



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2019 – 09:44 PM EDT

PDB ID : 1E7Q
Title : GDP 4-keto-6-deoxy-D-mannose epimerase reductase S107A
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

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 : 1.8.0 (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

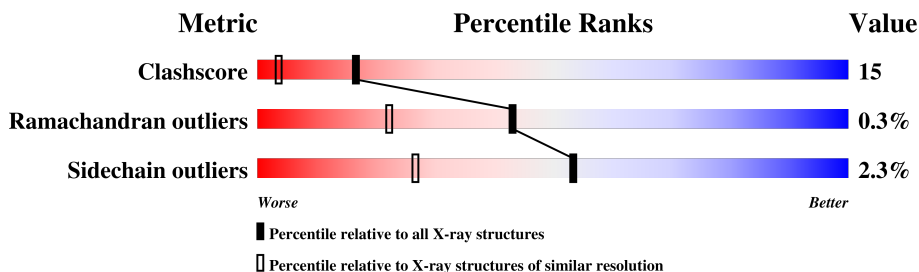
1 Overall quality at a glance

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 ≥ 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
5	TRS	A	1323	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2887 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.

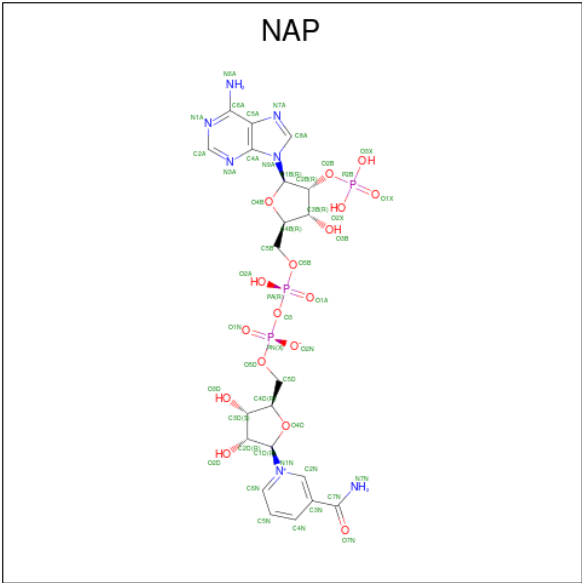
- Molecule 1 is a protein called GDP-FUCOSE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2489	1573	444	460	12	26	4	0

There are 2 discrepancies between the modelled and reference sequences:

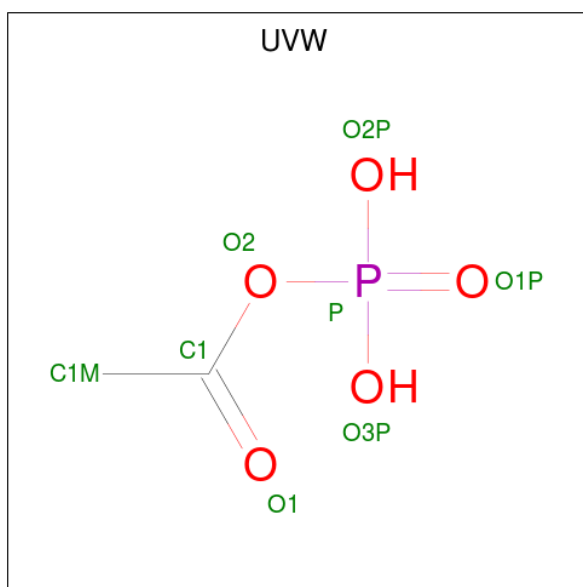
Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ALA	SER	engineered mutation	UNP P32055
A	195	SER	ASN	conflict	UNP P32055

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



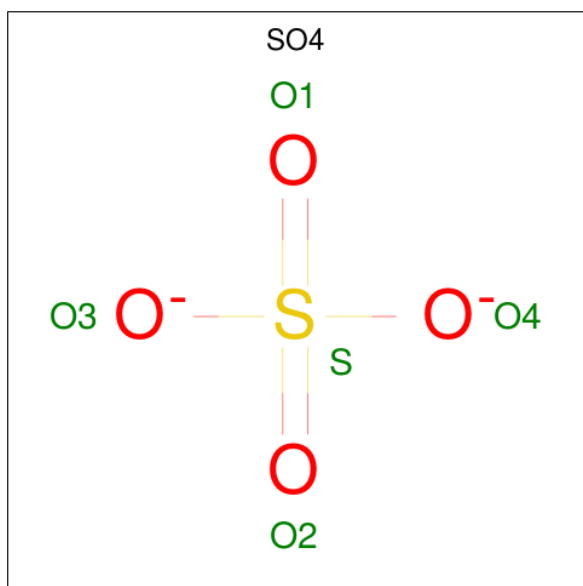
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	3	0

- Molecule 3 is ACETYLPHOSPHATE (three-letter code: UVW) (formula: C₂H₅O₅P).



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

- Molecule 4 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



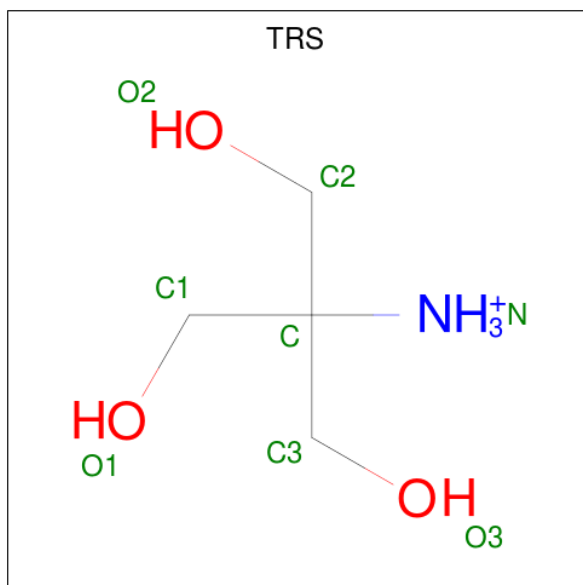
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

- Molecule 5 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
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is water.

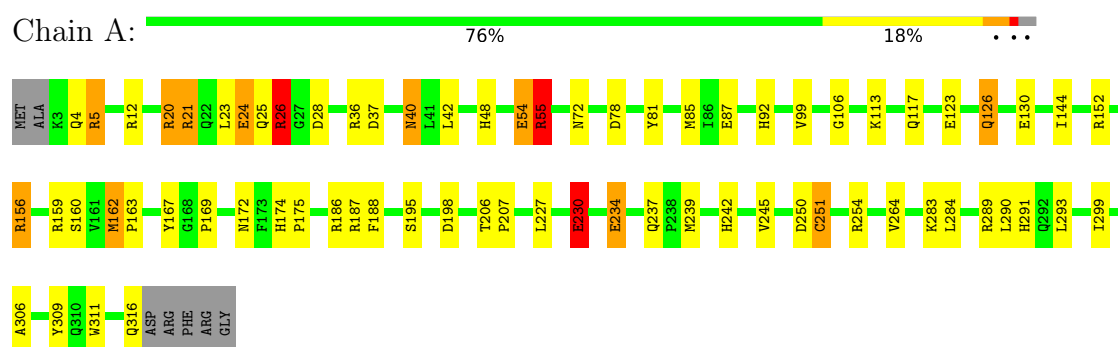
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	314	Total	O	0	0
			314	314		

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. 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



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, α , β , γ	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)	98.8 (10.00-1.60)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.138 , 0.182	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2887	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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	0.83	4/2568 (0.2%)	1.64	40/3487 (1.1%)

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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	ARG	CB-CG	-10.16	1.25	1.52
1	A	113	LYS	CG-CD	-5.84	1.32	1.52
1	A	160	SER	CA-CB	5.28	1.60	1.52
1	A	26	ARG	CD-NE	-5.06	1.37	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ARG	CD-NE-CZ	35.45	173.23	123.60
1	A	55	ARG	CA-CB-CG	-17.94	73.93	113.40
1	A	289	ARG	NE-CZ-NH2	-13.39	113.61	120.30
1	A	289	ARG	NE-CZ-NH1	-13.31	113.64	120.30
1	A	289	ARG	NH1-CZ-NH2	12.14	132.75	119.40
1	A	187	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	A	152	ARG	NE-CZ-NH1	11.59	126.10	120.30
1	A	152	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	A	87	GLU	CG-CD-OE1	10.10	138.50	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ARG	NE-CZ-NH2	10.00	125.30	120.30
1	A	54	GLU	C-N-CA	-9.27	98.52	121.70
1	A	186	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	A	78	ASP	CB-CG-OD2	-8.69	110.48	118.30
1	A	5	ARG	CD-NE-CZ	8.64	135.70	123.60
1	A	26	ARG	CG-CD-NE	-8.11	94.77	111.80
1	A	250	ASP	CB-CA-C	-7.63	95.14	110.40
1	A	21	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	A	87	GLU	CG-CD-OE2	-7.39	103.53	118.30
1	A	159	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	162[A]	MET	CG-SD-CE	6.55	110.68	100.20
1	A	162[B]	MET	CG-SD-CE	6.55	110.68	100.20
1	A	26	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	A	254	ARG	CD-NE-CZ	-6.51	114.49	123.60
1	A	123	GLU	OE1-CD-OE2	-6.49	115.51	123.30
1	A	55	ARG	CA-C-N	6.37	131.22	117.20
1	A	195	SER	N-CA-CB	6.27	119.90	110.50
1	A	167	TYR	CB-CG-CD1	6.22	124.73	121.00
1	A	24	GLU	CB-CG-CD	-5.97	98.09	114.20
1	A	289	ARG	CG-CD-NE	-5.76	99.69	111.80
1	A	198	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	36	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	37	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	130	GLU	OE1-CD-OE2	5.61	130.03	123.30
1	A	37	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	5	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	A	156	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	20	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	234	GLU	CA-CB-CG	5.12	124.67	113.40
1	A	230	GLU	OE1-CD-OE2	5.08	129.40	123.30
1	A	12	ARG	NE-CZ-NH1	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	GLN	Mainchain
1	A	55	ARG	Mainchain

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	2489	0	2447	65	0
2	A	48	0	24	9	0
3	A	8	0	3	3	0
4	A	20	0	0	0	0
5	A	8	0	12	4	0
6	A	314	0	0	33	5
All	All	2887	0	2486	76	5

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 (76) 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:309:TYR:HB3	6:A:2284:HOH:O	1.40	1.18
1:A:5:ARG:NE	1:A:55:ARG:HB3	1.61	1.15
1:A:5:ARG:HE	1:A:55:ARG:HB3	1.10	1.08
3:A:1318:UVW:H1M1	6:A:2305:HOH:O	1.53	1.06
1:A:54:GLU:O	1:A:55:ARG:CB	1.96	1.03
1:A:48:HIS:HE1	1:A:92:HIS:HD2	1.07	0.99
1:A:99:VAL:O	6:A:2115:HOH:O	1.81	0.97
1:A:48:HIS:CE1	1:A:92:HIS:HD2	1.89	0.90
2:A:1317:NAP:O3X	6:A:2296:HOH:O	1.90	0.87
1:A:316:GLN:O	6:A:2294:HOH:O	1.91	0.86
1:A:299:ILE:HD13	6:A:2080:HOH:O	1.76	0.86
2:A:1317:NAP:O2N	2:A:1317:NAP:O2A	1.92	0.86
2:A:1317:NAP:H4N	6:A:2302:HOH:O	1.76	0.85
1:A:283:LYS:HE2	6:A:2124:HOH:O	1.78	0.83
1:A:311:TRP:HB3	6:A:2176:HOH:O	1.80	0.82
1:A:48:HIS:HE1	1:A:92:HIS:CD2	1.97	0.82
1:A:24:GLU:HG3	6:A:2022:HOH:O	1.80	0.80
1:A:163:PRO:HG2	2:A:1317:NAP:H2N	1.66	0.77
5:A:1323:TRS:H21	6:A:2314:HOH:O	1.85	0.77
1:A:54:GLU:O	1:A:55:ARG:HB2	1.83	0.77
1:A:4:GLN:OE1	6:A:2003:HOH:O	2.01	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:HD2	6:A:2115:HOH:O	1.87	0.75
5:A:1323:TRS:O2	5:A:1323:TRS:O3	1.97	0.74
1:A:5:ARG:HE	1:A:55:ARG:CB	1.97	0.74
1:A:156:ARG:NE	6:A:2115:HOH:O	2.25	0.70
1:A:106:GLY:HA3	1:A:162[A]:MET:CE	2.22	0.70
1:A:156:ARG:CD	6:A:2115:HOH:O	2.41	0.69
1:A:156:ARG:CZ	6:A:2115:HOH:O	2.41	0.69
1:A:311:TRP:CB	6:A:2176:HOH:O	2.40	0.65
1:A:299:ILE:CD1	6:A:2080:HOH:O	2.42	0.64
1:A:72:ASN:O	6:A:2073:HOH:O	2.15	0.63
1:A:92:HIS:HE1	6:A:2102:HOH:O	1.83	0.61
3:A:1318:UVW:C1M	6:A:2305:HOH:O	2.28	0.61
1:A:291:HIS:HE1	6:A:2275:HOH:O	1.84	0.61
1:A:106:GLY:HA3	1:A:162[A]:MET:HE2	1.84	0.60
1:A:169:PRO:HA	6:A:2176:HOH:O	1.99	0.60
1:A:188:PHE:HB3	1:A:264:VAL:HG21	1.83	0.60
5:A:1323:TRS:H22	6:A:2312:HOH:O	2.02	0.59
1:A:163:PRO:HG2	2:A:1317:NAP:C2N	2.32	0.59
1:A:227:LEU:HD13	1:A:293:LEU:HD22	1.85	0.59
1:A:106:GLY:HA3	1:A:162[A]:MET:HE1	1.85	0.58
1:A:169:PRO:CA	6:A:2176:HOH:O	2.54	0.54
1:A:251:CYS:HB3	6:A:2232:HOH:O	2.07	0.53
1:A:5:ARG:CD	1:A:55:ARG:HB3	2.35	0.53
1:A:239:MET:SD	6:A:2157:HOH:O	0.94	0.53
1:A:306:ALA:O	6:A:2284:HOH:O	2.18	0.52
1:A:144:ILE:HD11	1:A:162[A]:MET:HE1	1.92	0.52
1:A:163:PRO:CG	2:A:1317:NAP:H2N	2.37	0.51
1:A:230:GLU:O	1:A:234:GLU:HG2	2.10	0.51
1:A:291:HIS:HD2	6:A:2270:HOH:O	1.94	0.51
1:A:21:ARG:HD3	5:A:1323:TRS:H31	1.93	0.50
2:A:1317:NAP:C3B	2:A:1317:NAP:O3X	2.58	0.50
1:A:174:HIS:CG	1:A:175:PRO:HD2	2.48	0.48
1:A:117:GLN:NE2	1:A:284:LEU:H	2.12	0.47
1:A:81:TYR:CZ	1:A:85:MET:HG3	2.50	0.46
1:A:163:PRO:CG	2:A:1317:NAP:C2N	2.93	0.46
1:A:48:HIS:CE1	1:A:92:HIS:CD2	2.82	0.45
1:A:242:HIS:CD2	1:A:242:HIS:H	2.35	0.45
1:A:23:LEU:O	1:A:26:ARG:HB2	2.16	0.45
1:A:26:ARG:HD2	1:A:28:ASP:OD1	2.17	0.45
1:A:299:ILE:CG1	6:A:2080:HOH:O	2.65	0.45
1:A:283:LYS:HB2	1:A:283:LYS:HE3	1.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1318:UVW:C1M	3:A:1318:UVW:O3P	2.64	0.44
1:A:20:ARG:O	1:A:24:GLU:HB2	2.17	0.43
1:A:206:THR:N	1:A:207:PRO:CD	2.81	0.43
1:A:117:GLN:HE22	1:A:284:LEU:H	1.67	0.43
1:A:237:GLN:NE2	6:A:2222:HOH:O	2.51	0.42
1:A:40:ASN:ND2	1:A:42:LEU:H	2.17	0.42
1:A:126:GLN:NE2	6:A:2139:HOH:O	2.52	0.42
1:A:144:ILE:HD11	1:A:162[A]:MET:CE	2.49	0.42
1:A:172:ASN:C	1:A:172:ASN:ND2	2.74	0.41
1:A:245:VAL:HA	1:A:290:LEU:HD22	2.03	0.41
2:A:1317:NAP:H6N	2:A:1317:NAP:O5D	2.21	0.41
1:A:169:PRO:HG3	6:A:2176:HOH:O	2.20	0.41

All (5) 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:2137:HOH:O	6:A:2137:HOH:O[5_555]	0.75	1.45
6:A:2099:HOH:O	6:A:2099:HOH:O[5_555]	0.89	1.31
6:A:2085:HOH:O	6:A:2162:HOH:O[5_555]	1.73	0.47
6:A:2073:HOH:O	6:A:2154:HOH:O[5_555]	2.02	0.18
6:A:2046:HOH:O	6:A:2046:HOH:O[5_555]	2.16	0.04

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	316/321 (98%)	310 (98%)	5 (2%)	1 (0%)	43 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ARG

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	268/269 (100%)	262 (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	55	ARG
1	A	126	GLN
1	A	230	GLU
1	A	251	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	48	HIS
1	A	92	HIS
1	A	117	GLN
1	A	126	GLN
1	A	133	ASN
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 ⓘ

7 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	1.35	5 (11%)	53,80,80	2.53	18 (33%)
3	UVW	A	1318	-	6,7,7	3.67	3 (50%)	7,10,10	2.30	2 (28%)
4	SO4	A	1319	-	4,4,4	0.89	0	6,6,6	0.37	0
4	SO4	A	1320	-	4,4,4	0.74	0	6,6,6	0.24	0
4	SO4	A	1321	-	4,4,4	0.74	0	6,6,6	0.31	0
4	SO4	A	1322	-	4,4,4	0.50	0	6,6,6	1.63	1 (16%)
5	TRS	A	1323	-	7,7,7	2.23	3 (42%)	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	-	-	9/27/67/67	0/5/5/5
3	UVW	A	1318	-	-	0/3/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TRS	A	1323	-	-	8/9/9/9	-

All (11) 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	O1-C1	4.90	1.39	1.20
5	A	1323	TRS	O1-C1	4.04	1.55	1.42
2	A	1317	NAP	P2B-O2B	-3.81	1.52	1.59
5	A	1323	TRS	C3-C	2.88	1.59	1.52
2	A	1317	NAP	C2N-C3N	2.67	1.43	1.39
2	A	1317	NAP	O4D-C1D	2.59	1.44	1.41
5	A	1323	TRS	C2-C	2.35	1.58	1.52
3	A	1318	UVW	P-O2P	-2.34	1.45	1.54
2	A	1317	NAP	C6N-C5N	-2.17	1.33	1.38
2	A	1317	NAP	C8A-N7A	-2.15	1.30	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1323	TRS	C1-C-N	15.07	139.77	107.73
5	A	1323	TRS	O1-C1-C	11.69	144.32	110.47
2	A	1317	NAP	C4B-O4B-C1B	-9.12	100.32	109.83
5	A	1323	TRS	C2-C-N	-7.52	91.74	107.73
5	A	1323	TRS	C3-C-N	-6.77	93.32	107.73
2	A	1317	NAP	O3X-P2B-O1X	-5.24	89.86	110.53
2	A	1317	NAP	O4B-C4B-C3B	5.04	115.09	105.14
2	A	1317	NAP	O3X-P2B-O2X	-5.01	88.09	107.57
3	A	1318	UVW	O1-C1-C1M	-4.15	109.59	124.81
2	A	1317	NAP	O3X-P2B-O2B	-3.91	88.49	105.99
2	A	1317	NAP	C5N-C4N-C3N	3.89	125.00	120.34
2	A	1317	NAP	O2X-P2B-O1X	3.71	125.17	110.53
2	A	1317	NAP	PN-O3-PA	-3.65	120.98	132.57
3	A	1318	UVW	O3P-P-O2	3.64	116.90	105.37
2	A	1317	NAP	O7N-C7N-N7N	-3.30	117.90	122.60
4	A	1322	SO4	O4-S-O3	-3.24	94.69	108.98
2	A	1317	NAP	O4B-C1B-C2B	3.07	111.91	106.60
2	A	1317	NAP	O2X-P2B-O2B	2.95	119.22	105.99
2	A	1317	NAP	O2B-C2B-C3B	2.94	122.33	111.68
2	A	1317	NAP	O4B-C4B-C5B	2.91	119.04	109.38
2	A	1317	NAP	C3N-C2N-N1N	-2.77	117.59	120.40
2	A	1317	NAP	O2A-PA-O1A	2.58	125.17	112.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1317	NAP	O7N-C7N-C3N	2.57	122.73	119.62
2	A	1317	NAP	O5B-C5B-C4B	-2.50	100.36	108.99
2	A	1317	NAP	O2A-PA-O5B	2.48	119.26	107.75
5	A	1323	TRS	C2-C-C1	-2.08	105.17	111.06

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1323	TRS	C2-C-C1-O1
5	A	1323	TRS	C3-C-C1-O1
5	A	1323	TRS	N-C-C1-O1
5	A	1323	TRS	C1-C-C2-O2
5	A	1323	TRS	C3-C-C2-O2
5	A	1323	TRS	C1-C-C3-O3
5	A	1323	TRS	C2-C-C3-O3
2	A	1317	NAP	O4B-C4B-C5B-O5B
5	A	1323	TRS	N-C-C2-O2
2	A	1317	NAP	C3B-C4B-C5B-O5B
2	A	1317	NAP	C3B-C2B-O2B-P2B
2	A	1317	NAP	C1B-C2B-O2B-P2B
2	A	1317	NAP	C2B-O2B-P2B-O1X
2	A	1317	NAP	C5B-O5B-PA-O3
2	A	1317	NAP	C2N-C3N-C7N-O7N
2	A	1317	NAP	C2N-C3N-C7N-N7N
2	A	1317	NAP	C2B-O2B-P2B-O3X

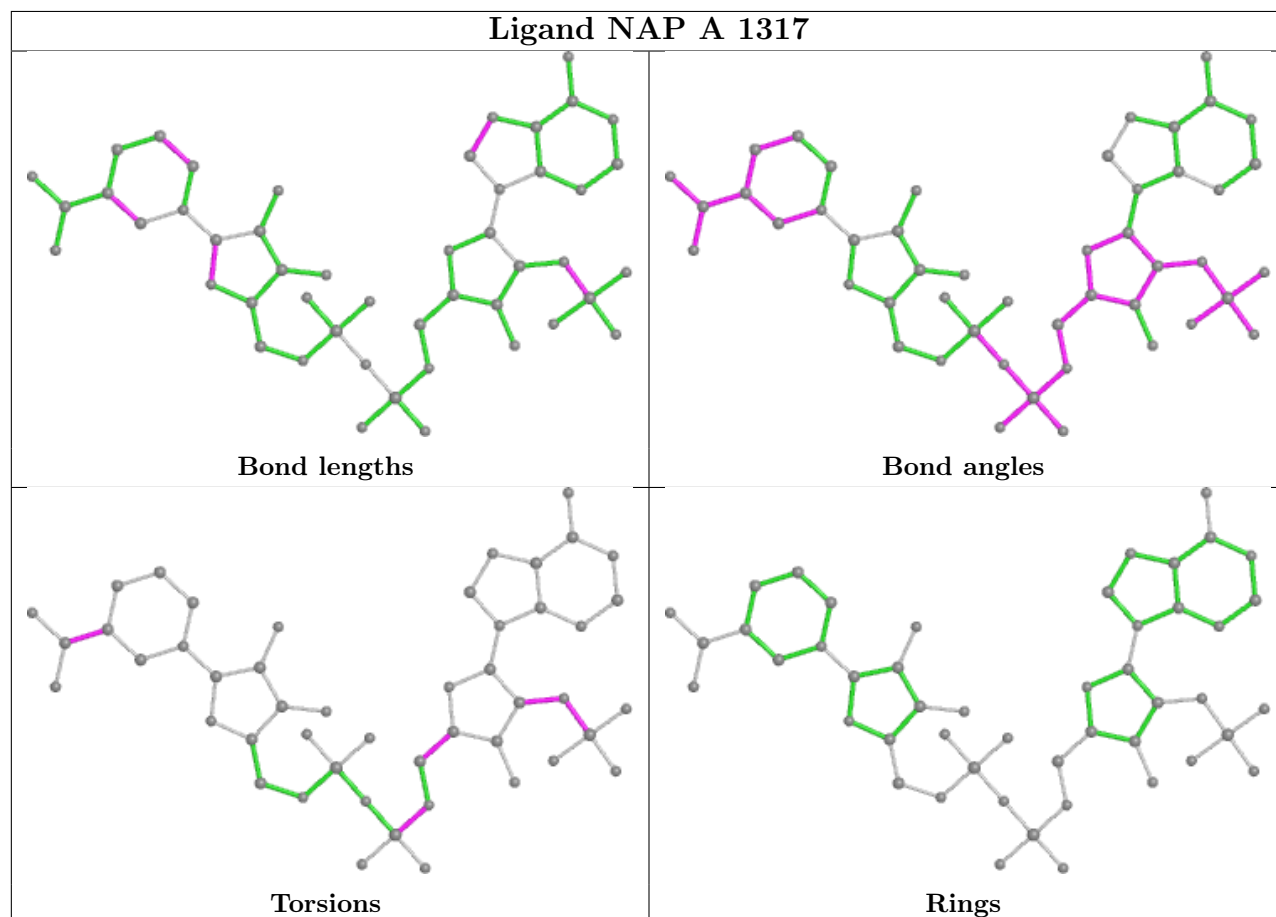
There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1317	NAP	9	0
3	A	1318	UVW	3	0
5	A	1323	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.