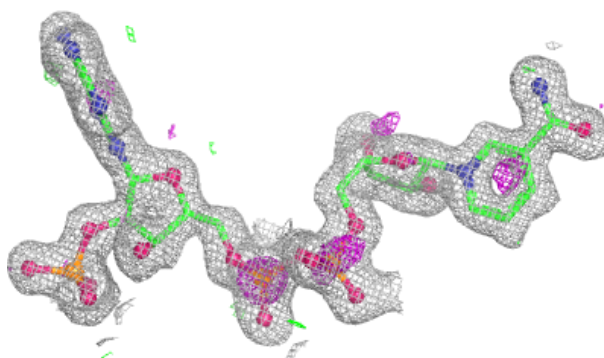
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP A 1367:**

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

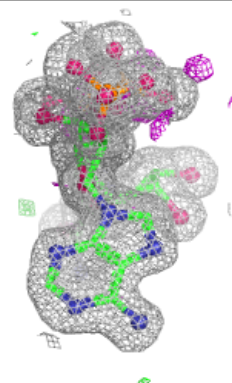
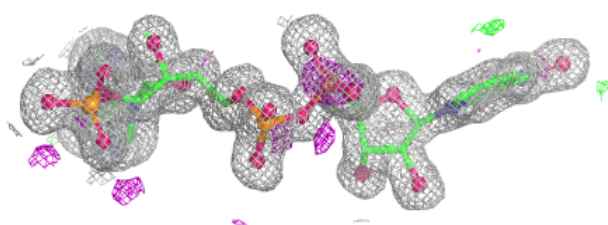
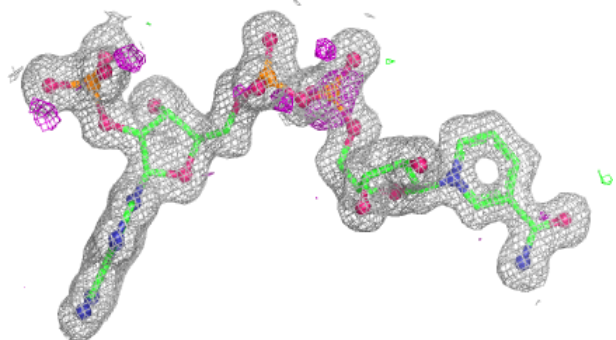
**Electron density around NAP B 1368:**

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

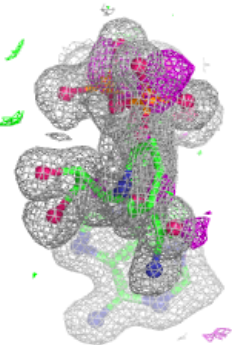
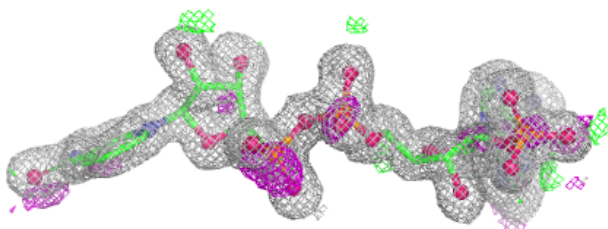
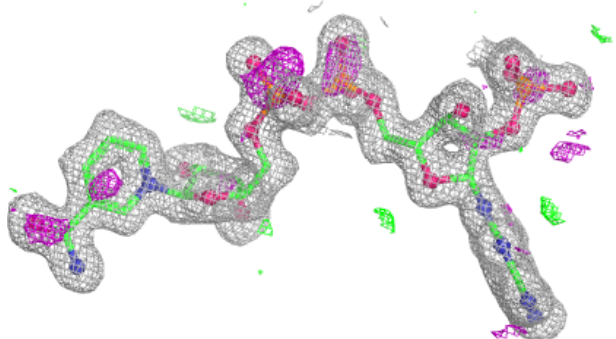


**Electron density around NAP C 1368:**

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

**Electron density around NAP D 1368:**

$2mF_o-DF_c$  (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.