



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2019 – 09:42 PM EDT

PDB ID : 1E7R  
Title : GDP 4-keto-6-deoxy-D-mannose epimerase reductase Y136E  
Authors : Rosano, C.; Izzo, G.; Bolognesi, M.  
Deposited on : 2000-09-07  
Resolution : 1.60 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

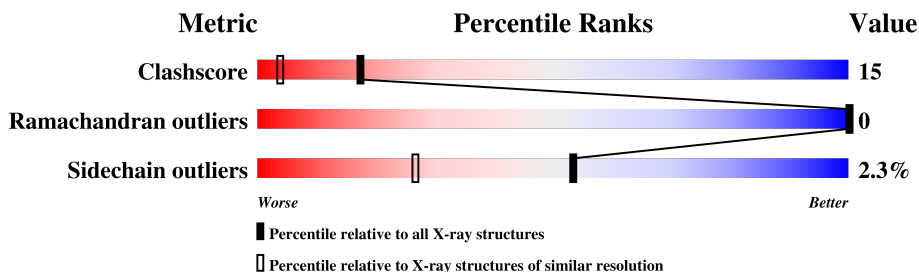
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	122126	3202 (1.60-1.60)
Ramachandran outliers	120053	3117 (1.60-1.60)
Sidechain outliers	120020	3116 (1.60-1.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	321	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UVW	A	1318	-	-	X	-
4	TRS	A	1319	-	X	-	-
4	TRS	A	1322	-	X	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2917 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.

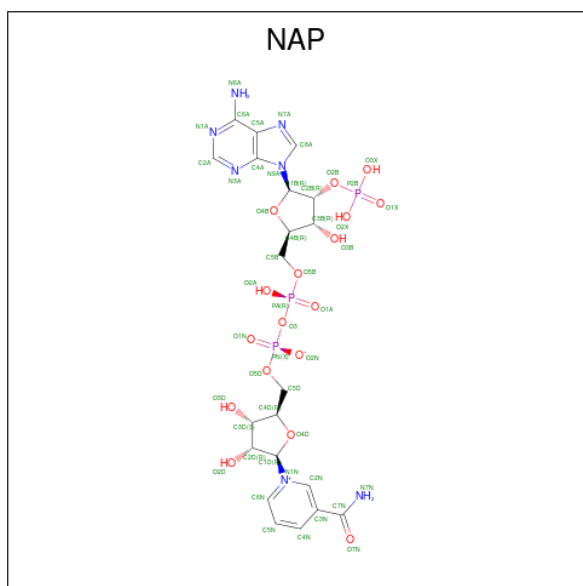
- Molecule 1 is a protein called GDP-FUCOSE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2488	1569	447	459	13	38	2	0

There are 2 discrepancies between the modelled and reference sequences:

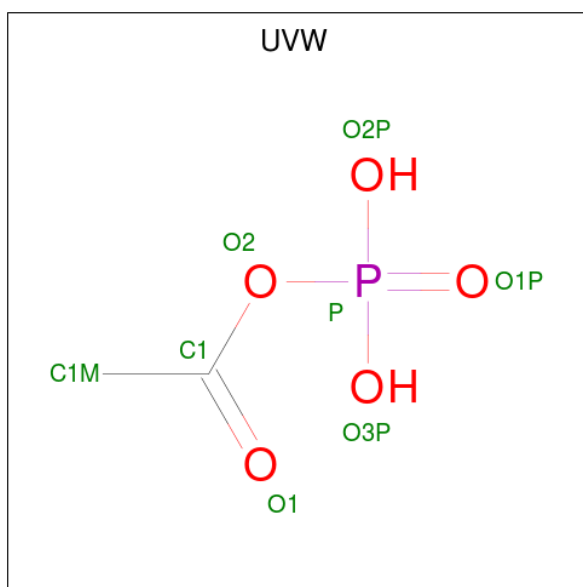
Chain	Residue	Modelled	Actual	Comment	Reference
A	136	GLU	TYR	engineered mutation	UNP P32055
A	195	SER	ASN	conflict	UNP P32055

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



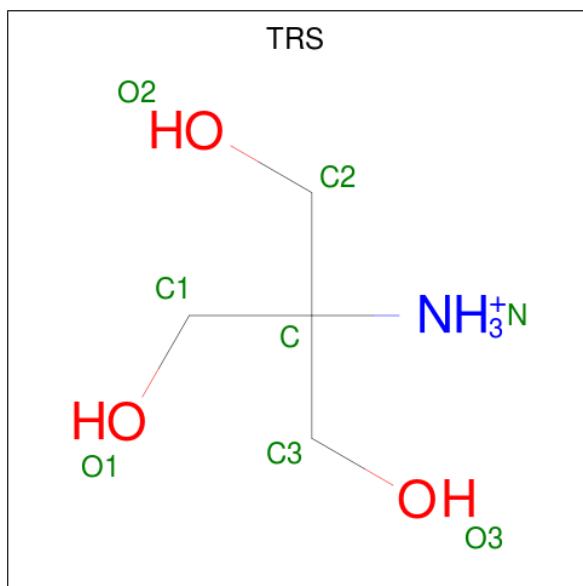
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is ACETYLPHOSPHATE (three-letter code: UVW) (formula:  $C_2H_5O_5P$ ).



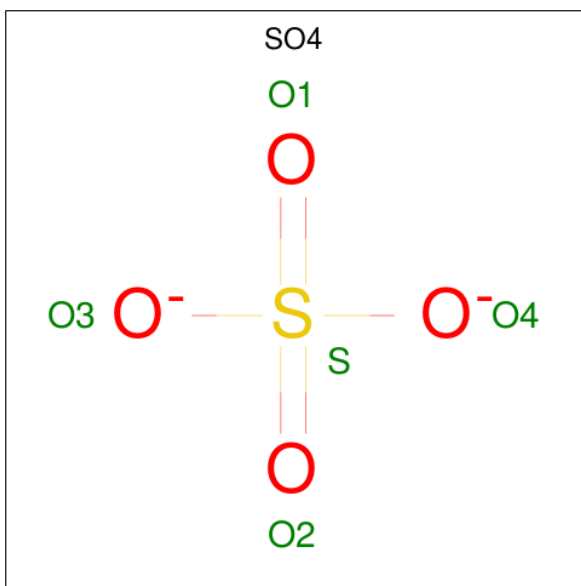
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			8	2	5	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	347	Total	O	0	0
			347	347		

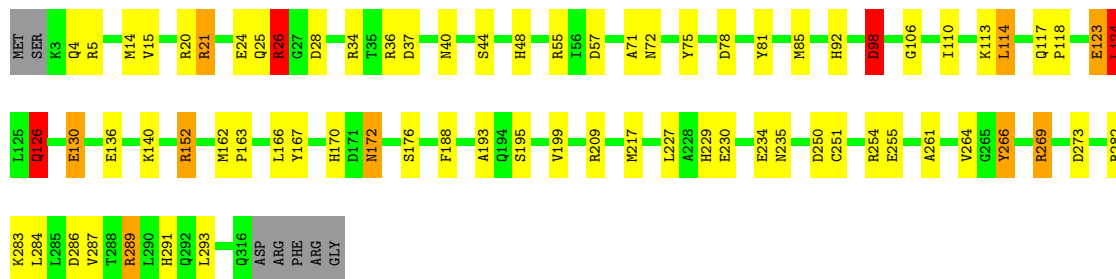
### 3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

#### • Molecule 1: GDP-FUCOSE SYNTHETASE

Chain A: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.30Å 103.30Å 75.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 1.60	Depositor
% Data completeness (in resolution range)	98.6 (10.00-1.60)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.139 , 0.180	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	2.77	8/2555 (0.3%)	1.82	53/3466 (1.5%)

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	A	0	8

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	GLU	CG-CD	131.81	3.49	1.51
1	A	283	LYS	CD-CE	9.93	1.76	1.51
1	A	113	LYS	CD-CE	-9.45	1.27	1.51
1	A	55	ARG	CG-CD	8.25	1.72	1.51
1	A	114	LEU	CG-CD1	7.11	1.78	1.51
1	A	234	GLU	CB-CG	-6.57	1.39	1.52
1	A	251	CYS	CB-SG	-6.02	1.72	1.82
1	A	269	ARG	CD-NE	-5.24	1.37	1.46

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ARG	NE-CZ-NH2	-32.40	104.10	120.30
1	A	230	GLU	CB-CG-CD	-29.42	34.77	114.20
1	A	26	ARG	CD-NE-CZ	15.59	145.42	123.60
1	A	289	ARG	NE-CZ-NH2	-15.21	112.69	120.30
1	A	114	LEU	CB-CG-CD1	-14.99	85.52	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	LEU	CB-CG-CD2	14.34	135.38	111.00
1	A	152	ARG	NE-CZ-NH2	-14.02	113.29	120.30
1	A	26	ARG	NE-CZ-NH1	12.87	126.73	120.30
1	A	230	GLU	CG-CD-OE1	-12.47	93.36	118.30
1	A	230	GLU	CG-CD-OE2	11.18	140.67	118.30
1	A	266	TYR	CB-CG-CD1	11.07	127.64	121.00
1	A	34	ARG	NE-CZ-NH2	-10.96	114.82	120.30
1	A	289	ARG	NH1-CZ-NH2	10.89	131.38	119.40
1	A	152	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	A	209	ARG	NE-CZ-NH2	-10.03	115.29	120.30
1	A	98	ASP	CB-CG-OD2	-9.86	109.43	118.30
1	A	273	ASP	CB-CG-OD2	-9.20	110.02	118.30
1	A	289	ARG	NE-CZ-NH1	-9.09	115.76	120.30
1	A	36	ARG	NE-CZ-NH1	-8.98	115.81	120.30
1	A	21	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	5	ARG	CD-NE-CZ	8.79	135.90	123.60
1	A	26	ARG	NH1-CZ-NH2	8.56	128.82	119.40
1	A	37	ASP	CB-CG-OD1	8.25	125.73	118.30
1	A	37	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	A	209	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	A	251	CYS	N-CA-CB	-6.94	98.10	110.60
1	A	20[A]	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	20[B]	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	130	GLU	OE1-CD-OE2	6.84	131.51	123.30
1	A	195	SER	N-CA-CB	6.59	120.39	110.50
1	A	167	TYR	CB-CG-CD1	6.58	124.95	121.00
1	A	289	ARG	CG-CD-NE	-6.56	98.03	111.80
1	A	167	TYR	CB-CG-CD2	-6.16	117.30	121.00
1	A	286	ASP	CB-CG-OD1	-6.16	112.76	118.30
1	A	250	ASP	CB-CA-C	-5.92	98.57	110.40
1	A	124	LEU	CA-CB-CG	5.89	128.85	115.30
1	A	282	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	266	TYR	CZ-CE2-CD2	-5.79	114.59	119.80
1	A	37	ASP	CA-CB-CG	-5.73	100.79	113.40
1	A	269	ARG	CD-NE-CZ	5.67	131.54	123.60
1	A	124	LEU	CD1-CG-CD2	-5.66	93.51	110.50
1	A	57	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	283	LYS	CG-CD-CE	-5.32	95.94	111.90
1	A	75	TYR	CB-CG-CD2	5.23	124.14	121.00
1	A	114	LEU	CD1-CG-CD2	5.19	126.08	110.50
1	A	4	GLN	OE1-CD-NE2	5.19	133.84	121.90
1	A	254	ARG	NE-CZ-NH1	-5.16	117.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ASP	CA-CB-CG	-5.13	102.11	113.40
1	A	266	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	A	78	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	123	GLU	CG-CD-OE2	-5.06	108.19	118.30
1	A	20[A]	ARG	NH1-CZ-NH2	5.02	124.93	119.40
1	A	20[B]	ARG	NH1-CZ-NH2	5.02	124.93	119.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	GLU	Sidechain
1	A	126	GLN	Sidechain
1	A	176	SER	Mainchain
1	A	199	VAL	Mainchain
1	A	25	GLN	Mainchain
1	A	255	GLU	Sidechain
1	A	266	TYR	Sidechain
1	A	98	ASP	Sidechain

## 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	2488	0	2451	62	0
2	A	48	0	24	6	0
3	A	8	0	3	5	0
4	A	16	0	23	7	0
5	A	10	0	0	0	0
6	A	347	0	0	28	3
All	All	2917	0	2501	74	3

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 15.

All (74) 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:114:LEU:CD1	1:A:114:LEU:CG	1.78	1.59
1:A:110:ILE:HD12	1:A:124:LEU:CD2	1.30	1.53
1:A:110:ILE:CD1	1:A:124:LEU:HD22	1.61	1.28
1:A:114:LEU:CB	1:A:114:LEU:CD1	2.26	1.13
1:A:193:ALA:HB2	6:A:2204:HOH:O	1.49	1.13
1:A:110:ILE:CD1	1:A:124:LEU:CD2	2.25	1.05
4:A:1319:TRS:O1	6:A:2338:HOH:O	1.77	0.98
1:A:15:VAL:HG13	1:A:217[B]:MET:HE1	1.46	0.97
1:A:48:HIS:CE1	1:A:92:HIS:HD2	1.81	0.97
1:A:110:ILE:HD12	1:A:124:LEU:HD21	1.47	0.96
1:A:48:HIS:HE1	1:A:92:HIS:HD2	0.97	0.94
1:A:284:LEU:HA	6:A:2292:HOH:O	1.67	0.94
1:A:48:HIS:HE1	1:A:92:HIS:CD2	1.87	0.92
2:A:1317:NAP:O2N	2:A:1317:NAP:O2A	1.90	0.90
1:A:287:VAL:HG13	6:A:2294:HOH:O	1.72	0.90
1:A:26:ARG:HG3	1:A:28:ASP:OD1	1.72	0.88
1:A:15:VAL:HG13	1:A:217[B]:MET:CE	2.04	0.86
1:A:110:ILE:HD12	1:A:124:LEU:HD22	0.87	0.85
1:A:287:VAL:HG22	6:A:2294:HOH:O	1.84	0.77
1:A:261:ALA:HB3	6:A:2254:HOH:O	1.86	0.74
3:A:1318:UVW:H1M1	6:A:2335:HOH:O	1.87	0.73
1:A:172:ASN:HD22	1:A:172:ASN:C	1.93	0.71
1:A:114:LEU:HB2	1:A:114:LEU:CD1	2.19	0.68
1:A:287:VAL:N	6:A:2294:HOH:O	2.27	0.67
1:A:291:HIS:HD2	6:A:2123:HOH:O	1.76	0.67
1:A:136:GLU:HG3	1:A:140:LYS:HE2	1.76	0.66
1:A:152:ARG:NH2	6:A:2174:HOH:O	2.21	0.65
1:A:26:ARG:CG	1:A:28:ASP:OD1	2.45	0.65
1:A:269:ARG:HD3	6:A:2270:HOH:O	1.95	0.64
1:A:72:ASN:O	6:A:2085:HOH:O	2.15	0.64
1:A:193:ALA:CB	6:A:2204:HOH:O	2.25	0.63
1:A:48:HIS:CE1	1:A:92:HIS:CD2	2.71	0.63
1:A:126:GLN:NE2	6:A:2154:HOH:O	2.34	0.61
1:A:188:PHE:HB3	1:A:264:VAL:HG21	1.84	0.59
4:A:1322:TRS:O3	6:A:2346:HOH:O	2.17	0.59
1:A:110:ILE:CG1	1:A:124:LEU:HD22	2.31	0.58
1:A:193:ALA:CA	6:A:2204:HOH:O	2.51	0.57
1:A:130:GLU:OE1	6:A:2160:HOH:O	2.17	0.57
1:A:170:HIS:NE2	4:A:1322:TRS:H32	2.20	0.56
3:A:1318:UVW:C1M	6:A:2335:HOH:O	2.50	0.56
4:A:1319:TRS:H12	6:A:2342:HOH:O	2.06	0.56
4:A:1319:TRS:O2	6:A:2341:HOH:O	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1317:NAP:O3B	6:A:2330:HOH:O	2.15	0.54
1:A:291:HIS:HE1	6:A:2309:HOH:O	1.90	0.53
3:A:1318:UVW:C1M	3:A:1318:UVW:O3P	2.54	0.52
1:A:110:ILE:HD12	1:A:124:LEU:HD23	1.67	0.52
3:A:1318:UVW:H1M1	3:A:1318:UVW:O3P	2.10	0.52
1:A:26:ARG:HH11	1:A:26:ARG:HG2	1.74	0.52
1:A:44:SER:O	1:A:48:HIS:HD2	1.93	0.51
2:A:1317:NAP:C3B	2:A:1317:NAP:O3X	2.59	0.50
1:A:106:GLY:HA3	1:A:162:MET:SD	2.52	0.50
1:A:163:PRO:HB3	1:A:217[A]:MET:SD	2.52	0.50
1:A:163:PRO:HG2	2:A:1317:NAP:C6N	2.41	0.49
1:A:81:TYR:CZ	1:A:85:MET:HG3	2.47	0.49
1:A:114:LEU:HB2	1:A:114:LEU:HD12	1.92	0.49
1:A:227:LEU:HD13	1:A:293:LEU:HD22	1.95	0.48
1:A:289:ARG:HG2	6:A:2300:HOH:O	2.14	0.47
1:A:166:LEU:HB2	2:A:1317:NAP:N7N	2.31	0.46
1:A:44:SER:HB2	6:A:2111:HOH:O	2.15	0.45
1:A:172:ASN:C	1:A:172:ASN:ND2	2.62	0.45
1:A:71:ALA:HB2	3:A:1318:UVW:H1M2	1.98	0.44
1:A:14:MET:N	2:A:1317:NAP:O2A	2.43	0.44
1:A:114:LEU:HB3	1:A:114:LEU:CD1	2.36	0.43
1:A:24:GLU:OE1	6:A:2025:HOH:O	2.21	0.43
1:A:21:ARG:HD3	4:A:1322:TRS:H31	2.00	0.43
1:A:193:ALA:N	6:A:2204:HOH:O	2.52	0.42
4:A:1322:TRS:O2	4:A:1322:TRS:O3	2.36	0.42
1:A:117:GLN:NE2	1:A:284:LEU:H	2.17	0.41
1:A:229:HIS:HE1	6:A:2183:HOH:O	2.04	0.41
1:A:235:ASN:HB2	1:A:293:LEU:HD21	2.02	0.41
1:A:117:GLN:HA	1:A:118:PRO:C	2.41	0.41
1:A:110:ILE:HD11	1:A:162:MET:HG3	2.03	0.40
1:A:287:VAL:CG1	6:A:2294:HOH:O	2.49	0.40

All (3) 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)
6:A:2110:HOH:O	6:A:2110:HOH:O[5_555]	0.92	1.28
6:A:2111:HOH:O	6:A:2111:HOH:O[5_555]	1.84	0.36
6:A:2164:HOH:O	6:A:2168:HOH:O[5_555]	2.13	0.07

## 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	314/321 (98%)	308 (98%)	6 (2%)	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	267/271 (98%)	261 (98%)	6 (2%)	55	28

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	40	ASN
1	A	98	ASP
1	A	124	LEU
1	A	126	GLN
1	A	172	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	48	HIS

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Mol	Chain	Res	Type
1	A	92	HIS
1	A	117	GLN
1	A	172	ASN
1	A	229	HIS
1	A	237	GLN
1	A	242	HIS
1	A	291	HIS
1	A	315	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

6 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	NAP	A	1317	-	43,52,52	1.28	6 (13%)	53,80,80	2.53	19 (35%)
3	UVW	A	1318	-	6,7,7	3.97	3 (50%)	7,10,10	1.97	2 (28%)
4	TRS	A	1319	-	7,7,7	2.17	2 (28%)	9,9,9	5.53	5 (55%)
5	SO4	A	1320	-	4,4,4	0.73	0	6,6,6	0.34	0
5	SO4	A	1321	-	4,4,4	0.55	0	6,6,6	1.34	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	TRS	A	1322	-	7,7,7	1.94	2 (28%)	9,9,9	7.28	5 (55%)

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
2	NAP	A	1317	-	-	5/27/67/67	0/5/5/5
3	UVW	A	1318	-	-	0/3/5/5	-
4	TRS	A	1319	-	-	5/9/9/9	-
4	TRS	A	1322	-	-	8/9/9/9	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1318	UVW	P-O2	-6.56	1.48	1.59
3	A	1318	UVW	C1M-C1	-6.46	1.27	1.49
4	A	1319	TRS	C3-C	3.59	1.61	1.52
4	A	1319	TRS	O1-C1	3.51	1.54	1.42
2	A	1317	NAP	C2N-C3N	3.48	1.44	1.39
4	A	1322	TRS	O1-C1	3.22	1.53	1.42
2	A	1317	NAP	C3B-C2B	-2.54	1.47	1.52
3	A	1318	UVW	P-O2P	-2.34	1.45	1.54
4	A	1322	TRS	C2-C	2.26	1.58	1.52
2	A	1317	NAP	C2D-C3D	-2.19	1.47	1.53
2	A	1317	NAP	C5A-C4A	-2.13	1.35	1.40
2	A	1317	NAP	PA-O1A	-2.03	1.43	1.50
2	A	1317	NAP	O4B-C1B	2.00	1.44	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1322	TRS	C1-C-N	13.65	136.75	107.73
4	A	1322	TRS	O1-C1-C	13.22	148.75	110.47
4	A	1319	TRS	C1-C-N	12.34	133.97	107.73
2	A	1317	NAP	C4B-O4B-C1B	-9.12	100.32	109.83
4	A	1319	TRS	C3-C-N	-7.97	90.79	107.73
4	A	1322	TRS	C2-C-N	-7.86	91.02	107.73
4	A	1319	TRS	O1-C1-C	6.50	129.28	110.47
4	A	1322	TRS	C3-C-N	-6.20	94.55	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1317	NAP	O3X-P2B-O1X	-5.50	88.85	110.53
2	A	1317	NAP	O3X-P2B-O2X	-4.83	88.82	107.57
2	A	1317	NAP	O4B-C4B-C3B	4.67	114.37	105.14
2	A	1317	NAP	O7N-C7N-N7N	-3.75	117.26	122.60
2	A	1317	NAP	O3X-P2B-O2B	-3.74	89.23	105.99
2	A	1317	NAP	O2X-P2B-O1X	3.74	125.27	110.53
3	A	1318	UVW	O3P-P-O2	3.64	116.90	105.37
4	A	1322	TRS	O3-C3-C	3.63	120.98	110.47
2	A	1317	NAP	O4B-C1B-C2B	3.51	112.67	106.60
2	A	1317	NAP	C3N-C2N-N1N	-3.50	116.85	120.40
2	A	1317	NAP	PN-O3-PA	-3.33	121.99	132.57
2	A	1317	NAP	O2A-PA-O1A	3.23	128.39	112.21
2	A	1317	NAP	O7N-C7N-C3N	3.16	123.44	119.62
2	A	1317	NAP	O2X-P2B-O2B	3.13	120.01	105.99
2	A	1317	NAP	O5B-C5B-C4B	-3.10	98.29	108.99
2	A	1317	NAP	O2B-C2B-C3B	2.90	122.18	111.68
2	A	1317	NAP	C5N-C4N-C3N	2.81	123.71	120.34
3	A	1318	UVW	O1-C1-C1M	2.74	134.84	124.81
2	A	1317	NAP	O4B-C4B-C5B	2.69	118.31	109.38
4	A	1319	TRS	O3-C3-C	-2.44	103.40	110.47
5	A	1321	SO4	O4-S-O3	-2.38	98.49	108.98
2	A	1317	NAP	O2A-PA-O5B	2.32	118.54	107.75
4	A	1319	TRS	C3-C-C1	-2.27	104.62	111.06
2	A	1317	NAP	C5B-C4B-C3B	2.07	123.00	115.21

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1322	TRS	C2-C-C1-O1
4	A	1322	TRS	C3-C-C1-O1
4	A	1322	TRS	C1-C-C2-O2
4	A	1322	TRS	C3-C-C2-O2
4	A	1322	TRS	C1-C-C3-O3
4	A	1322	TRS	C2-C-C3-O3
4	A	1319	TRS	C2-C-C1-O1
4	A	1319	TRS	C3-C-C1-O1
4	A	1319	TRS	N-C-C1-O1
4	A	1319	TRS	C1-C-C2-O2
4	A	1319	TRS	C3-C-C2-O2
2	A	1317	NAP	O4B-C4B-C5B-O5B
2	A	1317	NAP	C3B-C4B-C5B-O5B

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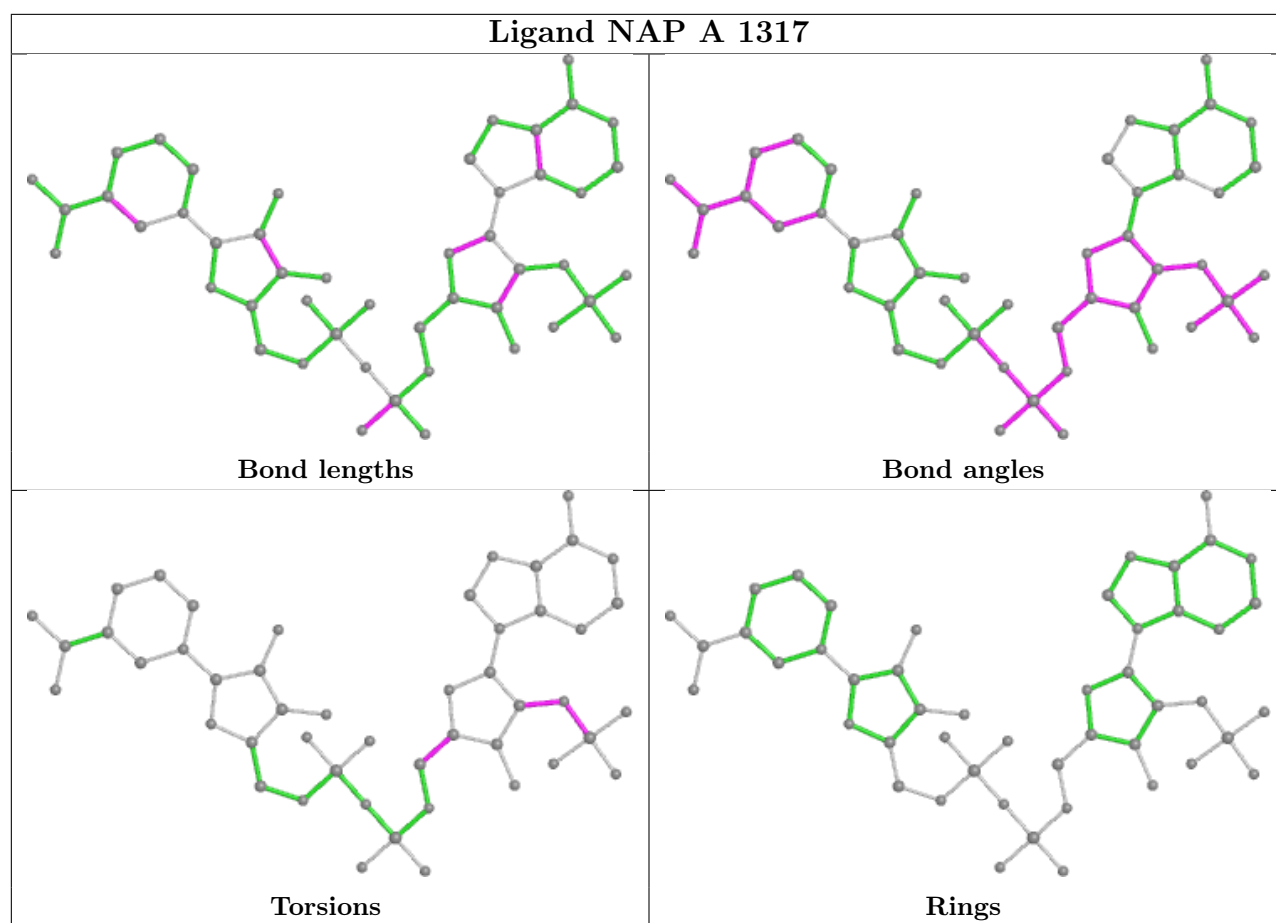
Mol	Chain	Res	Type	Atoms
2	A	1317	NAP	C3B-C2B-O2B-P2B
4	A	1322	TRS	N-C-C1-O1
4	A	1322	TRS	N-C-C2-O2
2	A	1317	NAP	C1B-C2B-O2B-P2B
2	A	1317	NAP	C2B-O2B-P2B-O3X

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1317	NAP	6	0
3	A	1318	UVW	5	0
4	A	1319	TRS	3	0
4	A	1322	TRS	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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.