



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:55 PM UTC

PDB ID : 1PGN / pdb_00001pgn
Title : CRYSTALLOGRAPHIC STUDY OF COENZYME, COENZYME ANALOGUE AND SUBSTRATE BINDING IN 6-PHOSPHOGLUCONATE DEHYDROGENASE: IMPLICATIONS FOR NADP SPECIFICITY AND THE ENZYME MECHANISM
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Deposited on : 1994-07-18
Resolution : 2.30 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](#) ①) 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

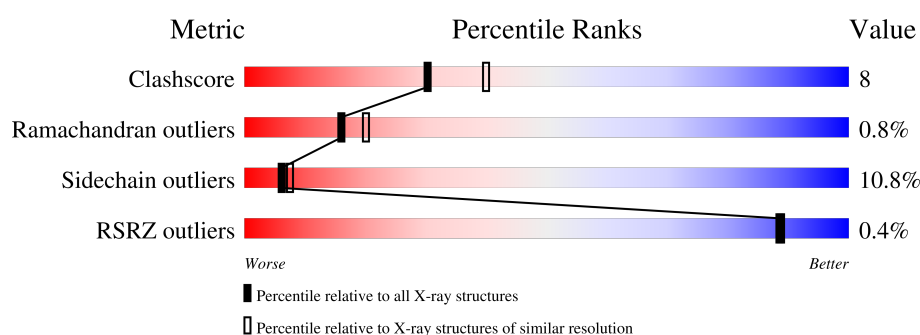
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	482	 67% 26% . . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4142 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.

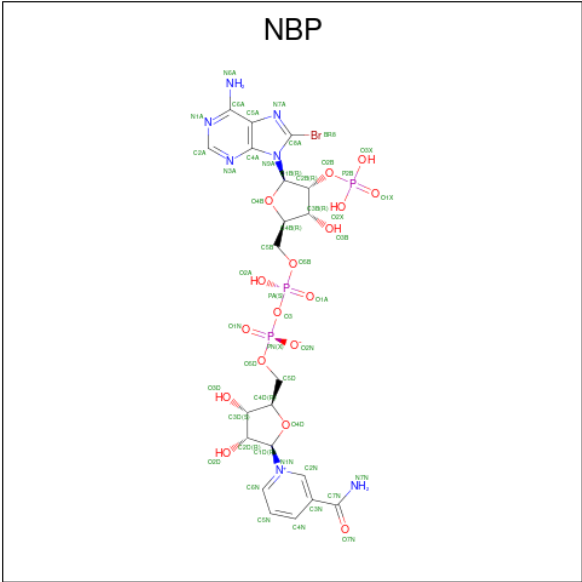
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	473	3654	2332	634	666	22	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is NICOTINAMIDE 8-BROMO-ADENINE DINUCLEOTIDE PHOSPHATE (CCD ID: NBP) (formula: C₂₁H₂₇BrN₇O₁₇P₃).

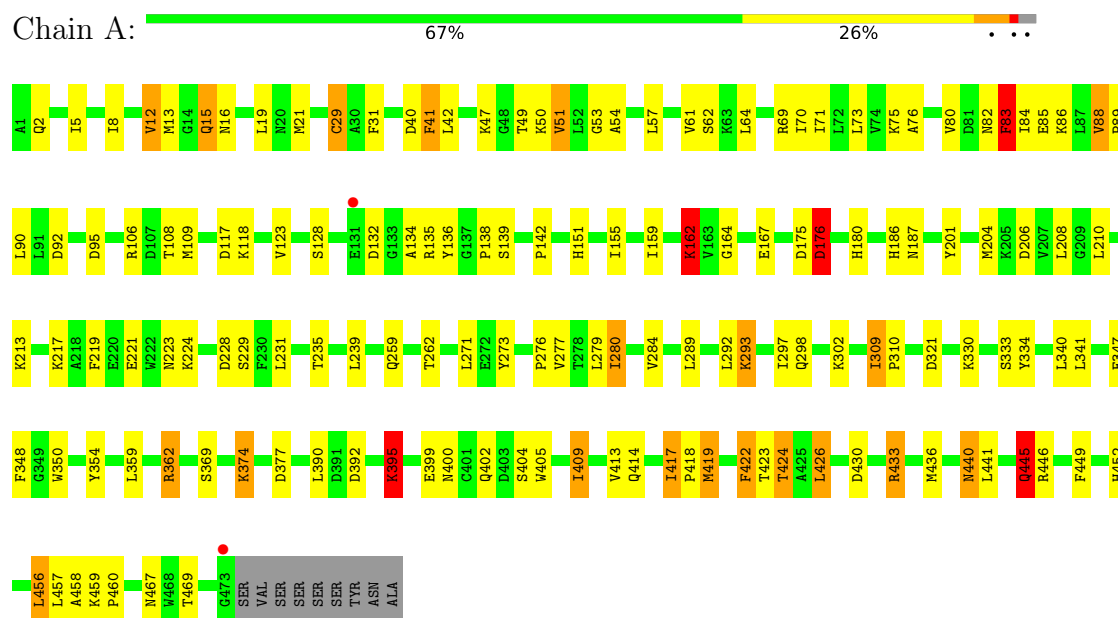


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	420	Total 420	O 420	0	0

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	72.74Å 148.40Å 102.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30 74.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30) 77.3 (74.20-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.30Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.204 , (Not available) 0.202 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 94.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4142	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NBP, POP, 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	0.73	2/3731 (0.1%)	1.64	46/5028 (0.9%)

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	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	VAL	CA-CB	7.07	1.62	1.54
1	A	88	VAL	CA-CB	5.34	1.57	1.54

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ASP	CA-CB-CG	10.62	123.22	112.60
1	A	176	ASP	CA-CB-CG	9.41	122.01	112.60
1	A	433	ARG	CA-CB-CG	8.35	130.81	114.10
1	A	83	PHE	CA-CB-CG	-8.08	105.72	113.80
1	A	458	ALA	N-CA-C	-7.89	99.90	110.55
1	A	64	LEU	N-CA-C	7.61	121.54	110.28
1	A	132	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	155	ILE	N-CA-C	-7.22	104.17	110.74
1	A	395	LYS	CA-CB-CG	7.18	128.45	114.10
1	A	175	ASP	N-CA-C	6.77	118.74	110.41
1	A	75	LYS	O-C-N	6.58	130.77	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	THR	N-CA-C	6.54	118.41	111.28
1	A	15	GLN	N-CA-CB	-6.43	100.69	110.01
1	A	409	ILE	CB-CA-C	-6.43	103.46	112.14
1	A	15	GLN	CA-CB-CG	6.31	126.72	114.10
1	A	40	ASP	CA-CB-CG	6.25	118.86	112.60
1	A	309	ILE	N-CA-C	-6.24	100.19	107.61
1	A	151	HIS	CA-CB-CG	-6.19	107.61	113.80
1	A	440	ASN	CA-CB-CG	6.10	118.70	112.60
1	A	377	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	259	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	A	467	ASN	N-CA-C	-5.85	99.00	108.41
1	A	452	HIS	N-CA-C	5.78	119.59	112.54
1	A	41	PHE	CA-CB-CG	5.73	119.53	113.80
1	A	29	CYS	N-CA-C	-5.71	99.11	108.41
1	A	228	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	162	LYS	CA-CB-CG	5.65	125.39	114.10
1	A	433	ARG	CB-CA-C	-5.63	100.22	110.63
1	A	139	SER	CA-CB-OG	5.61	122.33	111.10
1	A	118	LYS	CA-CB-CG	-5.53	103.05	114.10
1	A	206	ASP	N-CA-C	5.53	118.23	111.82
1	A	277	VAL	N-CA-CB	-5.52	106.76	112.28
1	A	426	LEU	N-CA-C	-5.51	104.92	111.69
1	A	82	ASN	CA-CB-CG	-5.50	107.10	112.60
1	A	139	SER	N-CA-C	-5.49	100.74	109.59
1	A	440	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	A	445	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	A	422	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	417	ILE	CA-C-O	5.36	122.31	119.15
1	A	223	ASN	CB-CG-ND2	5.30	124.36	116.40
1	A	424	THR	CB-CA-C	-5.26	100.90	110.63
1	A	419	MET	CA-C-N	5.25	124.70	119.24
1	A	419	MET	C-N-CA	5.25	124.70	119.24
1	A	423	THR	CA-C-O	-5.16	115.38	120.70
1	A	95	ASP	O-C-N	5.04	128.59	122.85
1	A	50	LYS	CG-CD-CE	-5.01	99.76	111.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	TYR	Sidechain
1	A	273	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	354	TYR	Sidechain
1	A	83	PHE	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	3654	0	3661	62	0
2	A	10	0	0	0	0
3	A	49	0	24	3	0
4	A	9	0	0	1	0
5	A	420	0	0	10	0
All	All	4142	0	3685	62	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 (62) 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:229:SER:HB3	1:A:369:SER:HB3	1.60	0.83
1:A:362:ARG:HH11	1:A:362:ARG:HG2	1.52	0.75
1:A:5:ILE:HG21	1:A:21:MET:HE1	1.76	0.66
1:A:83:PHE:CE2	3:A:499:NBP:H2A	2.32	0.64
1:A:204:MET:HE1	1:A:219:PHE:CE2	2.32	0.64
1:A:430:ASP:HA	1:A:433:ARG:HD3	1.81	0.63
1:A:436:MET:HE3	1:A:440:ASN:ND2	2.15	0.61
1:A:108:THR:OG1	1:A:180:HIS:HD2	1.83	0.60
1:A:128:SER:HA	4:A:506:POP:O5	2.02	0.59
1:A:83:PHE:HE2	3:A:499:NBP:H2A	1.67	0.59
1:A:405:TRP:O	1:A:409:ILE:HG12	2.01	0.59
1:A:446:ARG:HG2	1:A:446:ARG:HH11	1.70	0.57
1:A:229:SER:CB	1:A:369:SER:HB3	2.35	0.56
1:A:109:MET:HE1	1:A:348:PHE:CD1	2.42	0.55
1:A:13:MET:HE3	1:A:134:ALA:HB2	1.88	0.55
1:A:369:SER:HB2	5:A:606:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:THR:OG1	1:A:51:VAL:HG12	2.08	0.53
1:A:29:CYS:SG	1:A:54:ALA:HB2	2.49	0.53
1:A:109:MET:HG2	1:A:176:ASP:HB3	1.90	0.52
1:A:15:GLN:HG3	1:A:41:PHE:CE1	2.44	0.52
1:A:399:GLU:HA	1:A:402:GLN:HG2	1.91	0.52
1:A:57:LEU:HD21	1:A:83:PHE:HE1	1.74	0.52
1:A:57:LEU:O	1:A:61:VAL:HG23	2.10	0.51
1:A:459:LYS:N	1:A:460:PRO:HD3	2.25	0.51
1:A:279:LEU:HD13	1:A:333:SER:HB2	1.94	0.49
1:A:42:LEU:HD11	1:A:53:GLY:HA3	1.95	0.49
1:A:449:PHE:HA	5:A:841:HOH:O	2.10	0.49
1:A:280:ILE:O	1:A:284:VAL:HG23	2.12	0.49
1:A:86:LYS:O	1:A:89:PRO:HD2	2.13	0.48
1:A:231:LEU:HB2	5:A:605:HOH:O	2.12	0.48
1:A:16:ASN:HD22	1:A:135:ARG:HD3	1.78	0.47
1:A:213:LYS:HG3	5:A:636:HOH:O	2.14	0.47
1:A:392:ASP:HA	1:A:395:LYS:HG3	1.96	0.47
1:A:12:VAL:HG23	3:A:499:NBP:O7N	2.14	0.47
1:A:441:LEU:O	1:A:445:GLN:HG2	2.14	0.47
1:A:5:ILE:HD11	1:A:71:ILE:HD11	1.96	0.47
1:A:350:TRP:HA	5:A:598:HOH:O	2.15	0.47
1:A:419:MET:HB3	1:A:422:PHE:HB2	1.97	0.46
1:A:89:PRO:HB2	1:A:90:LEU:HD22	1.97	0.46
1:A:162:LYS:HA	1:A:167:GLU:O	2.17	0.45
1:A:186:HIS:HD2	1:A:187:ASN:OD1	2.00	0.44
1:A:374:LYS:N	1:A:374:LYS:HD2	2.32	0.44
1:A:84:ILE:O	1:A:88:VAL:HG23	2.16	0.44
1:A:47:LYS:HA	5:A:537:HOH:O	2.17	0.44
1:A:330:LYS:O	1:A:334:TYR:HD1	2.00	0.44
1:A:302:LYS:HD2	5:A:1146:HOH:O	2.18	0.43
1:A:106:ARG:HB2	5:A:1086:HOH:O	2.19	0.42
1:A:280:ILE:HD13	1:A:280:ILE:N	2.35	0.42
1:A:456:LEU:HD12	1:A:456:LEU:HA	1.88	0.42
1:A:90:LEU:HD12	5:A:767:HOH:O	2.20	0.42
1:A:321:ASP:HA	1:A:404:SER:HB3	2.00	0.42
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.80	0.41
1:A:293:LYS:HE2	1:A:297:ILE:HD11	2.02	0.41
1:A:417:ILE:HA	1:A:418:PRO:HD2	1.87	0.41
1:A:235:THR:O	1:A:239:LEU:HD13	2.20	0.41
1:A:80:VAL:O	1:A:84:ILE:HG13	2.21	0.41
1:A:409:ILE:HD12	1:A:422:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:TYR:HA	1:A:204:MET:HE3	2.02	0.41
1:A:309:ILE:HB	5:A:1131:HOH:O	2.21	0.41
1:A:409:ILE:O	1:A:413:VAL:HG23	2.20	0.41
1:A:8:ILE:HG12	1:A:31:PHE:HB3	2.03	0.40
1:A:21:MET:HG2	1:A:159:ILE:HG21	2.04	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	471/482 (98%)	437 (93%)	30 (6%)	4 (1%)	16 20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	GLY
1	A	469	THR
1	A	76	ALA
1	A	310	PRO

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	378/386 (98%)	337 (89%)	41 (11%)	6 7

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	12	VAL
1	A	19	LEU
1	A	62	SER
1	A	69	ARG
1	A	70	ILE
1	A	83	PHE
1	A	85	GLU
1	A	92	ASP
1	A	123	VAL
1	A	138	PRO
1	A	142	PRO
1	A	162	LYS
1	A	176	ASP
1	A	208	LEU
1	A	210	LEU
1	A	217	LYS
1	A	221	GLU
1	A	224	LYS
1	A	271	LEU
1	A	276	PRO
1	A	280	ILE
1	A	289	LEU
1	A	292	LEU
1	A	293	LYS
1	A	298	GLN
1	A	340	LEU
1	A	341	LEU
1	A	347	GLU
1	A	359	LEU
1	A	362	ARG
1	A	374	LYS
1	A	390	LEU
1	A	395	LYS
1	A	400	ASN
1	A	414	GLN
1	A	424	THR
1	A	426	LEU

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Mol	Chain	Res	Type
1	A	445	GLN
1	A	456	LEU
1	A	457	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	102	ASN
1	A	151	HIS
1	A	180	HIS
1	A	186	HIS
1	A	298	GLN
1	A	440	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	POP	A	506	-	6,8,8	1.20	0	12,13,13	2.47	2 (16%)
2	SO4	A	508	-	4,4,4	0.62	0	6,6,6	0.27	0
3	NBP	A	499	-	51,53,53	1.66	8 (15%)	71,82,82	2.25	14 (19%)
2	SO4	A	505	-	4,4,4	0.70	0	6,6,6	0.26	0

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	POP	A	506	-	-	0/6/6/6	-
3	NBP	A	499	-	-	10/35/67/67	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	499	NBP	C2N-N1N	6.57	1.42	1.35
3	A	499	NBP	C5A-N7A	-4.10	1.32	1.39
3	A	499	NBP	O4D-C1D	4.09	1.46	1.40
3	A	499	NBP	C8A-N9A	-3.19	1.33	1.38
3	A	499	NBP	C6N-N1N	2.93	1.42	1.35
3	A	499	NBP	C8A-N7A	2.58	1.34	1.29
3	A	499	NBP	C4A-N9A	-2.42	1.35	1.38
3	A	499	NBP	C3N-C7N	2.32	1.54	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	499	NBP	C6A-C5A-N7A	-7.88	123.92	131.72
3	A	499	NBP	N3A-C4A-N9A	7.87	138.68	127.33
3	A	499	NBP	C5A-C4A-N3A	-6.37	117.94	126.72
3	A	499	NBP	N9A-C8A-N7A	-5.93	110.44	115.04
4	A	506	POP	O2-P1-O	-5.78	85.26	104.64
4	A	506	POP	O3-P1-O	5.14	121.87	104.64
3	A	499	NBP	C6A-C5A-C4A	4.16	122.86	117.18
3	A	499	NBP	C6N-N1N-C2N	-3.88	118.58	121.88
3	A	499	NBP	N3A-C2A-N1A	-3.74	122.93	128.58
3	A	499	NBP	C5A-C4A-N9A	-3.68	103.31	105.63
3	A	499	NBP	P2B-O2B-C2B	-3.58	113.86	123.43
3	A	499	NBP	O4B-C1B-C2B	-3.25	100.99	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	499	NBP	C2A-N3A-C4A	3.19	119.63	111.83
3	A	499	NBP	BR8-C8A-N9A	2.77	124.72	121.97
3	A	499	NBP	C4A-C5A-N7A	2.14	113.11	110.91
3	A	499	NBP	O7N-C7N-C3N	2.13	122.20	119.60

There are no chirality outliers.

All (10) torsion outliers are listed below:

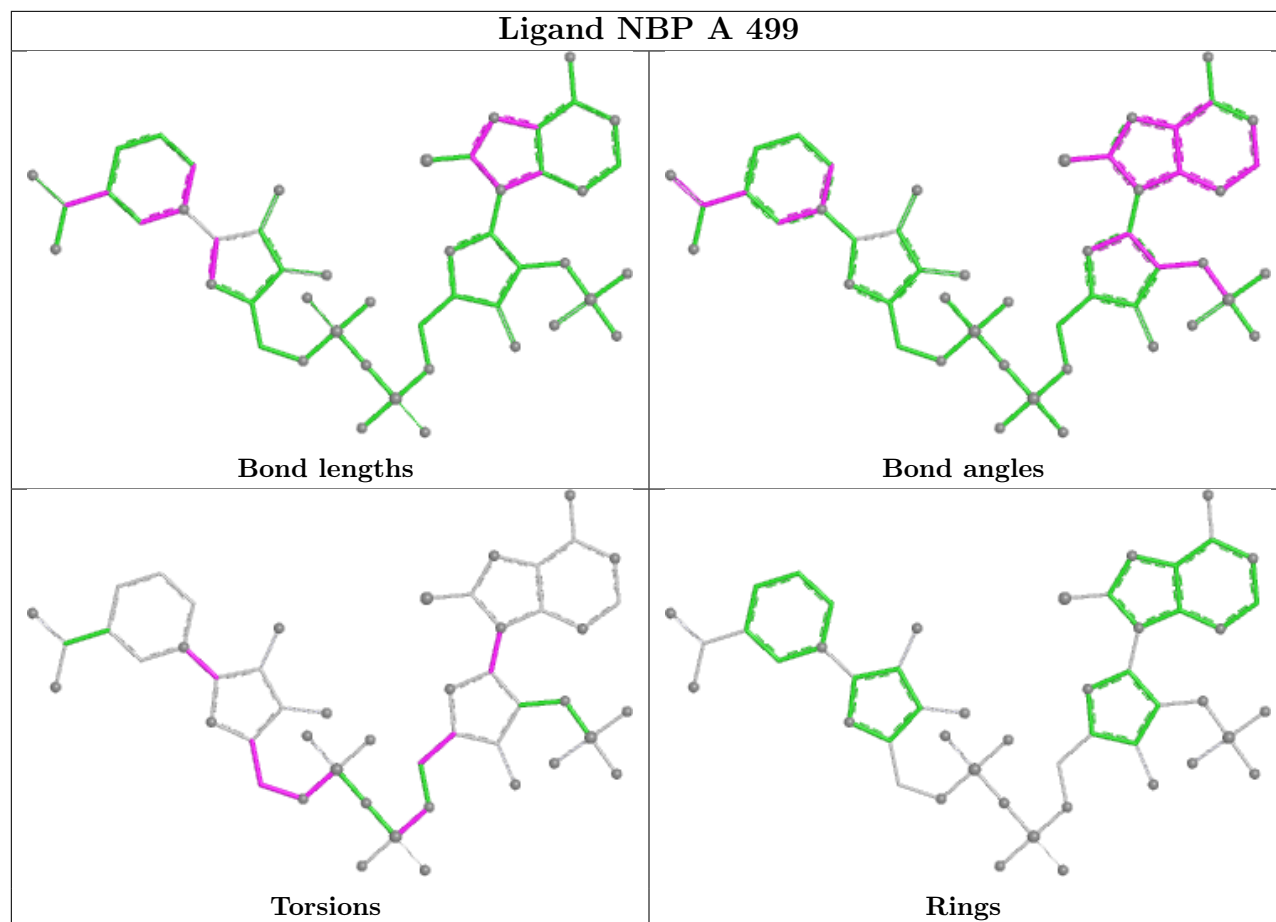
Mol	Chain	Res	Type	Atoms
3	A	499	NBP	C5B-O5B-PA-O1A
3	A	499	NBP	C5B-O5B-PA-O2A
3	A	499	NBP	C5B-O5B-PA-O3
3	A	499	NBP	C2D-C1D-N1N-C2N
3	A	499	NBP	O4D-C4D-C5D-O5D
3	A	499	NBP	C3D-C4D-C5D-O5D
3	A	499	NBP	C4D-C5D-O5D-PN
3	A	499	NBP	C5D-O5D-PN-O1N
3	A	499	NBP	O4B-C1B-N9A-C8A
3	A	499	NBP	C3B-C4B-C5B-O5B

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	506	POP	1	0
3	A	499	NBP	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	473/482 (98%)	-0.04	2 (0%) 88 89	12, 33, 47, 64	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	473	GLY	2.6
1	A	131	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.

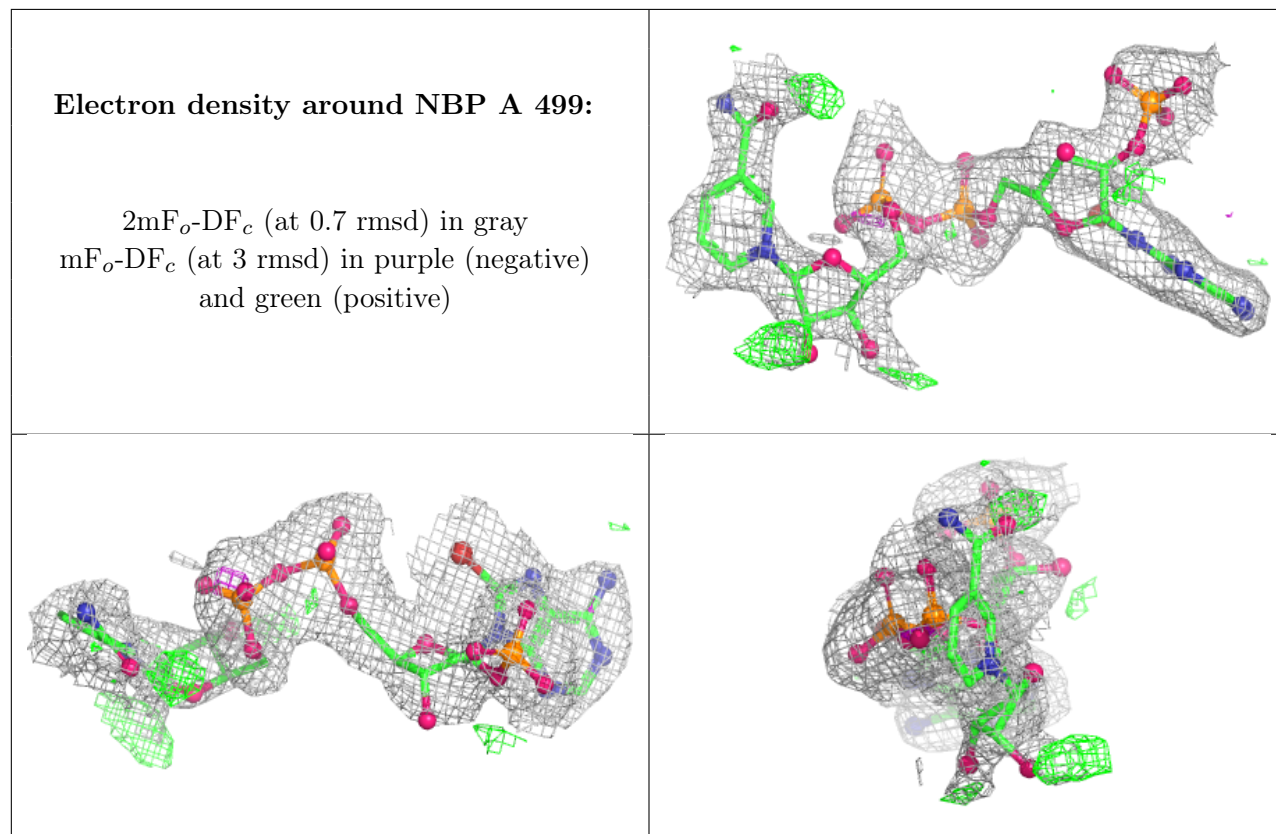
6.4 Ligands [i](#)

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	SO4	A	508	5/5	0.88	0.14	57,58,58,58	0
3	NBP	A	499	49/49	0.91	0.12	29,39,47,49	48
4	POP	A	506	9/9	0.91	0.10	55,59,60,60	0
2	SO4	A	505	5/5	0.96	0.07	31,35,36,38	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 [i](#)

There are no such residues in this entry.