



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 04:31 AM UTC

PDB ID : 2GR9 / pdb_00002gr9
Title : Crystal structure of P5CR complexed with NADH
Authors : Meng, Z.; Lou, Z.; Liu, Z.; Rao, Z.
Deposited on : 2006-04-23
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (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

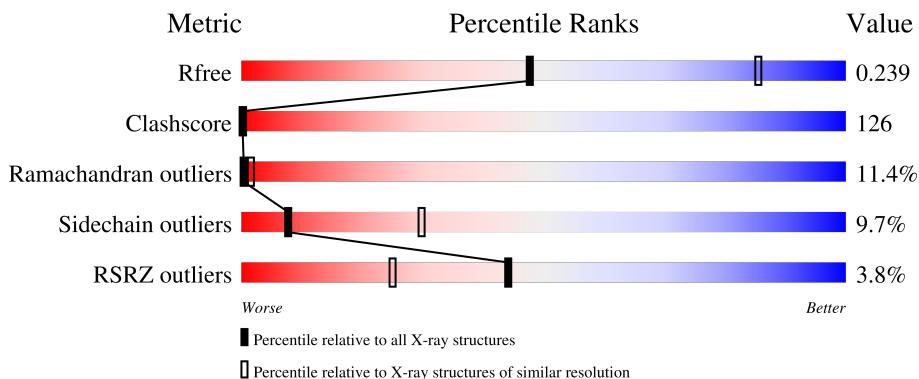
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	277	 18% 59% 21% .
1	B	277	 6% 17% 63% 19% .
1	C	277	 9% 16% 67% 16% .
1	D	277	 18% 66% 15% .
1	E	277	 2% 14% 66% 20% .

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	NAI	A	1300	X	X	X	-
2	NAI	B	2300	X	-	X	-
2	NAI	C	3300	X	-	X	-
2	NAI	D	4300	X	-	X	-
2	NAI	E	5300	X	X	X	-
3	GLU	A	1301	-	-	X	-
3	GLU	B	2301	-	-	X	-
3	GLU	C	3301	-	-	X	-
3	GLU	D	4301	-	-	X	-
3	GLU	E	5301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11077 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.

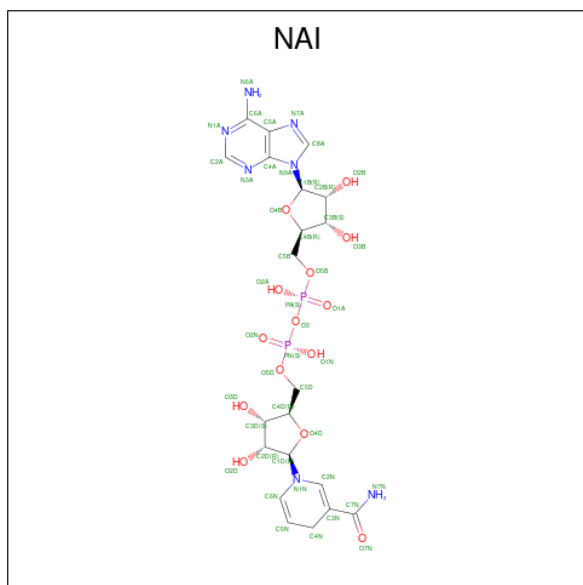
- Molecule 1 is a protein called Pyrroline-5-carboxylate reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	2038	1279	363	383	13	0	0	0
1	B	276	2023	1270	358	382	13	0	0	0
1	C	277	2032	1276	360	383	13	0	0	0
1	D	277	2038	1279	363	383	13	0	0	0
1	E	277	2038	1279	363	383	13	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

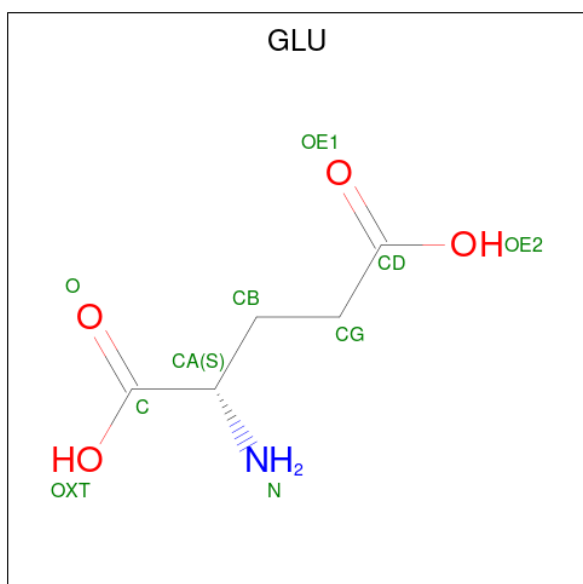
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	cloning artifact	UNP P32322
A	0	GLY	-	cloning artifact	UNP P32322
B	-1	ARG	-	cloning artifact	UNP P32322
B	0	GLY	-	cloning artifact	UNP P32322
C	-1	ARG	-	cloning artifact	UNP P32322
C	0	GLY	-	cloning artifact	UNP P32322
D	-1	ARG	-	cloning artifact	UNP P32322
D	0	GLY	-	cloning artifact	UNP P32322
E	-1	ARG	-	cloning artifact	UNP P32322
E	0	GLY	-	cloning artifact	UNP P32322

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
2	A	1	Total	43	21	6	14	2	0	0
2	B	1	Total	43	21	6	14	2	0	0
2	C	1	Total	43	21	6	14	2	0	0
2	D	1	Total	43	21	6	14	2	0	0
2	E	1	Total	43	21	6	14	2	0	0

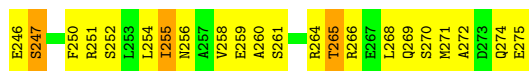
- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



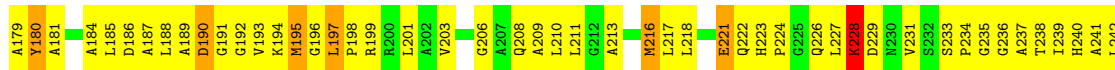
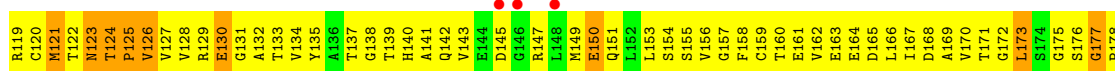
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	C	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		
3	E	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	141	Total	O	0	0
			141	141		
4	B	93	Total	O	0	0
			93	93		
4	C	116	Total	O	0	0
			116	116		
4	D	155	Total	O	0	0
			155	155		
4	E	138	Total	O	0	0
			138	138		



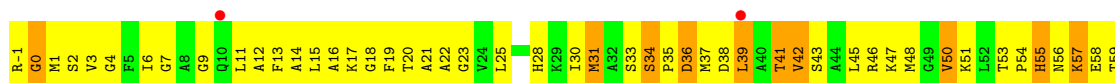
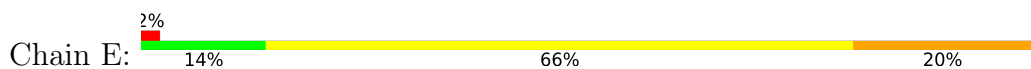
● Molecule 1: Pyrroline-5-carboxylate reductase 1



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V60	C120	Y180	A241	F250	G206	Q206	Q269
Q61	M121	A181	L242	R251	A207	Q208	A272
H62	T122	F182	H243	S252	R147	A209	D273
S63	N123	T183	V244	L253	L148	L210	Q274
D64	T124	A184	L245	L254	M149	L211	E275
V65	P125	L185	E246	L255	E150	G212	
L66	V126	D186	S247	M196	Q151	A213	
F67	V127	A187		A196	L152	A214	
L68	V128	L188		G197	L153	K215	
A69	R129	A189		L197	S154	M216	
V70	E130	D190		G198	S155	V156	
K71	G131	G191		F198	G96	A97	
P72	A132	G192		R199	G157	F98	
H73	T133	V193		R200	F158	C159	
I74	V134	K194		L201	S220	T160	
I75	Y135	M195		A202	E221	E161	
P76	A136	G196		V203	H223	V162	
F77	T137	L197			F224	S102	
I78	G138	P198			G225	S103	
L79	T139	R199			Q226	I104	
D80	H140	R200			L227	E105	
E81	A141	L201			K228	K106	
I82	Q142	R264			D229	L107	
I83	V143	T265			M230	L108	
A84	F144	R266			V231	S109	
D85	D145				S232	A110	
I86	G146				S233	F111	
E87	R147				P234	R112	
D88	L148				G235	P113	
R89	M149				A237	A114	
H90	E150				A238	P115	
I91	Q151				T239	R116	
Y92	L152				H240	V117	
S94	S153					I118	
C95	S154					R119	
A96	S155						
A97	V156						
G98	G157						
V99	F158						
T100	C159						
I101	T160						
S102	E161						
S103	V162						
I104	E163						
E105	E164						
K106	D165						
L107	L166						
L108	I167						
S109	D168						
A110	A169						
F111	V170						
R112	T171						
P113	G172						
A114	L173						
P115	S174						
R116	G175						
V117	S176						
I118	G177						
R119	P178						
	A179						

4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.18Å 122.64Å 120.71Å 90.00° 122.03° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 97.2 (50.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.80Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.278 0.236 , 0.239	Depositor DCC
R_{free} test set	3139 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtrriage
Anisotropy	0.443	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 102.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.017 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.026 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11077	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: NAI

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	0.53	0/2069	1.09	20/2800 (0.7%)
1	B	0.47	0/2053	1.08	15/2779 (0.5%)
1	C	0.50	0/2063	1.10	15/2793 (0.5%)
1	D	0.55	1/2069 (0.0%)	1.08	11/2800 (0.4%)
1	E	0.70	2/2069 (0.1%)	1.25	22/2800 (0.8%)
All	All	0.56	3/10323 (0.0%)	1.12	83/13972 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	129	ARG	C-N	18.38	1.59	1.33
1	E	128	VAL	C-N	-7.93	1.22	1.33
1	D	199	ARG	C-N	-7.34	1.24	1.33

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	128	VAL	O-C-N	19.16	146.53	122.57
1	E	128	VAL	CA-C-N	-13.71	99.30	122.89
1	E	128	VAL	C-N-CA	-13.71	99.30	122.89
1	E	39	LEU	N-CA-C	-11.42	98.73	112.89
1	D	245	LEU	N-CA-C	-10.81	99.50	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2038	0	2084	515	6
1	B	2023	0	2059	516	5
1	C	2032	0	2072	554	2
1	D	2038	0	2084	462	2
1	E	2038	0	2084	519	1
2	A	43	0	23	26	0
2	B	43	0	24	68	5
2	C	43	0	23	38	4
2	D	43	0	24	40	0
2	E	43	0	21	32	1
3	A	10	0	5	8	0
3	B	10	0	5	17	0
3	C	10	0	5	12	0
3	D	10	0	5	21	0
3	E	10	0	5	11	0
4	A	141	0	0	264	6
4	B	93	0	0	173	3
4	C	116	0	0	263	4
4	D	155	0	0	251	2
4	E	138	0	0	297	1
All	All	11077	0	10523	2646	22

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 126.

The worst 5 of 2646 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)
2:A:1300:NAI:C1D	2:A:1300:NAI:N1N	1.68	1.55
2:E:5300:NAI:O3	2:E:5300:NAI:PN	1.13	1.50
1:B:129:ARG:CZ	2:B:2300:NAI:H2N	1.48	1.40
2:E:5300:NAI:O5B	2:E:5300:NAI:C5B	1.71	1.36
2:D:4300:NAI:H1D	3:D:4301:GLU:N	1.41	1.36

The worst 5 of 22 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)
1:B:200:ARG:NH1	2:B:2300:NAI:N7A[2_555]	1.66	0.54
1:A:204:ARG:CB	2:C:3300:NAI:C3B[2_555]	1.75	0.45
1:B:204:ARG:CB	2:B:2300:NAI:C3B[2_555]	1.76	0.44
2:B:2300:NAI:O5B	4:B:2359:HOH:O[2_555]	1.88	0.32
1:D:204:ARG:CB	2:E:5300:NAI:C2B[2_555]	1.94	0.26

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	275/277 (99%)	189 (69%)	54 (20%)	32 (12%)	0	1
1	B	272/277 (98%)	168 (62%)	62 (23%)	42 (15%)	0	0
1	C	275/277 (99%)	198 (72%)	49 (18%)	28 (10%)	0	3
1	D	275/277 (99%)	190 (69%)	64 (23%)	21 (8%)	1	4
1	E	275/277 (99%)	178 (65%)	64 (23%)	33 (12%)	0	1
All	All	1372/1385 (99%)	923 (67%)	293 (21%)	156 (11%)	0	1

5 of 156 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	36	ASP
1	A	39	LEU
1	A	107	LYS
1	A	129	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	215/215 (100%)	185 (86%)	30 (14%)	3	15
1	B	213/215 (99%)	197 (92%)	16 (8%)	12	39
1	C	214/215 (100%)	197 (92%)	17 (8%)	11	37
1	D	215/215 (100%)	192 (89%)	23 (11%)	6	25
1	E	215/215 (100%)	199 (93%)	16 (7%)	13	40
All	All	1072/1075 (100%)	970 (90%)	102 (10%)	8	30

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	190	ASP
1	D	120	CYS
1	E	211	LEU
1	C	216	MET
1	D	37	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	28	HIS
1	D	140	HIS
1	E	269	GLN
1	D	61	GLN
1	D	219	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](#)

10 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
3	GLU	C	3301	-	8,9,9	1.92	2 (25%)	8,11,11	5.91	1 (12%)
3	GLU	A	1301	-	8,9,9	1.62	1 (12%)	8,11,11	5.89	1 (12%)
3	GLU	B	2301	-	8,9,9	1.92	2 (25%)	8,11,11	5.91	1 (12%)
3	GLU	D	4301	-	8,9,9	1.43	1 (12%)	8,11,11	1.76	1 (12%)
2	NAI	D	4300	-	46,47,48	5.81	26 (56%)	61,71,73	4.17	27 (44%)
2	NAI	B	2300	-	46,47,48	5.80	26 (56%)	61,71,73	4.15	27 (44%)
2	NAI	A	1300	-	46,47,48	5.79	30 (65%)	61,71,73	5.74	37 (60%)
2	NAI	E	5300	-	46,47,48	8.97	30 (65%)	61,71,73	6.44	40 (65%)
2	NAI	C	3300	-	46,47,48	5.81	25 (54%)	61,71,73	4.16	27 (44%)
3	GLU	E	5301	-	8,9,9	1.44	1 (12%)	8,11,11	0.85	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLU	C	3301	-	-	5/9/9/9	-
3	GLU	A	1301	-	-	5/9/9/9	-
3	GLU	B	2301	-	-	5/9/9/9	-
3	GLU	D	4301	-	-	2/9/9/9	-
2	NAI	D	4300	-	1/1/13/16	13/29/72/72	0/5/5/5
2	NAI	B	2300	-	1/1/13/16	13/29/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	A	1300	-	2/2/13/16	15/29/72/72	0/5/5/5
2	NAI	E	5300	-	3/3/13/16	16/29/72/72	0/5/5/5
2	NAI	C	3300	-	1/1/13/16	13/29/72/72	0/5/5/5
3	GLU	E	5301	-	-	2/9/9/9	-

The worst 5 of 144 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5300	NAI	PN-O3	-43.08	1.13	1.59
2	E	5300	NAI	PA-O3	19.02	1.80	1.59
2	C	3300	NAI	C8A-N7A	16.99	1.64	1.31
2	B	2300	NAI	C8A-N7A	16.98	1.64	1.31
2	D	4300	NAI	C8A-N7A	16.95	1.64	1.31

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5300	NAI	C1D-N1N-C6N	-19.57	79.40	120.77
2	E	5300	NAI	C1D-N1N-C2N	18.73	151.99	121.14
2	A	1300	NAI	C1B-N9A-C8A	-17.24	88.84	127.09
3	C	3301	GLU	CB-CG-CD	16.46	156.40	112.49
3	B	2301	GLU	CB-CG-CD	16.46	156.38	112.49

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1300	NAI	C1D
2	A	1300	NAI	C4D
2	B	2300	NAI	C4D
2	C	3300	NAI	C4D
2	D	4300	NAI	C4D

5 of 89 torsion outliers are listed below:

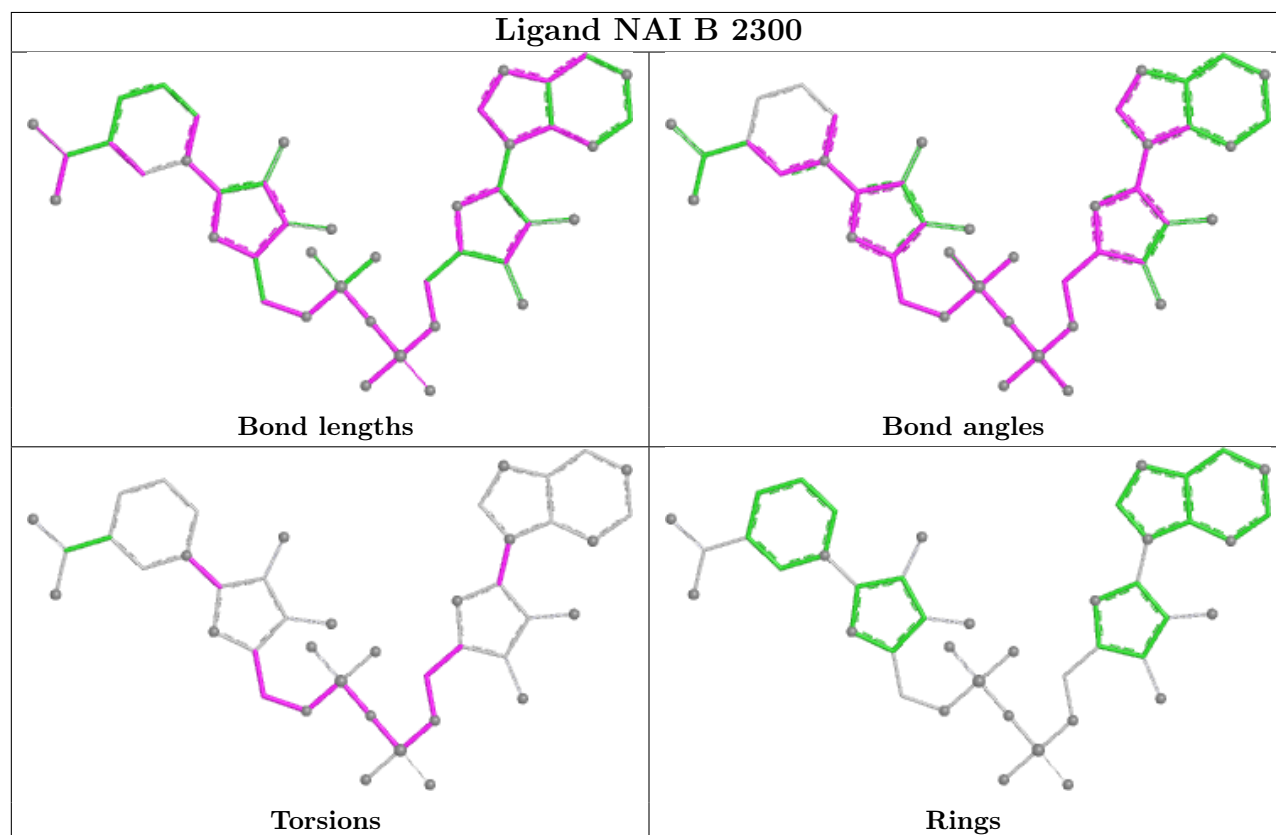
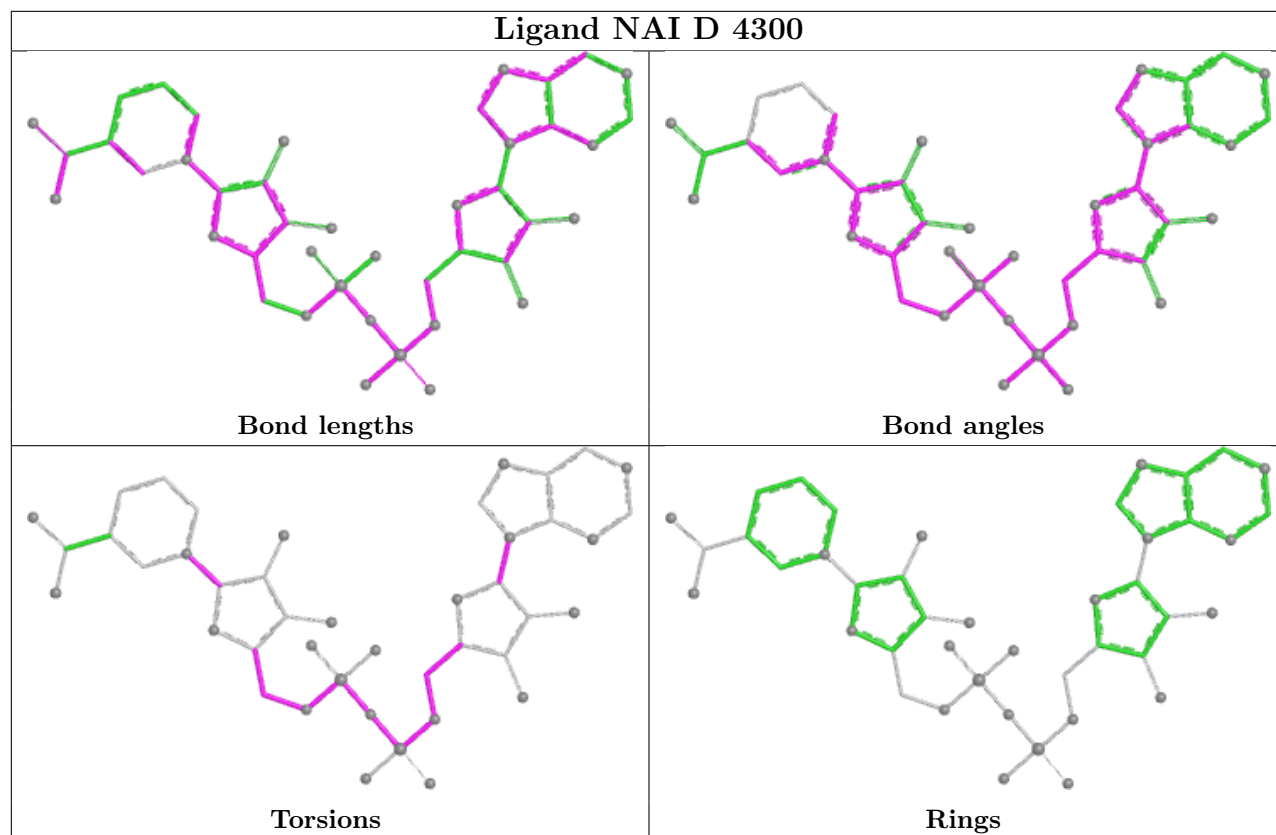
Mol	Chain	Res	Type	Atoms
2	A	1300	NAI	C5B-O5B-PA-O2A
2	A	1300	NAI	C5B-O5B-PA-O3
2	A	1300	NAI	O4B-C4B-C5B-O5B
2	A	1300	NAI	C5D-O5D-PN-O1N
2	A	1300	NAI	C4D-C5D-O5D-PN

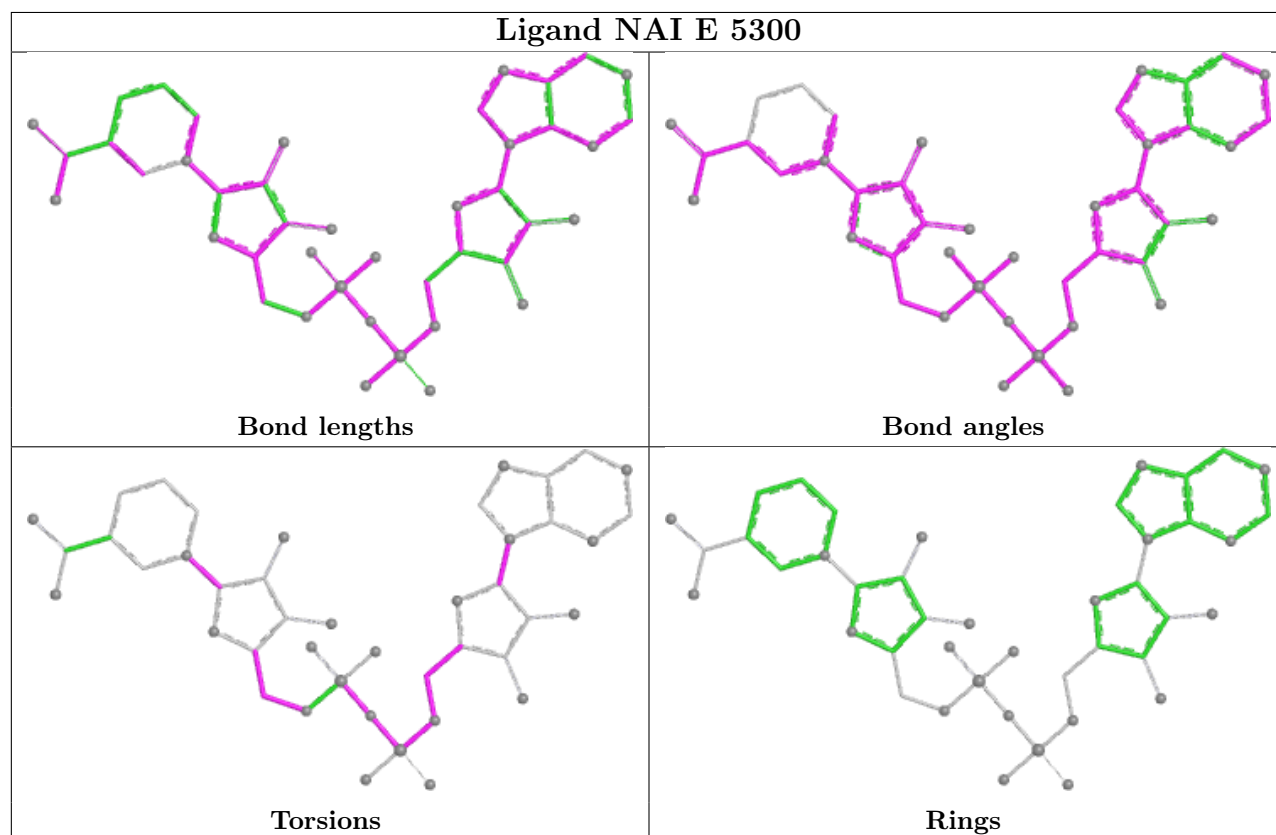
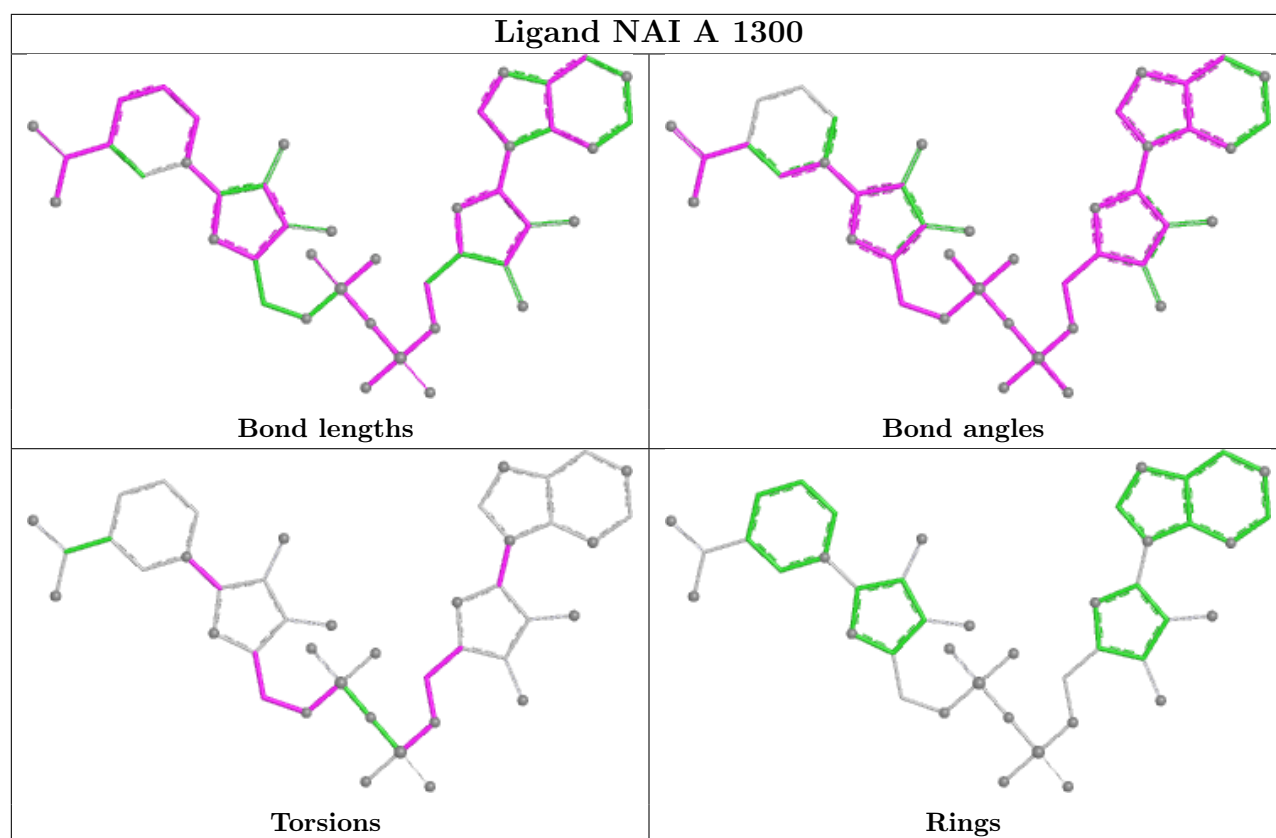
There are no ring outliers.

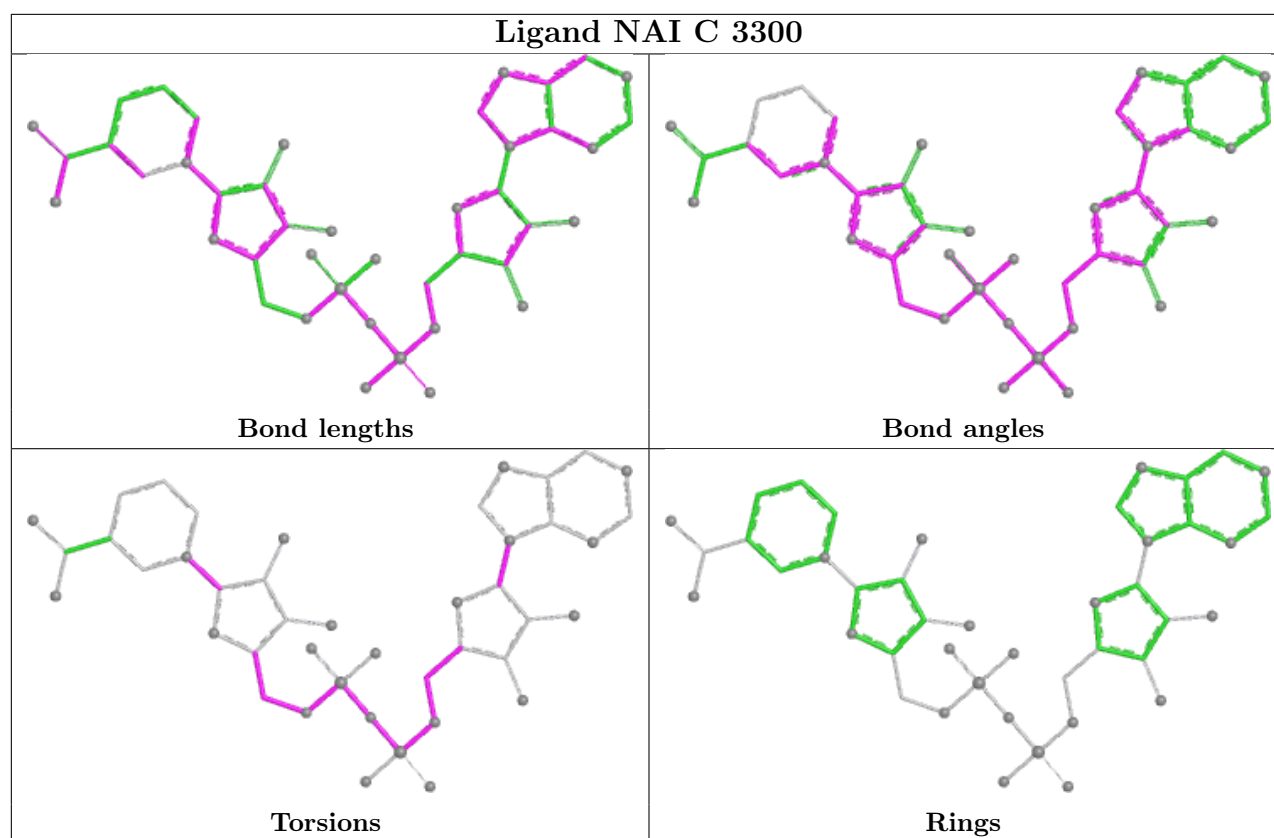
10 monomers are involved in 231 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3301	GLU	12	0
3	A	1301	GLU	8	0
3	B	2301	GLU	17	0
3	D	4301	GLU	21	0
2	D	4300	NAI	40	0
2	B	2300	NAI	68	5
2	A	1300	NAI	26	0
2	E	5300	NAI	32	1
2	C	3300	NAI	38	4
3	E	5301	GLU	11	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	277/277 (100%)	0.06	3 (1%) 78 59	32, 82, 117, 153	0
1	B	276/277 (99%)	0.49	18 (6%) 25 13	39, 129, 183, 200	0
1	C	277/277 (100%)	0.51	24 (8%) 16 9	31, 125, 181, 195	0
1	D	277/277 (100%)	0.02	2 (0%) 84 68	34, 76, 118, 191	0
1	E	277/277 (100%)	0.14	6 (2%) 62 41	24, 80, 128, 142	0
All	All	1384/1385 (99%)	0.24	53 (3%) 44 25	24, 87, 168, 200	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	96	ALA	4.5
1	C	32	ALA	3.8
1	A	8	ALA	3.7
1	C	97	ALA	3.7
1	C	70	VAL	3.6

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.

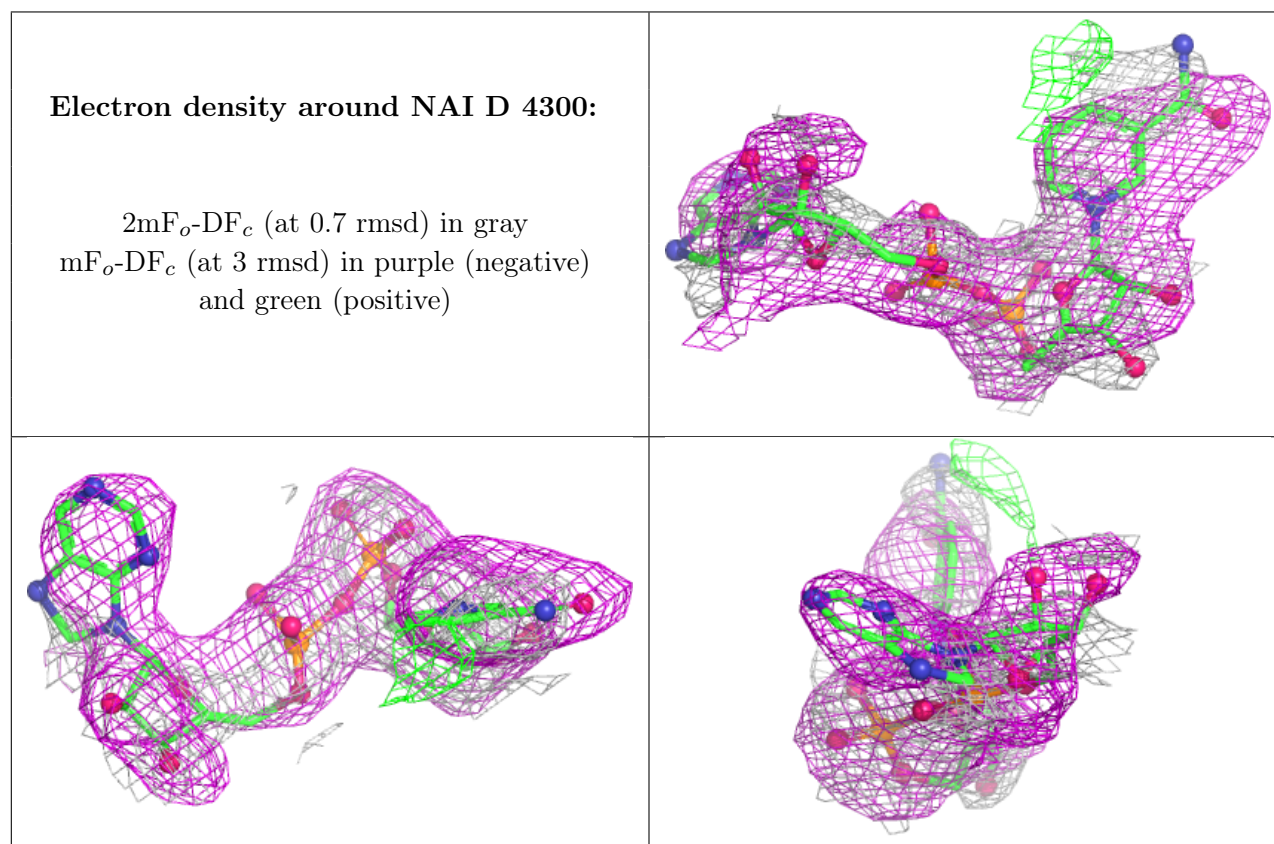
6.4 Ligands [i](#)

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.

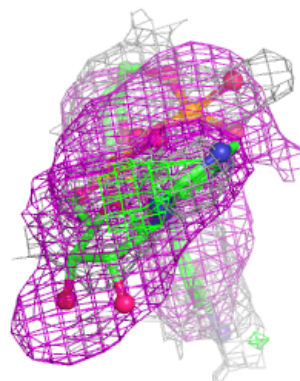
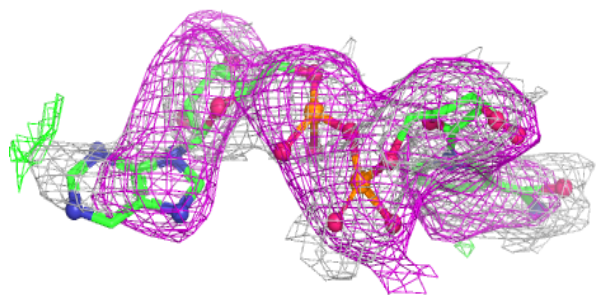
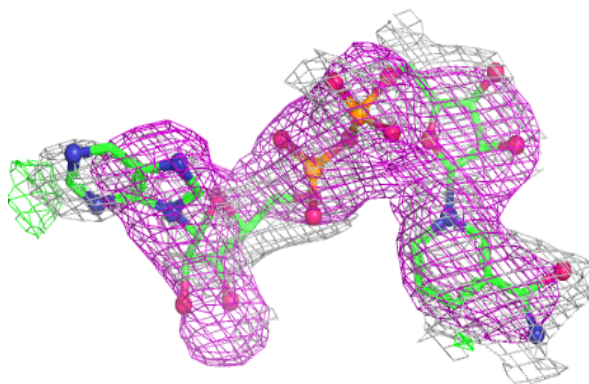
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLU	C	3301	10/10	0.13	0.20	200,200,200,200	0
3	GLU	A	1301	10/10	0.16	0.20	120,131,140,140	0
3	GLU	B	2301	10/10	0.26	0.19	192,200,200,200	0
3	GLU	E	5301	10/10	0.34	0.28	195,200,200,200	0
2	NAI	D	4300	43/44	0.44	0.23	81,91,95,95	0
2	NAI	A	1300	43/44	0.52	0.19	63,93,95,95	0
2	NAI	E	5300	43/44	0.52	0.21	69,94,95,95	0
2	NAI	C	3300	43/44	0.55	0.26	189,195,195,195	0
3	GLU	D	4301	10/10	0.58	0.21	182,193,196,198	0
2	NAI	B	2300	43/44	0.63	0.19	192,195,195,195	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.

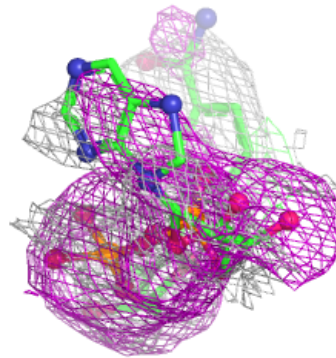
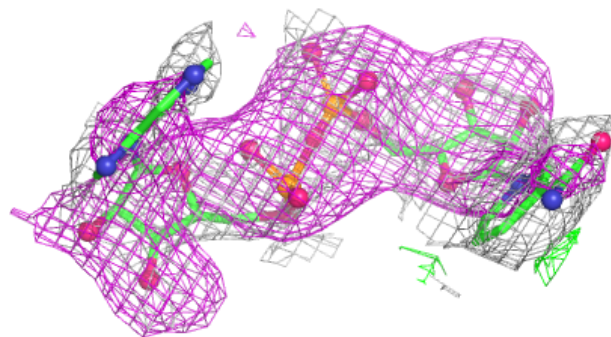
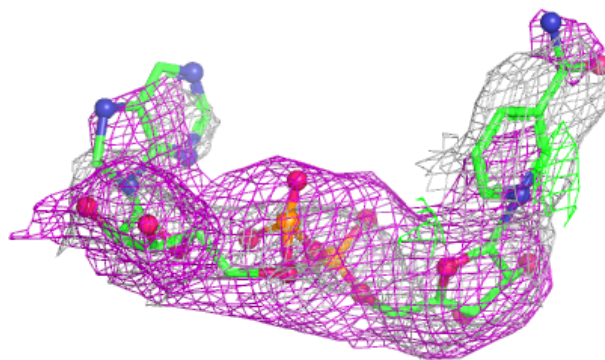


Electron density around NAI A 1300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

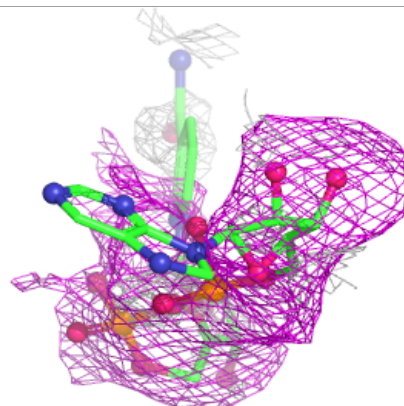
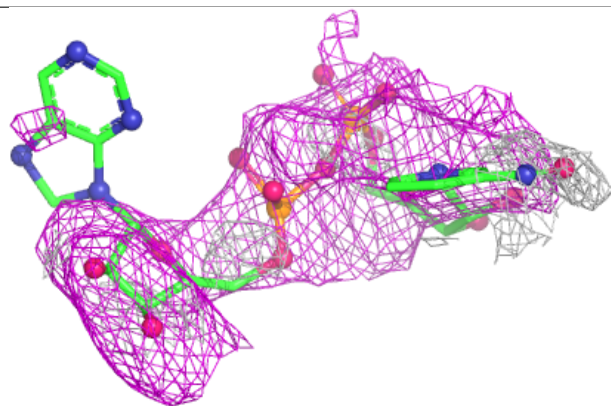
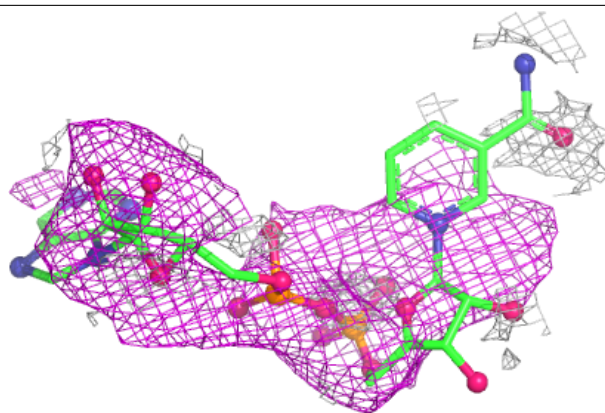
**Electron density around NAI E 5300:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

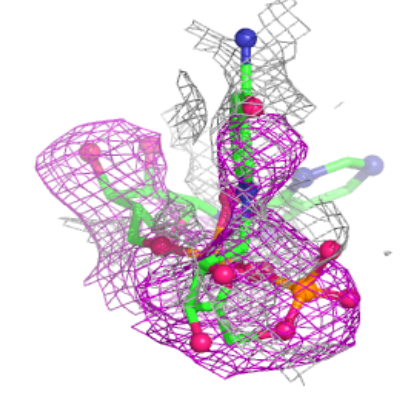
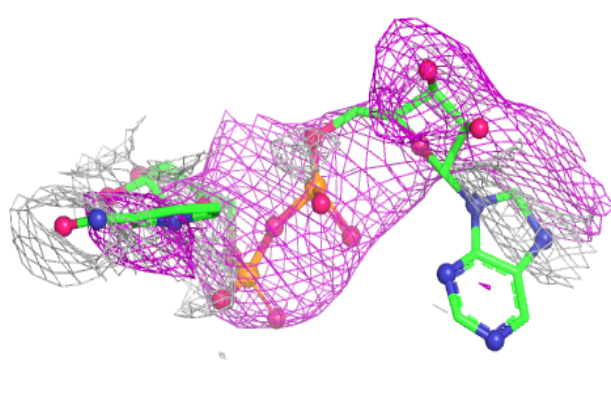
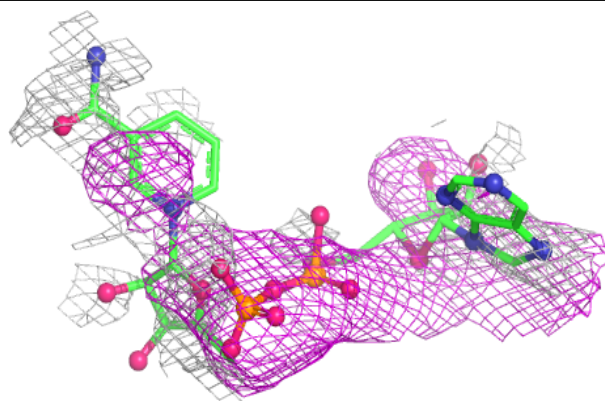


Electron density around NAI C 3300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAI B 2300:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.