



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:22 AM UTC

PDB ID : 7RM6 / pdb_00007rm6
Title : Horse liver alcohol dehydrogenase in complex with NADH and N-cylcohexyl formamide
Authors : Zheng, C.; Boxer, S.G.
Deposited on : 2021-07-26
Resolution : 1.43 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

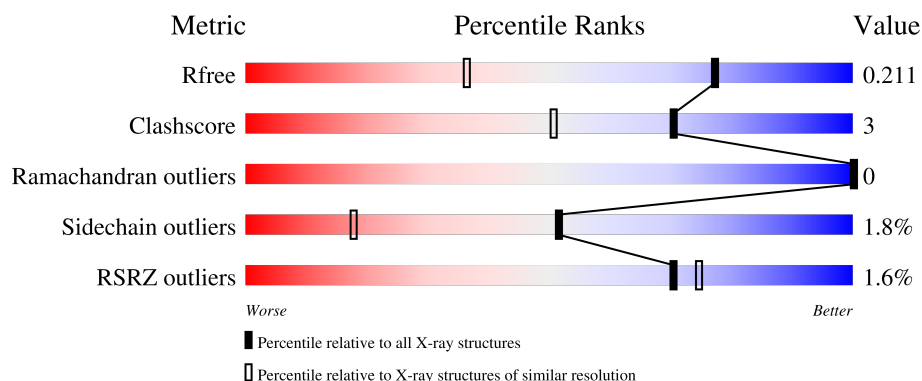
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	377	2% 46% 51% ..
1	B	377	2% 46% 50% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6466 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 Alcohol dehydrogenase E chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2785	1769	472	521	23			
1	B	374	Total	C	N	O	S	0	2	0
			2794	1775	473	523	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P00327
A	-1	ALA	-	expression tag	UNP P00327
A	0	GLY	-	expression tag	UNP P00327
B	-2	GLY	-	expression tag	UNP P00327
B	-1	ALA	-	expression tag	UNP P00327
B	0	GLY	-	expression tag	UNP P00327

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			9	7	1	1		

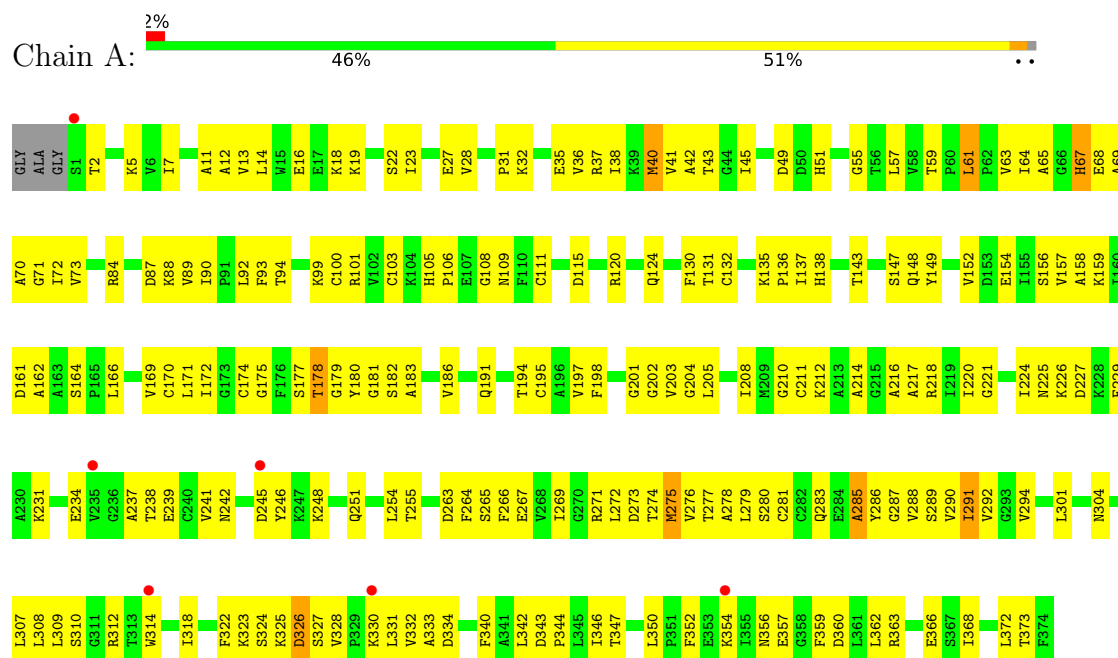
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	420	Total	O	0	0
			420	420		
5	B	357	Total	O	0	0
			357	357		

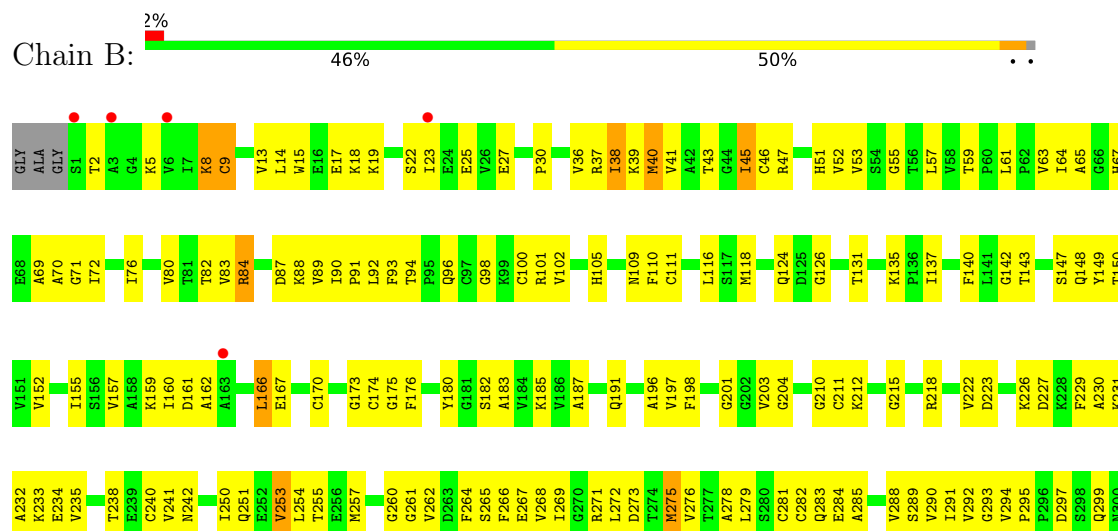
3 Residue-property plots

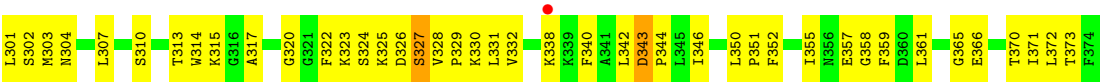
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alcohol dehydrogenase E chain



• Molecule 1: Alcohol dehydrogenase E chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.14Å 50.98Å 92.86Å 92.41° 103.03° 108.94°	Depositor
Resolution (Å)	37.94 – 1.43 37.94 – 1.43	Depositor EDS
% Data completeness (in resolution range)	85.8 (37.94-1.43) 73.5 (37.94-1.43)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.43Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.190 , 0.208 0.204 , 0.211	Depositor DCC
R_{free} test set	5892 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.6	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	6466	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% 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: ZN, CXF, 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	2.19	173/2837 (6.1%)	1.15	11/3834 (0.3%)
1	B	2.23	178/2852 (6.2%)	1.20	16/3854 (0.4%)
All	All	2.21	351/5689 (6.2%)	1.17	27/7688 (0.4%)

All (351) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	ASP	C-O	-10.27	1.14	1.24
1	A	328	VAL	C-O	-9.94	1.15	1.24
1	B	302[A]	SER	CA-C	9.22	1.63	1.52
1	B	302[B]	SER	CA-C	9.22	1.63	1.52
1	A	318	ILE	C-O	-9.09	1.14	1.24
1	A	350	LEU	C-O	-8.97	1.16	1.24
1	A	136	PRO	C-O	-8.75	1.14	1.23
1	B	266	PHE	C-O	-8.75	1.14	1.23
1	B	328	VAL	C-O	-8.65	1.17	1.24
1	A	291	ILE	C-O	-8.60	1.14	1.24
1	A	38	ILE	C-O	-8.55	1.15	1.24
1	A	59	THR	C-O	-8.49	1.15	1.24
1	A	266	PHE	C-O	-8.38	1.14	1.24
1	A	332	VAL	C-O	-8.36	1.14	1.24
1	B	84	ARG	C-O	-8.35	1.16	1.24
1	A	84	ARG	C-O	-8.32	1.16	1.24
1	A	65	ALA	C-O	-8.22	1.15	1.23
1	B	304	ASN	C-O	-8.21	1.13	1.24
1	B	140	PHE	C-O	-8.20	1.14	1.24
1	B	288	VAL	C-O	-8.02	1.15	1.24
1	B	61	LEU	C-O	-7.99	1.16	1.24
1	A	111	CYS	C-O	-7.99	1.14	1.23
1	A	31	PRO	C-O	-7.98	1.15	1.23
1	B	260	GLY	C-O	-7.97	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	ASP	C-O	-7.93	1.15	1.24
1	A	234	GLU	C-O	-7.92	1.14	1.24
1	A	331	LEU	C-O	-7.91	1.14	1.24
1	B	314	TRP	C-O	-7.87	1.14	1.24
1	B	278	ALA	C-O	-7.85	1.14	1.24
1	B	294	VAL	C-O	-7.84	1.14	1.24
1	B	157	VAL	C-O	-7.81	1.15	1.23
1	A	290	VAL	C-O	-7.78	1.15	1.24
1	B	230	ALA	C-O	-7.76	1.15	1.24
1	A	158	ALA	C-O	-7.74	1.14	1.23
1	B	38	ILE	C-O	-7.71	1.15	1.24
1	B	235	VAL	C-O	-7.66	1.15	1.24
1	B	91	PRO	C-O	-7.64	1.15	1.23
1	A	288	VAL	C-O	-7.57	1.16	1.24
1	A	273	ASP	C-O	-7.51	1.15	1.24
1	A	69	ALA	C-O	-7.48	1.15	1.23
1	A	276	VAL	C-O	-7.46	1.15	1.24
1	B	282	CYS	C-O	-7.43	1.14	1.23
1	B	152	VAL	C-O	-7.41	1.15	1.23
1	A	203	VAL	C-O	-7.39	1.15	1.24
1	B	232	ALA	C-O	-7.38	1.15	1.24
1	B	241	VAL	C-O	-7.34	1.16	1.24
1	A	310	SER	C-O	-7.31	1.14	1.24
1	B	161	ASP	C-O	-7.28	1.15	1.23
1	B	331	LEU	C-O	-7.27	1.15	1.24
1	B	94	THR	C-O	-7.26	1.16	1.24
1	B	19	LYS	C-O	-7.23	1.16	1.24
1	A	289	SER	C-O	-7.23	1.15	1.24
1	B	69	ALA	C-O	-7.22	1.16	1.23
1	A	226	LYS	C-O	-7.18	1.14	1.24
1	A	269	ILE	C-O	-7.18	1.15	1.24
1	A	64	ILE	C-O	-7.17	1.16	1.24
1	A	100	CYS	C-O	-7.17	1.14	1.23
1	B	231	LYS	C-O	-7.15	1.15	1.24
1	A	265	SER	C-O	-7.15	1.14	1.23
1	B	343	ASP	C-O	-7.14	1.18	1.24
1	B	101	ARG	C-O	-7.14	1.15	1.24
1	A	14	LEU	C-O	-7.12	1.15	1.24
1	A	41	VAL	C-O	-7.06	1.16	1.23
1	B	355	ILE	C-O	-7.04	1.15	1.24
1	A	285	ALA	C-O	-7.01	1.14	1.24
1	B	76	ILE	C-O	-7.01	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	VAL	C-O	-7.00	1.15	1.24
1	B	271	ARG	C-O	-6.97	1.15	1.23
1	B	299[A]	GLN	CA-C	6.95	1.61	1.52
1	B	299[B]	GLN	CA-C	6.95	1.61	1.52
1	B	147	SER	C-O	-6.95	1.15	1.23
1	B	301	LEU	C-O	-6.95	1.14	1.23
1	B	80	VAL	C-O	-6.94	1.16	1.24
1	B	276	VAL	C-O	-6.92	1.16	1.24
1	A	89	VAL	C-O	-6.83	1.16	1.23
1	A	16	GLU	C-O	-6.81	1.15	1.23
1	B	285	ALA	C-O	-6.81	1.15	1.24
1	A	42	ALA	C-O	-6.81	1.15	1.23
1	A	322	PHE	C-O	-6.80	1.15	1.24
1	A	308	LEU	C-O	-6.80	1.15	1.24
1	B	361	LEU	C-O	-6.80	1.16	1.24
1	A	57	LEU	C-O	-6.79	1.16	1.24
1	B	182	SER	C-O	-6.78	1.16	1.24
1	B	143	THR	C-O	-6.77	1.15	1.24
1	A	108	GLY	C-O	-6.75	1.16	1.23
1	A	254	LEU	C-O	-6.72	1.16	1.24
1	A	37	ARG	C-O	-6.69	1.16	1.24
1	B	291	ILE	C-O	-6.68	1.16	1.24
1	B	59	THR	C-O	-6.67	1.17	1.24
1	B	92	LEU	C-O	-6.66	1.16	1.24
1	A	172	ILE	C-O	-6.66	1.15	1.24
1	B	15	TRP	C-O	-6.66	1.15	1.24
1	B	265	SER	C-O	-6.64	1.15	1.23
1	A	326	ASP	C-O	-6.64	1.16	1.24
1	A	51	HIS	C-O	-6.63	1.15	1.24
1	A	210	GLY	C-O	-6.61	1.16	1.23
1	B	71	GLY	C-O	-6.59	1.17	1.23
1	A	177	SER	C-O	-6.58	1.16	1.24
1	A	274	THR	C-O	-6.58	1.15	1.24
1	A	275	MET	C-O	-6.58	1.16	1.24
1	B	67	HIS	C-O	-6.58	1.15	1.24
1	A	130	PHE	C-O	-6.57	1.16	1.24
1	B	196	ALA	C-O	-6.57	1.16	1.24
1	B	233	LYS	C-O	-6.56	1.16	1.24
1	A	43	THR	C-O	-6.54	1.15	1.23
1	A	101	ARG	C-O	-6.50	1.15	1.24
1	A	72	ILE	C-O	-6.50	1.17	1.24
1	B	198	PHE	C-O	-6.49	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	SER	C-O	-6.47	1.16	1.24
1	B	315	LYS	C-O	-6.46	1.15	1.23
1	A	197	VAL	C-O	-6.46	1.17	1.24
1	B	37	ARG	C-O	-6.46	1.16	1.24
1	A	309	LEU	C-O	-6.46	1.16	1.24
1	B	110	PHE	C-O	-6.45	1.16	1.23
1	B	203	VAL	C-O	-6.45	1.16	1.24
1	B	173	GLY	C-O	-6.42	1.16	1.24
1	B	303	MET	C-O	-6.42	1.16	1.23
1	A	205	LEU	C-O	-6.40	1.16	1.24
1	B	27	GLU	C-O	-6.39	1.16	1.24
1	B	234	GLU	C-O	-6.38	1.16	1.24
1	B	251	GLN	C-O	-6.34	1.16	1.24
1	A	11	ALA	C-O	-6.33	1.16	1.23
1	A	279	LEU	C-O	-6.32	1.16	1.24
1	B	187	ALA	C-O	-6.32	1.16	1.24
1	B	289	SER	C-O	-6.31	1.16	1.24
1	B	45	ILE	C-O	-6.28	1.17	1.24
1	A	159	LYS	C-O	-6.28	1.16	1.24
1	A	120	ARG	C-O	-6.25	1.15	1.23
1	B	332	VAL	C-O	-6.25	1.16	1.24
1	A	208	ILE	C-O	-6.23	1.16	1.24
1	A	137	ILE	C-O	-6.22	1.17	1.24
1	B	350	LEU	C-O	-6.21	1.17	1.24
1	B	250	ILE	C-O	-6.20	1.15	1.24
1	B	340	PHE	C-O	-6.16	1.16	1.23
1	B	372	LEU	C-O	-6.16	1.16	1.24
1	B	357	GLU	C-O	-6.16	1.17	1.24
1	A	186	VAL	C-O	-6.15	1.18	1.24
1	A	344	PRO	C-O	-6.15	1.16	1.24
1	B	325	LYS	C-O	-6.15	1.16	1.24
1	A	366	GLU	C-O	-6.15	1.16	1.24
1	A	28	VAL	C-O	-6.14	1.17	1.24
1	A	216	ALA	C-O	-6.14	1.16	1.23
1	A	152	VAL	C-O	-6.14	1.17	1.24
1	B	100	CYS	C-O	-6.13	1.15	1.23
1	B	160	ILE	C-O	-6.12	1.16	1.23
1	A	304	ASN	C-O	-6.12	1.16	1.24
1	A	307	LEU	C-O	-6.11	1.16	1.24
1	B	93	PHE	C-O	-6.10	1.16	1.24
1	B	324	SER	C-O	-6.10	1.17	1.24
1	A	357	GLU	C-O	-6.09	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	ILE	C-O	-6.08	1.17	1.24
1	A	237	ALA	C-O	-6.08	1.16	1.23
1	A	373	THR	C-O	-6.08	1.16	1.24
1	B	297	ASP	C-O	-6.07	1.16	1.23
1	A	73	VAL	C-O	-6.07	1.18	1.24
1	A	352	PHE	C-O	-6.07	1.17	1.24
1	A	156	SER	C-O	-6.06	1.15	1.23
1	B	310	SER	C-O	-6.06	1.16	1.24
1	A	218	ARG	C-O	-6.05	1.17	1.24
1	B	137	ILE	C-O	-6.05	1.17	1.24
1	A	182	SER	C-O	-6.04	1.16	1.24
1	B	180	TYR	C-O	-6.04	1.17	1.24
1	B	253	VAL	C-O	-6.03	1.17	1.24
1	B	323	LYS	C-O	-6.03	1.17	1.24
1	A	340	PHE	C-O	-6.02	1.16	1.23
1	B	72	ILE	C-O	-6.00	1.17	1.24
1	B	197	VAL	C-O	-6.00	1.17	1.24
1	A	170	CYS	C-O	-6.00	1.16	1.24
1	A	220	ILE	C-O	-6.00	1.17	1.24
1	B	292	VAL	C-O	-6.00	1.17	1.23
1	B	201	GLY	C-O	-5.98	1.18	1.23
1	A	135	LYS	C-O	-5.97	1.16	1.24
1	B	53	VAL	C-O	-5.97	1.17	1.24
1	A	359	PHE	C-O	-5.96	1.16	1.24
1	A	225	ASN	C-O	-5.96	1.17	1.24
1	B	281	CYS	C-O	-5.95	1.16	1.24
1	B	358	GLY	C-O	-5.95	1.16	1.23
1	A	227	ASP	C-O	-5.93	1.16	1.24
1	A	280	SER	C-O	-5.93	1.16	1.24
1	B	43	THR	C-O	-5.92	1.16	1.23
1	B	211	CYS	C-O	-5.92	1.17	1.24
1	B	371	ILE	C-O	-5.91	1.17	1.24
1	A	138	HIS	C-O	-5.89	1.16	1.23
1	A	157	VAL	C-O	-5.89	1.17	1.23
1	B	111	CYS	C-O	-5.89	1.17	1.23
1	A	325	LYS	C-O	-5.87	1.16	1.24
1	A	224	ILE	C-O	-5.86	1.16	1.24
1	B	159	LYS	C-O	-5.86	1.16	1.24
1	B	2	THR	C-O	-5.85	1.16	1.24
1	B	183	ALA	C-O	-5.85	1.17	1.24
1	A	238	THR	C-O	-5.82	1.16	1.24
1	A	356	ASN	C-O	-5.81	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	THR	C-O	-5.80	1.17	1.24
1	B	329	PRO	C-O	-5.79	1.16	1.24
1	B	352	PHE	C-O	-5.78	1.17	1.24
1	B	283	GLN	C-O	-5.78	1.16	1.23
1	B	9	CYS	C-O	-5.78	1.17	1.23
1	A	238	THR	C-N	-5.78	1.26	1.33
1	A	281	CYS	C-O	-5.78	1.16	1.24
1	B	105	HIS	C-O	-5.77	1.16	1.23
1	A	194	THR	C-O	-5.76	1.17	1.24
1	A	162	ALA	C-O	-5.76	1.16	1.24
1	B	90	ILE	C-O	-5.75	1.17	1.23
1	A	201	GLY	C-O	-5.73	1.18	1.23
1	B	148	GLN	C-O	-5.73	1.16	1.24
1	A	272	LEU	C-O	-5.73	1.17	1.24
1	B	142	GLY	C-O	-5.72	1.16	1.24
1	A	149	TYR	C-O	-5.72	1.17	1.23
1	B	65	ALA	C-O	-5.72	1.17	1.23
1	B	46	CYS	C-O	-5.71	1.17	1.23
1	A	178	THR	C-O	-5.71	1.17	1.24
1	B	254	LEU	C-O	-5.70	1.17	1.24
1	B	272	LEU	C-O	-5.69	1.17	1.24
1	B	87	ASP	C-O	-5.69	1.16	1.23
1	B	346	ILE	C-O	-5.69	1.17	1.23
1	B	365	GLY	C-O	-5.69	1.16	1.24
1	A	214	ALA	C-O	-5.68	1.16	1.24
1	B	70	ALA	C-O	-5.67	1.17	1.23
1	B	261	GLY	C-O	-5.67	1.16	1.23
1	A	148	GLN	C-O	-5.66	1.17	1.24
1	A	278	ALA	C-O	-5.66	1.17	1.24
1	A	124	GLN	C-O	-5.65	1.17	1.24
1	B	14	LEU	C-O	-5.65	1.17	1.23
1	A	161	ASP	C-O	-5.65	1.17	1.23
1	A	105	HIS	C-O	-5.64	1.16	1.23
1	A	2	THR	C-O	-5.63	1.16	1.24
1	B	170	CYS	C-O	-5.63	1.17	1.24
1	B	342	LEU	C-O	-5.63	1.16	1.23
1	B	210	GLY	C-O	-5.63	1.17	1.23
1	A	92	LEU	C-O	-5.62	1.17	1.24
1	A	175	GLY	C-O	-5.62	1.17	1.23
1	B	222	VAL	C-O	-5.61	1.18	1.24
1	A	372	LEU	C-O	-5.61	1.17	1.24
1	B	149	TYR	C-O	-5.60	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	ILE	C-O	-5.60	1.18	1.23
1	A	195	CYS	C-O	-5.59	1.16	1.23
1	A	143	THR	C-O	-5.59	1.16	1.23
1	A	55	GLY	C-O	-5.59	1.16	1.24
1	A	198	PHE	C-O	-5.58	1.17	1.24
1	B	255	THR	C-O	-5.57	1.17	1.24
1	A	71	GLY	C-O	-5.54	1.17	1.23
1	B	155	ILE	C-O	-5.54	1.17	1.24
1	A	271	ARG	C-O	-5.53	1.16	1.23
1	B	175	GLY	C-O	-5.52	1.17	1.23
1	A	12	ALA	C-O	-5.52	1.17	1.24
1	A	287	GLY	C-O	-5.50	1.16	1.23
1	B	313	THR	C-O	-5.50	1.17	1.24
1	B	174	CYS	C-O	-5.49	1.17	1.24
1	A	70	ALA	C-O	-5.48	1.17	1.23
1	B	273	ASP	C-O	-5.48	1.17	1.24
1	A	109	ASN	C-O	-5.48	1.18	1.24
1	B	351	PRO	C-O	-5.48	1.17	1.23
1	A	241	VAL	C-O	-5.47	1.18	1.24
1	A	147	SER	C-O	-5.47	1.17	1.23
1	B	102	VAL	C-O	-5.45	1.17	1.24
1	B	55	GLY	C-O	-5.44	1.16	1.24
1	A	264	PHE	C-O	-5.44	1.17	1.23
1	B	322	PHE	C-O	-5.43	1.17	1.23
1	B	89	VAL	C-O	-5.43	1.17	1.23
1	A	87	ASP	C-O	-5.43	1.17	1.23
1	B	320	GLY	C-O	-5.43	1.16	1.23
1	A	248	LYS	C-N	-5.42	1.26	1.33
1	B	264	PHE	C-O	-5.41	1.17	1.24
1	A	36	VAL	C-O	-5.41	1.18	1.24
1	A	202	GLY	C-O	-5.41	1.17	1.23
1	A	333	ALA	C-O	-5.40	1.17	1.24
1	B	215	GLY	C-O	-5.40	1.17	1.24
1	A	67	HIS	C-O	-5.40	1.17	1.24
1	B	36	VAL	C-O	-5.39	1.18	1.24
1	A	22	SER	C-O	-5.38	1.17	1.24
1	B	176	PHE	C-O	-5.38	1.17	1.24
1	A	362	LEU	C-O	-5.38	1.18	1.24
1	B	83	VAL	C-O	-5.38	1.18	1.23
1	A	93	PHE	C-O	-5.37	1.17	1.24
1	B	275	MET	C-O	-5.37	1.17	1.24
1	A	179	GLY	C-O	-5.37	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	VAL	C-O	-5.36	1.17	1.23
1	B	242	ASN	C-O	-5.36	1.18	1.24
1	B	279	LEU	C-O	-5.35	1.18	1.24
1	A	45	ILE	C-O	-5.35	1.18	1.24
1	A	217	ALA	C-O	-5.35	1.17	1.24
1	B	223	ASP	C-O	-5.35	1.17	1.23
1	A	327	SER	C-O	-5.35	1.17	1.24
1	B	290	VAL	C-O	-5.34	1.18	1.24
1	B	39	LYS	C-O	-5.34	1.17	1.24
1	A	23	ILE	C-O	-5.33	1.18	1.23
1	B	118	MET	C-O	-5.31	1.18	1.24
1	A	231	LYS	C-O	-5.31	1.17	1.24
1	B	13	VAL	C-O	-5.31	1.17	1.24
1	A	346	ILE	C-O	-5.30	1.17	1.23
1	B	116	LEU	C-O	-5.29	1.17	1.23
1	B	262	VAL	C-O	-5.29	1.16	1.23
1	A	174	CYS	C-O	-5.29	1.17	1.24
1	B	82	THR	C-O	-5.29	1.17	1.24
1	B	269	ILE	C-O	-5.28	1.17	1.24
1	B	51	HIS	C-O	-5.27	1.17	1.24
1	B	212	LYS	C-O	-5.26	1.18	1.24
1	A	347	THR	C-O	-5.26	1.17	1.24
1	A	229	PHE	C-O	-5.26	1.17	1.24
1	A	342	LEU	C-O	-5.26	1.16	1.23
1	B	126	GLY	C-O	-5.25	1.16	1.24
1	A	49	ASP	C-O	-5.25	1.17	1.24
1	B	226	LYS	C-O	-5.24	1.17	1.24
1	A	61	LEU	C-O	-5.24	1.18	1.24
1	B	295	PRO	C-O	-5.23	1.18	1.24
1	A	132	CYS	C-O	-5.22	1.17	1.23
1	B	359	PHE	C-O	-5.22	1.17	1.24
1	B	47	ARG	C-O	-5.22	1.17	1.24
1	B	52	VAL	C-O	-5.20	1.18	1.24
1	A	277	THR	C-O	-5.19	1.18	1.24
1	A	360	ASP	C-O	-5.19	1.18	1.24
1	B	8	LYS	C-O	-5.19	1.17	1.24
1	B	227	ASP	C-O	-5.19	1.17	1.24
1	A	169	VAL	C-O	-5.18	1.16	1.24
1	B	96	GLN	C-O	-5.16	1.17	1.23
1	B	109	ASN	C-O	-5.16	1.17	1.24
1	B	373	THR	C-O	-5.15	1.17	1.24
1	B	124	GLN	C-O	-5.15	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	GLY	C-O	-5.14	1.16	1.23
1	A	211	CYS	C-O	-5.14	1.18	1.24
1	B	40	MET	C-N	-5.14	1.27	1.33
1	A	212	LYS	C-O	-5.14	1.18	1.24
1	B	41	VAL	C-O	-5.14	1.17	1.24
1	B	218	ARG	C-O	-5.14	1.18	1.24
1	A	246	TYR	C-O	-5.13	1.17	1.23
1	A	368	ILE	C-O	-5.12	1.18	1.24
1	A	13	VAL	C-O	-5.12	1.17	1.24
1	B	240	CYS	C-O	-5.11	1.17	1.23
1	A	180	TYR	C-O	-5.11	1.18	1.24
1	B	167	GLU	C-O	-5.10	1.17	1.24
1	A	154	GLU	C-O	-5.09	1.18	1.24
1	A	334	ASP	C-O	-5.09	1.18	1.24
1	A	221	GLY	C-O	-5.08	1.16	1.23
1	B	204	GLY	C-O	-5.08	1.17	1.23
1	B	307	LEU	C-O	-5.08	1.17	1.24
1	A	106	PRO	C-O	-5.06	1.18	1.24
1	A	181	GLY	C-O	-5.06	1.17	1.23
1	B	326	ASP	C-O	-5.06	1.18	1.24
1	A	255	THR	C-O	-5.06	1.18	1.24
1	A	323	LYS	C-O	-5.06	1.18	1.24
1	A	363	ARG	C-O	-5.05	1.17	1.24
1	B	162	ALA	C-O	-5.05	1.17	1.24
1	A	103	CYS	C-O	-5.05	1.17	1.24
1	B	98	GLY	C-O	-5.05	1.17	1.24
1	B	166	LEU	C-O	-5.04	1.17	1.24
1	A	115	ASP	C-O	-5.04	1.17	1.24
1	B	317	ALA	C-O	-5.03	1.17	1.23
1	A	312	ARG	C-O	-5.01	1.17	1.23
1	B	229	PHE	C-O	-5.01	1.18	1.24
1	A	183	ALA	C-O	-5.00	1.18	1.24
1	A	204	GLY	C-O	-5.00	1.18	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	SER	N-CA-C	8.56	120.23	111.07
1	A	324	SER	N-CA-C	7.87	119.49	111.07
1	B	69	ALA	N-CA-C	7.78	118.88	108.38
1	A	327	SER	N-CA-C	7.01	120.32	111.69
1	B	284	GLU	N-CA-C	6.96	119.71	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	THR	CA-C-N	6.96	134.16	121.85
1	B	238	THR	C-N-CA	6.96	134.16	121.85
1	B	327	SER	N-CA-C	6.76	120.01	111.69
1	A	69	ALA	N-CA-C	6.59	117.27	108.38
1	A	108	GLY	N-CA-C	6.44	118.89	111.36
1	A	323	LYS	N-CA-C	-6.08	100.65	109.59
1	A	246	TYR	N-CA-C	6.00	119.33	109.85
1	A	239	GLU	O-C-N	-5.82	116.84	123.48
1	B	229	PHE	N-CA-C	5.79	117.68	111.36
1	B	323	LYS	N-CA-C	-5.75	100.86	109.15
1	A	238	THR	CA-C-N	5.54	131.94	121.69
1	A	238	THR	C-N-CA	5.54	131.94	121.69
1	B	30	PRO	O-C-N	5.45	123.71	121.15
1	B	64	ILE	N-CA-C	-5.37	99.42	107.37
1	B	366	GLU	N-CA-C	5.31	118.92	112.23
1	B	175	GLY	N-CA-C	5.25	118.99	112.64
1	B	299[A]	GLN	CA-C-O	5.20	126.90	120.92
1	B	299[B]	GLN	CA-C-O	5.20	126.90	120.92
1	A	38	ILE	N-CA-C	5.17	115.35	108.11
1	B	302[A]	SER	CA-C-O	5.12	125.89	120.36
1	B	302[B]	SER	CA-C-O	5.12	125.89	120.36
1	A	18	LYS	N-CA-C	5.08	118.75	112.24

There are no chirality outliers.

There are no planarity outliers.

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	2785	0	2848	20	0
1	B	2794	0	2861	19	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	27	1	0
3	B	44	0	27	0	0
4	A	9	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	9	0	13	1	0
5	A	420	0	0	2	0
5	B	357	0	0	3	0
All	All	6466	0	5789	39	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 3.

All (39) 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:B:17:GLU:HG3	1:B:18:LYS:HG3	1.62	0.80
1:B:185:LYS:NZ	5:B:501:HOH:O	2.20	0.72
1:B:38:ILE:HG22	1:B:40:MET:HE2	1.73	0.69
1:A:291:ILE:HD11	1:A:314:TRP:CZ2	2.27	0.68
1:A:178:THR:HG21	3:A:403:NAI:H4N	1.78	0.66
1:A:88:LYS:HG2	1:A:166:LEU:HD11	1.79	0.65
1:B:330:LYS:NZ	5:B:506:HOH:O	2.28	0.65
1:A:242:ASN:HB3	1:A:245:ASP:OD2	1.99	0.61
1:A:68:GLU:OE1	1:A:171:LEU:HD23	2.04	0.57
1:B:253:VAL:O	1:B:257:MET:HG3	2.06	0.55
1:A:267:GLU:HG3	1:A:275:MET:HA	1.89	0.55
1:B:38:ILE:CG2	1:B:40:MET:CE	2.86	0.54
1:A:68:GLU:OE1	1:A:171:LEU:CD2	2.56	0.54
1:A:40:MET:HE2	1:A:40:MET:CA	2.40	0.51
1:B:267:GLU:HG3	1:B:275:MET:HA	1.91	0.51
1:B:38:ILE:CG2	1:B:40:MET:HE2	2.41	0.50
1:B:45:ILE:HD12	1:B:370:THR:HB	1.93	0.50
1:A:283:GLN:HG3	1:A:286:TYR:CZ	2.47	0.49
1:B:8:LYS:HB3	1:B:25:GLU:OE1	2.13	0.49
1:A:301:LEU:HD12	1:A:301:LEU:C	2.38	0.48
1:A:294:VAL:HG21	4:A:404:CXF:H52	1.95	0.48
1:A:99:LYS:HD3	5:A:550:HOH:O	2.14	0.47
1:B:88:LYS:HG2	1:B:166:LEU:HD11	1.96	0.47
1:B:38:ILE:HG22	1:B:40:MET:CE	2.43	0.46
1:A:326:ASP:O	1:A:330:LYS:HE2	2.16	0.46
1:B:40:MET:HE3	1:B:150:THR:HG22	1.98	0.46
1:B:84:ARG:NH1	5:B:516:HOH:O	2.49	0.45
1:A:61:LEU:HD22	1:A:63:VAL:HG12	1.98	0.45
1:B:343:ASP:N	1:B:344:PRO:CD	2.81	0.43
1:A:40:MET:HE2	1:A:40:MET:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLN:OE1	1:A:285:ALA:HB3	2.18	0.43
1:A:19:LYS:NZ	5:A:519:HOH:O	2.50	0.43
1:A:67:HIS:CD2	4:A:404:CXF:H7	2.54	0.42
1:A:32:LYS:O	1:A:35:GLU:HB2	2.20	0.42
1:A:27:GLU:HB2	1:A:131:THR:HB	2.01	0.42
1:B:327:SER:HA	1:B:330:LYS:HE2	2.01	0.41
1:B:131:THR:HA	1:B:135:LYS:O	2.21	0.41
1:B:57:LEU:HD11	4:B:404:CXF:H51	2.03	0.40
1:B:9:CYS:O	1:B:25:GLU:HA	2.22	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	372/377 (99%)	358 (96%)	14 (4%)	0	100	100
1	B	374/377 (99%)	364 (97%)	10 (3%)	0	100	100
All	All	746/754 (99%)	722 (97%)	24 (3%)	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	308/308 (100%)	302 (98%)	6 (2%)	50	16
1	B	310/308 (101%)	305 (98%)	5 (2%)	55	21
All	All	618/616 (100%)	607 (98%)	11 (2%)	51	18

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	40	MET
1	A	164	SER
1	A	191	GLN
1	A	251	GLN
1	A	354	LYS
1	B	5	LYS
1	B	23	ILE
1	B	191	GLN
1	B	268	VAL
1	B	338	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	244	GLN
1	B	34	HIS
1	B	138	HIS
1	B	191	GLN
1	B	244	GLN

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

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	NAI	A	403	-	47,48,48	2.00	15 (31%)	64,73,73	1.65	9 (14%)
3	NAI	B	403	-	47,48,48	0.51	0	64,73,73	0.56	0
4	CXF	A	404	2	9,9,9	0.55	0	9,10,10	0.33	0
4	CXF	B	404	2	9,9,9	0.30	0	9,10,10	0.28	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
3	NAI	A	403	-	-	5/29/72/72	0/5/5/5
3	NAI	B	403	-	-	4/29/72/72	0/5/5/5
4	CXF	A	404	2	-	0/3/11/11	0/1/1/1
4	CXF	B	404	2	-	0/3/11/11	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	NAI	C4A-N9A	-4.26	1.28	1.37
3	A	403	NAI	C5A-N7A	-4.26	1.31	1.39
3	A	403	NAI	PN-O1N	-4.14	1.36	1.55
3	A	403	NAI	O7N-C7N	-3.75	1.15	1.24
3	A	403	NAI	C8A-N9A	-3.37	1.31	1.37
3	A	403	NAI	C2A-N1A	-3.27	1.28	1.33
3	A	403	NAI	PA-O1A	-3.14	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	NAI	PA-O2A	-2.59	1.43	1.55
3	A	403	NAI	C6N-N1N	-2.41	1.31	1.37
3	A	403	NAI	C6A-N1A	-2.39	1.29	1.35
3	A	403	NAI	C4A-N3A	-2.34	1.30	1.34
3	A	403	NAI	C5A-C6A	2.34	1.47	1.41
3	A	403	NAI	O3D-C3D	-2.21	1.37	1.43
3	A	403	NAI	C4N-C5N	-2.14	1.43	1.49
3	A	403	NAI	O4B-C4B	-2.06	1.40	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	NAI	C5A-C4A-N3A	-6.30	118.05	126.72
3	A	403	NAI	C2A-N3A-C4A	4.32	122.38	111.83
3	A	403	NAI	N3A-C4A-N9A	4.20	134.31	127.17
3	A	403	NAI	C4A-C5A-N7A	-3.79	106.25	110.58
3	A	403	NAI	N3A-C2A-N1A	-3.29	123.60	128.58
3	A	403	NAI	C6A-C5A-N7A	3.04	137.95	132.09
3	A	403	NAI	O4B-C1B-C2B	-2.76	100.72	106.62
3	A	403	NAI	C5A-N7A-C8A	2.36	107.16	103.45
3	A	403	NAI	O4D-C1D-C2D	-2.21	101.89	106.62

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	NAI	C2D-C1D-N1N-C2N
3	A	403	NAI	O4D-C1D-N1N-C2N
3	B	403	NAI	C2D-C1D-N1N-C2N
3	B	403	NAI	O4D-C1D-N1N-C2N
3	A	403	NAI	C2D-C1D-N1N-C6N
3	B	403	NAI	C2D-C1D-N1N-C6N
3	A	403	NAI	C2B-C1B-N9A-C8A
3	B	403	NAI	C2N-C3N-C7N-O7N
3	A	403	NAI	O4B-C4B-C5B-O5B

There are no ring outliers.

3 monomers are involved in 4 short contacts:

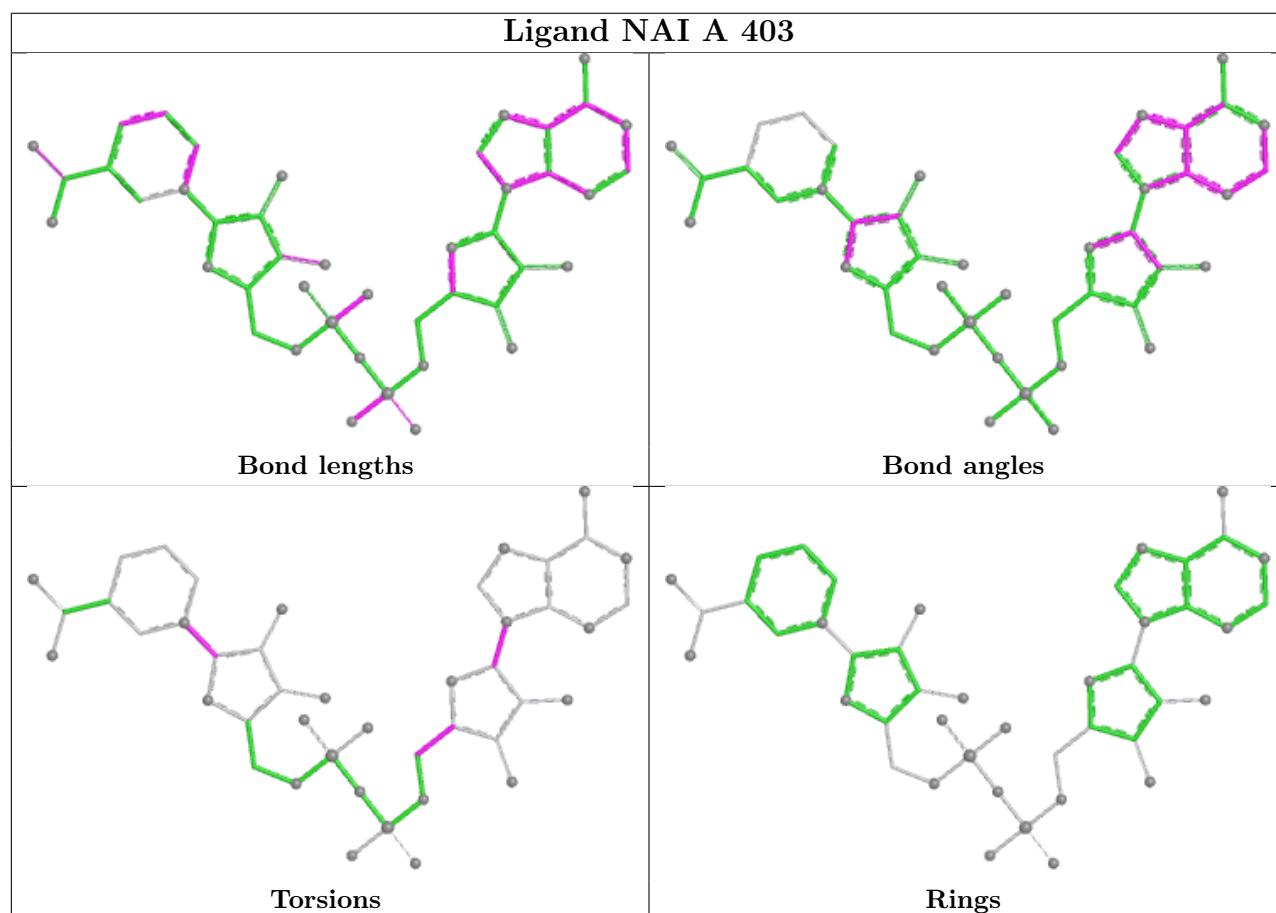
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	NAI	1	0

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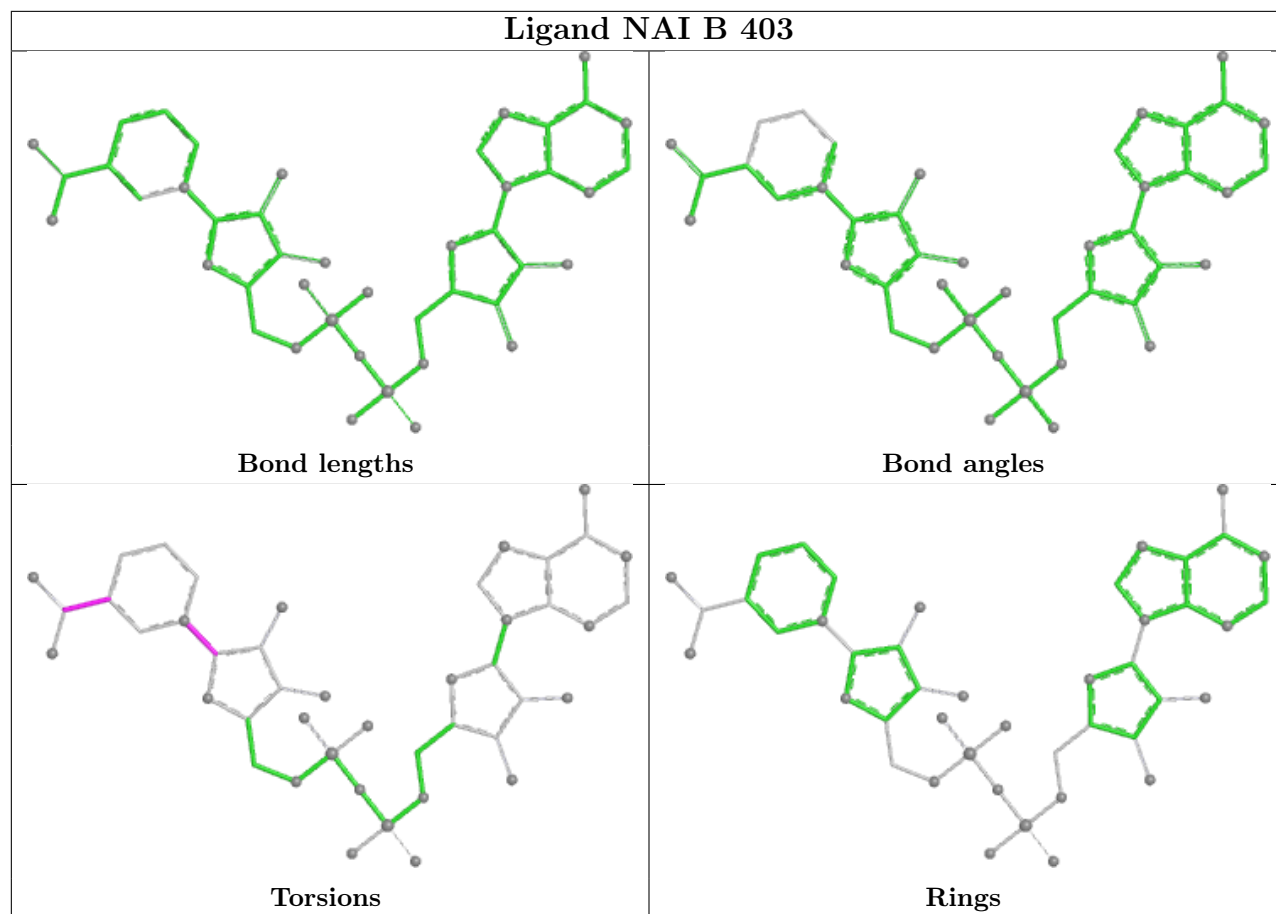
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	CXF	2	0
4	B	404	CXF	1	0

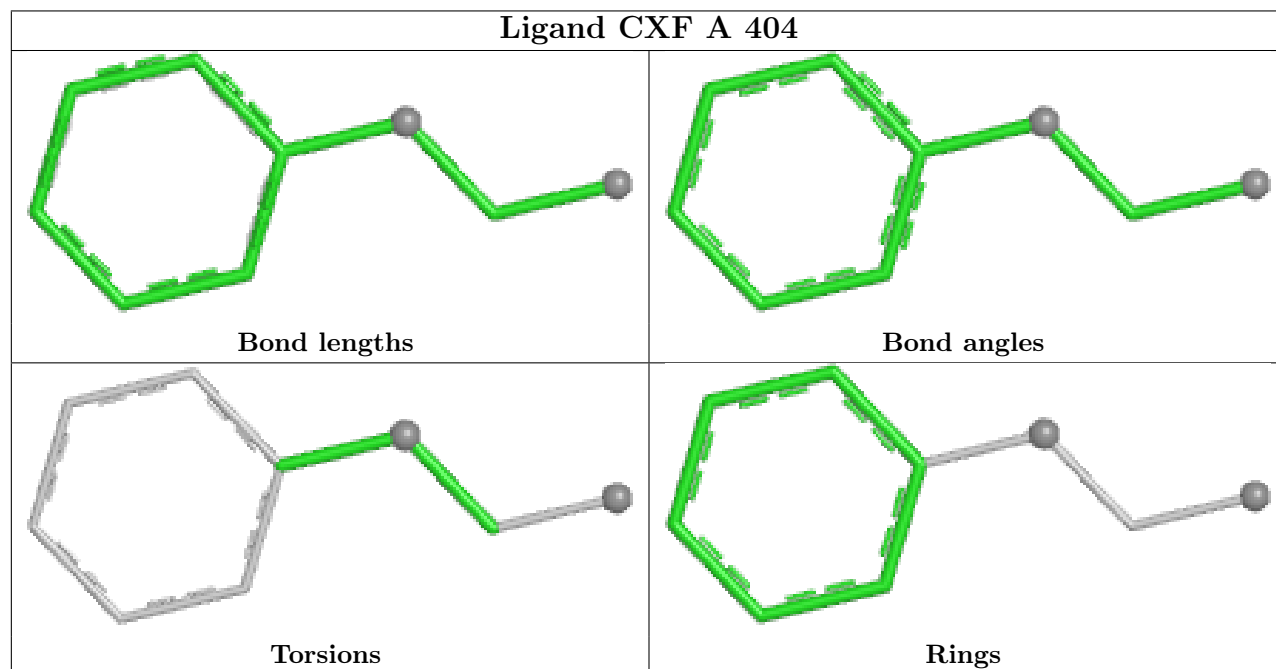
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

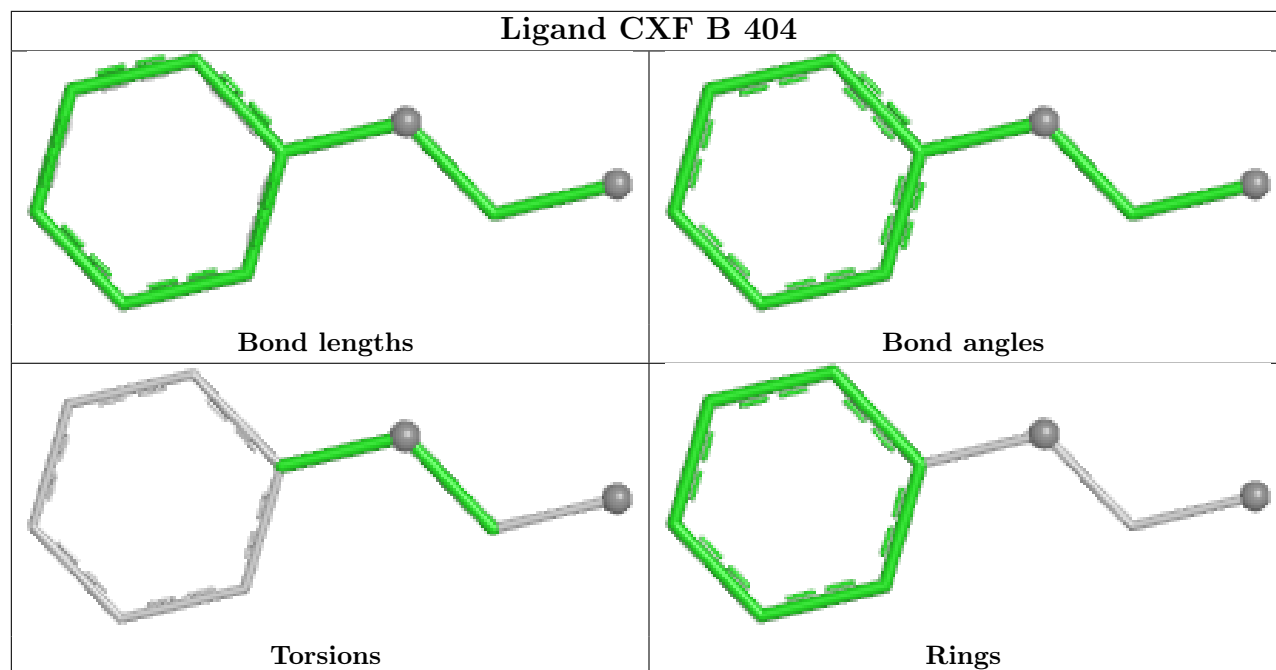


Ligand NAI B 403



Ligand CXF A 404





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	374/377 (99%)	0.35	6 (1%) 70 75	18, 25, 36, 47	0
1	B	374/377 (99%)	0.43	6 (1%) 70 75	18, 28, 40, 55	2 (0%)
All	All	748/754 (99%)	0.39	12 (1%) 70 75	18, 26, 39, 55	2 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	TRP	4.7
1	A	354	LYS	3.7
1	A	245	ASP	3.6
1	B	1	SER	2.7
1	B	23	ILE	2.5
1	A	1	SER	2.3
1	B	163	ALA	2.1
1	B	3	ALA	2.1
1	A	330	LYS	2.0
1	B	338	LYS	2.0
1	B	6	VAL	2.0
1	A	235	VAL	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](#)

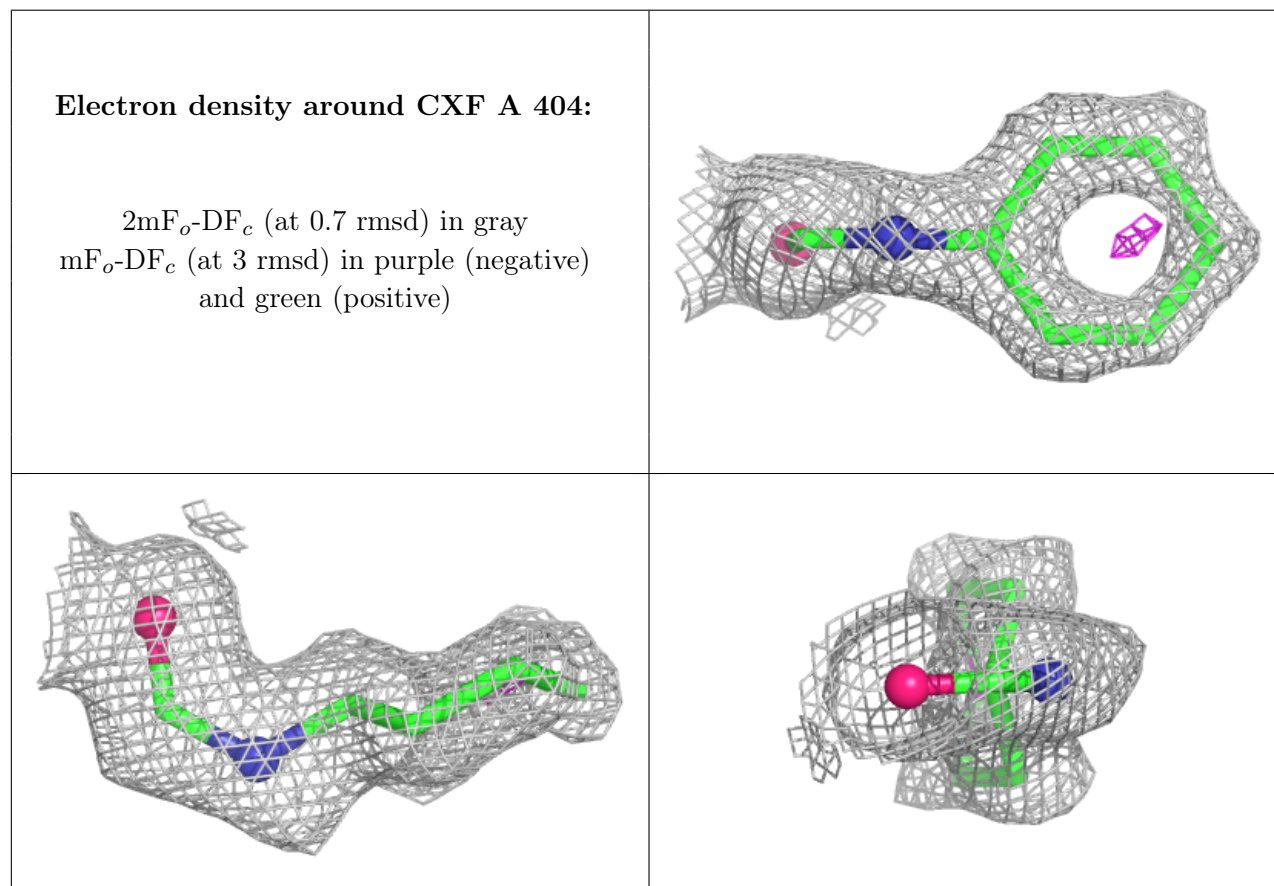
There are no oligosaccharides in this entry.

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.

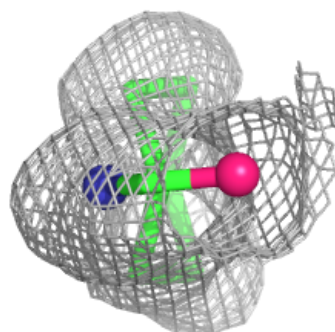
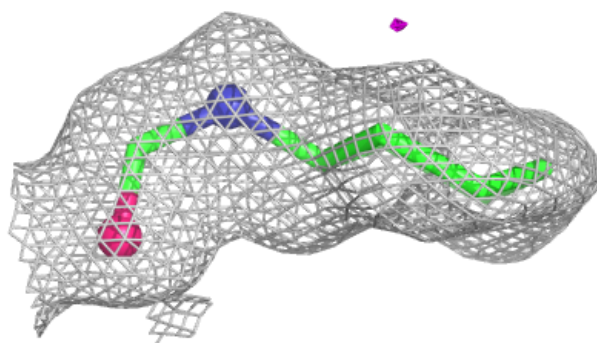
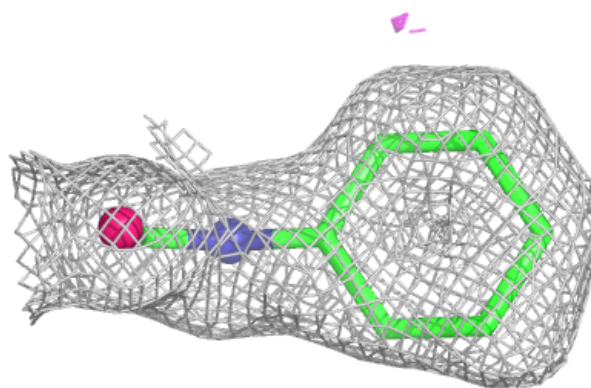
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CXF	A	404	9/9	0.94	0.09	20,21,23,24	0
4	CXF	B	404	9/9	0.95	0.08	22,24,29,31	0
3	NAI	A	403	44/44	0.97	0.06	16,19,26,37	0
3	NAI	B	403	44/44	0.97	0.06	19,22,28,33	0
2	ZN	B	401	1/1	0.99	0.02	23,23,23,23	0
2	ZN	B	402	1/1	0.99	0.02	25,25,25,25	0
2	ZN	A	401	1/1	1.00	0.01	20,20,20,20	0
2	ZN	A	402	1/1	1.00	0.01	22,22,22,22	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.

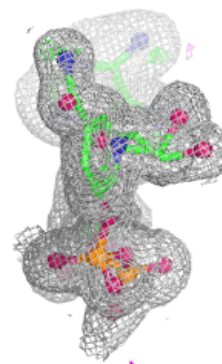
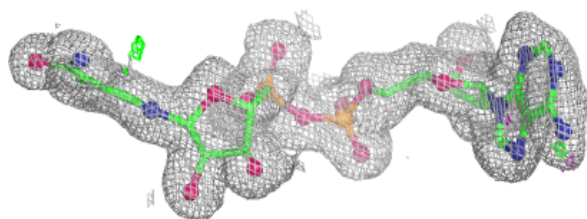
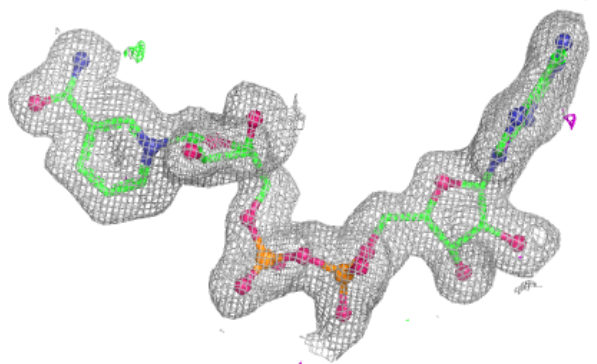


Electron density around CXF B 404:

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

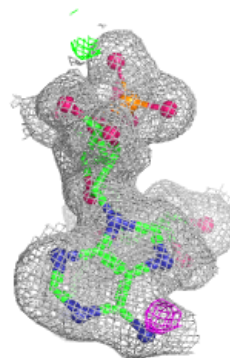
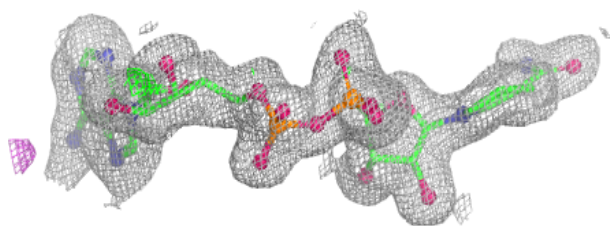
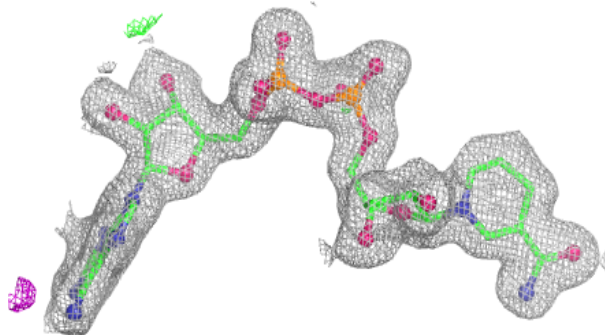
**Electron density around NAI A 403:**

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



Electron density around NAI B 403:

$2mF_o-DF_c$ (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.