



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:42 PM UTC

PDB ID : 1CX9 / pdb_00001cx9
Title : CRYSTAL STRUCTURE OF THE COMPLEX OF BACTERIAL TRYPTOPHAN SYNTHASE WITH THE TRANSITION STATE ANALOGUE INHIBITOR 4-(2-AMINOPHENYLTHIO)-BUTYLPHOSPHONIC ACID
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Deposited on : 1999-08-29
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

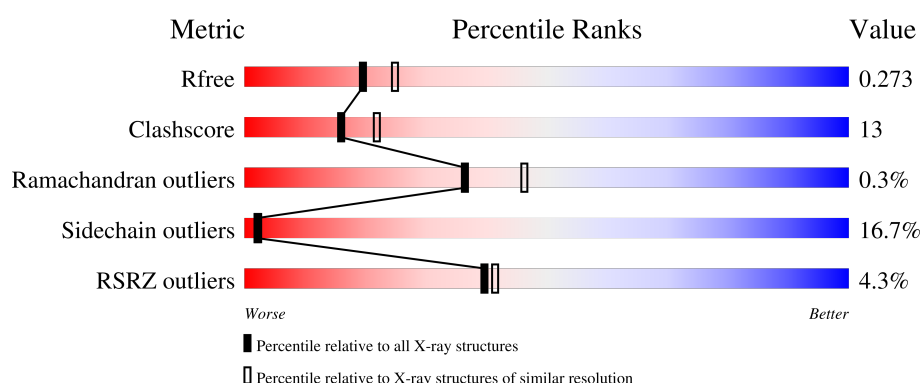
1 Overall quality at a glance

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))
R_{free}	180053	6319 (2.30-2.30)
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	268	7% 65% 26% 6%
2	B	397	2% 65% 24% 7%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5115 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.

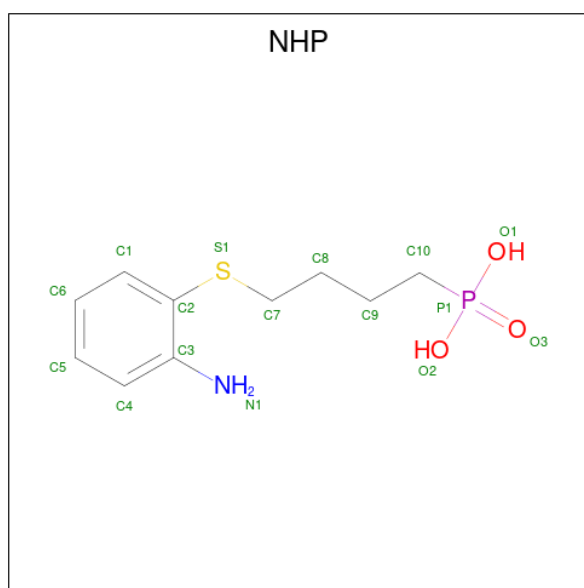
- Molecule 1 is a protein called TRYPTOPHAN SYNTHASE (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			1992	1264	348	373	7			

- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	387	Total	C	N	O	S	0	0	0
			2934	1843	516	556	19			

- Molecule 3 is 4-(2-AMINOPHENYLTHIO)-BUTYLPHOSPHONIC ACID (CCD ID: NHP) (formula: C₁₀H₁₆NO₃PS).

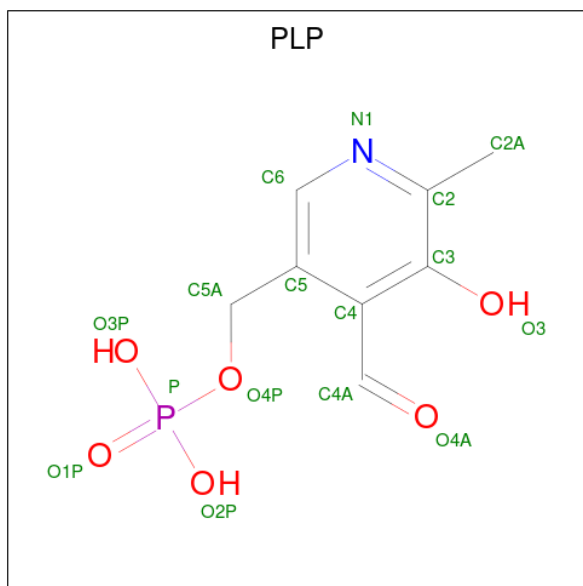


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			16	10	1	3	1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

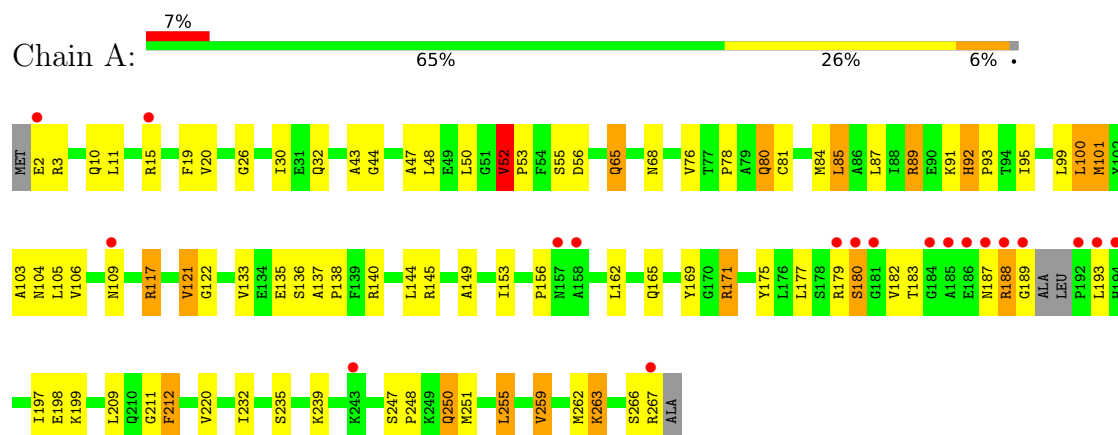
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	52	Total	O	0	0
			52	52		
6	B	105	Total	O	0	0
			105	105		

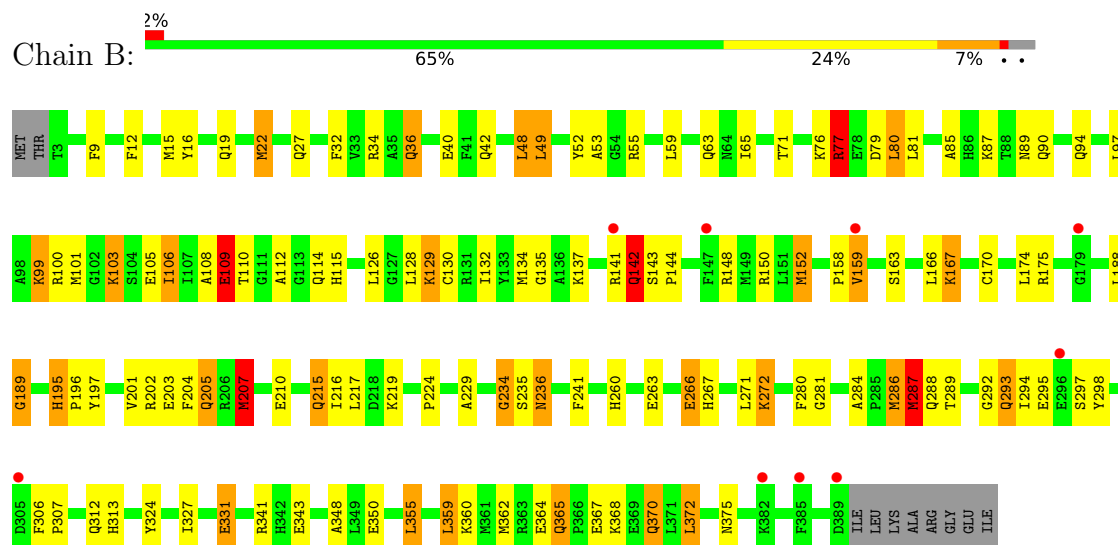
3 Residue-property plots

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: TRYPTOPHAN SYNTHASE (ALPHA CHAIN)



• Molecule 2: TRYPTOPHAN SYNTHASE (BETA CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.65Å 59.34Å 67.30Å 90.00° 94.50° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-2.30) 92.0 (30.00-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.27Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.210 , 0.276 0.210 , 0.273	Depositor DCC
R_{free} test set	3036 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.7	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	0.92	EDS
Total number of atoms	5115	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% 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: PLP, NHP, NA

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	0.57	0/2031	1.14	11/2757 (0.4%)
2	B	0.61	0/2992	1.19	22/4042 (0.5%)
All	All	0.59	0/5023	1.17	33/6799 (0.5%)

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
2	B	0	1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	341	ARG	N-CA-C	7.79	120.86	111.82
1	A	180	SER	N-CA-C	-7.05	99.80	109.95
1	A	103	ALA	N-CA-C	7.03	119.55	111.11
1	A	92	HIS	CA-C-N	7.02	126.63	119.19
1	A	92	HIS	C-N-CA	7.02	126.63	119.19
2	B	195	HIS	N-CA-C	-6.87	100.29	109.84
2	B	286	MET	N-CA-C	6.75	119.59	108.99
2	B	77	ARG	N-CA-C	6.54	119.79	109.39
2	B	207	MET	CB-CA-C	-6.33	100.67	110.81
2	B	12	PHE	N-CA-C	6.20	120.38	109.96
2	B	235	SER	N-CA-C	6.16	118.07	111.36
1	A	136	SER	N-CA-C	6.14	120.61	113.18
1	A	93	PRO	N-CA-C	5.95	121.36	113.57
1	A	44	GLY	N-CA-C	5.81	123.15	114.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	197	TYR	N-CA-C	5.78	121.36	113.16
2	B	234	GLY	N-CA-C	5.55	123.00	115.00
2	B	241	PHE	N-CA-C	5.50	116.96	111.07
2	B	130	CYS	N-CA-C	5.45	117.84	109.07
2	B	284	ALA	N-CA-C	5.42	113.10	108.22
1	A	65	GLN	N-CA-C	-5.37	105.33	111.07
2	B	109	GLU	N-CA-CB	-5.22	102.38	110.57
2	B	350	GLU	N-CA-C	-5.20	105.53	111.14
2	B	287	MET	N-CA-C	-5.19	99.31	108.23
2	B	114	GLN	N-CA-C	5.18	116.93	111.28
2	B	289	THR	N-CA-C	-5.18	103.08	110.59
2	B	306	PHE	CA-C-N	5.16	126.29	119.84
2	B	306	PHE	C-N-CA	5.16	126.29	119.84
2	B	348	ALA	N-CA-C	-5.14	103.25	110.50
1	A	100	LEU	N-CA-C	-5.10	100.41	108.73
2	B	189	GLY	N-CA-C	5.09	123.96	115.66
1	A	52	VAL	CA-C-N	5.08	126.19	119.84
1	A	52	VAL	C-N-CA	5.08	126.19	119.84
2	B	142	GLN	N-CA-C	5.02	116.46	110.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	298	TYR	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	1992	0	1995	59	0
2	B	2934	0	2902	76	0
3	A	16	0	14	4	0
4	B	1	0	0	0	0
5	B	15	0	7	0	0
6	A	52	0	0	2	0
6	B	105	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5115	0	4918	130	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 13.

All (130) 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:89:ARG:HD2	1:A:122:GLY:HA3	1.53	0.90
1:A:182:VAL:HG11	2:B:175:ARG:HG2	1.56	0.84
2:B:135:GLY:HA2	2:B:159:VAL:HG22	1.64	0.80
1:A:133:VAL:H	2:B:19:GLN:HE22	1.29	0.79
1:A:183:THR:HB	3:A:270:NHP:H101	1.66	0.77
1:A:89:ARG:HG3	1:A:89:ARG:HH21	1.51	0.76
2:B:202:ARG:HH21	2:B:312:GLN:HE22	1.32	0.76
2:B:202:ARG:HD3	2:B:312:GLN:HE22	1.51	0.75
2:B:77:ARG:HG2	2:B:80:LEU:HD22	1.68	0.74
2:B:15:MET:HB3	2:B:22:MET:HE1	1.68	0.72
2:B:267:HIS:CE1	2:B:287:MET:HE1	2.24	0.71
2:B:142:GLN:HG3	6:B:1071:HOH:O	1.90	0.70
2:B:112:ALA:O	2:B:142:GLN:HG2	1.93	0.69
2:B:89:ASN:HD22	2:B:205:GLN:NE2	1.91	0.69
2:B:202:ARG:HH21	2:B:312:GLN:NE2	1.90	0.69
2:B:108:ALA:HB3	2:B:132:ILE:HG12	1.72	0.69
2:B:327:ILE:HG23	2:B:331:GLU:HB3	1.75	0.68
2:B:89:ASN:HB2	2:B:205:GLN:HE22	1.60	0.67
2:B:87:LYS:HG2	6:B:1046:HOH:O	1.95	0.66
1:A:255:LEU:O	1:A:259:VAL:HG13	1.97	0.65
2:B:99:LYS:NZ	2:B:126:LEU:HB3	2.10	0.65
1:A:211:GLY:O	1:A:212:PHE:HB2	1.95	0.64
2:B:134:MET:O	2:B:158:PRO:HA	2.00	0.62
2:B:77:ARG:HG3	2:B:79:ASP:OD2	2.00	0.61
1:A:179:ARG:HG3	1:A:189:GLY:HA2	1.80	0.61
2:B:216:ILE:HG21	2:B:224:PRO:HD3	1.83	0.61
1:A:212:PHE:HA	3:A:270:NHP:O3	2.01	0.60
1:A:85:LEU:HB3	1:A:121:VAL:CG1	2.32	0.60
1:A:183:THR:HG22	1:A:212:PHE:CE2	2.38	0.59
1:A:53:PRO:HA	1:A:68:ASN:HD22	1.67	0.59
2:B:288:GLN:HE21	2:B:292:GLY:HA2	1.67	0.59
2:B:109:GLU:O	2:B:115:HIS:HD2	1.87	0.58
2:B:59:LEU:HD22	2:B:215:GLN:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:ASN:HD22	2:B:205:GLN:HE22	1.51	0.57
1:A:43:ALA:HB3	1:A:259:VAL:HG22	1.85	0.57
2:B:137:LYS:O	2:B:141:ARG:HB2	2.04	0.57
2:B:106:ILE:HD13	2:B:128:LEU:HD13	1.86	0.57
1:A:55:SER:HB3	2:B:293:GLN:HG3	1.86	0.56
2:B:106:ILE:CD1	2:B:128:LEU:HD13	2.37	0.55
1:A:140:ARG:HD2	1:A:169:TYR:HB3	1.87	0.55
1:A:248:PRO:HA	1:A:251:MET:HE3	1.87	0.55
1:A:56:ASP:OD2	2:B:167:LYS:HD3	2.08	0.54
2:B:236:ASN:HD22	2:B:375:ASN:HD22	1.56	0.54
2:B:137:LYS:HE2	2:B:163:SER:O	2.08	0.54
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.90	0.54
1:A:52:VAL:CG2	1:A:101:MET:HE1	2.38	0.52
1:A:76:VAL:HA	1:A:80:GLN:HE21	1.74	0.52
1:A:149:ALA:HB1	1:A:171:ARG:HB3	1.91	0.52
2:B:77:ARG:CG	2:B:80:LEU:HD22	2.39	0.52
1:A:104:ASN:HD21	2:B:288:GLN:NE2	2.07	0.52
1:A:78:PRO:HD3	6:B:1036:HOH:O	2.11	0.51
1:A:53:PRO:HA	1:A:68:ASN:ND2	2.26	0.50
2:B:297:SER:OG	2:B:307:PRO:HA	2.12	0.50
2:B:355:LEU:HD22	2:B:359:LEU:HD13	1.93	0.50
2:B:272:LYS:HD3	2:B:324:TYR:HB2	1.92	0.50
2:B:15:MET:CB	2:B:22:MET:HE1	2.38	0.50
2:B:260:HIS:HD2	2:B:266:GLU:HG2	1.77	0.49
2:B:32:PHE:O	2:B:36:GLN:HB2	2.12	0.49
1:A:43:ALA:CB	1:A:259:VAL:HG22	2.43	0.49
1:A:153:ILE:HD11	3:A:270:NHP:H6	1.94	0.49
1:A:263:LYS:HE2	1:A:266:SER:OG	2.13	0.49
1:A:85:LEU:HB3	1:A:121:VAL:HG11	1.93	0.49
1:A:89:ARG:HG3	1:A:89:ARG:NH2	2.20	0.49
2:B:370:GLN:HG2	6:B:1122:HOH:O	2.12	0.49
2:B:234:GLY:O	2:B:313:HIS:HE1	1.95	0.48
2:B:89:ASN:HB2	2:B:205:GLN:NE2	2.28	0.48
2:B:313:HIS:HD2	2:B:324:TYR:OH	1.96	0.48
1:A:117:ARG:NH2	6:A:1114:HOH:O	2.45	0.48
2:B:148:ARG:O	2:B:152:MET:HE2	2.13	0.48
2:B:204:PHE:C	2:B:207:MET:HE1	2.39	0.47
2:B:263:GLU:H	2:B:263:GLU:CD	2.22	0.47
2:B:16:TYR:O	2:B:281:GLY:HA2	2.13	0.47
2:B:71:THR:CB	2:B:362:MET:HG3	2.44	0.47
1:A:52:VAL:HG21	1:A:101:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:LEU:O	2:B:53:ALA:HB3	2.15	0.47
1:A:177:LEU:HD21	6:B:1125:HOH:O	2.15	0.47
1:A:235:SER:O	1:A:239:LYS:HB2	2.14	0.46
2:B:71:THR:OG1	2:B:362:MET:HG3	2.15	0.46
1:A:89:ARG:NH1	1:A:95:ILE:O	2.48	0.46
1:A:100:LEU:C	1:A:100:LEU:HD13	2.40	0.46
2:B:110:THR:HG23	2:B:134:MET:HG3	1.98	0.46
1:A:91:LYS:HB3	1:A:92:HIS:CD2	2.51	0.46
2:B:195:HIS:HD2	6:B:1006:HOH:O	2.00	0.46
2:B:48:LEU:O	2:B:52:TYR:HB3	2.16	0.45
2:B:205:GLN:NE2	2:B:205:GLN:HA	2.31	0.45
1:A:89:ARG:NH2	1:A:92:HIS:O	2.49	0.45
1:A:193:LEU:O	1:A:197:ILE:HG13	2.17	0.45
2:B:109:GLU:HG3	2:B:170:CYS:SG	2.57	0.45
1:A:20:VAL:HG22	1:A:47:ALA:HB3	1.99	0.45
2:B:109:GLU:OE2	2:B:170:CYS:SG	2.72	0.45
1:A:175:TYR:OH	3:A:270:NHP:H72	2.17	0.45
2:B:76:LYS:HA	2:B:76:LYS:HD2	1.53	0.44
1:A:52:VAL:CG1	1:A:101:MET:HE1	2.47	0.44
2:B:195:HIS:CD2	2:B:196:PRO:HA	2.51	0.44
2:B:229:ALA:HB1	2:B:236:ASN:HD21	1.83	0.44
1:A:19:PHE:CE1	1:A:262:MET:HG2	2.53	0.44
2:B:27:GLN:HE22	2:B:103:LYS:NZ	2.16	0.44
2:B:34:ARG:HG2	2:B:100:ARG:HH11	1.83	0.44
2:B:167:LYS:NZ	2:B:294:ILE:O	2.50	0.44
2:B:9:PHE:CD2	2:B:312:GLN:HG3	2.53	0.43
2:B:81:LEU:HD23	2:B:85:ALA:O	2.17	0.43
1:A:30:ILE:HD11	1:A:80:GLN:HG2	1.99	0.43
2:B:135:GLY:CA	2:B:159:VAL:HG22	2.42	0.43
1:A:85:LEU:HB3	1:A:121:VAL:HG13	2.00	0.43
1:A:137:ALA:HB3	1:A:138:PRO:CD	2.48	0.43
2:B:129:LYS:HE3	2:B:129:LYS:HB2	1.79	0.43
2:B:143:SER:HB2	2:B:144:PRO:HD3	2.01	0.43
2:B:271:LEU:HD12	2:B:271:LEU:O	2.18	0.43
1:A:81:CYS:O	1:A:84:MET:HB2	2.19	0.43
1:A:19:PHE:CZ	1:A:262:MET:HG2	2.54	0.43
1:A:145:ARG:NH1	6:A:1057:HOH:O	2.51	0.43
1:A:43:ALA:HB3	1:A:259:VAL:CG2	2.49	0.42
1:A:188:ARG:HB3	1:A:189:GLY:H	1.67	0.42
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.54	0.42
2:B:365:GLN:NE2	6:B:1016:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:VAL:O	1:A:232:ILE:HA	2.19	0.42
1:A:199:LYS:HD2	1:A:199:LYS:HA	1.79	0.42
2:B:201:VAL:O	2:B:205:GLN:HB2	2.20	0.42
1:A:52:VAL:HA	1:A:53:PRO:HD3	1.92	0.41
1:A:156:PRO:HD3	1:A:177:LEU:HB3	2.02	0.41
1:A:211:GLY:O	1:A:212:PHE:CB	2.68	0.41
1:A:247:SER:HB2	1:A:250:GLN:HB2	2.03	0.41
2:B:87:LYS:HD3	2:B:115:HIS:HA	2.01	0.41
2:B:100:ARG:HH21	2:B:100:ARG:HG3	1.85	0.41
2:B:360:LYS:O	2:B:364:GLU:HB2	2.20	0.41
1:A:2:GLU:O	1:A:2:GLU:HG2	2.21	0.41
2:B:71:THR:HG23	2:B:372:LEU:HD22	2.03	0.41
1:A:30:ILE:CD1	1:A:80:GLN:HG2	2.51	0.40
2:B:174:LEU:HD11	2:B:280:PHE:CE1	2.57	0.40
1:A:20:VAL:HG21	1:A:209:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

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	260/268 (97%)	247 (95%)	11 (4%)	2 (1%)	16	20
2	B	385/397 (97%)	372 (97%)	13 (3%)	0	100	100
All	All	645/665 (97%)	619 (96%)	24 (4%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE
1	A	188	ARG

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	206/208 (99%)	172 (84%)	34 (16%)	2	2
2	B	303/311 (97%)	252 (83%)	51 (17%)	2	2
All	All	509/519 (98%)	424 (83%)	85 (17%)	2	2

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	10	GLN
1	A	11	LEU
1	A	15	ARG
1	A	32	GLN
1	A	48	LEU
1	A	50	LEU
1	A	52	VAL
1	A	65	GLN
1	A	80	GLN
1	A	85	LEU
1	A	87	LEU
1	A	89	ARG
1	A	99	LEU
1	A	101	MET
1	A	105	LEU
1	A	106	VAL
1	A	109	ASN
1	A	117	ARG
1	A	121	VAL
1	A	135	GLU
1	A	144	LEU
1	A	162	LEU
1	A	165	GLN
1	A	171	ARG
1	A	180	SER
1	A	187	ASN

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Mol	Chain	Res	Type
1	A	198	GLU
1	A	220	VAL
1	A	250	GLN
1	A	255	LEU
1	A	259	VAL
1	A	263	LYS
1	A	267	ARG
2	B	22	MET
2	B	36	GLN
2	B	40	GLU
2	B	42	GLN
2	B	48	LEU
2	B	49	LEU
2	B	55	ARG
2	B	63	GLN
2	B	65	ILE
2	B	77	ARG
2	B	80	LEU
2	B	90	GLN
2	B	94	GLN
2	B	97	LEU
2	B	99	LYS
2	B	101	MET
2	B	103	LYS
2	B	105	GLU
2	B	106	ILE
2	B	109	GLU
2	B	129	LYS
2	B	142	GLN
2	B	150	ARG
2	B	152	MET
2	B	159	VAL
2	B	166	LEU
2	B	167	LYS
2	B	188	LEU
2	B	203	GLU
2	B	205	GLN
2	B	207	MET
2	B	210	GLU
2	B	215	GLN
2	B	217	LEU
2	B	219	LYS

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Mol	Chain	Res	Type
2	B	236	ASN
2	B	266	GLU
2	B	272	LYS
2	B	286	MET
2	B	287	MET
2	B	293	GLN
2	B	295	GLU
2	B	331	GLU
2	B	343	GLU
2	B	355	LEU
2	B	359	LEU
2	B	365	GLN
2	B	367	GLU
2	B	368	LYS
2	B	370	GLN
2	B	372	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	68	ASN
1	A	80	GLN
1	A	244	ASN
2	B	19	GLN
2	B	27	GLN
2	B	44	GLN
2	B	63	GLN
2	B	64	ASN
2	B	90	GLN
2	B	94	GLN
2	B	171	ASN
2	B	185	HIS
2	B	195	HIS
2	B	205	GLN
2	B	215	GLN
2	B	236	ASN
2	B	273	HIS
2	B	288	GLN
2	B	312	GLN
2	B	313	HIS
2	B	342	HIS

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Mol	Chain	Res	Type
2	B	365	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NHP	A	270	-	16,16,16	1.58	2 (12%)	21,21,21	1.85	5 (23%)
5	PLP	B	900	2	15,15,16	1.81	5 (33%)	21,22,23	5.09	10 (47%)

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
3	NHP	A	270	-	-	2/9/9/9	0/1/1/1
5	PLP	B	900	2	-	0/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	270	NHP	P1-C10	-4.86	1.73	1.78
5	B	900	PLP	C4A-C4	-3.21	1.45	1.51
5	B	900	PLP	C3-C2	-2.74	1.38	1.41
3	A	270	NHP	P1-O1	-2.57	1.49	1.55
5	B	900	PLP	P-O2P	-2.48	1.45	1.54
5	B	900	PLP	O4P-C5A	-2.19	1.36	1.44
5	B	900	PLP	P-O3P	-2.02	1.47	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	900	PLP	C4A-C4-C5	15.54	136.96	120.94
5	B	900	PLP	C4A-C4-C3	-8.57	106.23	120.52
5	B	900	PLP	O4P-P-O1P	8.34	128.98	106.44
5	B	900	PLP	O2P-P-O4P	-5.88	91.34	106.67
5	B	900	PLP	C6-C5-C4	5.41	122.53	118.10
5	B	900	PLP	C3-C4-C5	-5.35	112.17	118.59
5	B	900	PLP	C5A-C5-C6	-5.14	110.99	119.36
3	A	270	NHP	C7-S1-C2	4.56	112.54	103.05
3	A	270	NHP	O1-P1-O3	-3.56	103.18	112.39
5	B	900	PLP	C4-C3-C2	3.47	125.08	119.89
3	A	270	NHP	O2-P1-C10	3.38	114.98	106.91
3	A	270	NHP	O2-P1-O3	-3.11	104.34	112.39
5	B	900	PLP	O3P-P-O4P	-2.85	99.24	106.67
3	A	270	NHP	O1-P1-C10	2.81	113.62	106.91
5	B	900	PLP	O4P-C5A-C5	-2.37	104.91	109.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

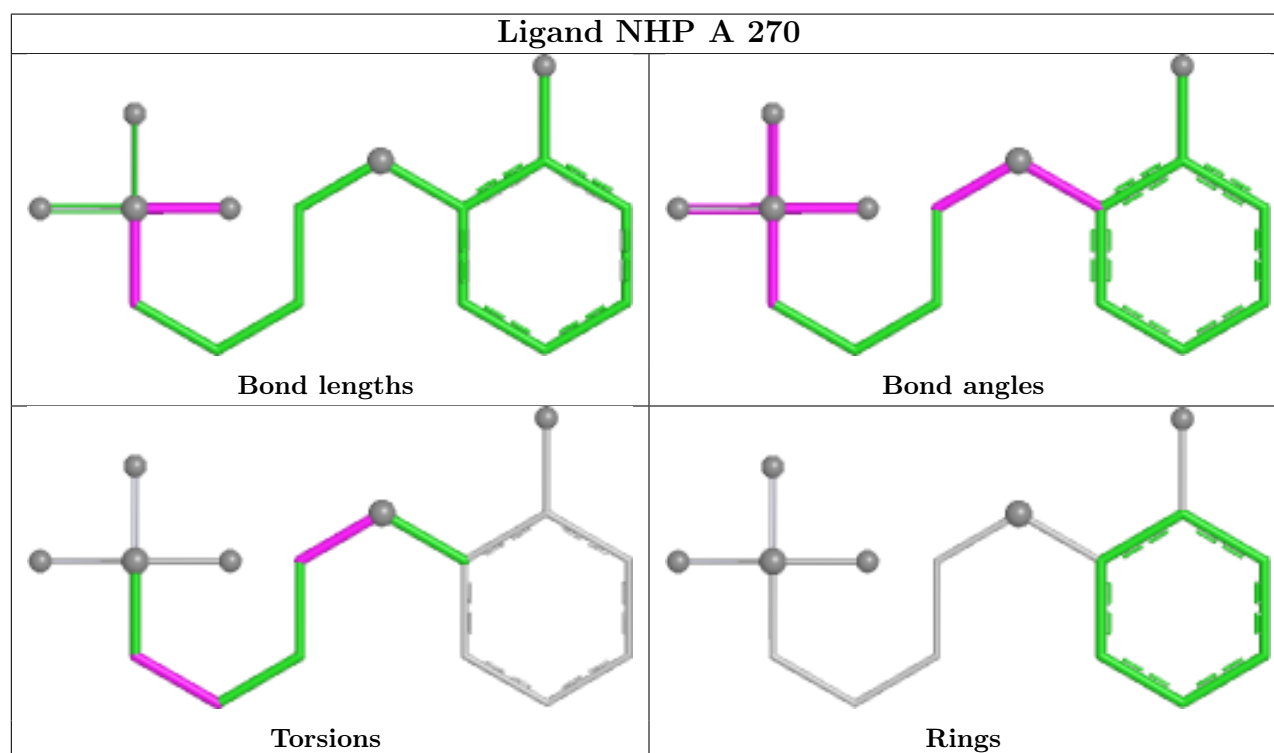
Mol	Chain	Res	Type	Atoms
3	A	270	NHP	C8-C7-S1-C2
3	A	270	NHP	P1-C10-C9-C8

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	270	NHP	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

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	264/268 (98%)	0.37	19 (7%) 21 23	7, 18, 46, 77	0
2	B	387/397 (97%)	0.02	9 (2%) 61 63	3, 12, 30, 56	0
All	All	651/665 (97%)	0.16	28 (4%) 40 41	3, 15, 36, 77	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	GLY	5.4
1	A	187	ASN	3.5
1	A	188	ARG	3.4
1	A	185	ALA	3.2
2	B	385	PHE	3.0
1	A	109	ASN	3.0
1	A	186	GLU	3.0
1	A	192	PRO	2.8
1	A	267	ARG	2.8
1	A	193	LEU	2.7
2	B	389	ASP	2.6
1	A	2	GLU	2.6
2	B	382	LYS	2.6
1	A	157	ASN	2.6
2	B	147	PHE	2.6
1	A	184	GLY	2.5
2	B	159	VAL	2.5
2	B	141	ARG	2.4
1	A	180	SER	2.4
1	A	194	HIS	2.3
2	B	179	GLY	2.3
1	A	179	ARG	2.2
1	A	243	LYS	2.2
2	B	305	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	181	GLY	2.2
1	A	158	ALA	2.2
2	B	296	GLU	2.0
1	A	15	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

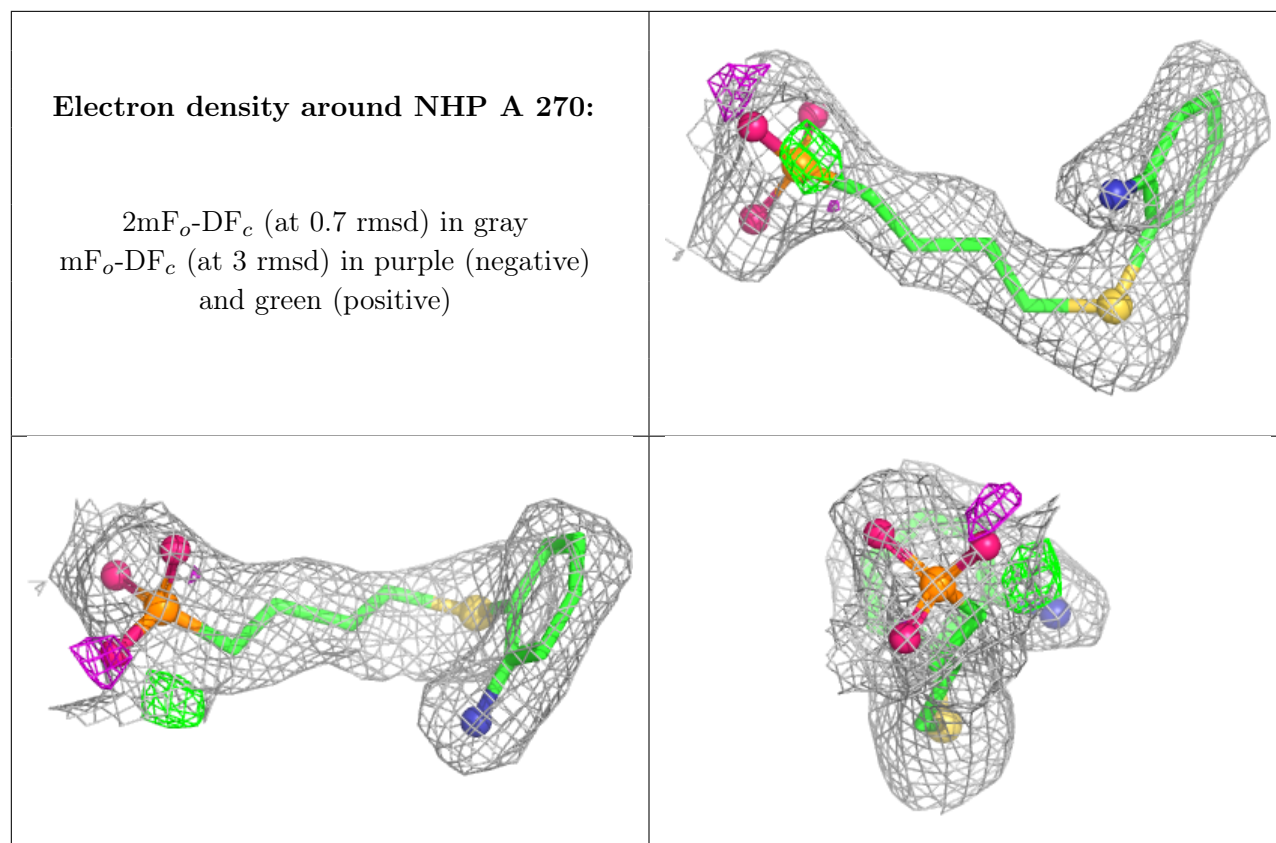
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
4	NA	B	1162	1/1	0.89	0.08	13,13,13,13	0
3	NHP	A	270	16/16	0.90	0.12	19,23,38,41	0
5	PLP	B	900	15/16	0.96	0.08	10,17,22,23	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.