



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:38 AM UTC

PDB ID : 5XVH / pdb_00005xvh
Title : Crystal structure of the NADP⁺ and tartrate-bound complex of L-serine 3-dehydrogenase from the hyperthermophilic archaeon *Pyrobaculum calidifontis*
Authors : Yoneda, K.; Sakuraba, H.; Ohshima, T.
Deposited on : 2017-06-28
Resolution : 1.57 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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)
Xtriage (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

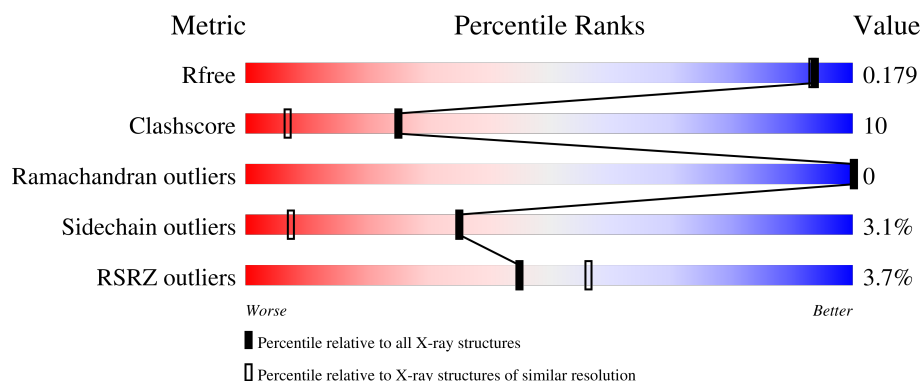
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

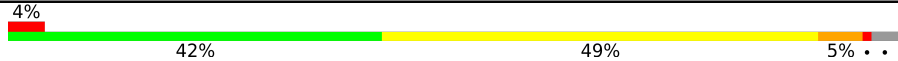
The reported resolution of this entry is 1.57 Å.

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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	306	

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
2	TLA	A	301	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	304	-	X	-	-
5	SO4	A	305	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2601 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.

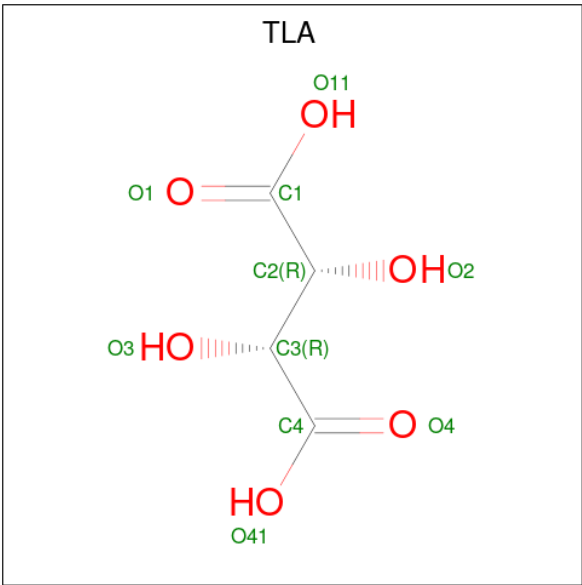
- Molecule 1 is a protein called 6-phosphogluconate dehydrogenase, NAD-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2229	1431	387	399	12	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

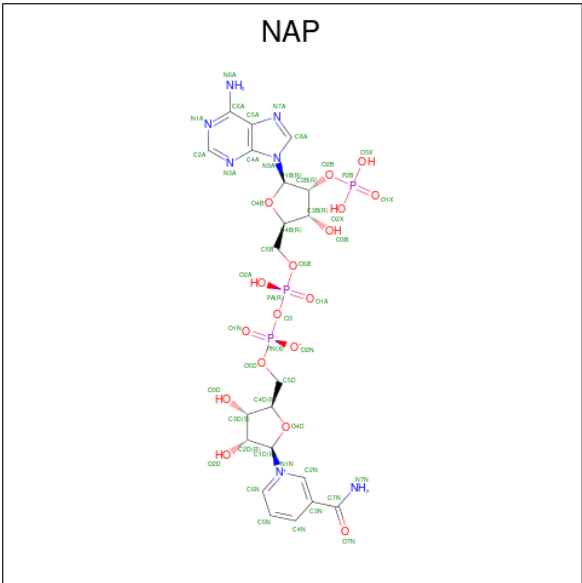
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A3MU08
A	-18	GLY	-	expression tag	UNP A3MU08
A	-17	SER	-	expression tag	UNP A3MU08
A	-16	SER	-	expression tag	UNP A3MU08
A	-15	HIS	-	expression tag	UNP A3MU08
A	-14	HIS	-	expression tag	UNP A3MU08
A	-13	HIS	-	expression tag	UNP A3MU08
A	-12	HIS	-	expression tag	UNP A3MU08
A	-11	HIS	-	expression tag	UNP A3MU08
A	-10	HIS	-	expression tag	UNP A3MU08
A	-9	SER	-	expression tag	UNP A3MU08
A	-8	SER	-	expression tag	UNP A3MU08
A	-7	GLY	-	expression tag	UNP A3MU08
A	-6	LEU	-	expression tag	UNP A3MU08
A	-5	VAL	-	expression tag	UNP A3MU08
A	-4	PRO	-	expression tag	UNP A3MU08
A	-3	ARG	-	expression tag	UNP A3MU08
A	-2	GLY	-	expression tag	UNP A3MU08
A	-1	SER	-	expression tag	UNP A3MU08
A	0	HIS	-	expression tag	UNP A3MU08

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		

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



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

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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		

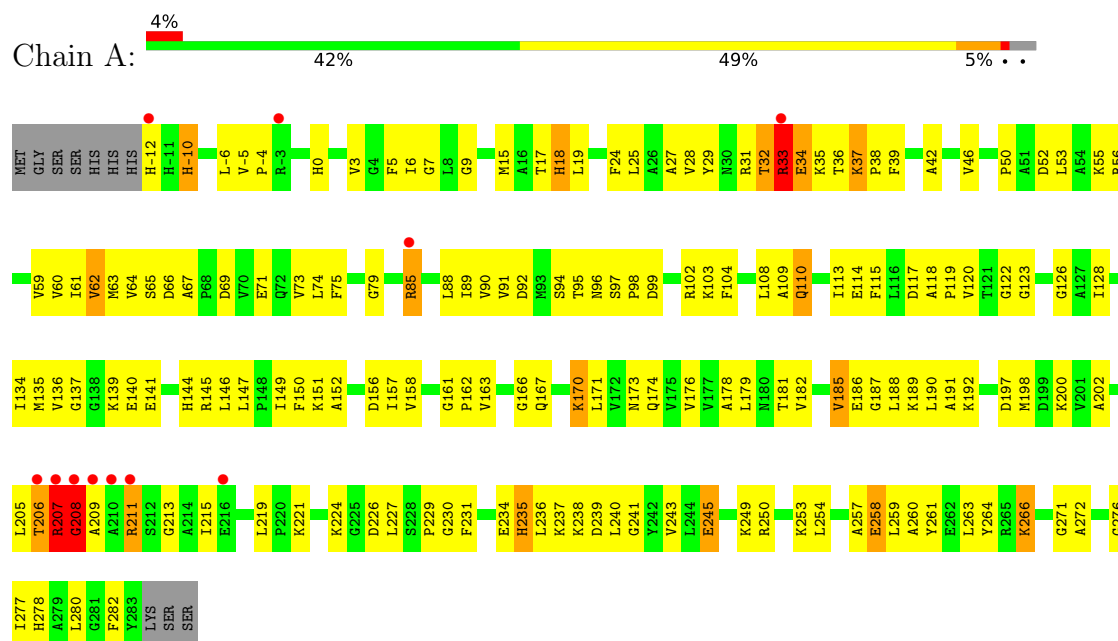
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	300	Total 300	O 300	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: 6-phosphogluconate dehydrogenase, NAD-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.97Å 57.51Å 56.41Å 90.00° 106.91° 90.00°	Depositor
Resolution (Å)	28.70 – 1.57 28.70 – 1.57	Depositor EDS
% Data completeness (in resolution range)	96.5 (28.70-1.57) 96.5 (28.70-1.57)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.57Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.173 , 0.179 0.174 , 0.179	Depositor DCC
R_{free} test set	2490 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2601	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, TLA, ACY, 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	2.19	148/2272 (6.5%)	1.09	6/3065 (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	A	0	2

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	ARG	C-O	-10.21	1.13	1.24
1	A	67	ALA	C-O	-9.26	1.15	1.24
1	A	147	LEU	C-O	-9.10	1.15	1.24
1	A	208	GLY	C-O	-8.80	1.11	1.23
1	A	113	ILE	C-O	-8.26	1.14	1.24
1	A	60	VAL	C-O	-8.16	1.15	1.24
1	A	257	ALA	C-O	-8.16	1.14	1.24
1	A	5	PHE	C-O	-7.92	1.14	1.24
1	A	219	LEU	C-O	-7.86	1.17	1.24
1	A	221	LYS	C-O	-7.86	1.15	1.24
1	A	254	LEU	C-O	-7.78	1.15	1.24
1	A	32	THR	C-O	-7.64	1.14	1.24
1	A	97	SER	C-O	-7.59	1.14	1.24
1	A	59	VAL	C-O	-7.52	1.16	1.24
1	A	173	ASN	C-O	-7.45	1.15	1.24
1	A	234	GLU	C-O	-7.25	1.15	1.24
1	A	-5	VAL	C-O	-7.16	1.17	1.23
1	A	3	VAL	C-O	-7.14	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	MET	C-O	-7.13	1.16	1.24
1	A	237	LYS	C-O	-7.09	1.15	1.24
1	A	66	ASP	C-O	-7.07	1.14	1.23
1	A	259	LEU	C-O	-7.05	1.15	1.24
1	A	171	LEU	C-O	-6.85	1.16	1.24
1	A	231	PHE	C-O	-6.85	1.16	1.24
1	A	166	GLY	C-O	-6.82	1.15	1.23
1	A	89	ILE	C-O	-6.80	1.16	1.24
1	A	136	VAL	C-O	-6.79	1.16	1.24
1	A	179	LEU	C-O	-6.79	1.15	1.24
1	A	0	HIS	CG-ND1	-6.77	1.30	1.38
1	A	150	PHE	C-O	-6.76	1.16	1.24
1	A	200	LYS	C-O	-6.72	1.16	1.24
1	A	104	PHE	C-O	-6.67	1.16	1.24
1	A	63	MET	C-O	-6.59	1.15	1.23
1	A	278	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	134	ILE	C-O	-6.54	1.17	1.24
1	A	161	GLY	C-O	-6.52	1.15	1.24
1	A	90	VAL	C-O	-6.51	1.16	1.24
1	A	157	ILE	C-O	-6.50	1.17	1.24
1	A	42	ALA	C-O	-6.47	1.15	1.24
1	A	280	LEU	C-O	-6.46	1.16	1.23
1	A	19	LEU	C-O	-6.44	1.16	1.24
1	A	264	TYR	C-O	-6.44	1.16	1.24
1	A	236	LEU	C-O	-6.42	1.16	1.24
1	A	253	LYS	C-O	-6.39	1.16	1.24
1	A	167	GLN	C-O	-6.36	1.16	1.24
1	A	162	PRO	C-O	-6.34	1.15	1.24
1	A	39	PHE	C-O	-6.31	1.16	1.24
1	A	36	THR	C-O	-6.31	1.15	1.24
1	A	95	THR	C-O	-6.30	1.16	1.24
1	A	28	VAL	C-O	-6.30	1.17	1.24
1	A	272	ALA	C-O	-6.25	1.16	1.24
1	A	-10	HIS	CG-ND1	-6.24	1.31	1.38
1	A	149	ILE	C-O	-6.23	1.16	1.24
1	A	170	LYS	C-O	-6.22	1.16	1.24
1	A	119	PRO	C-O	-6.18	1.16	1.23
1	A	62	VAL	C-O	-6.18	1.17	1.24
1	A	235	HIS	CG-ND1	-6.16	1.31	1.38
1	A	205	LEU	C-O	-6.14	1.16	1.24
1	A	141	GLU	C-O	-6.14	1.17	1.24
1	A	176	VAL	C-O	-6.13	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	ALA	C-O	-6.12	1.16	1.23
1	A	24	PHE	C-O	-6.11	1.16	1.24
1	A	140	GLU	C-O	-6.10	1.16	1.24
1	A	25	LEU	C-O	-6.09	1.16	1.24
1	A	71	GLU	C-O	-6.09	1.17	1.24
1	A	7	GLY	C-O	-6.09	1.15	1.23
1	A	163	VAL	C-O	-6.07	1.18	1.24
1	A	79	GLY	C-O	-6.06	1.16	1.23
1	A	178	ALA	C-O	-5.99	1.17	1.24
1	A	151	LYS	C-O	-5.96	1.16	1.24
1	A	64	VAL	C-O	-5.96	1.17	1.24
1	A	103	LYS	C-O	-5.93	1.17	1.24
1	A	85	ARG	C-O	-5.92	1.16	1.23
1	A	190	LEU	C-O	-5.90	1.17	1.24
1	A	91	VAL	C-O	-5.88	1.17	1.24
1	A	96	ASN	C-O	-5.88	1.16	1.24
1	A	29	TYR	C-O	-5.88	1.17	1.24
1	A	282	PHE	C-O	-5.87	1.16	1.24
1	A	207	ARG	CA-C	5.84	1.58	1.53
1	A	6	ILE	C-O	-5.82	1.17	1.24
1	A	278	HIS	CG-ND1	-5.82	1.31	1.38
1	A	94	SER	C-O	-5.81	1.16	1.23
1	A	15	MET	C-O	-5.79	1.17	1.24
1	A	98	PRO	C-O	-5.77	1.17	1.24
1	A	9	GLY	C-O	-5.73	1.17	1.24
1	A	239	ASP	C-O	-5.73	1.17	1.24
1	A	88	LEU	C-O	-5.69	1.16	1.23
1	A	146	LEU	C-O	-5.68	1.16	1.24
1	A	191	ALA	C-O	-5.67	1.17	1.24
1	A	120	VAL	C-O	-5.67	1.17	1.23
1	A	69	ASP	C-O	-5.66	1.17	1.24
1	A	263	LEU	C-O	-5.65	1.17	1.24
1	A	75	PHE	C-O	-5.64	1.16	1.24
1	A	117	ASP	C-O	-5.63	1.17	1.24
1	A	266	LYS	C-O	-5.60	1.17	1.24
1	A	-4	PRO	C-O	-5.58	1.17	1.23
1	A	37	LYS	C-O	-5.58	1.19	1.24
1	A	260	ALA	C-O	-5.57	1.17	1.24
1	A	158	VAL	C-O	-5.57	1.18	1.24
1	A	50	PRO	C-O	-5.56	1.17	1.24
1	A	227	LEU	C-O	-5.55	1.16	1.24
1	A	235	HIS	C-O	-5.53	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	GLY	C-O	-5.53	1.16	1.24
1	A	52	ASP	C-O	-5.51	1.17	1.24
1	A	152	ALA	C-O	-5.50	1.17	1.24
1	A	258	GLU	C-O	-5.49	1.17	1.24
1	A	33	ARG	C-O	-5.49	1.17	1.24
1	A	-10	HIS	CD2-NE2	-5.46	1.31	1.37
1	A	115	PHE	C-O	-5.45	1.17	1.23
1	A	145	ARG	C-O	-5.44	1.17	1.24
1	A	241	GLY	C-O	-5.44	1.17	1.23
1	A	245	GLU	C-O	-5.44	1.17	1.24
1	A	126	GLY	C-O	-5.38	1.17	1.23
1	A	137	GLY	C-O	-5.37	1.16	1.23
1	A	18	HIS	CG-ND1	-5.36	1.32	1.38
1	A	31	ARG	C-O	-5.35	1.18	1.24
1	A	215	ILE	C-O	-5.35	1.18	1.24
1	A	182	VAL	C-O	-5.34	1.18	1.24
1	A	277	ILE	C-O	-5.31	1.17	1.24
1	A	74	LEU	C-O	-5.30	1.17	1.24
1	A	185	VAL	C-O	-5.29	1.17	1.24
1	A	197	ASP	C-O	-5.27	1.17	1.24
1	A	144	HIS	CG-ND1	-5.26	1.32	1.38
1	A	92	ASP	C-O	-5.26	1.17	1.24
1	A	108	LEU	C-O	-5.25	1.18	1.24
1	A	56	ARG	C-O	-5.24	1.16	1.24
1	A	109	ALA	C-O	-5.24	1.17	1.24
1	A	156	ASP	CG-OD2	-5.24	1.15	1.25
1	A	118	ALA	C-O	-5.22	1.17	1.23
1	A	240	LEU	C-O	-5.20	1.17	1.24
1	A	139	LYS	C-O	-5.19	1.17	1.23
1	A	46	VAL	C-O	-5.17	1.18	1.24
1	A	17	THR	C-O	-5.16	1.18	1.24
1	A	186	GLU	C-O	-5.15	1.18	1.24
1	A	53	LEU	C-O	-5.14	1.18	1.24
1	A	123	GLY	C-O	-5.14	1.14	1.23
1	A	226	ASP	C-O	-5.12	1.17	1.23
1	A	114	GLU	C-O	-5.11	1.17	1.23
1	A	276	GLY	C-O	-5.10	1.16	1.23
1	A	-6	LEU	C-O	-5.10	1.17	1.24
1	A	73	VAL	C-O	-5.09	1.17	1.24
1	A	61	ILE	C-O	-5.08	1.18	1.24
1	A	189	LYS	C-O	-5.08	1.18	1.24
1	A	187	GLY	C-O	-5.08	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	THR	C-O	-5.07	1.18	1.24
1	A	261	TYR	C-O	-5.04	1.18	1.24
1	A	243	VAL	C-O	-5.01	1.18	1.24
1	A	213	GLY	C-O	-5.00	1.17	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	SER	N-CA-C	9.63	121.72	111.03
1	A	207	ARG	N-CA-C	8.68	124.70	108.65
1	A	208	GLY	N-CA-C	-7.57	103.22	111.93
1	A	206	THR	CB-CA-C	5.72	120.94	110.36
1	A	238	LYS	CA-CB-CG	5.15	124.40	114.10
1	A	97	SER	N-CA-C	5.07	112.79	108.22

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	GLY	Peptide
1	A	211	ARG	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	2229	0	2302	42	0
2	A	10	0	4	3	0
3	A	48	0	25	0	0
4	A	4	0	3	1	0
5	A	10	0	0	0	0
6	A	300	0	0	23	0
All	All	2601	0	2334	45	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 10.

All (45) 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)
4:A:303:ACY:H1	6:A:533:HOH:O	1.34	1.24
1:A:209:ALA:HB3	6:A:608:HOH:O	1.41	1.21
1:A:35:LYS:HE3	6:A:429:HOH:O	1.53	1.06
1:A:62:VAL:HG12	6:A:538:HOH:O	1.71	0.89
1:A:245:GLU:O	1:A:249:LYS:HG3	1.76	0.84
1:A:249:LYS:HD2	6:A:616:HOH:O	1.85	0.75
1:A:99:ASP:OD1	1:A:102:ARG:NH2	2.20	0.75
1:A:266:LYS:HE3	6:A:434:HOH:O	1.86	0.73
1:A:188:LEU:HD11	1:A:198:MET:CE	2.19	0.72
1:A:188:LEU:HD11	1:A:198:MET:HE1	1.70	0.72
1:A:192:LYS:HG2	1:A:198:MET:HE2	1.71	0.71
1:A:32:THR:HG22	1:A:34:GLU:HG2	1.73	0.71
1:A:35:LYS:CE	6:A:429:HOH:O	2.25	0.70
1:A:33:ARG:HD3	6:A:628:HOH:O	1.93	0.67
1:A:32:THR:HG22	1:A:34:GLU:CG	2.31	0.61
1:A:188:LEU:CD1	1:A:198:MET:HE1	2.31	0.60
1:A:-10:HIS:CE1	1:A:55:LYS:HE3	2.36	0.60
1:A:235:HIS:HD2	6:A:505:HOH:O	1.84	0.59
2:A:301:TLA:H2	6:A:511:HOH:O	2.01	0.59
1:A:211:ARG:HD3	6:A:524:HOH:O	2.03	0.57
1:A:122:GLY:H	2:A:301:TLA:C4	2.18	0.57
1:A:202:ALA:O	1:A:206:THR:HG23	2.06	0.55
1:A:192:LYS:CG	1:A:198:MET:HE2	2.37	0.55
1:A:110:GLN:HG3	6:A:565:HOH:O	2.06	0.55
1:A:192:LYS:CG	1:A:198:MET:CE	2.84	0.55
1:A:192:LYS:HG3	1:A:198:MET:HE1	1.89	0.55
1:A:208:GLY:N	6:A:404:HOH:O	2.39	0.53
1:A:34:GLU:HG3	6:A:569:HOH:O	2.08	0.52
1:A:250:ARG:HH11	1:A:250:ARG:HG3	1.74	0.51
1:A:249:LYS:HE2	6:A:588:HOH:O	2.11	0.51
1:A:249:LYS:HG2	6:A:588:HOH:O	2.09	0.51
1:A:18:HIS:HE1	1:A:128:ILE:O	1.96	0.48
1:A:258:GLU:HG3	6:A:437:HOH:O	2.13	0.47
1:A:208:GLY:CA	6:A:404:HOH:O	2.64	0.45
1:A:170:LYS:O	1:A:174:GLN:HG2	2.17	0.45
1:A:192:LYS:HG3	1:A:198:MET:CE	2.47	0.44
1:A:258:GLU:HG2	6:A:423:HOH:O	2.19	0.43
1:A:37:LYS:HB3	1:A:38:PRO:HD3	2.01	0.43
1:A:85:ARG:NH2	6:A:410:HOH:O	2.52	0.43
1:A:229:PRO:HA	1:A:230:GLY:HA3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:O	1:A:208:GLY:C	2.61	0.41
1:A:249:LYS:HE3	6:A:616:HOH:O	2.21	0.41
2:A:301:TLA:C4	2:A:301:TLA:O1	2.68	0.40
1:A:208:GLY:HA3	6:A:404:HOH:O	2.21	0.40
1:A:235:HIS:CD2	6:A:505:HOH:O	2.67	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	294/306 (96%)	288 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/236 (96%)	220 (97%)	7 (3%)	35	7

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-12	HIS

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Mol	Chain	Res	Type
1	A	33	ARG
1	A	34	GLU
1	A	110	GLN
1	A	185	VAL
1	A	207	ARG
1	A	224	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-10	HIS
1	A	180	ASN
1	A	235	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	ACY	A	303	-	3,3,3	1.30	1 (33%)	3,3,3	0.83	0
2	TLA	A	301	-	9,9,9	4.40	3 (33%)	12,12,12	3.55	7 (58%)
5	SO4	A	305	-	4,4,4	1.38	1 (25%)	6,6,6	2.44	3 (50%)
3	NAP	A	302	-	50,52,52	1.71	11 (22%)	71,80,80	1.48	9 (12%)
5	SO4	A	304	-	4,4,4	1.97	2 (50%)	6,6,6	2.12	3 (50%)

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	TLA	A	301	-	-	9/12/12/12	-
3	NAP	A	302	-	-	8/35/67/67	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	TLA	C3-C4	-12.21	1.35	1.52
3	A	302	NAP	O7N-C7N	-4.29	1.16	1.24
3	A	302	NAP	C5A-C4A	4.01	1.46	1.39
3	A	302	NAP	P2B-O3X	-3.49	1.41	1.54
3	A	302	NAP	P2B-O1X	-3.25	1.40	1.50
3	A	302	NAP	C2N-N1N	-2.96	1.31	1.35
3	A	302	NAP	O4D-C4D	-2.87	1.38	1.45
2	A	301	TLA	O4-C4	-2.81	1.13	1.22
2	A	301	TLA	O41-C4	-2.76	1.21	1.30
5	A	305	SO4	O1-S	-2.68	1.29	1.44
3	A	302	NAP	PA-O2A	-2.61	1.43	1.55
5	A	304	SO4	O4-S	2.52	1.68	1.48
3	A	302	NAP	C8A-N9A	-2.49	1.33	1.37
3	A	302	NAP	C5A-N7A	-2.24	1.35	1.39
4	A	303	ACY	OXT-C	-2.19	1.20	1.30
3	A	302	NAP	C4A-N9A	-2.14	1.33	1.37
3	A	302	NAP	P2B-O2X	-2.12	1.46	1.54
5	A	304	SO4	O1-S	-2.08	1.32	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	TLA	O11-C1-C2	6.59	131.62	113.31
2	A	301	TLA	O1-C1-C2	-6.23	105.03	121.62
3	A	302	NAP	C5A-C4A-N3A	-6.00	118.46	126.72
2	A	301	TLA	O3-C3-C2	5.64	121.65	110.17
3	A	302	NAP	N3A-C4A-N9A	5.01	135.69	127.17
2	A	301	TLA	C2-C3-C4	-4.11	100.72	109.82
3	A	302	NAP	C4D-O4D-C1D	4.08	113.66	109.92
5	A	305	SO4	O4-S-O1	3.92	130.06	109.56
5	A	304	SO4	O4-S-O1	3.34	127.02	109.56
3	A	302	NAP	C2A-N3A-C4A	3.16	119.55	111.83
5	A	305	SO4	O3-S-O1	-3.12	93.23	109.56
5	A	305	SO4	O4-S-O3	-2.85	92.84	108.54
2	A	301	TLA	O2-C2-C3	2.65	115.55	110.17
5	A	304	SO4	O4-S-O2	-2.62	95.84	109.56
3	A	302	NAP	C3B-C2B-C1B	-2.50	98.02	102.81
2	A	301	TLA	O2-C2-C1	2.41	115.85	110.69
3	A	302	NAP	O3-PA-O1A	-2.21	104.05	110.70
3	A	302	NAP	O2N-PN-O1N	2.10	122.20	112.44
5	A	304	SO4	O3-S-O2	-2.09	98.65	109.56
3	A	302	NAP	N6A-C6A-N1A	2.07	122.99	118.38
3	A	302	NAP	C4A-C5A-N7A	-2.02	108.27	110.58
2	A	301	TLA	O41-C4-O4	2.00	128.63	124.08

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	TLA	O3-C3-C4-O4
3	A	302	NAP	O4D-C1D-N1N-C2N
3	A	302	NAP	O4D-C1D-N1N-C6N
3	A	302	NAP	C2D-C1D-N1N-C2N
3	A	302	NAP	C2D-C1D-N1N-C6N
2	A	301	TLA	O11-C1-C2-O2
2	A	301	TLA	O3-C3-C4-O41
2	A	301	TLA	O1-C1-C2-O2
2	A	301	TLA	C1-C2-C3-O3
2	A	301	TLA	O2-C2-C3-C4
2	A	301	TLA	C1-C2-C3-C4
2	A	301	TLA	O11-C1-C2-C3
3	A	302	NAP	C1B-C2B-O2B-P2B
2	A	301	TLA	O1-C1-C2-C3
3	A	302	NAP	C3B-C2B-O2B-P2B
3	A	302	NAP	C2B-O2B-P2B-O1X

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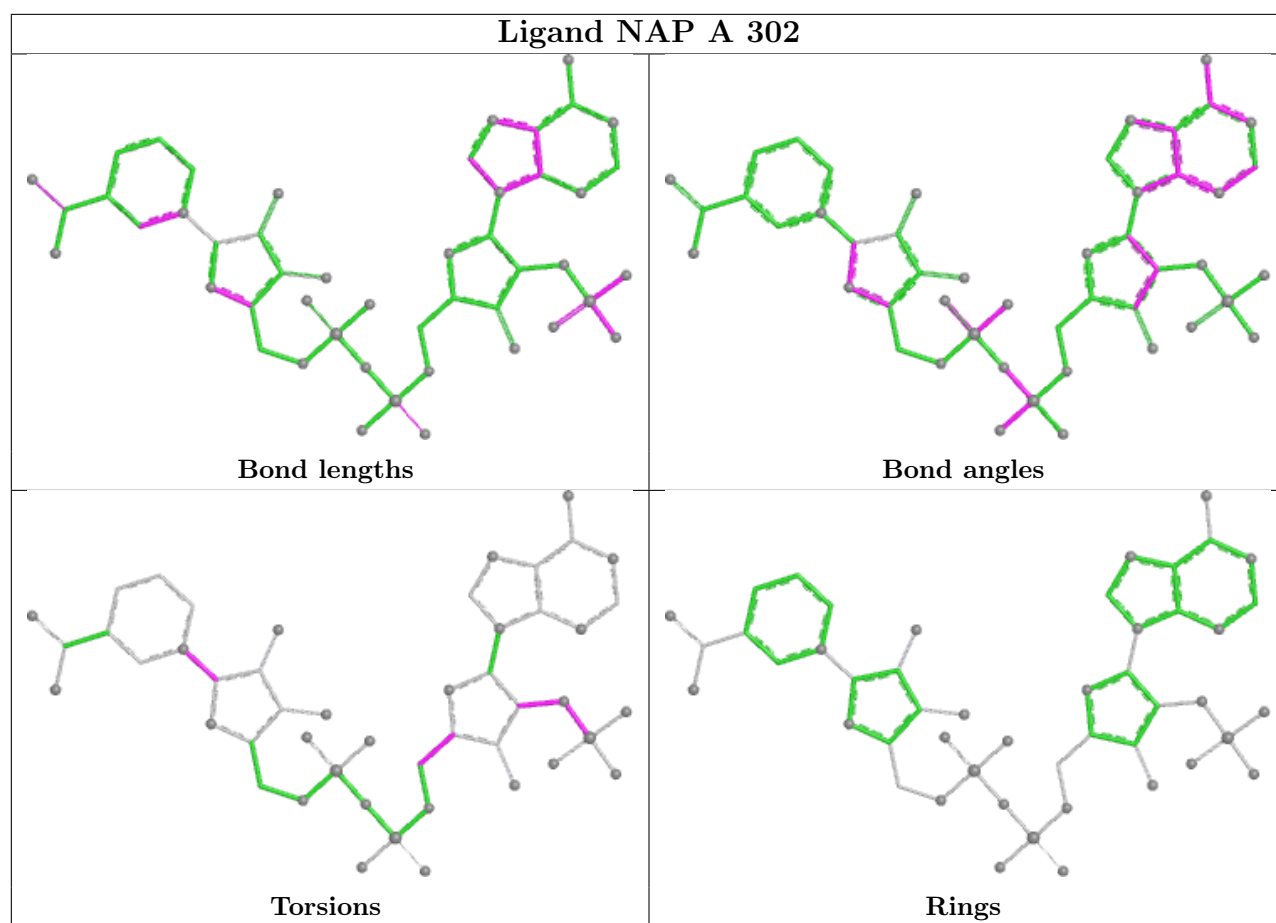
Mol	Chain	Res	Type	Atoms
3	A	302	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	ACY	1	0
2	A	301	TLA	3	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 [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	296/306 (96%)	-0.01	11 (3%) 45 56	8, 12, 25, 39	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	GLY	9.0
1	A	209	ALA	7.5
1	A	207	ARG	4.8
1	A	206	THR	3.8
1	A	-12	HIS	3.3
1	A	211	ARG	3.3
1	A	-3	ARG	2.7
1	A	33	ARG	2.7
1	A	210	ALA	2.5
1	A	85	ARG	2.3
1	A	216	GLU	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 oligosaccharides in this entry.

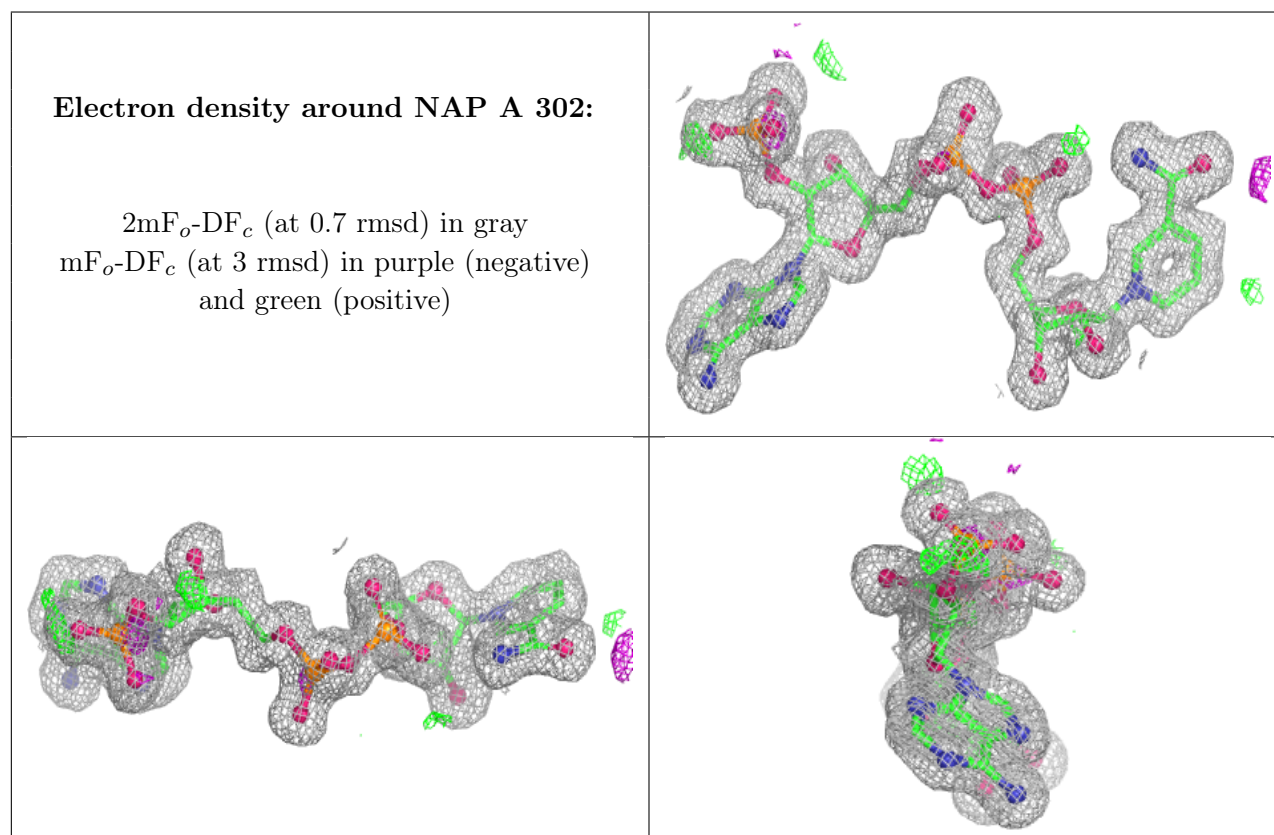
6.4 Ligands [i](#)

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, 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
2	TLA	A	301	10/10	0.77	0.19	25,30,34,37	0
5	SO4	A	304	5/5	0.94	0.10	27,27,31,38	0
5	SO4	A	305	5/5	0.94	0.20	22,22,25,27	0
3	NAP	A	302	48/48	0.98	0.04	7,10,11,12	0
4	ACY	A	303	4/4	0.99	0.04	13,13,14,14	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.